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Posted Date: 19 May 2026

doi: 10.20944/preprints202605.1191.v1

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Article

Digital Twin and Machine Learning-Based Diagnostics for PEM Electrolyzer

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Abstract

The degradation of the health state of Proton Exchange Membrane (PEM) water electrolyzer, caused by power supply variability, operating temperature changes, and other chemical factors, represents a major challenge for green hydrogen production efficiency. This paper presents an advanced hybrid system combining a digital twin and machine learning, enabling real-time anomaly detection of a PEM electrolyzer. This intelligent approach allows for the real-time prediction of operating parameters, namely current, voltage, and hydrogen flow rate, via *Azure Machine Learning*, and their visualization within the system's digital twin via *Azure Digital Twins*. Furthermore, the comparison between simulated data from the digital twin and those predicted by machine learning enables the anticipation of PEM electrolyzer anomalies. The selected prediction models rely on the *Extreme Random Trees* algorithm for current and voltage estimation, and on the *Elastic Net* algorithm for hydrogen flow rate prediction. The obtained results confirm the robustness of the proposed approach, with coefficients of determination R^2 of 0.99820, 0.99693, and 0.99665 for current, voltage, and hydrogen flow rate respectively, associated with *Normalized Root Mean Square Errors (NRMSE)* of 0.00870, 0.011278, and 0.11087. This high accuracy provides the digital twin with the capability to anticipate failures and extend the PEM electrolyzer's lifespan, with a view to optimizing the global efficiency of green hydrogen production.

Keywords: anomaly; diagnostics; digital twin; PEM electrolyzer; machine learning

Introduction

In response to the growing global energy demand and the increasing urgency of environmental and climatic challenges, the adoption of low-carbon and environmentally friendly energy systems has gained significant attention. Green hydrogen, characterized by its eco-friendly nature and high energy density, is regarded as a promising energy source capable of mitigating greenhouse gas emissions [1]. Among green hydrogen production methods, Proton Exchange Membrane (PEM) water electrolysis remains the most prevalent technology due to its substantial advantages. These include high current density ($> 2 A/cm^2$), low ohmic losses, and a fast response time ($< 5 seconds$) to fluctuations in renewable energy sources. However, its limited lifespan and component degradation, primarily caused by power supply instability, continue to hinder its widespread commercial deployment, thereby affecting the overall efficiency of green hydrogen production [2,3]. Membrane degradation represents a major challenge, as it leads to reduced proton conductivity and increased ohmic resistance. This results in higher cell voltages and increased energy consumption for hydrogen production [3,4].

To address these challenges, an online diagnostic system capable of real-time monitoring of the electrolyzer's operating state is necessary to rapidly isolate faults by adjusting operating parameters [5].

In this context, the authors of [6] proposed a prediction method based on an Extended Kalman Filter for estimating the non-measurable degradation effects of a PEM electrolyzer. This filter provides an estimate of the catalyst and membrane states using only input (current) and output

(voltage) data. Going further, article [3] proposes a machine learning framework for membrane fault detection, relying on current-voltage characteristics and combining validated physical modeling with classification algorithms. In [5], the authors proposed a precise fault diagnosis system for Proton Exchange Membrane Fuel Cells, based on a hybrid deep learning network combining Residual Networks and Long Short-Term Memory (ResNet and LSTM) networks. Furthermore, the authors of [7] present a comparative study of machine learning algorithms to evaluate the impact of four key physical parameters, notably temperature, Porous Transport Layer (PTL) thickness, membrane thickness, and PEM electrolyzer voltage. In [8], a new diagnostic method is presented for estimating degradation parameters, based on the analysis of the linearized polarization curve. This approach defines and integrates two key parameters: the surface degradation rate and the membrane degradation rate.

The analysis of these works demonstrates that the use of Artificial Intelligence for data and fault prediction in electrolyzers is making significant strides toward improving efficiency. However, to make a major contribution to green hydrogen production systems, this paper presents a hybrid system combining Digital Twin technology and Machine Learning. This system enables real-time monitoring and comparison of predicted versus actual data from the PEM electrolyzer, with the aim of optimizing component health, extending the electrolyzer's lifespan, and improving the overall system efficiency.

