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Machine Learning Applications in Electrolyzer Systems: A Comprehensive Review of Process Control, Predictive Maintenance, and Optimization Strategies

Muhammad Asyraf Abdullah[a], Abu Bakar Sulong[a,b], Edy Herianto Majlan[a], Mohd Faisal Ibrahim[b], Ahmad Adam Danial Shahril[a], Maryam Jamilah Shabdin[a], Siti Haziyah Mohd Chachuli[a], Afifah Kamal[a] & Kean Long Lim[a*]

[a]*Fuel Cell Institute, Universiti Kebangsaan Malaysia,*
43600 UKM Bangi, Selangor, Malaysia;

[b]*Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia,*
43600 UKM Bangi, Selangor, Malaysia

[*]*Corresponding author: kllim@ukm.edu.my*

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ABSTRACT

Artificial intelligence (AI) has emerged as a transformative technology capable of addressing complex engineering challenges through advanced data-driven modeling, prediction, and optimization techniques. In the context of sustainable energy systems, hydrogen production via water electrolysis has attracted considerable attention as a promising pathway toward carbon-neutral energy generation. However, the widespread deployment of electrolyzer technologies remains constrained by challenges related to energy efficiency, operational stability, system degradation, and dynamic process control. In response, machine learning (ML) techniques have increasingly been integrated into electrolyzer systems to enhance performance prediction, adaptive control, predictive maintenance, and operational optimization. This review presents a comprehensive and engineering-oriented analysis of recent advancements in ML applications for hydrogen production via electrolysis. The study first outlines the fundamental principles of ML, including major learning paradigms, data processing approaches, and commonly adopted algorithms for electrochemical systems. Subsequently, the review critically examines ML-driven strategies for hydrogen production optimization, hyperparameter tuning, intelligent process control, system design enhancement, and degradation monitoring in electrolyzer technologies such as Proton Exchange Membrane Water Electrolyzers (PEMWE) and Anion Exchange Membrane Water Electrolyzers (AEMWE). Comparative analysis of algorithms including Artificial Neural Networks (ANN), Support Vector Machines (SVM), Reinforcement Learning (RL), and Physics-Informed Neural Networks (PINN) is also discussed from both electrochemical and engineering perspectives. Furthermore, current challenges involving data quality, model interpretability, computational complexity, and industrial deployment are critically evaluated. Overall, this review provides strategic insights into future intelligent electrolyzer systems and highlights critical research directions for scalable and sustainable green hydrogen production.

Keywords: Artificial Intelligence (AI); Machine Learning (ML); Control systems; Proton Exchange Membrane Water Electrolyzers (PEMWE); Anion Exchange Membrane Water Electrolyzer (AEMWE)

INTRODUCTION

Global dependence on fossil fuels continues to drive environmental concerns, with record levels of carbon dioxide emissions intensifying the urgency for clean and sustainable energy alternatives (Abiola et al. 2023). Among the promising solutions, hydrogen has emerged as a key enabler in the transition toward a carbon-neutral energy system. Its versatility as an energy carrier coupled with high energy density and zero carbon emissions during utilization makes hydrogen vital for decarbonizing industrial, transportation, and power sectors (Tao et al. 2025). In particular, hydrogen produced through water electrolysis powered by renewable electricity represents a pathway toward truly green hydrogen production, offering a route to bridge the gap between renewable power generation and energy storage (Yan, 2025). Water electrolysis, the process of splitting water into hydrogen and oxygen, has evolved into several major technologies: alkaline water electrolysis (AWE), proton-exchange-membrane water electrolysis (PEMWE), and anion-exchange-membrane water electrolysis (AEMWE) (Du et al. 2022). Each differs in electrolyte type, operating temperature, and material composition. While AWE remains commercially mature, PEMWE and AEMWE exhibit higher current densities and faster dynamic responses, aligning better with intermittent renewable sources such as solar and wind (Vedrtnam et al. 2025). However, these advanced systems face critical challenges including stack degradation, catalyst corrosion, gas crossover, and complex nonlinear dynamics which complicate operational control and limit efficiency (Spöri et al. 2017).

