Comprehensive Simulation and Validation of Green Hydrogen Value Chain in the KoNSTanZE Project: From Production to End-Use

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Abstract

The aim of this paper is to emphasize the development and validation of a simulation model for the KoNSTanZE project [1]. This last project is specifically concerned on green hydrogen in the Bosch Homburg plant, in Germany, through its value chain. This green hydrogen is generated on site exclusively with renewable energy, and its several roles in industrial process, transport and energy supply through the so called eH_2Cycle. The model is holding critical elements such as hydrogen generation, industrial application in the hardening shop, a multi-stage storage system and distribution to mobility sectors via refuelling stations were meticulously modelled based on their physical characteristics and safety operational parameters. Besides, the simulation includes the thermodynamic of hydrogen and dynamic operational factors. To perform accuracy of the model and its subsequent analysis, the calibration and validation were based on data from the real plant which is monitored. The model was validated to ensure that it can reflect the real behaviour of the system in the various operations scenarios. This work provided a robust numerical model of eH_2Cycle for optimising green hydrogen application, which is aligning with the current strategies for industrial decarbonisation and enhancement of sustainable energy solutions.

1. Introduction

The current global challenge of decarbonization of the global economy in order to decrease greenhouse gas emissions has put a focus on the avenues which are potential renewable energy sources and carrier for industrial, transport and energy sector. Among these renewable energies (RE), green hydrogen or H_2 generated from RE resources has emerged as a viable candidate [2]. Indeed, through its entire value chain, when produced and used across various sectors, green hydrogen presents possibilities for reducing global carbon emission and directly driving the transition towards a cleaner energy system and carbon neutral. More specifically, hydrogen is viewed as the critical solution to address sectors that remain hard to electrify such as carbon-intensive industries or long-distance transport. To this end, the European Union has provided goals to deploy green hydrogen as part of the EU Hydrogen Strategy. This strategy expects hydrogen to enable the economic sector reach carbon neutrality by 2050.

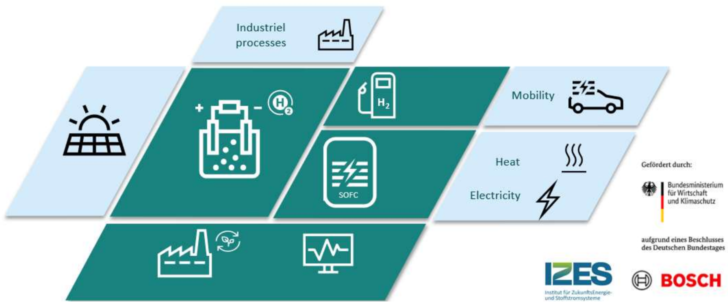

Figure 1: the KoNSTanZE project layout (Source: Robert Bosch GmbH)

In this purpose, the large-scale demonstration of such technologies is evident in the KoNSTanZE project, conducted at the Robert Bosch plant in Homburg, Germany. This project covers the entire value chain of green hydrogen, from the generation process through renewable power to its various utilisation. With the support of the German Federal Ministry of Economic Affairs and Climate Action (FKZ: 03EI3043A&B), the KoNSTanZE project is witnessing the commitment and aim of BOSCH for decarbonization of its industries. Moreover, this central system in which hydrogen is generated, stored, distributed and applied across various segments is called the eH_2Cycle. The green hydrogen is then used in industrial processes, for instance, the hardening shop, hence decreasing the carbon foot print of the plant. Moreover, this project comprises the integration of hydrogen in the mobility sector, through the refuelling stations that support different hydrogen-powered vehicles fleet. In fact, the logistic vehicles operating within the plant are powered by hydrogen. Additionally, one of the objectives of the project is the development of an accurate eH_2Cycle simulation model. It is worth mentioning that simulation modelling allows for a thorough analysis of multiple aspects of the entire hydrogen value chain, as it is highlighted by the recent research literature [3, 4]. Furthermore, this holistic approach underscores the project's ambition to cover the full spectrum of hydrogen utilization. The main goal of this paper is to introduce a highly accurate simulation model of the KoNSTanZE project, which incorporates key components such as the thermodynamics of hydrogen and its behaviour during production, storage, and distribution. The modelling is validated throughout the data collected through the monitored plant. This paper not only considers the technical and physical properties but also, asses the refuelling station under different weather conditions.

