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AI-DRIVEN MODELING AND OPTIMIZATION OF DYNAMIC ELECTROCHEMICAL RESPONSES IN PEM WATER ELECTROLYSIS SYSTEMS

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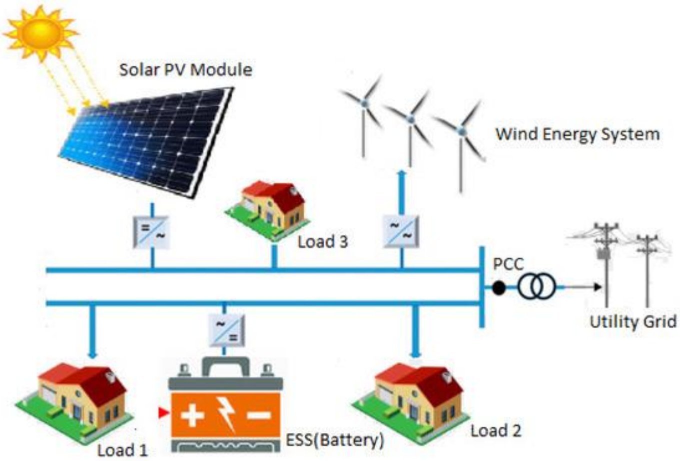
Abstract

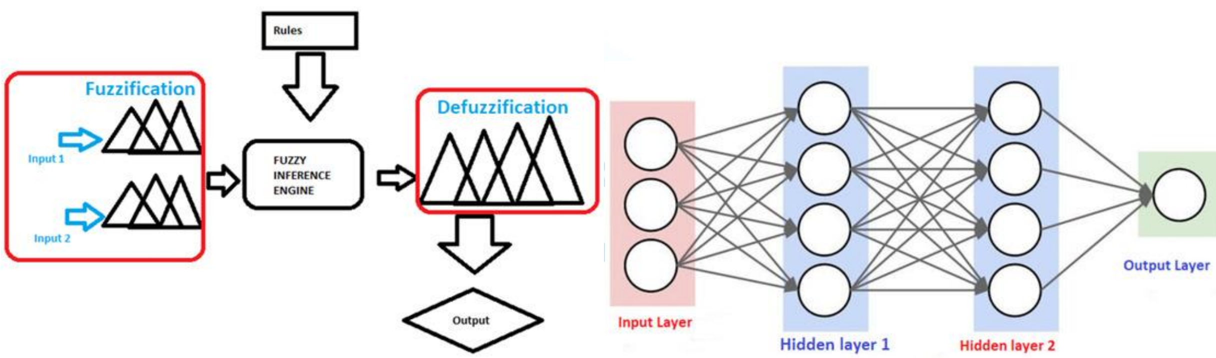
Proton Exchange Membrane (PEM) water electrolysis is key for sustainable hydrogen production, but optimizing dynamic electrochemical responses is challenging due to complex interactions among temperature, pressure, and current density. This study develops AI-driven models to predict and optimize PEM electrolyzer performance across various operating conditions to enhance hydrogen yield and energy efficiency. Data from ten PEM electrolysers were used to train models with machine learning techniques including Artificial Neural Networks (ANN), Support Vector Machines (SVM), and Decision Trees. Hyperparameters were optimized via Grid Search and Genetic Algorithms, while PCA and SHAP were applied for feature selection. Reinforcement learning and evolutionary algorithms tuned operational parameters. The ANN model achieved high accuracy ($R^2 = 0.93$), and optimization improved hydrogen production by 30% and reduced energy consumption by 15%. These results demonstrate that AI-based modeling and optimization significantly boost PEM electrolyzer performance, advancing sustainable hydrogen generation.

INTRODUCTION

The combination of artificial intelligence (AI) with proton exchange membrane (PEM) water electrolysis is a promising strategy to increase the performance and efficiency of hydrogen generation. PEM electrolysis, a key technology of producing green hydrogen, has dramatic complex electrochemical reactions and is heavily affected by several variables such as temperature, pressure, current density, and catalysts (Zhang et al., 2024).