II.1. PEM Electrolyzer Equivalent Circuit

The equivalent circuit is illustrated in Figure 1. The dynamic behavior of the cathode and anode is modeled by two RC branches. The amount of electric power converted into hydrogen is given by the product of the voltage E_{rev} and the current flowing through the electrolyzer, while the resistance R_m accounts for the losses in the membrane. The two capacitances can be considered equal, while the resistance R_c models the heat loss in the cathode, and R_a represents both the Gibbs energy and the heat loss in the anode [9].

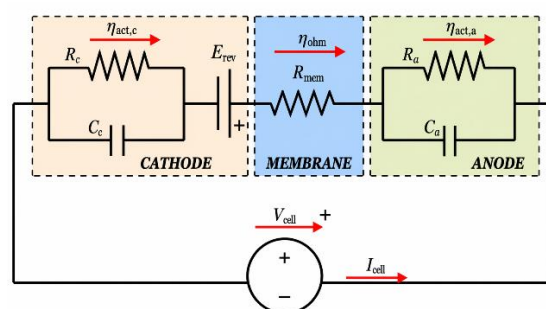


Figure 1. PEM electrolyzer equivalent circuit.

II.2. PEM Electrolyzer Modeling

The detailed electrochemical modeling accounts for the open-circuit voltage as well as three types of overvoltages: activation, ohmic, and concentration. To achieve the desired hydrogen production at a constant flow rate, multiple elementary cells are connected in series to form a PEM electrolyzer stack [10].

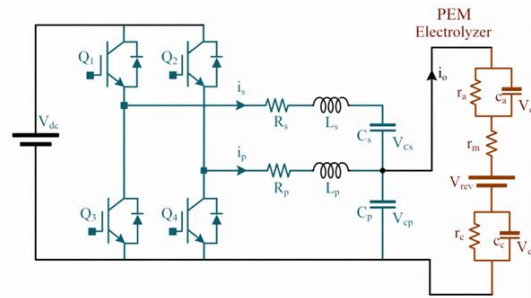


Figure 2. PEM electrolyzer associated with an interleaved buck converter.

The interleaved buck converter consists of two sub-circuits operating with phase interleaving, each controlled by two electronic switches, resulting in a total of four active switches. The timing diagram explains the switching operation, the switch activation times, as well as the evolution of the inductor currents in each phase. By applying Kirchhoff's laws to both sub-circuits during the various conduction phases, the input-state-output models of the system are derived [11].

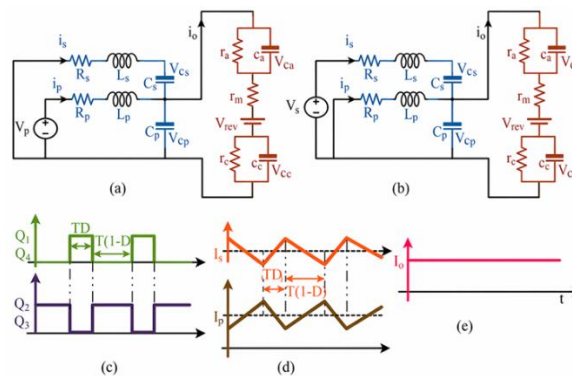


Figure 3. Operational timing diagram of the interleaved converter: (a) Mode I; (b) Mode II; (c) switching pulse; (d) inductor currents; (e) output current [11].

Mode 1: when Q_1, Q_4 are activated and Q_2, Q_3 are deactivated for $T < t \leq DT$

$$\left. \begin{aligned} L_p \frac{di_p}{dt} &= v_p - i_p \cdot R_p - v_{cp} \\ L_s \frac{di_s}{dt} &= -v_{cs} - i_s \cdot R_s - v_{cp} \\ C_s \frac{dv_{cs}}{dt} &= i_s \\ C_p \frac{dv_{cp}}{dt} &= i_p + i_s - \frac{v_{cp}}{r_m} + \frac{v_{ca}}{r_m} + \frac{v_{rev}}{r_m} + \frac{v_{cc}}{r_m} \\ C_a \frac{dv_{ca}}{dt} &= \frac{v_{cp}}{r_m} - \frac{v_{ca}}{r_m} - \frac{v_{rev}}{r_m} - \frac{v_{cc}}{r_m} - \frac{v_{ca}}{r_a} \\ C_c \frac{dv_{cc}}{dt} &= \frac{v_{cp}}{r_m} - \frac{v_{ca}}{r_m} - \frac{v_{rev}}{r_m} - \frac{v_{cc}}{r_m} - \frac{v_{cc}}{r_c} \end{aligned} \right\} \quad (1)$$