2. Methodology

The methodology for developing a highly accurate simulation model of the KoNSTanZE project is based on a systematic approach that includes the characterization, classification, and modelling of key components in the hydrogen value chain.

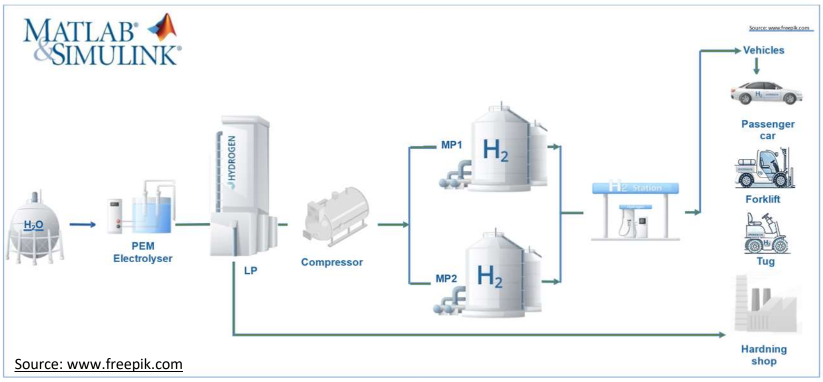

Figure 2 : The components involved in the hydrogen model value chain

Figure 2 shows the components involved in this project and their connections. For the development of this model, MATLAB Simulink was used using MATLAB Simulink to in order to enables integrated multi-domains system and a complex dynamical interaction modelling [5], such as the time-dependent behaviours of pressure, temperature, and gas flow rates. In addition, Simulink provides robust tools for control system design and optimization. The table below listed all the components modelled and the adopted approach used for this work.

Table 1 Modelling Approaches and Functions of Key Components in KoNSTanZE Project

Component	Function	Modelling Approach
PEM Electrolyser	splits water into hydrogen and oxygen using electricity from renewable sources.	Model electrical input, efficiency, thermodynamic properties (temperature, pressure), and energy consumption using data from NIST for hydrogen properties.
Compressor	Increases hydrogen pressure for storage in mid-pressure vessels.	Simulate compression process, and thermal behaviour during compression. Using the technical data sheet from the supplier.
Low-Pressure (LP) and Mid-Pressure Vessels (MP1 & MP2)	Store hydrogen at different pressure levels for later use.	Model hydrogen state changes over time (Filling and emptying). Focus on, pressure dynamics, and energy conservation, model thermal insulation incorporating material properties of vessels.
Hydrogen Distribution	Distributes hydrogen to the hardening shop and refuelling station.	Simulate hydrogen flow dynamics and pressure losses during distribution, considering pipeline thermodynamics and fluid behaviour to ensure efficiency in distribution.
Hydrogen-Powered Vehicles (Passenger Car, Forklift, Trolley)	Vehicles operating in the plant, powered by hydrogen fuel.	Simulate onboard hydrogen storage and thermodynamics during operation, including the refuelling time.
Hardening Shop	Uses hydrogen for industrial processes	Modelled as a constant consumer with a constant mass flow rate out, that comes from the low-pressure vessel directly (See figure 2).

2.1 Component Characterization and Classification

Table 2 presents the details of various components involved in hydrogen storage and distribution. Key parameters such as volume, initial pressure, maximal pressure, specific heat, and thermal conductivity are outlined for each component.