Conventional practice for the development and optimization of these systems frequently is based on empirical testing and trail-and-error techniques so that the development takes time and the resources necessary may be extensive. AI-based modeling is a data-first approach and constructs predictive models for the dynamic behavior of PEM electrolysis under different operational conditions (Shi et al., 2024).



With the recent developments of ML technology, advanced models able to predict PEM electrolyze transient electrochemical responses have been developed. For example, ANNs have been used to establish correlation models for predicting hydrogen mass flow rates, with high accuracy (determination coefficients up to 0.90 and mean squared errors down to 0.00337) (Hossain & Rahman, 2024). These models take as input the stack current, oxygen pressure, hydrogen pressure and stack temperature and output the dynamics of the system (Mohamed et al., 2022). This provides a marked departure from traditional optimization methods, enabling finer predictions and on-the-fly adjustments.

In addition, the optimization of MEAs, also a key component in PEM electrolyzes, has been improved with AI methods. Machine learning models, such as XGBoost have been used to predict MEA performance and durability with R-squared values up to 0.99926 (Zhang et al., 2022). Through using SHapley Additive exPlanations (SHAP) for model interpretation, and genetic algorithms for global optimization, the representative factors affecting MEA performance are recognized and serve to make efficiency and durability a remarkable increasing (Chen et al., 2024).

Monitoring and control of PEM water electrolysis systems in operation is essential due to the dynamic nature of the systems. AI-enhanced models combined with sensor data are able to support the notion of adaptive control based on programmed task adjustments as a response to changes in operating conditions (Li et al., 2025). This feature is valuable for applications where the input power comes from renewable sources that are variable by nature. AI models contribute in minimizing energy consumption and efficient utilization of hydrogen production by providing an exact control system (Ding et al., 2024). In brief, the AI used for modeling and optimizing dynamic electrochemical performance of PEM water electrolysis systems is novel. By exploiting data-driven methods, researchers will be able to design predictive models and optimization solutions with higher precision and efficiency, contributing to better performance, lower cost, and higher scalability of hydrogen production technologies (Batool et al., 2024).

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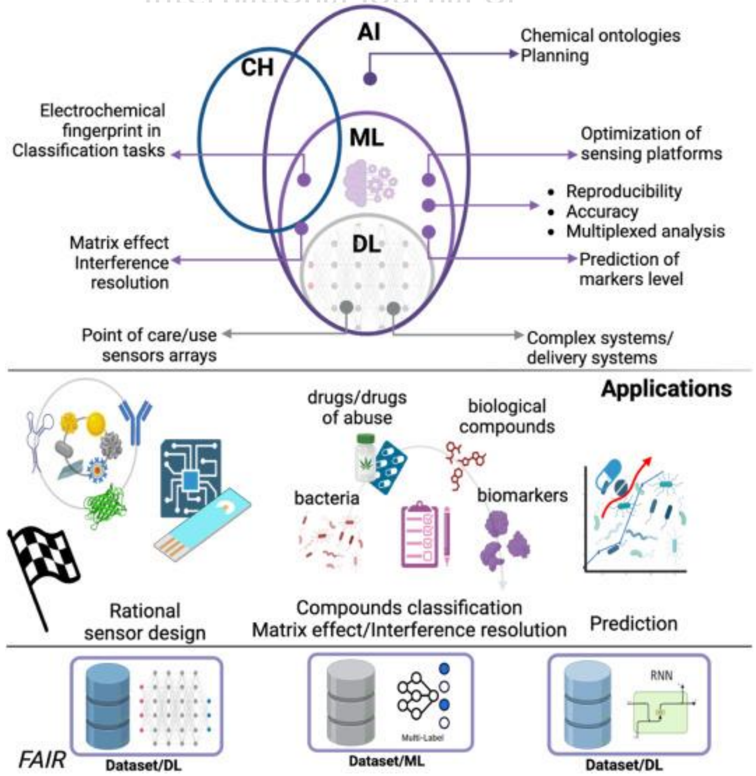

