IZES
Institut für ZukunftsEnergie- und Stoffstromsysteme

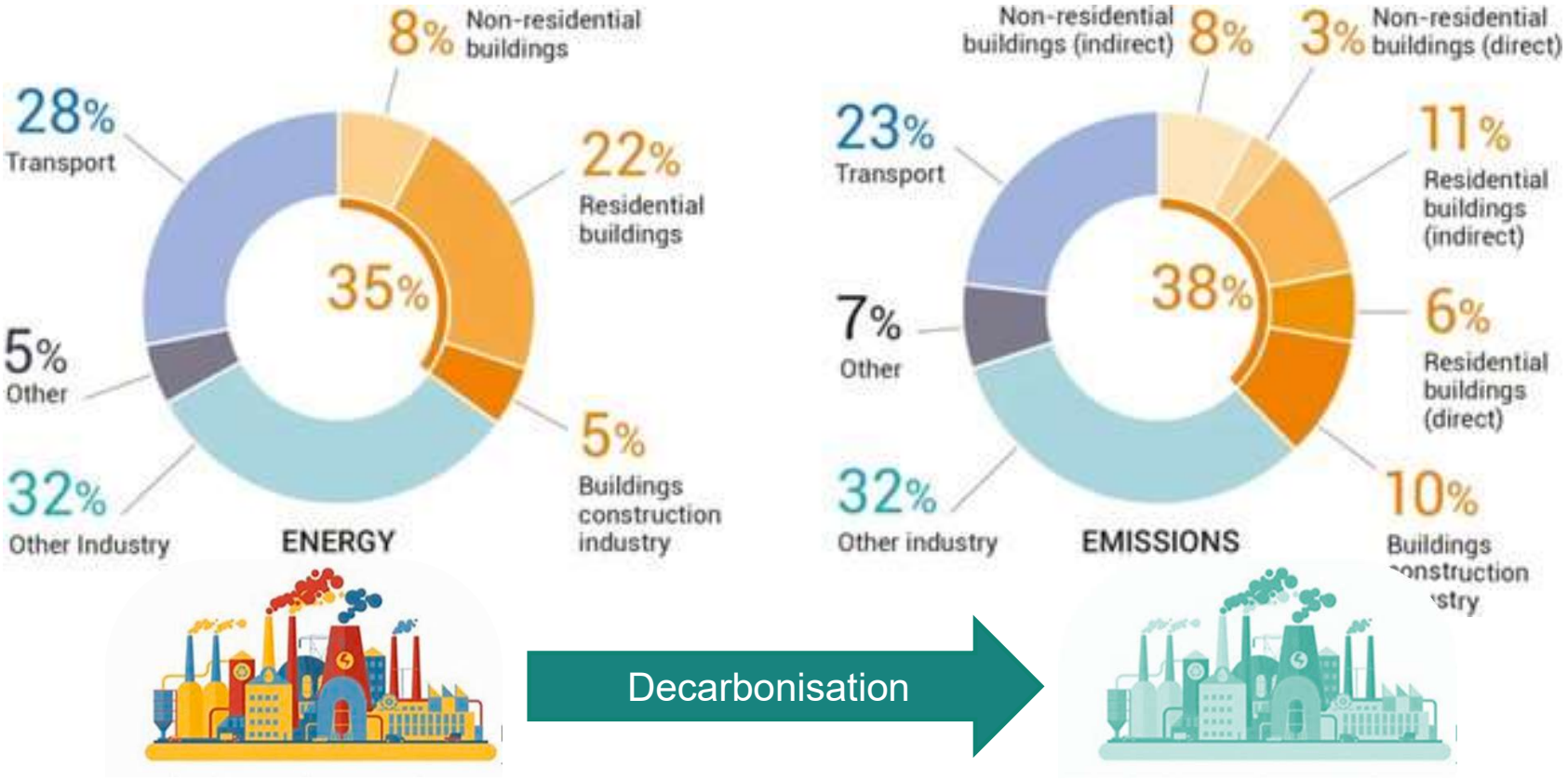
REGWA
Energie - Symposium
Nutzung regenerativer Energiequellen und Wasserstofftechnik

COMPREHENSIVE SIMULATION AND VALIDATION OF GREEN HYDROGEN VALUE CHAIN IN THE KONSTANZE PROJECT: FROM PRODUCTION TO END-USE

F. Mustapha , B. Groß, S, Fleming, M, Byrne, F. Kruchten , and M. Reinstädtler

Contexte / Objectives

Current Distribution of Energy Consumption & CO2 Emissions by Sector (2019)



Contexte / Objectives

Decarbonising Industry

Renawable Energies

Green Hydrogen

Gefördert durch:

Bundesministerium für Wirtschaft und Klimaschutz

aufgrund eines Beschlusses des Deutschen Bundestages

Projektträger Jülich
Forschungszentrum Jülich

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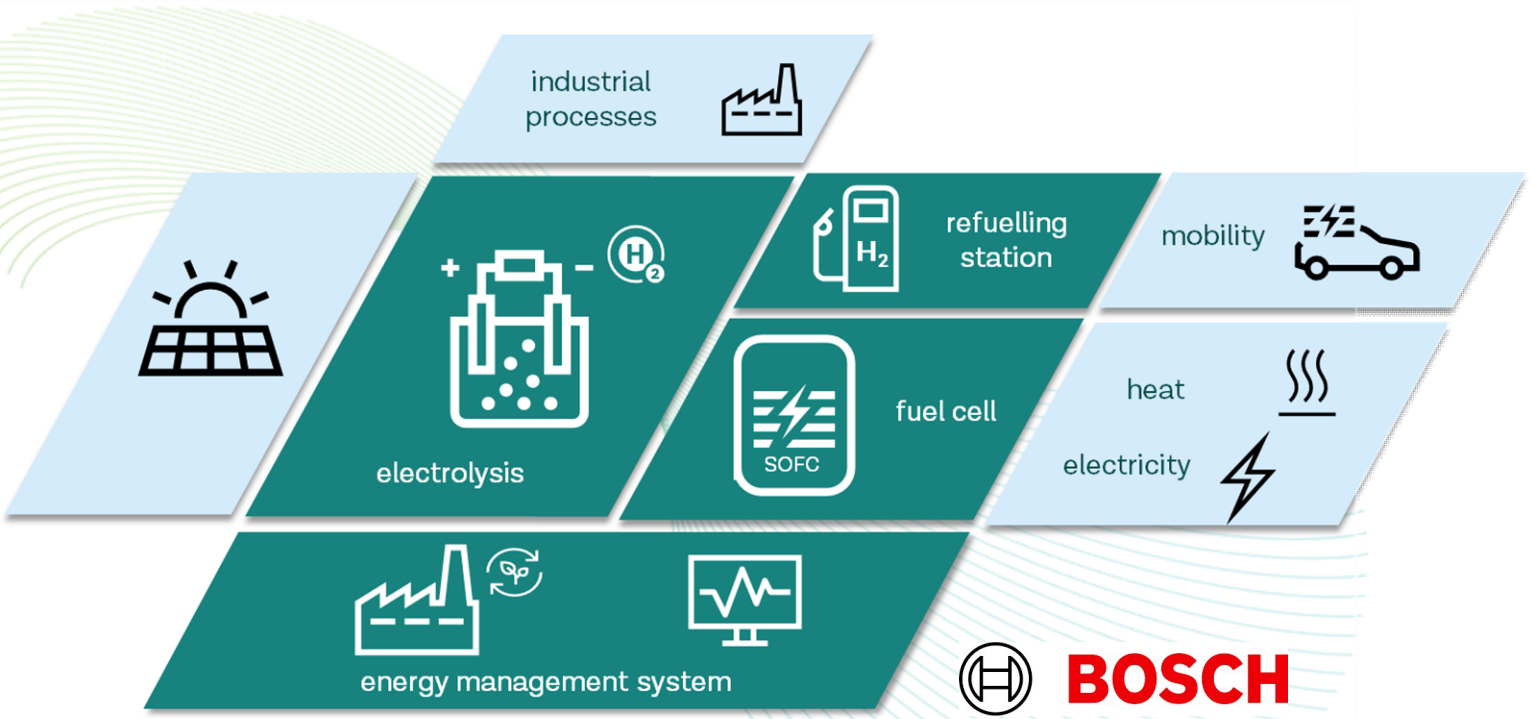
BOSCH