In recent years, the integration of machine learning (ML) has shown transformative potential to address these challenges. Electrolyzer systems generate vast amounts of operational data through sensors monitoring parameters such as voltage, current density, pressure, temperature, and gas purity. ML techniques ranging from supervised regression to deep reinforcement learning (DRL) can leverage these datasets to identify performance patterns, detect anomalies, predict degradation, and optimize operational parameters (Anny, 2024; Salehmin et al. 2024). For instance, ML-based predictive maintenance systems can detect early signs of membrane or catalyst degradation (Onwusa et al. 2025), while data-driven models can support real-time control and adaptive optimization under fluctuating power input (Feng et al. 2025). These capabilities enhance efficiency, reduce downtime, and extend electrolyzer lifetime. Moreover, the emergence of digital-twin frameworks and AIoT (Artificial Intelligence of Things) architectures enables the creation of virtual electrolyzer systems that replicate real-time operational behaviour (Feng et al. 2024). These hybrid “grey-box” systems integrate physics-based and ML models, improving forecasting, diagnostics, and control accuracy (Sharma et al. 2024). As illustrated in Figure 1, sensor data are collected, processed, and analyzed through ML algorithms to enable predictive control and system optimization.

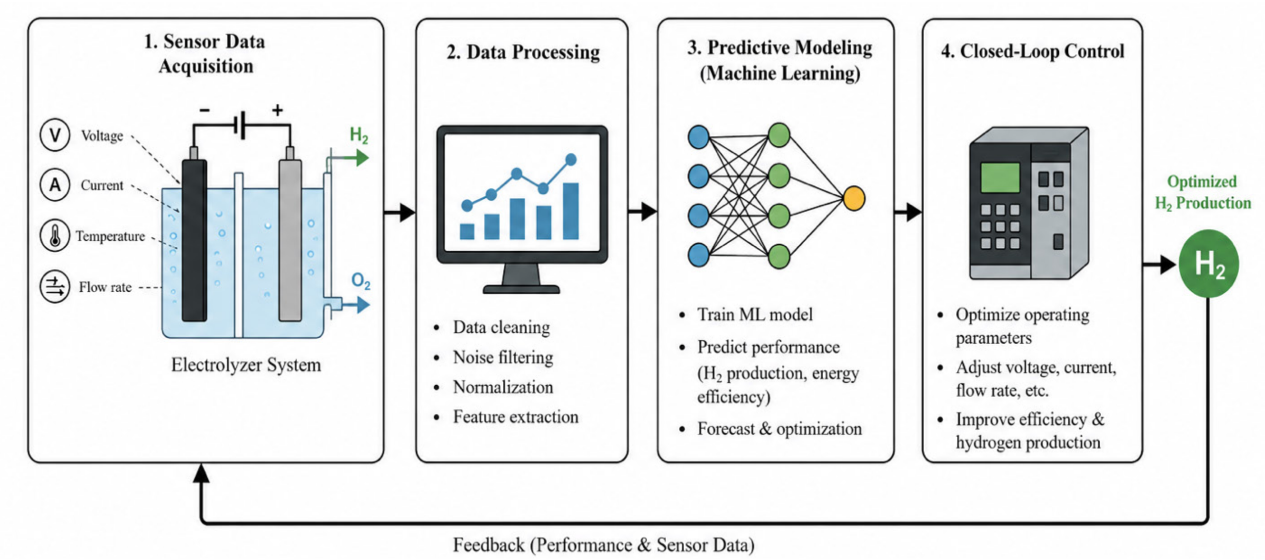

FIGURE 1. Conceptual framework of a machine learning-assisted electrolyzer system integrating sensor data acquisition, data processing, predictive modeling, and closed-loop control for optimized hydrogen production

The growing body of literature has demonstrated the application of ML in diverse aspects of hydrogen research from catalyst discovery and process modeling to system-level optimization and control. However, a focused synthesis of its role specifically in electrolyzer operation remains limited. Exploring ML integration across process control, predictive maintenance, and production optimization is therefore essential for advancing hydrogen technology. Table 1 summarizes machine learning applications and performance metrics in electrolyzer systems, highlighting ML-based approaches such as SVM, ANN, Deep Reinforcement Learning–Long Short-Term Memory (DRL–LSTM), Artificial Neural Network–Genetic Algorithm (ANN–GA), and Physics-Informed Neural Network (PINN), which have shown strong potential in overcoming operational, optimization, and degradation-related challenges in hydrogen production systems.