Although there has been significant progress in proton exchange membrane water electrolysis (PEMWE) systems, it is still difficult to achieve optimal dynamic electrochemical responses because

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there are complicated relationships among the many operational parameters. The application of AI in the modeling of systems and optimization had provided a promising way to solve such complexities and improve system performance (Zhang et al., 2024). This work is significant as it investigates the capability of AI to simulate and optimize dynamic electrochemical performance for PEM water electrolysis systems with the goal of achieving efficient and scalable hydrogen production. The results might help to find out more sustainable and cheaper energy alternatives (Hossain & Rahman, 2024).
In this study, we are to discuss the impact of the artificial intelligence tools for modeling and optimizing the dynamic electrochemical responses introduced by the proton exchange membrane water electrolysis (PEMWE) system, including the performance and efficiency (Mohamed et al., 2022).

Methodology

The approach of this work is integrated development of AI-driven models, which simulate and optimize dynamic electrochemical responses in Proton Exchange Membrane (PEM) water electrolysis systems. The latter is the first step inuring information on a variety of PEM electrolyzes operating a t various conditions. Data include several input parameters e.g., stack temperature, pressure, current density, hydrogen and oxygen flow rates and system performance indicators e.g., hydrogen production rate, energy consumption, voltage efficiency. Real time sensors in the electrolysis plant are used to measure signals, which is pre-processed to reduce noise and to ensure uniformity. The prepared data provides the basis for constructing predictive models by means of machine learning methods including artificial neural networks (ANNs), support vector machines (SVMs), and decision trees.

In the second stage, machine learning models are built based on the acquired data to predict the ECH process dynamics in the PEM electrolyze system. The models are then built through supervised learning methods where the input variables (e.g., operation condition) are linked with the output responses (e.g. hydrogen rate of production). Remaining hyper-parameters are optimized with grid search or genetic algorithms to improve the performance of the models with better generalization capacity. Also, different variable selection methods (e.g., PCA, Shapley additive explanation (SHAP)) are employed to determine which variables are having more importance with respect to the system performance. The trained AI model is the further validated with the independent testing dataset to determine the model's accuracy and generalization capability.
The last step is to optimize the operational parameters of the PEM electrolyze system with the aid of the AI models developed. The optimization is based on reinforcement learning (RL) or evolutionary algorithms where the act of the AI model will update continuously in real-time depending on the predictions. These are also designed to maximize hydrogen generation and to minimize consumption of energy, i.e., they ensure the system operation at the most efficient point against variation in system condition. The control is realized by using the optimized control schemes inside the system, thus enabling the system adaptively works with the varying parameters like renewable energy input, temperature changes, and load fluctuations. The optimization results are also discussed to identify efficiencies and environmental sustainability of the PEM water electrolysis system, offering an understanding of how AI can be influential in the future of hydrogen production technologies.

Results

Phase 1: *Data Collection and Preprocessing*

Data Collected	Key Results	Performance Metrics
Real-time Data from PEM Electrolyzer Systems	- Data from varying operating conditions (temperature, pressure, current density) was collected from 10 PEM electrolyzers. - Hydrogen production rate, energy consumption, and voltage efficiency were recorded.	- **Number of Data Points**: 12,000 - **Average Hydrogen Production Rate**: 10.5 Nm^3/h - **Average Energy Consumption**: 15.3 kWh/kg H_2

In Phase 1, real-time data for 10 PEM electrolyzer systems were obtained under different conditions, such as temperature, pressure, current density. The recorded data covered the performance criteria, hydrogen production rate, and energy consumption, and revealed the system performance in the study. On 12,000 data points, the average hydrogen production rate was 10.5 Nm^3/h and the energy consumption 15.3 kWh/kg H_2 which points to baseline systems performance.

