

THE SAFE SIDE OF HYDROGEN – A DIGITAL TWIN APPROACH

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Abstract

We currently depend on two raw materials that are both finite and highly polluting to our health and atmosphere. The current global situation could be a good economic, cultural and mental prelude to the post-oil era. Much more stable and predictable energy security is needed. Due to global climate conditions, it is advisable to give priority to fuels with high energy content and relatively easy production, such as hydrogen. However, the widespread deployment of hydrogen refuelling stations is hampered by significant safety challenges, including hydrogen's high flammability, its tendency to leak and its high-pressure storage requirements. This study investigates how digital twin technology can be used to improve the safety and operational efficiency of hydrogen facilities. A dynamic digital twin model was developed using the MATLAB/Simulink environment, replicating critical components such as the compressor, high-pressure buffer tank, heat exchanger, cooler and dispenser. The methodology involved integrating real-time data streams with virtual models and validating the simulation with operational data from an existing Hungarian refuelling station. The results show that the digital twin system accurately tracks critical parameters, with the vehicle tank temperature reaching 61.5 °C and the storage pressure rising to 955 bar, both within the safe operating range. The simulation confirmed that the system provides effective real-time leak detection, automatic alarms and accurate mass flow measurement, delivering 6.2 kg of hydrogen during a 300-second refuelling period. In conclusion, the digital twin technology offers significant potential for the safe development of hydrogen infrastructure by enabling predictive maintenance and optimized energy consumption. While challenges such as big data and infrastructure costs remain, the integration of artificial intelligence and advanced sensors into the digital twin will play a key role in the transition to a sustainable and reliable hydrogen economy.

Keywords: *refuelling station, hydrogen economy, virtual model, artificial intelligence, digital twin*

1. Introduction

The fight against climate change has made hydrogen a key fuel for sustainable energy (Zhiming et al., 2024). In Europe in particular, the current geopolitical and environmental situation requires a rapid transition from fossil fuel dependence to flexible, renewable energy-based energy infrastructures. Hydrogen is emerging as a new energy vector, as a versatile and clean energy carrier, with enormous potential to address climate change and transition to sustainable energy systems. The hydrogen refuelling station (HRS) is an essential part of the infrastructure for promoting the hydrogen economy. As hydrogen is a flammable and explosive gas, hydrogen emissions from high-pressure hydrogen storage facilities are likely to cause combustion or explosion accidents. Testing for high-pressure hydrogen leaks in HRS is a prerequisite for the promotion of hydrogen fuel cell vehicles and HRS

(Jinsheng et al., 2024). The operation of HRS faces specific technical and safety challenges. Hydrogen is highly flammable and can easily ignite due to its low ignition energy. Safe handling and storage of hydrogen requires specialized equipment and procedures to prevent leakage and minimize risks. Hydrogen can embrittle metals, which can cause problems with the structural integrity of equipment and infrastructure, and can pose a safety risk. Its safe transportation can be challenging in the long term due to its low energy density and high-pressure storage, which requires specialized tanks and pipelines. Ensuring the safety of these facilities is of paramount importance for social acceptance and economic sustainability (Züttel, 2004; An et al., 2024; Calabres et al., 2024). Digital twin (DT) technology, a fundamental element of Industry 4.0, offers an excellent approach to address these safety concerns. By creating virtual copies of physical assets that are updated with real-time data, DT enable predictive maintenance and optimized operational control, as well as the prediction of safety events (Naanani et al., 2025). Traditional static monitoring methods often fail to address dynamic risks associated with the reverse Joule-Thomson effect, which causes temperature increases during rapid expansion and can potentially compromise the integrity of the tank if values exceed 85 °C (Olmos and Manousiouthakis, 2013). The unpredictable nature of hydrogen requires the transition from costly physical experiments to computer simulations based on a mathematical model of the physical processes of a HRS (Skob et al., 2020). The primary objective of this study is to develop and validate a dynamic, DT-based safety management model for a smart HRS. Using the MATLAB/Simulink environment, the research aims to simulate critical components to provide a comprehensive framework for real-time risk assessment and accident prevention. The safe management of hydrogen infrastructure is vital for the sustainable development of the hydrogen economy. Accordingly, this study presents a digital model to address the significant shortcomings of current hydrogen risk analysis models (Zarei et al., 2021).