KoNSTanZE project

Contexte / Objectives



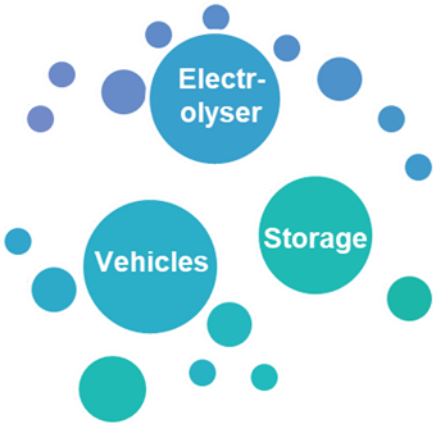
Schematic KoNSTanZE test field

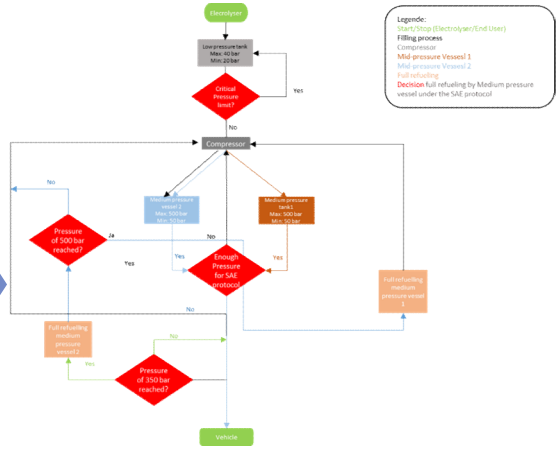
Simulation Model

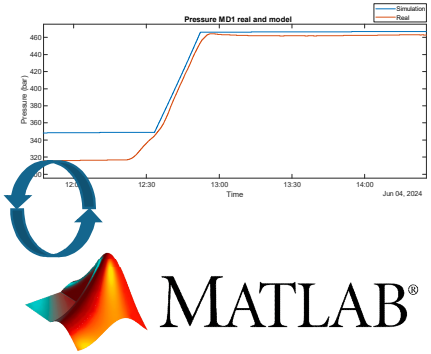
Contexte / Objectives

KoNSTanZE test field: BOSCH credit

Methodology





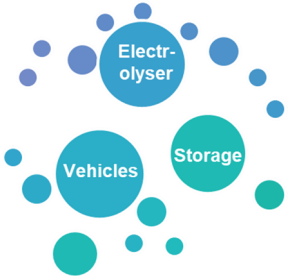


Modelling the components considering boundary conditions

Programming the management system and operating conditions

Validation process through the real data

Methodology: Modelling approach



Modelling the components considering boundary conditions

Source: www.freepik.com

MATLAB®

H_2O

PEM Electrolyser

HYDROGEN

LP

Compressor

MP1 H_2

MP2 H_2

H_2 Station

H_2 Vehicles

Passenger car

Forklift

Tug

Hardning shop

Production

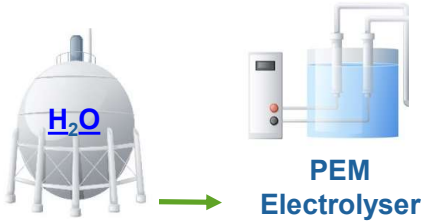
Storage and Distribution

Final End Use

Methodology: Modelling approach

Source: www.freepik.com

MATLAB®



Production

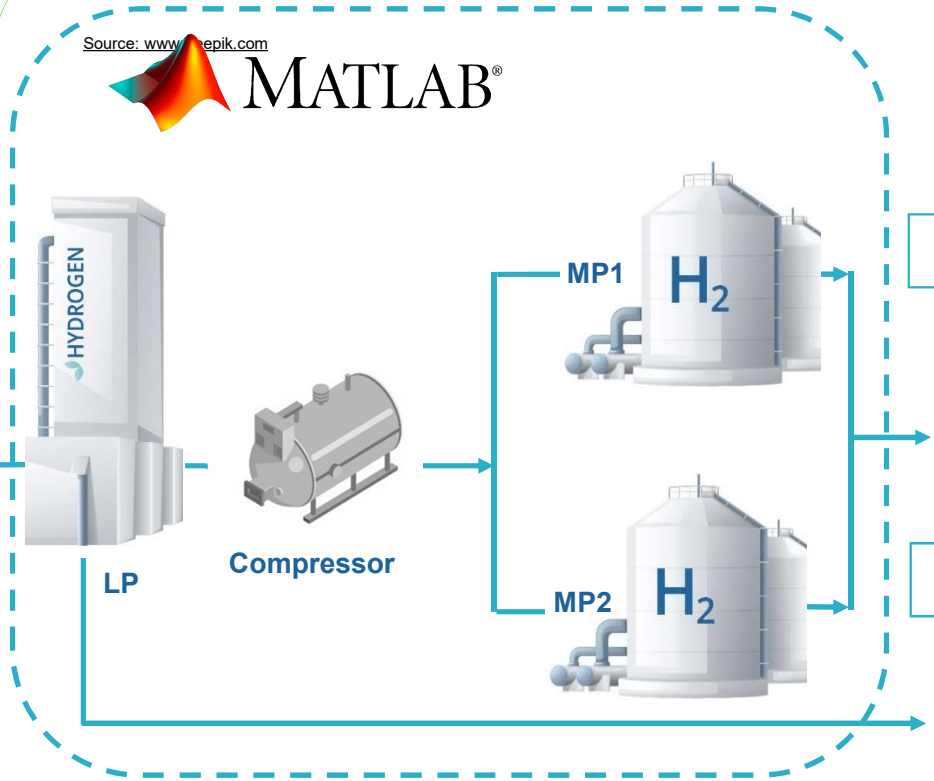
Function

Proton Exchange Membrane electrolyser splits water into hydrogen and oxygen using electricity from renewable sources.
Production rate of 2.5Kg/h

Modelling Approach

Model electrical input, efficiency, **thermodynamic properties** (temperature, pressure), and energy consumption using data from **NIST for hydrogen properties**.