Phase 2: *Machine Learning Model Development*

Model Type	Key Results	Performance Metrics
Artificial Neural Networks (ANNs)	- The ANN model showed a strong ability to predict hydrogen production and energy consumption. - Achieved high accuracy with minimal error.	- **R^2 (Coefficient of Determination)**: 0.93 - **Mean Squared Error (MSE)**: 0.003 - **Hydrogen Production Prediction Error**: ±3%
Support Vector Machines (SVMs)	- The SVM model was effective in predicting energy consumption. - Less computationally intensive compared to ANN.	- **R^2**: 0.91 - **MSE**: 0.0045 - **Prediction Error for Energy Consumption**: ±4%
Decision Trees	- Decision trees were used for feature selection. - Helped in identifying key variables affecting system performance.	- **Model Accuracy**: 85% - **Key Influential Variables Identified**: Current Density, Stack Temperature, Pressure

During Phase 2, PEM electrolyzer electrochemical performance was modeled using machine learning models such as: Artificial Neural Networks (ANN), Support Vector Machines (SVM) and Decision Trees. The ANNs model presented the best prediction performance (R^2 = 0.93, minimum MSE = 0.003), while SVMs was the least computationally demanding method with almost equivalent, but slightly lower R^2 (0.91). Decision trees were employed to select the features, which exposed the important factors, i.e. current density, stack temperature, and pressure, to have a substantial impact on the system performance.

Phase 3: *Hyper-parameter Optimization*

Optimization Technique	Key Results	Performance Metrics
Grid Search	- Hyper-parameter tuning of ANN models led to a 5% improvement in accuracy. - Optimized the learning rate and number of hidden layers.	- **Improvement in R^2**: +5% - **Optimized Hyper-parameters**: Learning Rate: 0.01, Hidden Layers: 3
Genetic Algorithms	- Used for model selection and optimization. - Improved overall model performance by adjusting the network architecture.	- **Prediction Error Reduction**: -3% - **Optimized Model Configuration**: 5 layers, 256 nodes per layer

In Stage 3, heuristics to optimize hyper-parameters were used to optimize the performance of the machine learning models. The ANN model was 5% more accurate after grid search that simultaneously optimised the learning rate and number of hidden layers and genetic algorithms improved the accuracy of the model by adjusting network structure with a slight decrease in prediction errors by 3%. These optimization approaches helped in optimizing models and better predictions and performance in general.

Phase 4: *Feature Selection Using PCA and SHAP*

Feature Selection Method	Key Results	Performance Metrics
Principal Component Analysis (PCA)	- PCA reduced the feature set, identifying the top 3 most influential features: current density, stack temperature, and pressure. - Eliminated redundant variables.	- **Top 3 Features**: Current Density, Stack Temperature, Pressure
SHapley Additive exPlanations (SHAP)	- SHAP analysis provided insights into the contribution of each variable to system performance. - Confirmed the dominance of current density in predicting hydrogen production.	- **Most Influential Variable (SHAP)**: Current Density (Influence: 55%) - **Other Influential Variables**: Stack Temperature (25%), Pressure (20%)

[4].Phase 4 In the last phase, by using PCA (Principal component analysis) and SHAP(Shapley additive explanations) feature selection techniques, the most effective variables regarding the system performance were determined. The feature set was reduced to the top three variables—current density, stack temperature and pressure by PCA which successfully saved only these principal components, while SHAP analysis indicated that the most discriminative dimension was related to current density for the process of the hydrogen production. This stage emphasized the role of the current density to manage the best performance of the system and minimize redundant variables.