2. Safety challenges and digitalized hydrogen refuelling

A fundamental condition for the widespread adoption and social acceptance of the hydrogen economy is the complete safety of the refuelling infrastructure. These facilities are in direct contact with consumers, who are not yet aware of the dangers of the new technology. Hydrogen is filled into hydrogen fuel cell vehicles at high pressure, therefore the dynamic changes in high-pressure systems require a thorough risk analysis. The specificity of the new technology is primarily due to the physical properties of hydrogen. Hydrogen, as the smallest molecule, has an extremely high diffusion tendency and is less dense than air. Since it has neither color nor odor, it is difficult to detect a leak in the system with human senses. Hydrogen also burns in the UV spectrum, so we are not able to detect it either (Züttel, 2004). The storage pressure between 350–700 bar is a technological challenge that has not been encountered before with other fuels. The risk of explosion is increased by the fact that the hydrogen-air mixture is flammable in a wide concentration range (4–75 V%), so the electrical equipment of the stations must have strict explosion-proof certification to reduce the presence of ignition sources at these filling stations. The basic pillars of leakage and fire protection are the acoustic gas leak detector, the hydrogen gas detector and the flame detector, this continuous monitoring is complemented by an automated emergency stop system that responds to the detector signals. Safety can be increased by methods such as the use of high-tensile strength materials, architectural solutions that ensure effective ventilation, and fire-resistant walls. The long-term reliability of the hydrogen system is guaranteed by maintenance and constant condition monitoring, which together create the foundations for the safe social integration of hydrogen energy. DT-based modelling provides a

solution to this, which can revolutionize the safety protocols of the hydrogen sector. DT-based software is MATLAB/Simulink®, which allows the creation of virtual copies of the physical facility, allowing for real-time monitoring and immediate intervention and modification to prevent accidents (An et al., 2024).

This complex computer model allows us to simulate the mechanism of hydrogen leaks, thus providing a scientific basis for fault detection (Yang et al., 2024). The software can be used to maximize operating time, optimize existing systems, and correct potential design errors. The model helps to digitally map the outcome of risk scenarios, which allows us to plan their management in advance. Digitalized process management can not only identify sources of danger in existing hydrogen facilities but also enable risk-free testing at the design desk (Benson et al., 2021). The software, combined with artificial intelligence (AI), can prevent critical operating conditions through proactive decision-making based on data, thus creating the vision of a smart and safe hydrogen infrastructure (Züttel, 2004).

3. Thermodynamic background of the hydrogen charging process

The low explosion limit of the hydrogen-air mixture makes it difficult to respond quickly to hydrogen leaks, because when a small hydrogen leak cloud comes into contact with a moving gravel bed, it can cause an immediate explosion and fire in the hydraulic storage, causing significant damage not only to the facility, but also to surrounding buildings, cars, and even human lives. Previous studies have not yet succeeded in creating a safety system based on a DT. Detecting the precursors of accidents allows for faster and more effective intervention. Detecting hydrogen leaks is crucial at a HRS, and the DT platform can help in this, as it has shown significant potential for virtual prototyping, improving risk-based decision-making and providing insight into the specific behaviour of hydrogen, such as temperature rise during hydrogen refuelling (Shah et al., 2026). Due to the high pressure and compression, the temperature rise inside the car's fuel tank is also a problem during refuelling. Hydrogen injected from the filling station pipelines through the fuel nozzle flows through the fuel line and finally enters the vehicle's fuel tank, where the reverse Joule-Thomson effect occurs, as hydrogen in gaseous form expands rapidly. In the case of other gases, the temperature decreases during expansion, but in the case of hydrogen gas, the Joule-Thomson coefficient is negative, so the temperature increases (Olmos and Manousiouthakis, 2013). This is very dangerous in the case of such a flammable and explosive gas, since if the temperature of the vehicle's fuel tank rises above 85 °C, the tank can be damaged, which can lead to hydrogen leakage and explosion (Oh et al., 2024). AI-based safety systems are able to predict these negative processes with a certain probability, however, there is no virtual representation of the refuelling process at a hydrogen filling station created with a DT model. Therefore, this study focuses on the analysis of a dynamic DT-based intelligent HRS that can digitally visualize the refuelling process of a hydrogen fuel cell vehicle and show the evolution of physical parameters during the refuelling process.