TABLE 1. Quantitative Summary of Machine Learning Applications and Performance Metrics in Electrolyzer Systems

ML Algorithm	Application Domain	Target Parameter	Performance Metric	Reported Value	Key Contribution	Reference
SVM	Performance prediction	Current density & hydrogen flowrate	MAE	0.0317	High prediction accuracy for PEM electrolyzer performance	(Ozdemir & Pektezel, 2024)
DRL–LSTM	Predictive maintenance	Degradation / failure	RMSE	0.1351	Reliable degradation prediction and maintenance scheduling	(Abiola et al. 2023)
ANN	Production optimization	Hydrogen flow rate	R^2	0.9093	Accurate prediction of hydrogen generation rate	(Tawalbeh et al. 2024)
ANN–GA	System optimization	Efficiency	MAE	0.04691	Hybrid model improves system efficiency prediction	(Boekfah et al. 2025)
PINN	System modeling	Temperature	RMSE	0.1232	Physics-informed modeling for dynamic temperature prediction	(Zerrougui et al. 2025)
SVM	Fault detection	Catalyst performance	Accuracy	83%	Reliable classification of catalyst performance data	(Arjmandi et al. 2023)

The convergence of artificial intelligence, electrochemical modeling, and energy systems engineering presents significant opportunities to accelerate the development of scalable, efficient, and intelligent hydrogen production infrastructure. Accordingly, this paper reviews recent advances in ML applications for electrolyzer systems, with particular emphasis on process control, predictive maintenance, and operational optimization. The review further examines the integration of ML with physics-based modeling and digital twin frameworks to enhance system performance, reliability, and sustainable hydrogen generation.

This narrative review provides a structured technical synthesis of current ML approaches applied to electrolyzer technologies. Unlike existing broad AI-focused hydrogen reviews, this work emphasizes quantitative and engineering-oriented evaluation of ML techniques based on predictive accuracy, computational complexity, electrochemical interpretability, and industrial deployment readiness. In addition, key technical challenges limiting real-world implementation are identified, and future research directions involving hybrid physics-informed ML, digital twin integration, and reinforcement learning-based autonomous control are discussed.

BACKGROUND AND FUNDAMENTALS OF ELECTROLYZER SYSTEMS

KEY OPERATIONAL PARAMETERS AND PERFORMANCE INDICATORS

Understanding the operational parameters and performance indicators of an electrolyzer is crucial for optimizing hydrogen production efficiency and ensuring long-term system reliability. These parameters provide insight into how electrical, chemical, and thermal conditions interact to influence the rate and cost of hydrogen generation. The most significant parameters include cell voltage, current density, efficiency, and energy consumption, all of which are interrelated and define the overall electrochemical performance of the electrolyzer stack (Ali et al. 2025). The cell voltage represents the total potential required to drive the electrolysis reaction, typically comprising the thermodynamic voltage (~1.23 V at 25 °C) plus several overpotentials due to activation, ohmic, and mass-transport losses (W. Li et al. 2022). As the current density increases, the cell voltage rises nonlinearly because of these voltage losses, which are captured in the polarization curve. The polarization curve serves as a fundamental performance indicator for any electrolyzer technology, illustrating how increasing current density boosts hydrogen output but simultaneously decreases efficiency due to additional energy losses (Chandrasekar et al. 2021)related indicator, current density, expresses the applied current normalized by electrode area (A cm^{-2}), and is directly proportional to hydrogen production rate according to Faraday's law (Wilcox & Gabe, 1992). While higher current densities increase hydrogen yield, they also accelerate degradation and elevate energy consumption. Optimal operating current densities for PEM electrolyzers generally range between 1–3 A cm^{-2}, balancing productivity and efficiency (Delargy, 2024). At these values, system efficiencies between 60–70 % (LHV basis) are typically achieved, with energy consumption around 50–60 kWh kg^{-1} H_2 (Annex, 2023). Efficiency in electrolyzers can be defined in several complementary ways: One, voltage efficiency, the ratio between the theoretical reversible voltage and actual operating voltage. Second, faradaic efficiency, the ratio between the actual hydrogen produced and the theoretical amount predicted by charge transfer. Third, energy efficiency, which accounts for both electrical and thermal energy inputs (Pashchenko, 2024). For practical operation, the energy efficiency (η_e) is often expressed as the ratio of the lower heating value (LHV) of hydrogen to the electrical energy consumed per kilogram of hydrogen produced:

$$n_e = \frac{LHV_{H_2}}{E_{consumed}} \times 100\% \quad (1)$$

Modern PEM systems reach 65% efficiency, depending on stack design, catalyst loading, and temperature, whereas alkaline electrolyzers achieve similar or slightly higher values at lower current densities (Caparrós Mancera et al. 2020). The specific energy consumption (E<consumed>) is another key metric, typically between 47–66 kWh kg^{-1} H_2 for present systems, with future targets below 45 kWh kg^{-1} H_2 (W. Li et al. 2024). Operational efficiency and energy consumption are further influenced by factors such as temperature, pressure, electrolyte conductivity, and material composition. Higher temperatures improve reaction kinetics and reduce ohmic losses, while elevated pressures allow for direct high-pressure hydrogen output, minimizing compression energy requirements (Zou et al. 2020). Materials with high proton conductivity, low resistance, and corrosion resistance such as perfluorosulfonic acid membranes and noble metal catalysts significantly enhance performance and longevity (Zatoń et al. 2017). Collectively, these operational parameters define the energy conversion efficiency, durability, and cost of hydrogen production systems. The interplay between voltage, current density, and energy efficiency forms the technical foundation upon which advanced optimization and control strategies such as machine learning-based modeling can be developed. A comprehensive understanding of these indicators is therefore essential for accurately assessing system performance and for guiding future advancements in intelligent electrolyzer design (Bhuiyan et al. 2025).

VOLTAGE–CURRENT CHARACTERISTICS AND POLARIZATION CURVE

The relationship between the applied cell voltage and the resulting current density is one of the most fundamental indicators of electrolyzer performance. This relationship is commonly represented by the polarization curve, which describes how the electrolyzer responds to increasing current densities under specific operating conditions (Williams et al. 2005). The curve typically shows three distinct regions of voltage loss: activation, ohmic, and concentration (or mass-transport) overpotentials (Figure 2). At low current densities, the activation region dominates, reflecting the energy required to initiate the electrochemical reactions at the anode and cathode. These losses are influenced by electrode materials, catalyst loading, and reaction kinetics (Alia et al. 2019). As the current increases, the ohmic region appears where voltage losses result from electrical resistance within the electrolyte, membrane, electrodes, and interconnects (Mennola et al. 2002). The slope of this region largely determines the internal resistance of the cell and can be minimized by improving material conductivity or reducing membrane thickness. At high current densities, mass-transport losses become significant due to limited reactant diffusion and gas bubble accumulation, which restricts ion and electron transfer (Zhang et al. 2025).

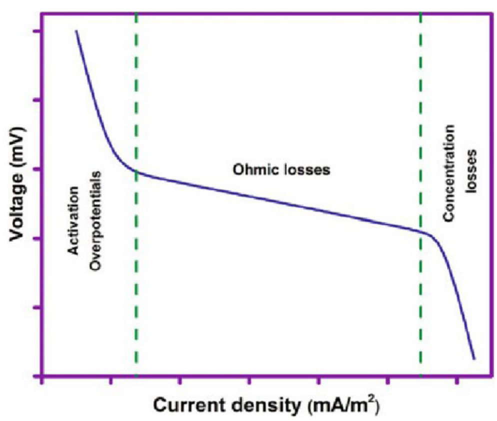

FIGURE 2. Typical polarization curve for a PEM electrolyzer, highlighting activation, ohmic, and concentration losses. Adapted with permission from Ref. (Venkata Mohan et al. 2013)

A low slope in the polarization curve indicates efficient electrochemical operation with minimal resistive losses. However, the operating point must be carefully selected: increasing current density accelerates hydrogen production but raises energy consumption and thermal stress on the components (Zeng & Zhang, 2010). Therefore, the polarization curve is often used to assess the trade-off between production rate and energy efficiency. For instance, Grigoriev et al. (2019) reported that increasing current density from 1 A cm^{-2} to 3 A cm^{-2} in a PEMWE increased hydrogen production rate by 200 % but also raised the required voltage by > 0.3 V, reducing voltage efficiency by 10 %.