Methodology: Modelling approach



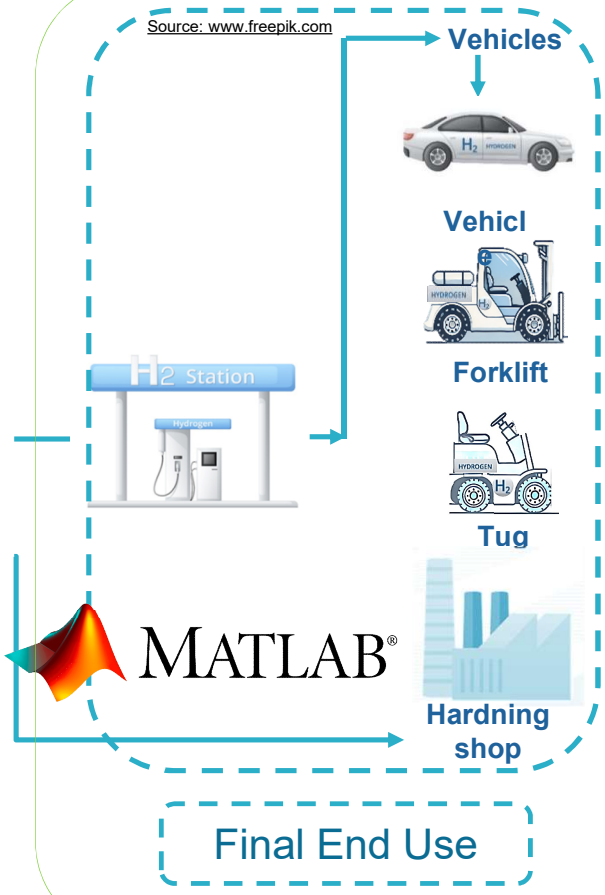
Function

Increases hydrogen pressure from low pressure (**40 bars**) storage to mid-pressure vessels (**500 bars**).
Store hydrogen at different pressure levels for later use.

Modelling Approach

Model the materials, efficiency, **thermodynamic** properties (**temperature, pressure**), and the thermal model of every tank including conduction and convection

Methodology: Modelling approach



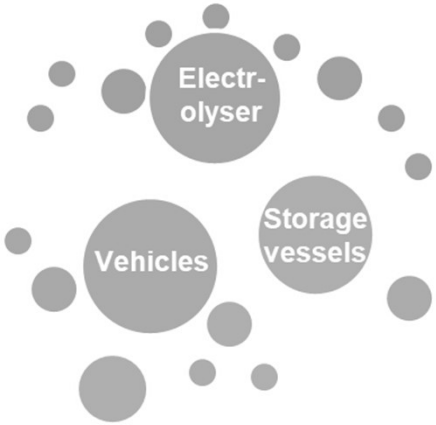
Function

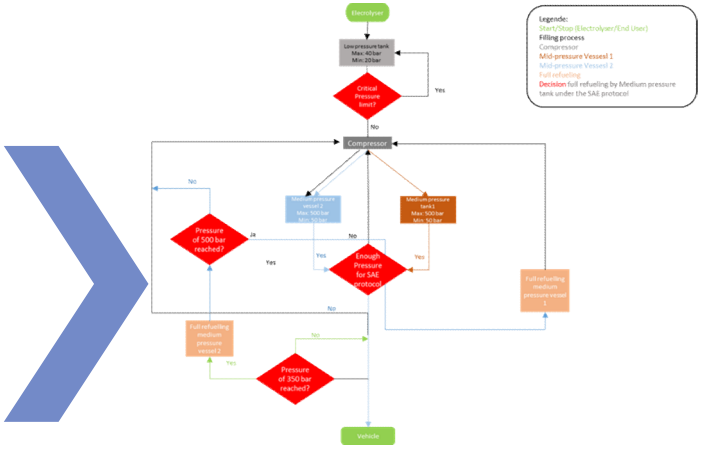
- Distributes hydrogen to the hardening shop and refuelling station According to the **SAE protocol**.
- Vehicles operating in the plant, powered by hydrogen fuel.
- Uses continuously hydrogen for industrial processes.

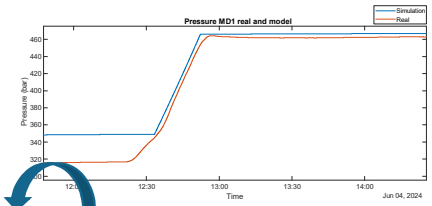
Modelling Approach

- Simulate hydrogen flow dynamics and pressure losses during distribution, considering **thermodynamics** and **fluid** behaviour to ensure efficiency in distribution.
- Simulate onboard hydrogen storage and thermodynamics during operation, including the **refuelling time**.
- Modelled as a **constant consumer** with a constant mass flow rate out, that comes from the low-pressure vessel directly.