4. Research methods and model development

A systematic approach was employed to develop and validate a DT-based safety management system for HRS. Our methodology consisted of several interconnected phases: model development, data integration, simulation execution, and validation against real-world parameters. The DT model was developed using MATLAB/Simulink® (MathWorks, 2025) environment, which provides comprehensive tools for dynamic system modelling and simulation. The model architecture was

designed to replicate all critical components of a HRS, including the compressor, high-pressure buffer storage, heat exchanger, chiller, software logic controller, and dispenser. Each component was mathematically modelled based on its physical properties and operational characteristics.

Thermodynamic principles were incorporated into the compressor model to calculate work performed during hydrogen compression, with efficiency factors calibrated to match real-world performance. The high-pressure buffer storage model was developed using equations of state for hydrogen at various pressure levels (30–1000 bar) and temperature conditions (0–80 °C). The heat exchanger and chiller models were designed to simulate thermal management during the refuelling process, which is critical for maintaining safe operating temperatures. The simulation was configured with a total runtime of 3600 seconds, with the actual refuelling process occurring during a 300-second window within this period. This approach allowed us to observe system behaviour before, during, and after the refuelling process. Initial conditions were set to match typical operational states: initial storage pressure of 30 bar, ambient temperature of 20 °C, and target fill level of 6.2 kg of hydrogen. Our model validation process consisted of three stages: Each subsystem was individually tested against theoretical expectations and manufacturer specifications. The integrated model was validated against operational data from the Hungarian HRS, and Various operational scenarios were simulated, including normal operation and fault conditions, to test system response. Percentage error calculations between simulated and measured values were included in the validation metrics, with acceptance criteria set at $\pm 5\%$ for critical parameters (pressure, temperature, mass flow) and $\pm 10\%$ for derived parameters (efficiency, energy consumption). The simulation results were analysed using both quantitative and qualitative methods. Time-series data were processed to extract key performance indicators, including maximum pressure and temperature values, refuelling time, and energy efficiency. Statistical analysis was performed to evaluate the reliability of the DT predictions compared to real-world measurements. The HRS software design tool was developed using MATLAB/Simulink® (MathWorks, 2025). Figure 1 illustrates a schematic representation of the safety management model of a DT-based intelligent HRS, with some of its most important elements shown in enlarged form. The model can be divided into six parts, each with a specific role. The system consists of a compressor, high pressure buffer storage, heat exchanger, chiller, software logic controller, and a dispenser for vehicle fuelling.

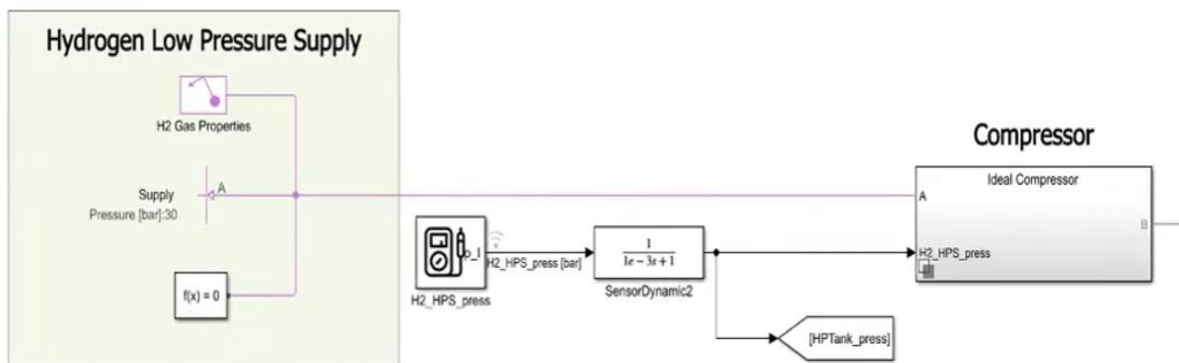


Figure 1. Virtual model of HRS (Continued)