EFFICIENCY, CURRENT DENSITY, AND ENERGY CONSUMPTION

Efficiency in an electrolyzer is typically expressed in several complementary ways: voltage efficiency, Faradaic efficiency, and energy consumption per kilogram of hydrogen produced. Faradaic efficiency refers to the fraction of electric charge that contributes to hydrogen evolution, whereas voltage efficiency relates the theoretical minimum voltage typically ~1.23 V for water splitting under standard conditions to the actual applied voltage (Yodwong et al. 2020). From an energy-consumption perspective, many state-of-the-art technologies operate around 47-66 kWh per kg H_2 for the stack level, with system-level targets below ~45 kWh/kg H_2 by 2050 for PEM electrolyzers (Chatenet et al. 2022). Current density strongly influences when increasing current density boosts hydrogen production rate per unit area, but also tends to increase voltage losses, thereby increasing energy consumption per unit hydrogen. For instance, one parametric study on PEM electrolysis found that the optimal energy consumption ~58.4 kWh/kg H_2 was achieved at ~200 mA/cm^2 and 70-80 °C, corresponding to a voltage efficiency of ~85% and energy efficiency of ~67.5 %.

Electrolyzer efficiency quantifies how effectively electrical energy is converted into chemical energy stored in hydrogen. It can be expressed through several related parameters: first, voltage efficiency, which compares the theoretical reversible voltage (~ 1.23 V) with the actual cell voltage; second, faradaic efficiency, which measures how much of the electrical charge contributes to hydrogen generation; and third energy efficiency, which considers the total energy input relative to the heating value of hydrogen (Yodwong et al. 2020). Modern PEM electrolyzers typically operate at cell voltages between 1.6 – 2.2 V, yielding voltage efficiencies of 65–75 % (Bessarabov & Millet, 2018). The total energy consumption (E_e) per kilogram of hydrogen can be expressed as:

$$E_e = \frac{V_{cell} \times I \times t}{m_{H_2}} \tag{2}$$

In practice, the average energy consumption ranges between 53 and 54.7 kWh/kg for PEM and alkaline systems (Aghakhani et al. 2023). Lowering this value is crucial to making green hydrogen economically viable. Future targets established by the World Nuclear Association aim for 50-55 kWh kg^{-1} H_2 (World Nuclear Association, 2024). Current density directly influences both production rate and efficiency. According to Faraday's law, hydrogen production is proportional to the applied current; however, higher current densities increase overpotentials and thus decrease overall efficiency (Koponen, 2020). A moderate current density typically 1 – 2 A cm^{-2} for PEMWE is often preferred to achieve an optimal balance between productivity and energy cost (Titheridge & Marshall, 2024). To provide a clearer comparison of the operational performance among different electrolyzer types, Table 2 summarizes the typical operating voltages, current densities, energy consumption, and efficiencies for electrolyzer as reported in recent literature.

TABLE 2. Typical operating parameters and efficiency metrics for the main electrolyzer technologies

Technology	Operating Voltage (V)	Current Density (A cm^{-2})	Specific energy consumption at stack (kWh Nm^{-3})	Efficiency (LHV %)	Typical Operating Temp (°C)	Ref
AWE	1.5 – 2.6	0.2 – 0.7	3.8 – 4.4	55 – 73	60 – 80	(Backurs et al. 2025; Benghanem et al. 2024)
PEMWE	1.4 – 2.3	0.6 – 2.0	4.53 – 7.3	55–75	50 – 80	(Benghanem et al. 2024)
AEMWE	1.8 – 2.3	0.2 – 1.5	4.8	60 – 70	40 – 70	(Backurs et al. 2025; Hou & Yang, 2024)

INFLUENCING FACTORS: TEMPERATURE, PRESSURE, AND MATERIAL PROPERTIES

The performance of an electrolyzer is significantly affected by temperature, pressure, and material characteristics. These parameters govern reaction kinetics, ionic conductivity, and system efficiency (Bazarah et al. 2022). Temperature strongly influences the rate of electrochemical reactions. Increasing operating temperature decreases activation overpotential and improves proton or hydroxide ion mobility within the electrolyte (Zhang et al. 2023). Research has demonstrated that optimizing the operating temperature of a PEM electrolyzer can substantially lower energy consumption. For instance, increasing the temperature from 25 °C to 80 °C has been shown to boost energy efficiency from 67.5% to 85% at a current density of 200 mA/cm² (Noor Azam et al. 2023). However, higher temperatures can accelerate material degradation, especially membrane thinning and catalyst dissolution, requiring optimized thermal management (Seselj et al. 2023). Pressure is another important operational parameter. Operating under higher pressures allows the production of high-pressure hydrogen directly within the cell, reducing the need for downstream compression. Nonetheless, pressurization can increase mechanical stress on cell components and alter bubble dynamics, potentially affecting gas purity and electrode performance. PEM electrolyzers are typically operated up to 30–50 bar, while next-generation systems aim for > 70 bar to improve storage integration (Hancke et al. 2022). Material properties including catalyst type, membrane conductivity, and electrode structure directly determine reaction kinetics and ohmic losses. High-performance catalysts such as IrO_2 (anode) and Pt (cathode) are widely used in PEMWE for their excellent activity and corrosion resistance (Zhang et al. 2022). For alkaline and AEM systems, non-precious alternatives such as NiFe, Co, and Mn-based oxides are under development to lower cost while maintaining performance (Tran Thi Ngoc, 2022). Meanwhile, thin-film membranes with high ionic conductivity and mechanical stability help minimize ohmic losses, improving polarization behavior and energy efficiency. Figure 3 illustrates the combined influence of temperature and current density on cell voltage, showing that higher temperature operation leads to lower cell voltage and improved performance efficiency.