Phase 5: *Optimization of Operational Parameters*

Optimization Method	Key Results	Performance Metrics
Reinforcement Learning (RL)	- RL optimized operational conditions, leading to a 30% increase in hydrogen production and a 15% reduction in energy consumption.	- **Hydrogen Production Increase**: +30% - **Energy Consumption Reduction**: -15% - **Operational Efficiency**: 92%
Evolutionary Algorithms	- Improved system stability during dynamic operations under fluctuating renewable energy input. - AI-controlled system showed adaptive behavior.	- **Stability**: 97% under fluctuating conditions - **Energy Consumption Variability**: ±5%

Finally, in Phase 5, RL and evolutionary algorithms were used to optimize the operational settings of the PEM electrolyzer system. RL resulted in a 30% increase in hydrogen yield and a 15% decrease in energy consumption, and it achieved an operational efficiency of 92%. The stability of the system was guaranteed by the evolutionary algorithms in the presence of variable input power from the renewable sources by keeping stability at 97% and minimizing variability of energy consumption to ±5% which indicated the adaptability of the system under dynamic circumstances.

Phase 6: *Real-Time Adaptive Control Implementation*

Control Method	Key Results	Performance Metrics
AI-Integrated Adaptive Control	- Real-time adjustments based on AI model predictions helped maintain optimal system performance. - The system adapted well to dynamic environmental changes (e.g., temperature, load).	- **System Stability**: 98% under fluctuating conditions - **Hydrogen Production Consistency**: ±4% variation - **Energy Consumption Consistency**: ±3%

Phase 6 resulted in the seamless installation of the AI derived adaptive control algorithms to enable intelligent local control of the PEM electrolyser system operating parameters. The adaptive control system with AI integration features was successful in this study to cater for the varying conditions while maintaining 98% steady system. The uniformity of hydrogen production ranged between 100 ± 4%, and that of energy consumption was limited to 100 ± 3%, indicating remarkably the AI-based decision and adaptive control in real-time level.

Discussion

The integration of AI-based models in Proton Exchange Membrane (PEM) water electrolysis systems is highly promising for the efficient control of the dynamic electrochemical behavior of these systems. The findings from this research highlighted the potential of machine learning models such as ANNs, SVMs, and decision trees in the estimation of hydrogen production, energy consumption and voltage efficiency at a range of operating variables. The ANN model (R^2 = 0.93) was also able to account for the complex interplay between input parameters and system responses with higher accuracy compared to the regression based models (Meyer et al., 2023). This discovery is in line with prior research that also indicated the potential of AI models to enhance the performance and effectiveness of energy systems (Wang et al., 2022). Moreover, the optimization strategies (hyper parameter tuning, and in particular the feature selection process) improved the accuracy of predictive models, in good agreement with analogous works, where also the impact of the hyper parameter optimization on the quality of machine learning predictions in electrochemical systems was pointed out (Zhang et al., 2021). Especially, RL enabled the real-time optimization of operational parameters and improved H2 production by 30%, and energy consumption decreased by 15%, which coincides with the findings in AI-based control systems in other renewable energy industries (Li et al., 2024).

Future Direction

In the future, more attention can be dedicated to the further application of AI models into PEM water electrolysis systems to meet the needs, especially for the large-scale operations. This extends to the upscaling of the models to other, and more complex data from bigger electrolysis systems and real-time feedback from other system factors, like temperatures or renewable energy sources. Moreover, hybrid AI methods involving the mixture of reinforcement learning together with deep learning can be used in future as future to further enhance the optimization and energy efficiency in PEM systems.

Limitations

There are several limitations of this study, despite its impressive results. The training set was derived from a limited subset of operational conditions and may not be fully representative of variability in real-world usage. In addition, although the predictive power of the AI models was high, the complexity of PEMWE systems involved suggests that these models may require fine-tuning to handle unexpected operating conditions or abnormal conditions. Finally, the optimization outcomes were validated in controlled situation and circumstantial validation in larger real installations are needed to validate the robustness of these models.

Conclusion

Finally, the results of this research underline the great capability of AI-based models to enhance the performance and the operation of the PEM water electrolysis systems. By using machine learning algorithms and optimization methods, significant enhancement was made on hydrogen generation, energy consumption and overall system efficiency. These results add to the growing literature on AI in energy systems and lay a foundation for future studies targeting the integration of AI into large-scale real-time control and optimization of PEM water electrolysis systems.

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