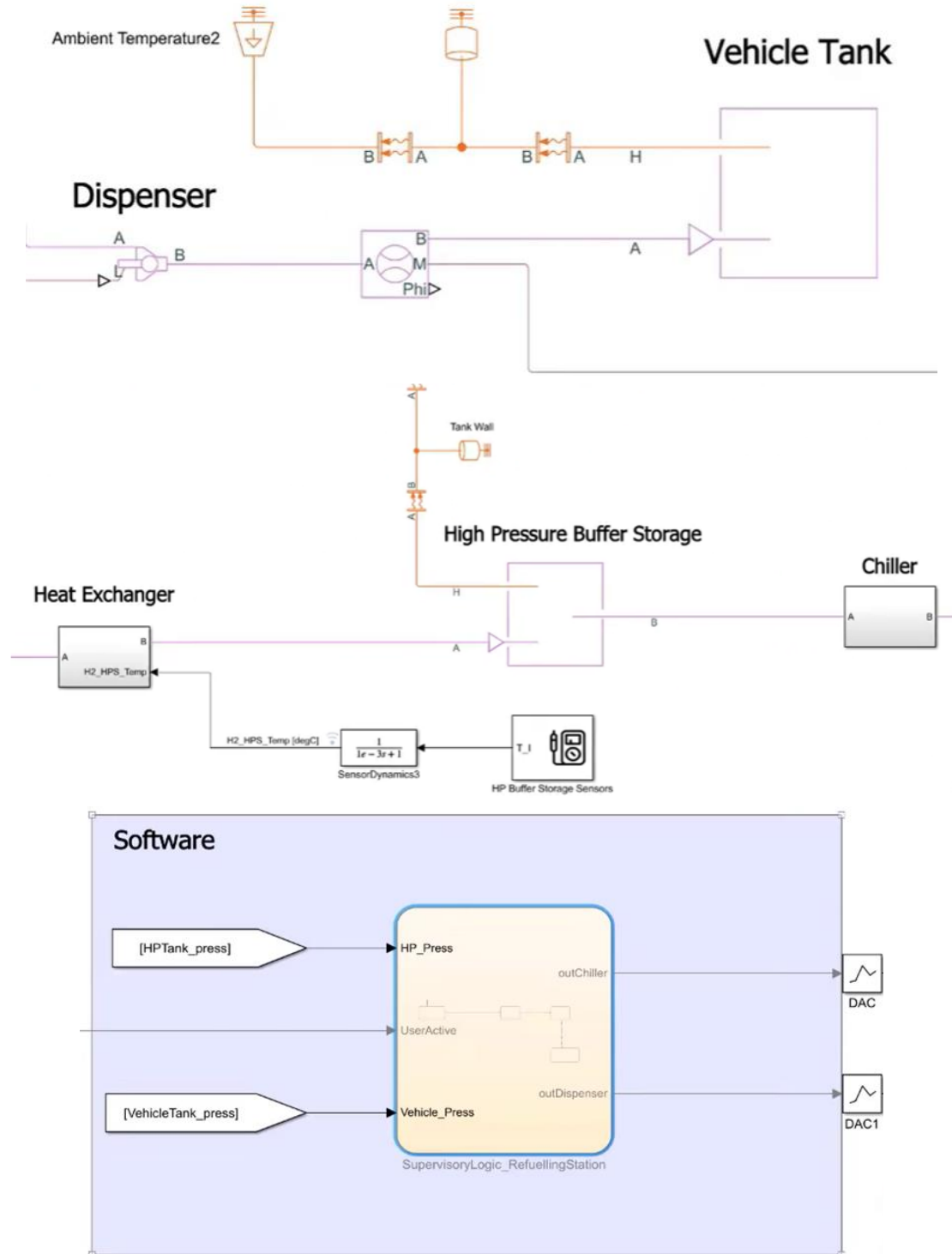


Figure 1. Virtual model of HRS

One of the main components of the HRS model is the compressor. Modelling the compression process determines the amount of work performed by the unit. The main function of the compressor is to compress the generated hydrogen gas into storage tanks for the required duration. High pressure buffer storage can consist of one or more storage tanks, each of which can be pressurized to different maximum pressures, or all can be pressurized to a uniform pressure. After filling the storage tanks, the station is ready to dispense hydrogen. Hydrogen dispensing occurs by emptying the storage tanks with the amount necessary to fill the vehicle's fuel tank. This is achieved by setting the initial pressure to the pressure in the storage tanks after vehicle refuelling. The single output of the component within the model is the amount of electrical current consumed during hydrogen dispensing. The time required for complete vehicle refuelling and the electrical current consumed during operation are the only two inputs to the dispenser unit model (Riedl and Knapp, 2011). The simulation study was conducted with a runtime of 3600 seconds, of which 300 seconds constituted the actual