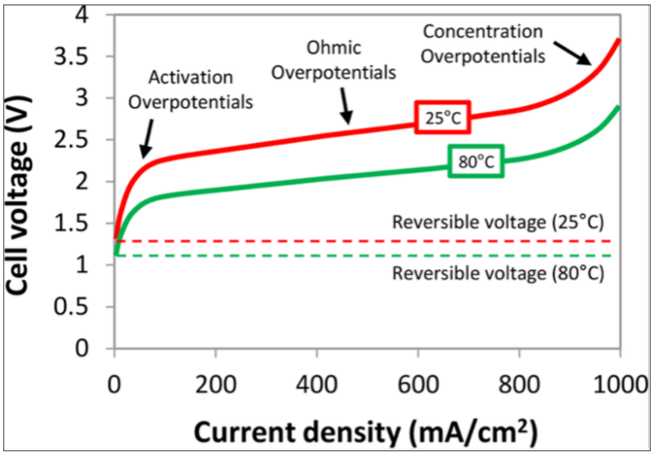

FIGURE 3. Influence of temperature and current density on cell voltage for a PEM electrolyzer. Adapted with permission from Ref. (Amores et al. 2017)

The synergy between these influencing factors defines the operational envelope of an electrolyzer. Managing temperature, pressure, and materials in a coordinated manner is essential to maximize durability, hydrogen yield, and efficiency. These insights form the fundamental baseline for integrating advanced modeling and machine learning approaches to further optimize electrolyzer operation under dynamic conditions.

MACHINE LEARNING APPLICATIONS IN ELECTROLYZER SYSTEMS

OPTIMIZATION OF PRODUCTION AND HYPERPARAMETER TUNING

The quest for enhanced efficiency and reduced cost in hydrogen production via electrolyzer necessitates precise optimization across a multitude of influencing factors, including the electrolyzer type, water purity, operating temperature and pressure, and the characteristics of the electricity source. Traditionally, optimizing these parameters has relied on manual adjustments and empirical techniques. While such conventional approaches can yield some effective results, their capacity for comprehensive optimization of complex, nonlinear electrochemical systems is inherently limited (Abou Houran et al. 2023; Wazirali et al. 2023). Moreover, these methods are typically labor-intensive and time-consuming, rendering them impractical for the demands of large-scale hydrogen production. In contrast, ML presents a compelling alternative for revolutionizing the electrolyzer process by leveraging data-driven models. ML algorithms are uniquely poised to identify intricate, non-linear relationships between diverse input parameters such as temperature, feed flow rate, voltage supply, and electrolyte concentration and critical system performance metrics like hydrogen production rate and energy efficiency (Bassey & Ibegbulam, 2023).

Various ML paradigms offer distinct advantages for the optimization of electrolyzer operation. Regression analysis, for instance, serves as a valuable tool for predicting electrolyzer efficiency by modeling the quantitative relationships between key input parameters, including electrical energy input, electrolyte concentration, temperature, and pressure, and the resultant system performance (Stanley et al. 2019; G. R. Yang & Wang, 2020). This quantification provides crucial insights into the principal factors governing electrolyzer efficiency (Bassey & Ibegbulam, 2023). Beyond linear relationships, Neural Networks (NNs) excel at identifying complex, non-linear patterns and interdependencies that may not be discernable through traditional analytical methods, enabling more precise predictions and subsequent process optimizations (Ukoba & Jen, 2022). Furthermore, Reinforcement Learning (RL) offers a dynamic and adaptive approach to optimizing electrolyzer in real time. By continuously adjusting process parameters based on environmental feedback and iteratively learning optimal policies, RL algorithms enhance both efficiency and cost-effectiveness over prolonged operational periods (Yan et al. 2021). Such RL algorithms have emerged as powerful tools for electrolyzer applications, enabling intelligent, real-time maintenance strategies that adaptively optimize system reliability and operational longevity based on environmental and performance feedback.