Mode 2: when Q_2, Q_3 are activated and Q_1, Q_4 are deactivated for $0 < t \leq (1 - D)T$

$$\left. \begin{aligned} L_p \frac{di_p}{dt} &= -i_p \cdot R_p - v_{cp} \\ L_s \frac{di_s}{dt} &= V_{in} - v_{cs} - i_s \cdot R_s - v_{cp} \\ C_s \frac{dv_{cs}}{dt} &= i_s \\ C_p \frac{dv_{cp}}{dt} &= i_p + i_s - \frac{v_{cp}}{r_m} + \frac{v_{ca}}{r_m} + \frac{v_{rev}}{r_m} + \frac{v_{cc}}{r_m} \\ C_a \frac{dv_{ca}}{dt} &= \frac{v_{cp}}{r_m} - \frac{v_{ca}}{r_m} - \frac{v_{rev}}{r_m} - \frac{v_{cc}}{r_m} - \frac{v_{ca}}{r_a} \\ C_c \frac{dv_{cc}}{dt} &= \frac{v_{cp}}{r_m} - \frac{v_{ca}}{r_m} - \frac{v_{rev}}{r_m} - \frac{v_{cc}}{r_m} - \frac{v_{cc}}{r_c} \end{aligned} \right\} \quad (2)$$

II.3. Control Strategy of the Interleaved Buck Converter

The primary objective of the control strategy for the stacked interleaved buck converter is to maintain the PEM electrolyzer voltage and current at stable and constant values. To achieve this, a dual-loop control technique is employed. It consists of an inner current loop and an outer voltage loop. The faster current loop controls the inductor dynamics, while the slower voltage loop regulates the electrolyzer supply voltage [12,13].

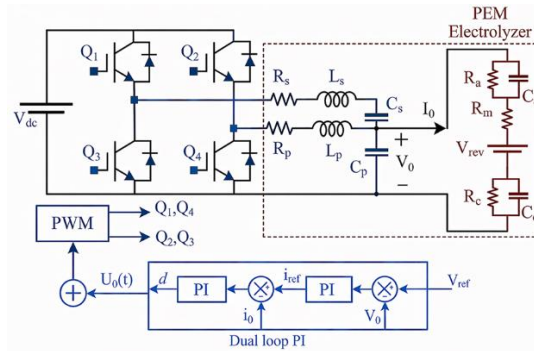


Figure 4. SIBC control strategy [11].

The difference between the measured and reference voltages is used to generate the current reference value, enabling a more precise response to power supply variations. A Proportional-Integral (PI) controller is employed to implement both control loops. The PI controller parameters are tuned based on the frequency response from the Bode plot, ensuring system stability and a fast response time while minimizing overshoot [13].

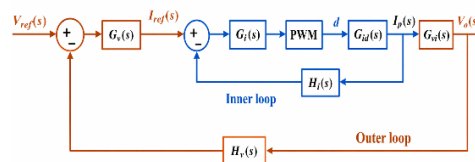


Figure 5. Block diagram of the dual-loop control.

The electrical model of the PEM electrolyzer used in this work is implemented and simulated within the MATLAB/Simulink environment. The data generated by this simulation, specifically the current and voltage at the electrolyzer terminals as well as the produced hydrogen flow rate, serve as the dataset used for training the machine learning algorithm via Azure Machine Learning (AML) and are visualized through the electrolyzer's digital twin designed using Azure Digital Twins.

Table 1.

Symbol	Quantity	Values and Units
Vdc	DC Bus Voltage	100 – 200 V
T	Temperature	50 – 80 °C
Icell	Cell current	0 – 60 A
Ra	Anode resistance	0.333 Ω
Rc	Cathode resistance	0.033 Ω
Ca	Anode capacitance	33.33 F

C_c	Cathode capacitance	33.33 F
N_{cell}	Number of cells	6
V_{rev}	Reversible voltage	1.23 V
R_{mem}	Membrane resistance	0.09 Ω
L_p, L_s	Primary and secondary inductances	450×10^{-6} H
R_p, R_s	Primary and secondary resistance	60×10^{-3} Ω
C_p	Primary capacitance	100×10^{-6} F
C_s	Secondary capacitance	10×10^{-6} F
N, D	Switching Frequency	100×10^3 Hz

Digital Twins

In an Internet of Things (IoT)-based green hydrogen production system, the key steps for data acquisition and digital twin model synchronization include acquisition, transmission, preprocessing, synchronization, and model update [14]. However, in the absence of a real physical green hydrogen production system, a simulation is performed within the *MATLAB/Simulink* environment. This enables the collection of operating parameters—specifically current, voltage, and hydrogen flow rate—for machine learning purposes and establishes communication with the system's digital twin developed using *Azure Digital Twins*.