Table 2 Hydrogen Storage and Distribution Components of KoNSTanZE Project

Components	Volume (m^3)	Initial Pressure (bar)	Maximal Pressure (bar)	Specific Heat J/(kg.K)	Thermal Conductivity ($W/m^2.K$)
The Low-Pressure Vessel	100	50	40	1200	30
The Mid Pressure Vessels	1,2	50	500	470	42.6
The Passenger Car	0.1224	60	350	1200	300
The Forklift	0.074	35	350	1553.9	6.5
The Trolley	0.029	35	350	1155	6.5

The system includes two key components: an electrolyser and a hardening shop. The electrolyser uses Proton Exchange Membrane (PEM) technology, operating with a mass flow rate of 2.5 kg/h and producing hydrogen at an outlet pressure of 40 bar. The hardening shop is modelled as a constant consumer with a fixed mass flow rate of 600 g/h.

2.2 Thermodynamic Modelling and NIST Data Integration

The model obeys the laws of thermodynamics, ensuring the faithful representation of hydrogen's physical behaviour during production, compression, storage, and distribution. The hydrogen's state variables, including temperature, pressure, enthalpy, and entropy, are based on the National Institute of Standards and Technology [6].

2.3 Operational conditions

The flowchart describes the work-flow for existing hydrogen refuelling station (See Figure 3), starting with an electrolyser delivering hydrogen at low pressure (20-40 bar). A check on a critical pressure limit is made. If the pressure exceeds the limit, the hydrogen is sent to a compressor, which increases the pressure and directs it to two medium-pressure vessels: The two Medium Pressure Vessels with pressure between 50-500 bar A decision point is made when there is sufficient pressure within the medium-pressure vessels to perform a refuelling according to the SAE Protocol until in the vehicle reaches 350 bars If this is not the case, the system goes back to pump from the dispenser. If the pressure is reached, the order goes to the compressor to continue the filling of the two medium pressure vessels, one by one, until the pressure max is reached. This SAE protocol guarantees a safe refuelling. Indeed, it determines the pressure ramp rate at the dispenser depending on the hydrogen temperature, the vehicle vessel's volume, its initial pressure, and the ambient temperature [7].