Methodology: Operational Conditions







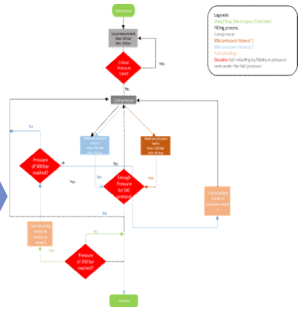
MATLAB®

Modelling the components considering boundary conditions

Programming the management system and operating conditions

Validation process through the real data

Methodology: Operational Conditions

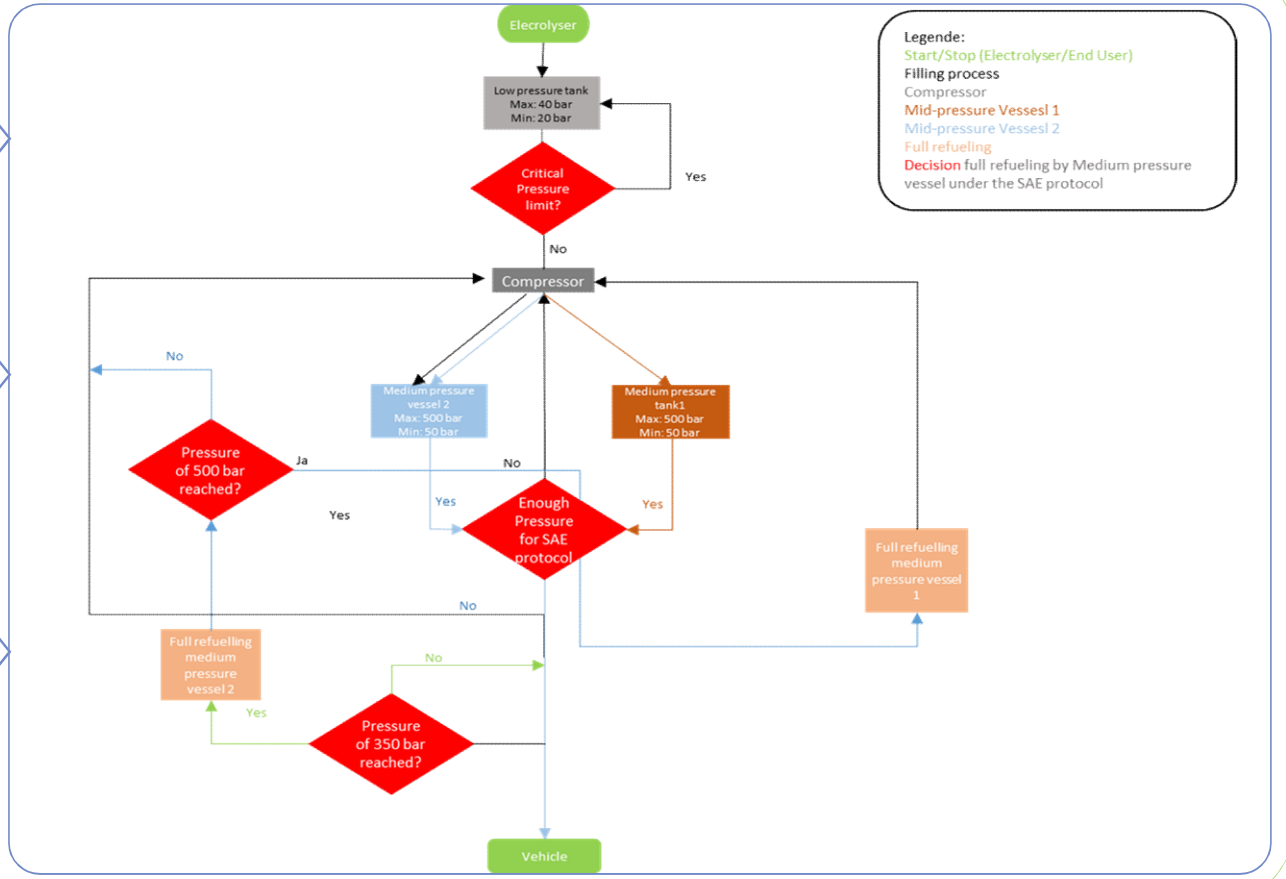


Programming the management system and operating conditions

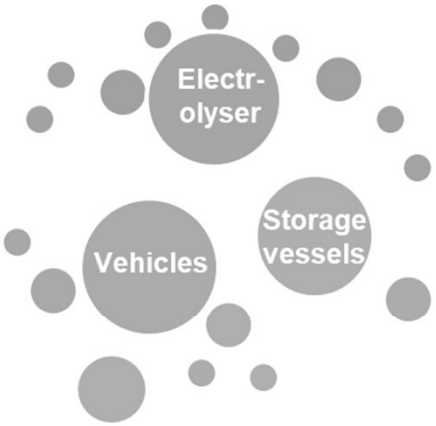
Filling Logic

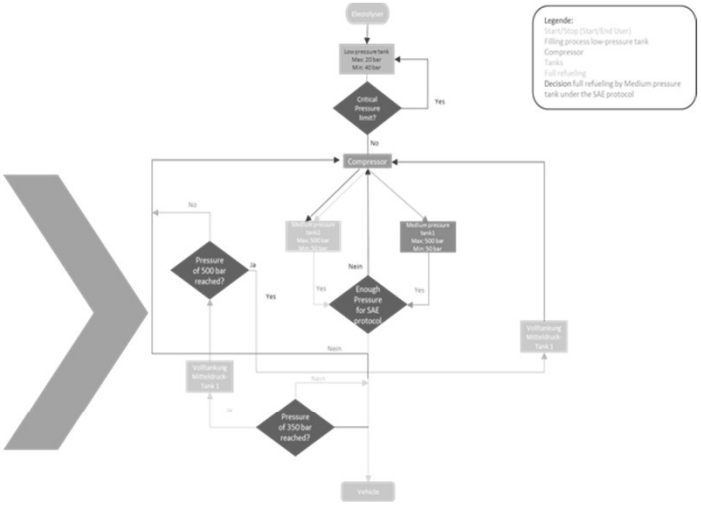
SAE Protocol

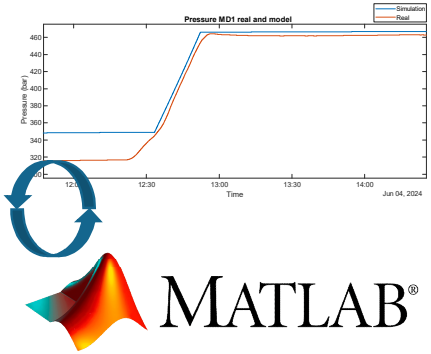
Management and Operational Conditions System.



Methodology: Validation Process







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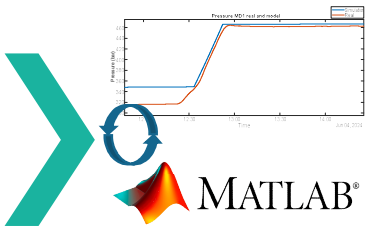