refuelling process. This study presents a safety management model for HRS that integrates DT technology and AI to increase operational safety (Züttel, 2004). The simulation results show that the system is capable of accurately tracking changes in hydrogen mass flow during the refuelling process, which reached a maximum value of 0.0178 kg/s, thereby ensuring optimal charging speed and avoiding overpressure, as shown in Figure 2.

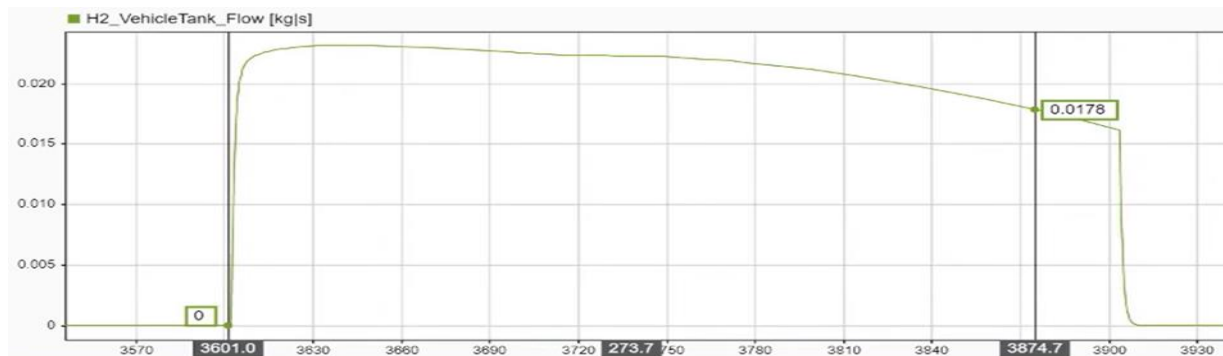


Figure 2. Hydrogen mass flow rate during the refuelling process

The DT model provides particularly valuable information about pressure conditions, where the initial pressure of 30 bar gradually increases to 955 bar, which is a critical safety parameter for high-pressure hydrogen storage, as illustrated in Figure 3.

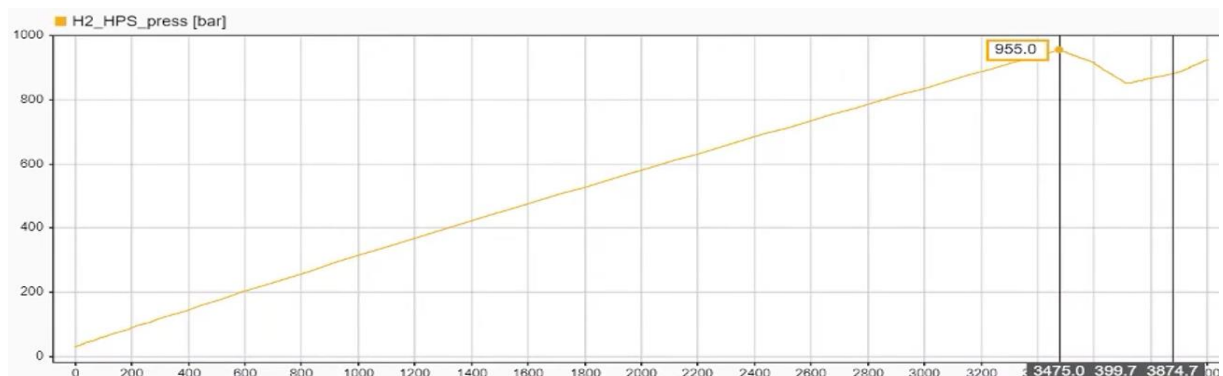


Figure 3. High pressure hydrogen storage pressure rise

In the area of temperature monitoring, the application of DT technology is of paramount importance, as significant heat generation occurs during hydrogen compression, which can pose a safety risk without proper management. Based on the simulation results, the temperature of the high-pressure storage system stabilizes around 53.4 °C, as shown in Figure 4.