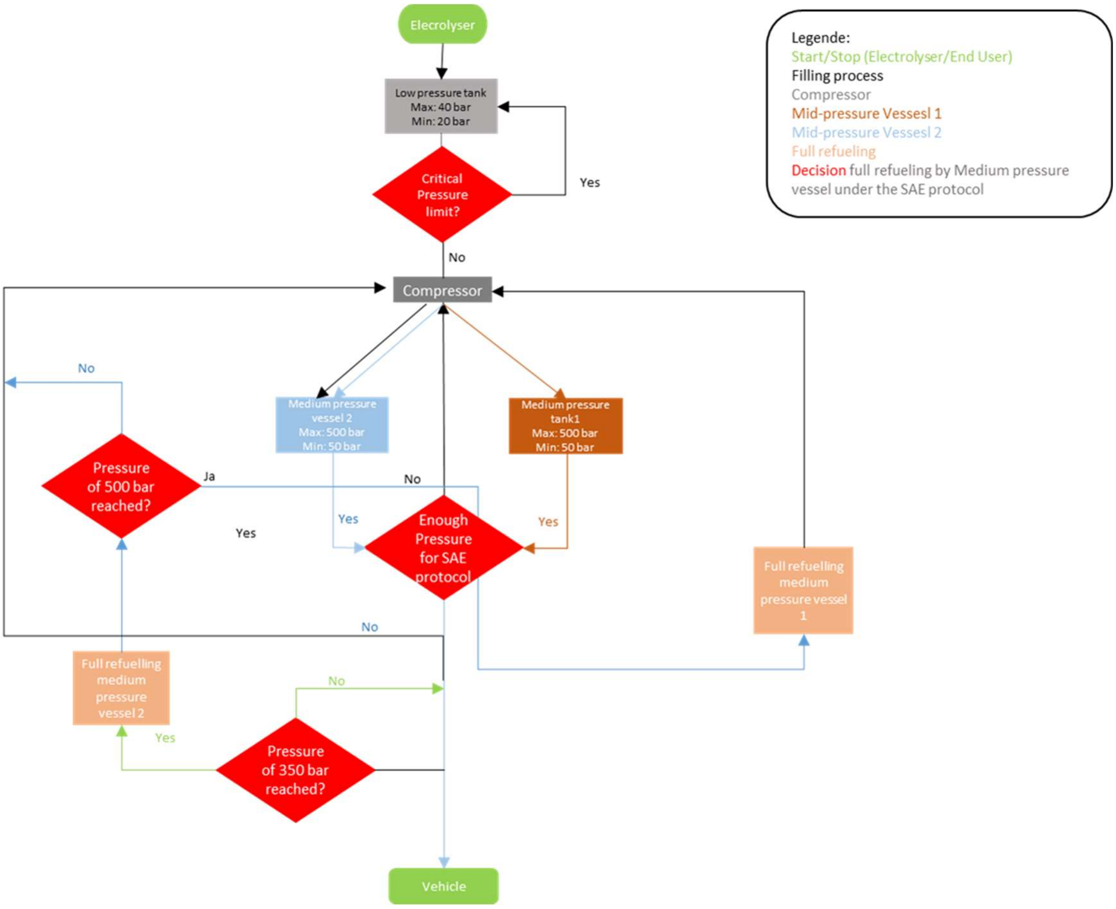

Figure 3 Hydrogen Refuelling Process Flow Diagram with Pressure Management

The accuracy of the simulation model is validated through real data gathered from the monitored plant. These data are compared through an iteration method to attain a high level of precision for the physical, thermal and chemical properties of the hydrogen as well as the components in the system.

3. Validation process

In this case, a comparative approach was used through defined measures between real and simulated data to evaluate the efficiency of the model. In fact, validation process influential measure is the Mean Squared Error (MSE), Correlation Coefficient and R2 figures. Ensuing metrics offered a vista of how the real dataset compared with the simulated one.

1. **Mean Squared Error (MSE)**: The MSE measures the average of the squares of the differences between the real and simulated data. It gives an idea of the overall magnitude of the error.

$$\mathrm{MSE}=\frac{1}{n}\sum_{i=1}^{n}(y_i-\hat{y}_i)^2 \qquad (1)$$

Where: y_i is out of real data point at index $_i$ y'_i is the simulated data point at index, and n represents number of data points.

2. **Correlation Coefficient (r)**: The correlation coefficient quantifies how closely the points match on the scatter plot and the sign that shows whether real and simulated data are directly or inversely related. It lies between -1 and 1, nearer to 1 represents positive linear relationship whereas nearer to 0 there is no linear relationship.

$$r=\frac{\sum_{i=1}^{n}(y_i-\bar{y})(\hat{y}_i-\bar{\hat{y}})}{\sqrt{\sum_{i=1}^{n}(y_i-\bar{y})^2}\sqrt{\sum_{i=1}^{n}\left(\hat{y}_i-\bar{\hat{y}}\right)^2}} \qquad (2)$$

Where: $\bar{y}$ Mean of the real data, and $\bar{\hat{y}}$ is Mean of the simulated data.

3. **R-squared (R^2)**: is the coefficient of determination, is the proportion of the real data variability that can be explained by the variability from the simulated data. Indeed, if R^2 is close to 1, this indicates that the simulation explains most of the variance in the real data, while a negative or low R^2 suggests poor prediction. It is calculated as:

$$R^2=1-\frac{\sum_{i=1}^{n}(y_i-\hat{y}_i)^2}{\sum_{i=1}^{n}(y_i-\bar{y})^2} \qquad (3)$$

Where: The numerator represents the residual sum of squares (the error between real and simulated data). The denominator is the total sum of squares (variance of the real data).

These metrics represents a clear and defined accuracy indicator of a model, and highlight the deviation location between the simulation and reality [8]. The table below summarises up cited metrics for different components of the electrolyser, comparing real and simulated data for hydrogen production, energy consumption, and pressure behaviour (See Table3).