Methodology: Validation Process



Validation process through the real data

Selected Validation Data

Mass of H_2 Produced | **Energy Consumed** | **Pressure**

Mean Squared Error (MSE) | **Correlation Coefficient (r)** | **R-squared (R^2)**

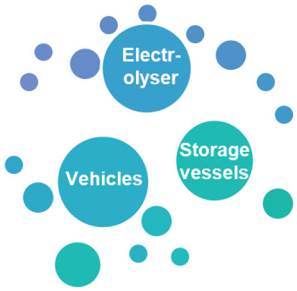
$$\mathbf{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

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

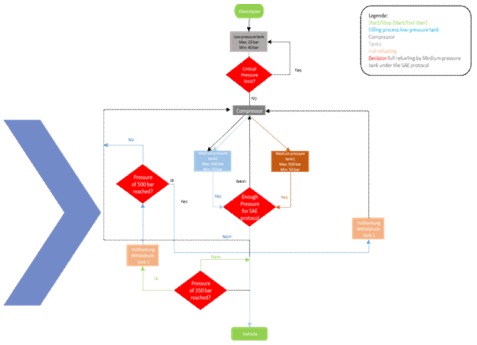
$$\mathbf{R^2} = 1 - \frac{\sum_{i=1}^{n}(y_i-\hat{y}_i)^2}{\sum_{i=1}^{n}(y_i-\bar{y})^2}$$

Methodology: Validation Process

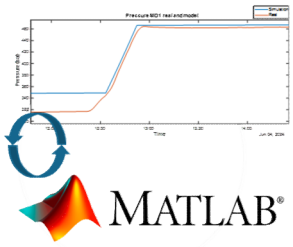
The methodology is applied to :