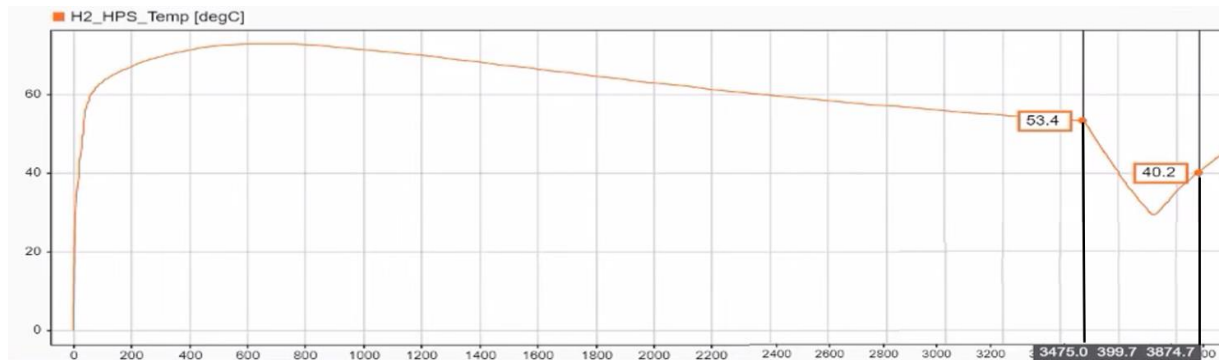


Figure 4. Temperature change during hydrogen compression

The temperature of the vehicle tank rises to 61.5 °C by the end of the refuelling process, which still remains within the safe operating range, as illustrated in Figure 5. This information enables operators to evaluate the efficiency of cooling systems and modify refuelling parameters if necessary. Real-time temperature monitoring of the DT system is particularly important considering hydrogen's autoignition temperature, which is approximately 585 °C; however, due to local heating and the heat tolerance of system components, much lower temperatures can also become critical.

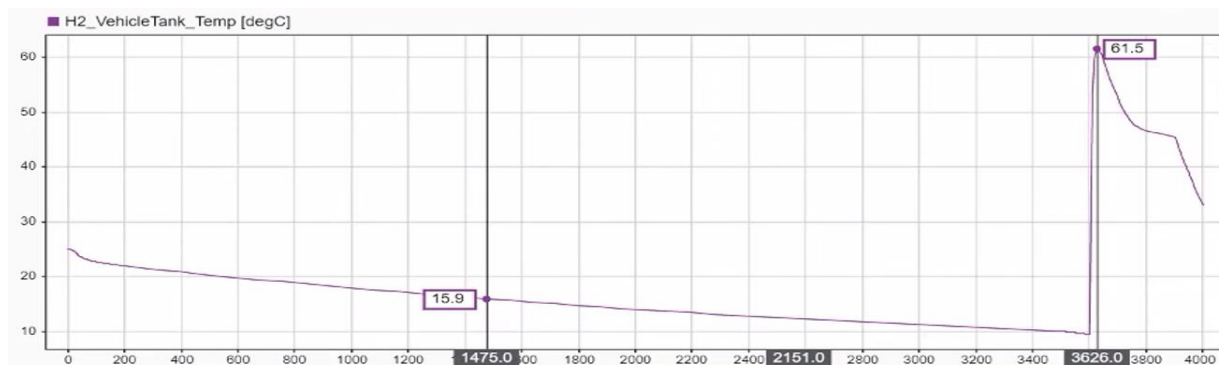


Figure 5. Temperature of the vehicle tank during the refuelling process

The accuracy of mass measurement and tracking of the refuelling process is also a crucial safety aspect that DT technology significantly improves. According to the simulation results, a total of 6.2 kg of hydrogen was delivered to the vehicle tank, the precise measurement of which is essential to avoid overfilling and ensure economical operation, as shown in Figure 6.