Table 3 Performance Metrics and Statistical Validation for KoNSTanZE Components

Component	Metrics	MSE	r	R^2
Electrolyser	Mass of H_2	13.7901	0.99981	0.99495
	Energy consumed	5699.4237	0.99979	0.99945
Mid-Pressure Vessel 1	Pressure	317.1198	0.99712	0.92749
Mid-Pressure Vessel 2		33.1112	0.99869	0.99291
Passenger car		138.5319	0.97098	0.62173

Figure 4 emphasises the electrolyser's performance, particularly hydrogen mass produces and its associated energy consumption. The mass of H_2 produced exhibited a high correlation. In addition, the electrolyser energy consumption shows excellent accuracy. This suggests that the simulation model is highly reliable in predicting the amount of hydrogen produced in real-world scenarios.

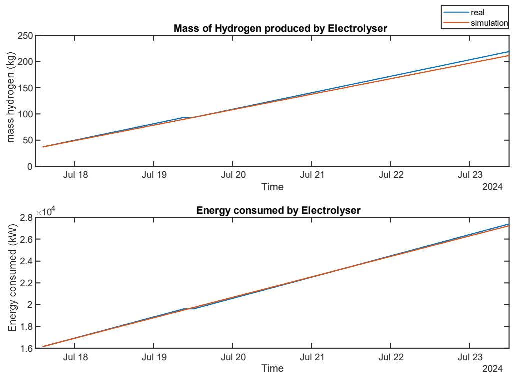

Figure 4 Comparison of Real and Simulated Data of The Electrolyser.

The level of correlation achieved by the simulation was generally very high for both pressure variables, but pressure into mid-pressure vessel 2 demonstrated an outstanding result. This implies that pressure behaviour in the system is well captured by the model. However, the pressure into mid-pressure vessel 1 had a higher MSE. This is attributed to an initial pressure difference in the simulation, which is due to a stop in filling in the real data, as observed in the figures. Despite this discrepancy, the model still exhibits strong predictive capabilities.

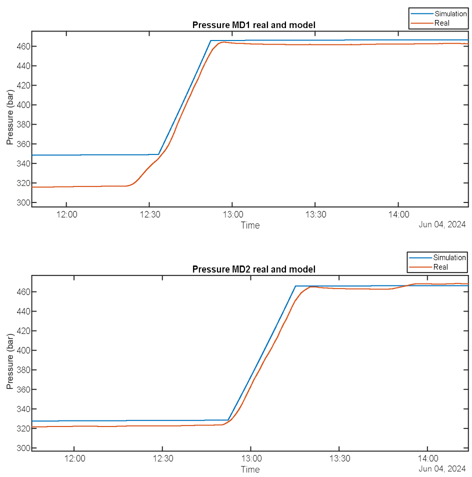

Figure 5 Comparison of Real and Simulated Pressure Profiles for Mid-Pressure Vessels Over Time

The passenger car´s MSE of 138.5319 reflects the fact that there is a consistent offset (approximately 10 bar) between the real and simulated pressure data (See Figure 6), particularly in the early stages. While this impacts the absolute error calculation, as in the validation of the mid-pressure vessel. Due to the difficulty in capturing the initial pressure of the final consumer vessel. Mainly, Figure 6 shows the overall trend of the pressure increase in the simulation, which closely aligns with the real data after this initial deviation.

Therefore, although the MSE, the model still provides a reasonable approximation, particularly for the pressure ramp that is managed by the SAE protocol. The primary issue lies in the starting offset, which, if corrected, would reduce the MSE significantly.