Modelling the components considering boundary conditions



Programming the management system and operating conditions



Validation process through the real data

PEM Electrolyser

Mid Pressure vessels

Passenger car

Mass of H_2 Produced

Energy Consumed

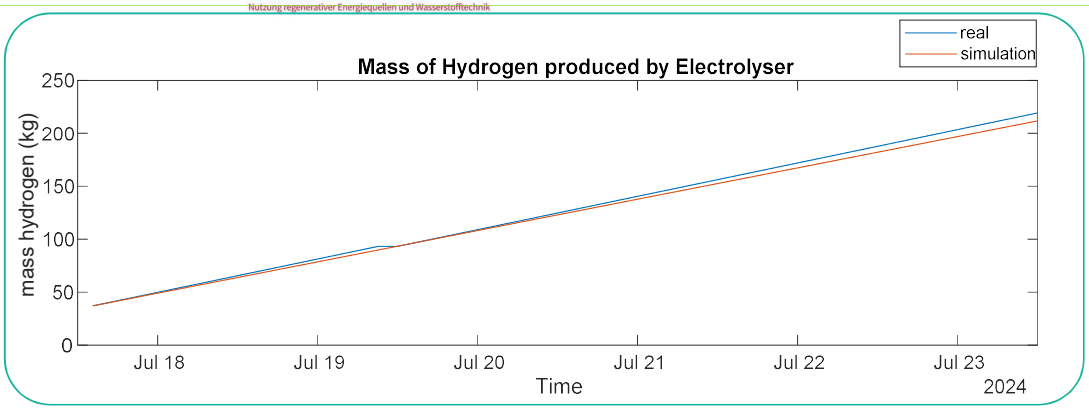
Pressure

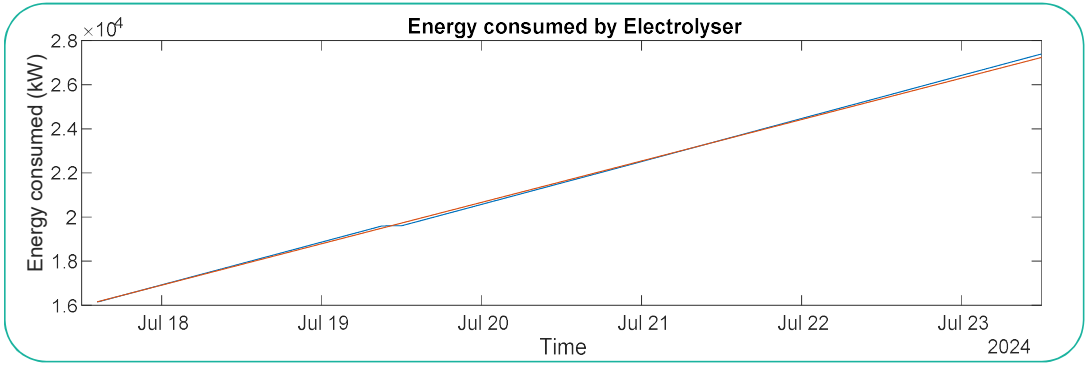
Results

PEM Electrolyser

Mass of H_2 Produced

Energy Consumed

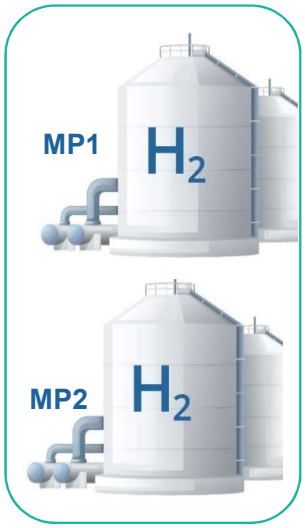




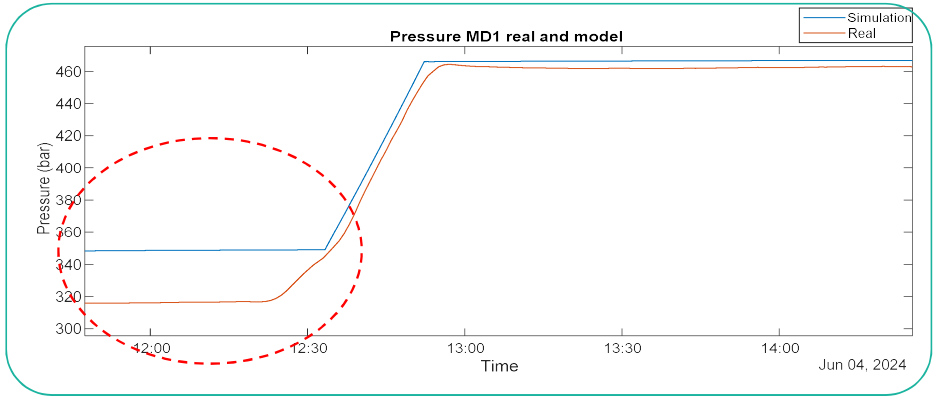
The simulation model accurately predicts hydrogen mass produced and associated energy consumption, showing high reliability in real-world applications.