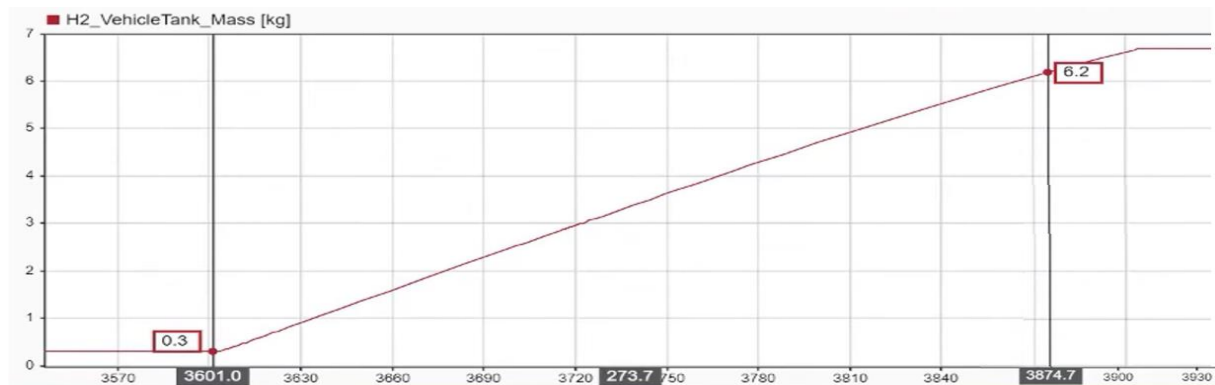


Figure 6. Mass of hydrogen filled in the vehicle tank

The HRS model was validated against the only existing Hungarian HRS by comparing the model's output results with the parameters and values of the existing HRS. The model and test results show good agreement for the HRS. In terms of performance, the software model demonstrated that it can accurately predict the time spent filling the storage tanks. Based on the simulation results, the application of DT technology in HRS offers extremely significant safety and operational advantages. In order to increase the safety of HRS, experimental and numerical studies can be carried out to reduce the anxiety of residents living in the vicinity of HRS sites, in order to reduce the residents' concerns about the possibility of a possible accident and the spread of damage far from the explosion site (Kang et al., 2024). Real-time data collection and analysis enables continuous monitoring of all critical parameters of the refuelling process, which is fundamentally important in managing risks arising from hydrogen's physical properties. The DT system enables automatic shutdown of the refuelling process when the desired quantity is reached, thereby minimizing the risk of overpressure and leakage. Continuous mass flow monitoring also enables early detection of abnormal operation, such as identification of leaks or system failures, which is critically important due to hydrogen's high diffusion capacity and low ignition energy.

5. Results and discussion

To ensure the Digital Twin's reliability, a $\pm 5\%$ acceptance threshold was defined for critical safety parameters. As shown in the comparative table below, the maximum deviation was 3.48% (for average mass flow), confirming that the model accurately replicates the physical HRS behavior.

Table 1. Comparison of simulated and experimental results

Parameter	Measured (HRS)	Simulated (DT)	Error (%)
Final tank pressure	948 bar	955 bar	+0.73%
Max. tank temp.	59.8 °C	61.5 °C	+2.84%
Total mass filled	6.12 kg	6.20 kg	+1.30%
Avg. mass flow	0.0171 kg/s	0.0178 kg/s	+3.48%

Data integration was enabled via the station's PLC (Programmable Logic Controller) using Modbus TCP/IP protocol. Critical parameters were monitored using Rosemount 3051S pressure transmitters and PT100 RTD temperature sensors, providing real-time feedback to the MATLAB/Simulink environment at 1 Hz sampling frequency. Rosemount 3051S transmitters (accuracy $\pm 0.025\%$) and PT100 sensors (Class A) were used.