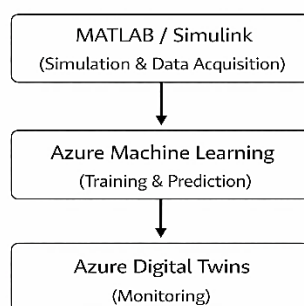


Figure 6. Communication architecture between MATLAB/Simulink, Azure Machine Learning, and Azure Digital Twins.

The Azure IoT platform is utilized for the modeling and cloud-based visualization of the digital twin. The transmission of the real-time telemetry data stream to the cloud (Azure IoT Hub) is ensured by a MATLAB/Simulink *MQTT Client Publish* block. This block initially connects to a local MQTT broker (Eclipse Mosquitto™), which subsequently publishes the data to their respective topics in Node-RED. Finally, SSL/TLS-secured MQTT connectors within Node-RED ensure the routing of data to the IoT Hub [15]. Simultaneously, the data generated by the system simulation in MATLAB/Simulink—specifically the electrolyzer current and voltage, as well as the green hydrogen flow rate—are utilized for machine learning via Azure Machine Learning. This enables real-time data prediction, which is also visualized by the PEM electrolyzer's digital twin.

IV.1. Azure Machine Learning

Azure Machine Learning (AML) is a Microsoft cloud service designed to accelerate and manage the lifecycle of machine learning (ML) projects. ML professionals, data scientists, and engineers use

it daily to train and deploy models and to manage machine learning operations (MLOps), thereby facilitating model monitoring, retraining, and redeployment [16]. The workspace environment for a machine learning project is Azure Machine Learning Studio.

IV.2. Azure Machine Learning Studio

Azure Machine Learning Studio is a web-based application that enables the creation, training, testing, and deployment of machine learning (ML) models. It facilitates rapid experimentation, hyperparameter optimization, pipeline creation, and interface management [16].

IV.3. Automated Machine Learning

Automated Machine Learning (AutoML) enables the training of regression models by rapidly iterating through numerous combinations of algorithms and hyperparameters. This approach identifies the optimal model based on a specific performance metric [16].

IV.4 Machine Learning Stages

- Data Assets

Data assets serve as the foundation for computations in Azure Machine Learning. They are created from datastores, local files, public URLs, or open datasets. In this paper, the parameters (currents, voltages, and flow rates) are obtained from the simulation of the PEM electrolyzer electrical model performed in MATLAB/Simulink and serve as the dataset for machine learning.

- Task Type: Regression

Azure Machine Learning offers several task types: classification, forecasting, regression, and computer vision. In this paper, we consider regression. This common supervised learning task is primarily used to predict numerical values, such as those simulated in MATLAB/Simulink for the PEM electrolyzer [17].

- Validation Type

Validation methods in Automated Machine Learning enable the evaluation and testing of various selected algorithms to identify the most accurate model. In this paper, Monte Carlo Cross-Validation was selected. This is a simple and efficient procedure that requires a sequence of observations for model training and validation [17].

- Data Prediction Algorithms

Automated Machine Learning (AutoML) evaluates various models and algorithms during the automation and tuning process. The specific task type determines the list of candidate algorithms. In this study, the *Extreme Random Trees* algorithm was selected for predicting current and voltage, while the *Elastic Net* algorithm was chosen for estimating the hydrogen flow rate. The prediction principle involves testing and validating different algorithms to select the optimal model based on performance metrics, the primary one being the Normalized Root Mean Squared Error (NRMSE).

V. Results and Discussion

V.1. Azure Machine Learning Results

- Actual and Predicted Current Values

Figure 7 illustrates the comparison between the actual (simulated) values and the values predicted by the Automated Machine Learning model. The histogram on the x-axis indicates that most current values utilized for prediction fall within the range of 4.04A and 58.81A. This represents a sample density significantly higher than that of the first interval [0 ; 4.04A] and the last interval [58.81A ; 58.9A]. The robustness of the *Extreme Random Trees* prediction algorithm is validated by a coefficient of determination R^2 of 0.9982 and a Normalized Root Mean Squared Error (NRMSE) of 0.00870, ensuring a prediction error of less than 1%.