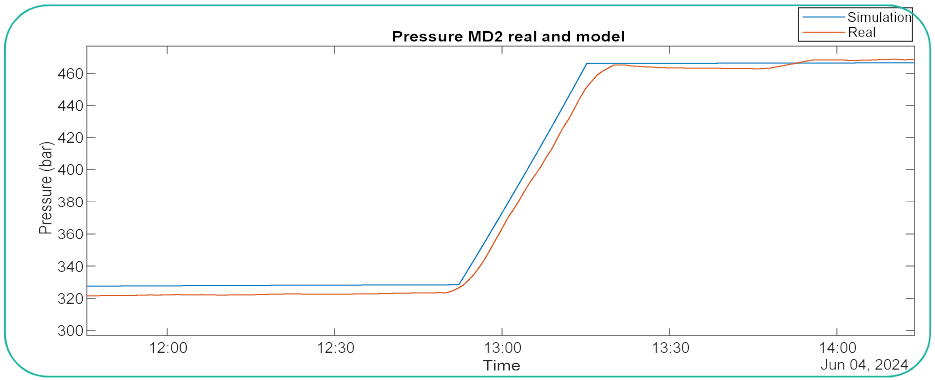
Component	Metrics	MSE	r	R^2
Electrolyser	Mass of H_2	13.7901	0.99981	0.99495
	Energy consumed	5699.4237	0.99979	0.99945

Results



Pressure





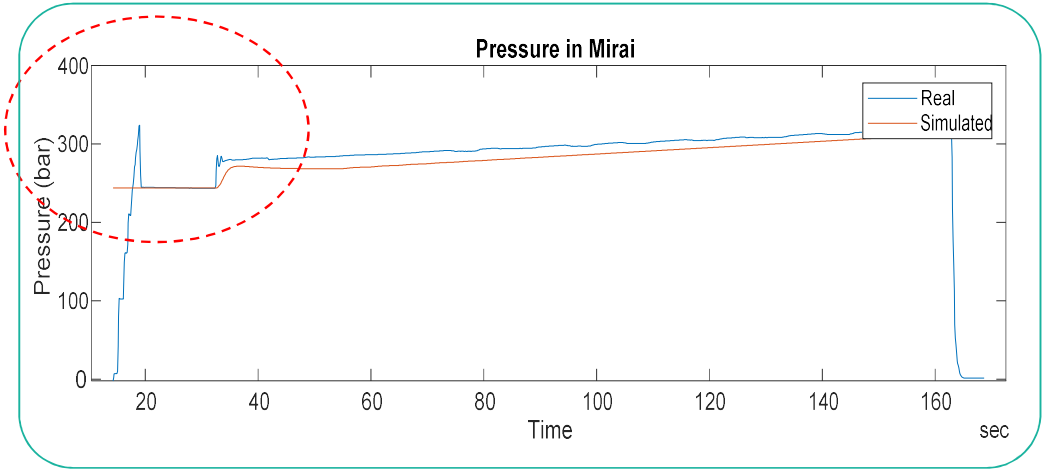
- **Pressure Deviation in Mid-Pressure vessel 1**: A higher Mean Squared Error (MSE) was noted for mid-pressure vessel 1 due to an initial pressure discrepancy caused by real data stops in filling. Despite this, the model's pressure predictions remain robust.

- **Pressure Prediction Accuracy**: The model demonstrates high correlation for pressure variables, especially with mid-pressure vessel 2, indicating strong predictive accuracy in pressure behaviors.

Component	Metrics	MSE	r	R^2
Mid-Pressure vessel 1	Pressure	317.1198	0.99712	0.92749
Mid-Pressure vessel 2		33.1112	0.99869	0.99291

Results

Pressure



Vehicle Pressure Offset:
The model has an MSE of **138.5319**, largely due to a consistent 10-bar offset in initial vehicle vessel pressure. This impacts the absolute error but shows good alignment with real data trends.
The model still provides a reasonable approximation, particularly for the pressure ramp that is managed by the SAE protocol.

Component	Metrics	MSE	r	R^2
Vehicle	Pressure	138.5319	0.97098	0.62173

Conclusion

•**Simulation Model**: A detailed simulation model was developed in MATLAB Simulink, covering **Key Components Simulated**, focusing on thermodynamics and operational functions.

•**Validation Methods**: For model validation, real-time data monitoring was used, with **performance metrics** including **Mean Squared Error (MSE), correlation coefficient (r), and coefficient of determination (R^2),** confirming high accuracy in hydrogen generationmass, energy utilisation, and pressure stability.

•**Observed Inconsistencies**: Minor inconsistencies were found, particularly in refueling pressure variation for vehicles; however, these were minimal and did not significantly impact model evaluation.

•**Long-term Potential**: The validated model serves as a versatile platform for optimizing the green hydrogen value chain, supporting scenario analysis and operational adjustments.

•**Future Research Directions**: Future work will expand the model to include additional components like bottling filling stations and mobile refuelers, with applications in broader industrial and transportation sectors for advancing a sustainable energy mix.

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