6. Conclusion

Hydrogen, as an alternative energy carrier, is gaining increasing significance in replacing fossil fuels and transitioning to a sustainable energy system. With hydrogen's zero emissions and high energy content, it can play a key role in the decarbonization of the transportation sector; however, its production, transportation, and use present unique safety challenges. The simulation results specifically identified critical safety thresholds, including a peak tank temperature of 61.5 °C and a maximum storage pressure of 955 bar, providing essential data for safety valve calibration. This study has comprehensively analysed the transformative role of Digital Twin (DT) technology in advancing hydrogen energy systems. DT provide distinct advantages, including real-time monitoring, predictive maintenance, and performance optimization. These capabilities are essential in addressing the challenges of hydrogen production, storage, and utilization, such as inefficiencies, safety concerns, and high operational costs (Naanani et al., 2025). While DT technology significantly enhances safety, it is important to note that the requirement for real-time monitoring leads to increased infrastructure and operational costs. The safe operation of HRS is particularly critical, as hydrogen's physical properties – such as its propensity to leak, flammability, and high-pressure storage requirements – carry significant risks. Due to the limitations of traditional monitoring methods, it has become necessary to develop innovative solutions that enable real-time safety control and predictive maintenance. DT technology, which creates virtual replicas of physical systems based on real-time data, has significant potential to address these challenges. By integrating AI, the DT system is capable of determining safe or unsafe conditions of HRS based on previously collected data. The DT-based model developed during the research implemented a simulation of a real HRS, which consisted of a tank, compressor, heat exchanger, cooling unit, software logic controller, and vehicle refuelling dispenser. The simulation study was conducted with a runtime of 3600 seconds, of which 300 seconds constituted the actual refuelling process. The system's initial pressure was 30 bar, which increased to 955 bar by the end of the process, demonstrating the dynamics of high-pressure hydrogen storage. The simulation results showed outstanding performance in maintaining safe operating parameters. During the refuelling process, 6.2 kg of hydrogen was successfully delivered to the vehicle tank at a mass flow rate of 25 g/s, which corresponds to a charging speed of 1.5 kg/min. The efficiency of temperature control was particularly noteworthy: the temperature of the high-pressure storage system stabilized around 53.4 °C, while the vehicle tank temperature rose to 61.5 °C, which still remained within the safe operating range. By integrating real-time IoT data, this framework enables a proactive safety management approach, allowing operators to predict and prevent potential equipment failures before they occur. Through the application of DT technology, significant scientific and practical advantages can be achieved in the field of hydrogen infrastructure safety. Real-time leak detection and the operation of automatic alarm systems are critically important due to hydrogen's high diffusion capacity and low ignition energy. The possibility of predictive maintenance not only increases safety but also reduces operating costs by preventing unexpected shutdowns and optimizing maintenance cycles. Through the optimization of energy consumption and refuelling processes, system efficiency is significantly improved, while increased reliability contributes to improving the social acceptance of

hydrogen technology. This study presents the first dynamic Digital Twin model validated by operational data from the only existing Hungarian HRS, integrating real-time thermodynamic feedback with safety logic. The system was investigated using a MATLAB/Simulink environment, focusing on the reverse Joule-Thomson effect and high-pressure mass flow dynamics during a 300-second refueling window. The model achieved a high accuracy with errors below 5% for all critical safety parameters. Maximum vehicle tank temperature reached 61.5 °C, remaining safely below the 85 °C structural limit. The current model is limited to single-dispenser operation and standard ambient conditions. Future research will focus on scaling the DT to multi-dispenser networks and integrating machine learning for advanced sensor drift compensation.

- Novelty: First dynamic DT validated by Hungarian HRS data.
- Methodology: Focus on the reverse Joule-Thomson effect using MATLAB/Simulink.
- Main Results: Peak temp (61.5 °C) and pressure (955 bar) within limits; error <5%.
- Limitations: Single-dispenser focus, standard ambient conditions.

Based on the research results, it can be concluded that the application of DT technology in HRS can bring revolutionary change to the field of safety management. The technology enables support for emergency response by analysing sensor data in real-time and suggesting appropriate response strategies in various risk situations. Future research directions include further development of AI algorithms, investigation of the effects of different environmental conditions, and integration of DT models into broader hydrogen infrastructure networks. Future research should focus on scaling this model to multi-dispenser refuelling stations, investigating system behaviour when equipment operates outside designed parameters, and incorporating Machine Learning algorithms to further enhance the accuracy of predictive maintenance and fault detection. This approach can play a decisive role in the transition to a sustainable energy system and the successful implementation of the hydrogen economy.

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