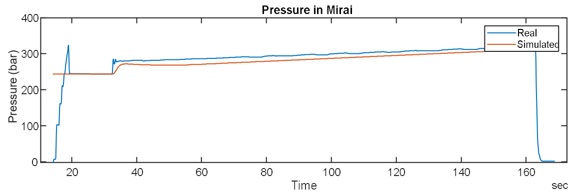

Figure 6 Comparison of Real and Simulated Pressure Profiles for Passenger Car Vessels over Time

4. CONCLUSION

The current research work demonstrates a detailed simulation and validation of the KoNSTanZE project located at the Bosch Homburg plant, with emphasis on the entirety of green hydrogen value chain. The developed simulation model in MATLAB Simulink has been reliable in establishing the significant components of hydrogen production, storage as well as distribution. The critical components specified as PEM electrolyser and storage vessels and hydrogen-powered vehicles and applications in the hardening shop were simulated with focus on the thermodynamics and function. For data validation of the model, information was collected in real-time monitoring. The process of validation applied widely-accepted performance criteria of Mean Squared Error, correlation coefficient (r), and coefficient of determination (R^2) to indicate high accuracy of the model in hydrogen generation, energy utilisation, and in pressure variations of storage and distribution lines. It must be noted some inconsistencies were observed. The first instance such as variation in the refuelling pressure of the vehicles. However, the disparities were not very large as to have a major impact on the evaluation capability of the model. In the long run, the simulation model notwithstanding, is a diverse platform for the green hydrogen value chain optimality hence scenario analysis and operations interferences. As part of the EU Hydrogen Strategy on industrial decarbonisation and the integration of hydrogen into the mobility sector, the KoNSTanZE project is conceived. Thus, this validated model also has a great research perspective in the future, as it can be applied and developed in other industrial and mobility sectors for contributing to the creation of the new, cleaner energy system of the world.

The future work will be dedicated to modelling of the remaining components, such as the bottling filling station and the mobile refueler. This extended model will help to global transformation towards more sustainable energy mix by elaborating hydrogen applications in industrial and transportation segments.

BIBLIOGRAPHY

[1] "KoNSTanZE – Kombinierte Nutzung von regenerativ hergestelltem Wasserstoff in den Sektoren Verkehr/Transport, Produktion und Energie im industriellen Umfeld mit dem Ziel der Entwicklung und mittelfristigen Etablierung CO2 neutraler Produktionsstandorte," [Online]. Available: http://www.projekt-konstanze.de.

[2] J. Rey, F. Segura and J. M. Andújar, "Green Hydrogen: Resources Consumption, Technological Maturity, and Regulatory Framework," *energies,* vol. 16, no. 17, p. 6222, 2023.

[3] M. Hugo, F. Ana Cristina, F. T. Senhorinha and T. José Carlos, "Green Hydrogen Value Chain: Modelling of a PV Power Plant Integrated with H2 Production for Industry Application," *energies,* vol. 17, no. 6, p. 1414, 2024.

[4] J. Riera, R. Lima and O. Knio, "A review of hydrogen production and supply chain modeling and optimization," *International Journal of Hydrogen Energy,* vol. 48, no. 37, pp. 13731-13755, 2023.

[5] W. Yongli, H. Tianliang, Y. Pengjun, L. Weichao and M. Songhua, "Study on the construction theory of digital twin mechanism model for mechatronics equipment," *The International Journal of Advanced Manufacturing Technology,* vol. 131, pp. 5383-5401, 2022.

[6] N. Ashby, T. P. Heavner, S. R. Jefferts, T. E. Parker, A. G. Radnaev and Y. O. Dudin, "Testing Local Position Invariance with Four Cesium-Fountain Primary Frequency Standards<? format?> and Four NIST Hydrogen Masers.," *Physical Review Letters,* vol. 98, no. 7, p. 070802, 2007.

[7] K. Reddi, A. Elgowainy, N. Rustagi and E. Gupta, "Impact of hydrogen SAE J2601 fueling methods on fueling time of light-duty fuel cell electric vehicles," *International Journal of Hydrogen Energy,* vol. 42, no. 26, pp. 16675-16685, 2017.

[8] S. Meduri and J. Nandanavanam, "Prediction of hydrogen uptake of metal organic frameworks using explainable machine learning," *Energy and AI,* vol. 12, p. 100230, 2023.