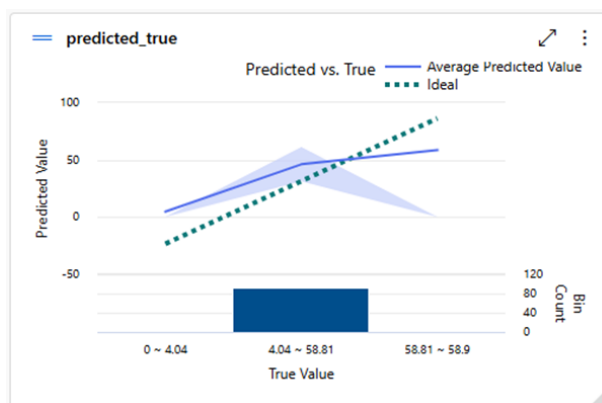


Figure 7. Comparison of simulated and predicted currents.

- Actual and Predicted Voltage Values

Figure 8 illustrates the actual and predicted values of the PEM electrolyzer voltage obtained via Automated Machine Learning. The dark blue histogram on the x-axis represents most of the training data used, specifically between $7.59V$ and $12V$. This data density enables high performance, as demonstrated by the predicted voltage curve (blue line), which closely tracks the actual values. The robustness of the *Extreme Random Trees* algorithm is validated by a Normalized Root Mean Squared Error (NRMSE) of 0.011278 and a coefficient of determination R^2 of 0.99693.

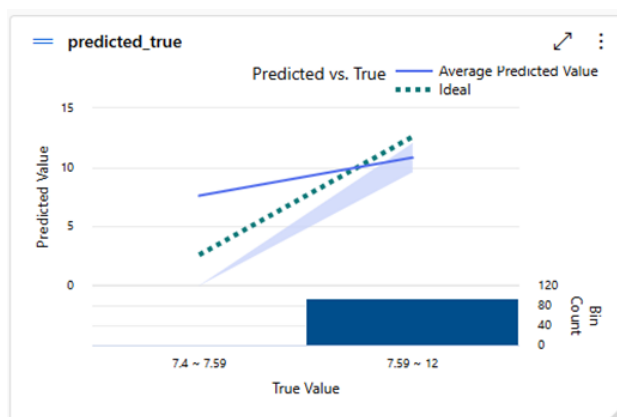


Figure 8. Actual and Predicted Voltage Values.

- Simulated and Predicted Flow Rate Values

Figure 9 illustrates the actual and predicted values of the hydrogen flow rate produced by the PEM electrolyzer. The results of the *Elastic Net* algorithm demonstrate high prediction performance, as indicated by the blue curve representing the mean predicted flow rate. The blue histogram covers nearly all training values, specifically within the interval $[0.19L/min ; 2.4L/min]$, highlighting a low data density at the beginning of the process (varying between 0 et $0.19L/min$). Despite this, the algorithm remains robust with a coefficient of determination R^2 of 0.99665—corresponding to 99.6% accuracy—and a Normalized Root Mean Squared Error (NRMSE) of 0.011087.

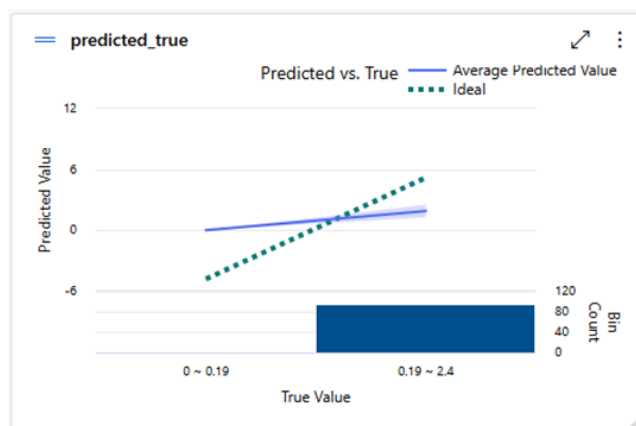


Figure 9. Simulated and Predicted Flow Rate Values.

V.2. Azure Digital Twins Results

• Predicted and Actual Current Values

Figure 10 illustrates the comparison between the simulated current values and those predicted via Azure Machine Learning, as well as the anomaly score, which quantifies the deviation between these two values. This visualization is rendered by the PEM electrolyzer's digital twin developed using Azure Digital Twins. The predicted and actual current curves closely overlap, exhibiting minimal difference. Consequently, the anomaly threshold is not breached, thereby validating the robustness of the *Extreme Random Trees* algorithm with a Normalized Root Mean Squared Error (NRMSE) of 0.00870, ensuring a prediction error of less than 1%.

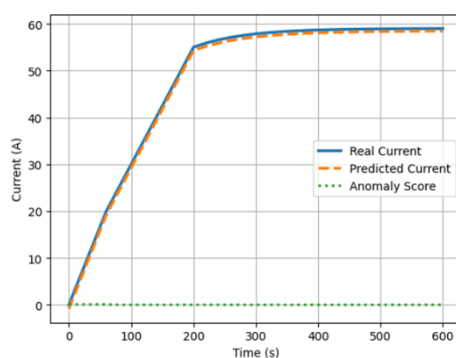


Figure 10. Comparison between the actual and predicted current of the PEM stack.

• Predicted and Actual Voltage Values

Figure 11 demonstrates the validation of the predicted voltage values, which closely track the measured values visualized in real-time via the PEM electrolyzer's digital twin. The anomaly score, representing the deviation between measured and predicted values, remains very low, as indicated by the curve hugging the x-axis. This performance is attributed to the robustness of the *Extreme Random Trees* prediction algorithm, which achieves a Normalized Root Mean Squared Error (NRMSE) of 0.011278.

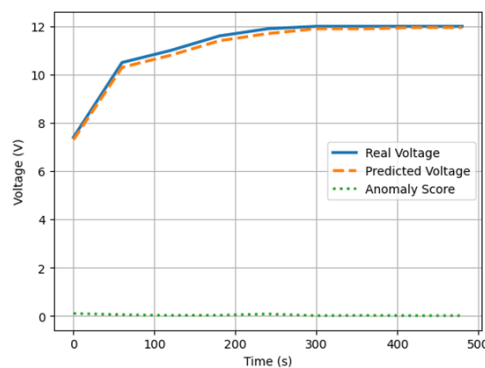


Figure 11. Comparison between actual and predicted voltage of the PEM stack.

- Predicted and Actual Flow Rate Values

Figure 12 illustrates the real-time measured and predicted values for green hydrogen flow rate. The alignment of these curves confirms the operability of the digital twin and the machine learning framework integrated with the PEM electrolyzer system simulated in *Matlab/Simulink*. Furthermore, the profile of the anomaly score curve highlights a negligible gap between the measured and predicted values. Despite this slight variance, no anomalies were detected, as the production flow rate remains directly dependent on the electrolyzer current. The robustness of the *Elastic Net* algorithm is further validated by a normalized mean squared error (*NMSE*) of 0.011087.

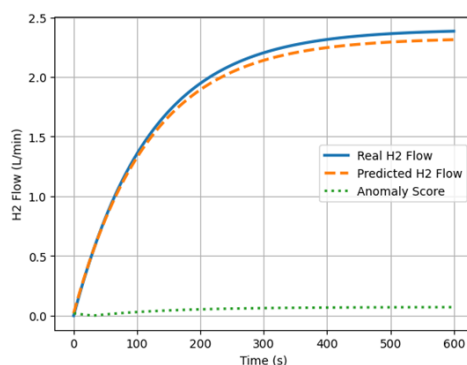


Figure 12. Comparison between actual and predicted hydrogen flow rate values.

VI. Conclusion and Future Work

This paper presents a system combining Digital Twin technology and Machine Learning to monitor the operating parameters of a green hydrogen production system, specifically the electrolyzer current, voltage, and produced hydrogen flow rate. Real-time data, derived from the mathematical model simulation in MATLAB/Simulink, are transmitted to Azure Machine Learning. To this end, Automated Machine Learning (AutoML) selected the highest-performing models: the *Extreme Random Trees* algorithm for current and voltage prediction, and the *Elastic Net* algorithm for hydrogen flow rate prediction.

Concurrently, the electrolyzer's digital twin facilitates real-time monitoring of the evolution of measured and predicted parameters, enabling early anomaly detection and the anticipation of component failures. The obtained results validate the robustness of each algorithm, exhibiting a Normalized Root Mean Squared Error (NRMSE) of less than 1 %. Furthermore, this work opens a significant perspective toward combining this hybrid Digital Twin and Machine Learning system with Quantum Computing to overcome the limitations of classical computing.

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