In the context of supervised learning for PEMWE optimization, a study by (Ozdemir & Pektezel, 2024) rigorously evaluated three prominent supervised ML models: Multilayer Perceptron (MLP), Support Vector Machine (SVM), and Random Forest (RF). These models were selected for their demonstrated capability in handling non-linear data and complex interdependencies among variables typical of electrochemical systems. Input parameters including cell voltage, temperature, torque, and water flow rate were provided to the models to predict two critical output variables: hydrogen flow rate and current density. Among the evaluated techniques, the SVM model demonstrated superior predictive accuracy, achieving a Mean Absolute Error (MAE) of 0.0317 for current density and 0.0671 for hydrogen flow rate in the test dataset (Ozdemir & Pektezel, 2024).

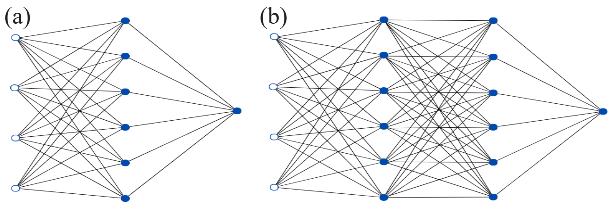

FIGURE 4. Illustration of optimal architecture of the (a) Artificial Neural Network (ANN), (b) Deep Neural Networks (DNN)

While SVM exhibited superior overall accuracy, the MLP model was recognized for its scalability and inherent suitability for real-time applications. A key advantage of MLP lies in its seamless integration with control systems in PEMWE, facilitating dynamic adjustments to operating conditions. This adaptability is instrumental in enhancing both hydrogen production rates and overall energy efficiency. Furthermore, the network architecture, conceptually illustrated in Figure 4 (a), highlights MLP's flexibility in supporting tailored solutions for real-time system control, positioning it as a viable candidate for advanced PEMWE operations. MLP thus holds substantial potential for refining and enhancing PEMWE system optimization, with its reliable predictive capabilities and capacity to model complex, non-linear relationships establishing it as an essential tool for advancing green hydrogen production technologies. Future research should prioritize hybrid modeling approaches that integrate MLP with complementary ML techniques or physics-based models, aiming to further improve predictive accuracy and operational efficiency in PEMWE systems.

Central to developing reliable and high-performing ML models for electrolyzer system simulations is hyperparameter optimization. Unlike model parameters, which are learned intrinsically during the training process, hyperparameters define the structural and functional aspects of an ML model and must be predetermined (Yang & Shami, 2020). These include essential configurations such as the number of hidden layers in a neural network, the learning rate that dictates the step size during optimization, the choice of activation functions, and the specific optimization algorithms employed. For instance, in Support Vector Machines (SVMs), the penalty parameter (C) controls the tolerance for errors, while in Artificial Neural Networks (ANNs), hyperparameters such as the neuron count per layer and the learning rate significantly impact both model accuracy and computational efficiency. Given that optimal hyperparameter configurations are highly specific to datasets and problem domains, meticulous fine-tuning of these settings is critical to ensure high predictive performance and effective generalization to unseen data (Akl et al. 2019). Various studies have explored methodologies for hyperparameter tuning to improve ANN performance. Common approaches include systematic techniques like grid search and probabilistic methods like random search, as well as heuristic-based evolutionary algorithms, all of which systematically evaluate different hyperparameter configurations to identify optimal settings. Research indicates that deep learning architectures, particularly those employing Rectified Linear Unit (ReLU) activation functions and multiple hidden layers, are highly effective for modeling the inherently non-linear electrochemical processes characteristic of electrolysis (Tawalbeh et al. 2024). However, overfitting remains a persistent challenge in ANN development, especially when an excessive number of neurons or layers leads to model memorization of training data rather than genuine pattern learning, ultimately reducing predictive accuracy on unseen data (Sun et al. 2010).

Recent advancements in automated hyperparameter optimization, such as Bayesian optimization and reinforcement learning-based strategies, offer more efficient tuning by dynamically adjusting model configurations based on real-time performance feedback, significantly reducing the computational burden associated with exhaustive searches. To ensure model reliability and mitigate overfitting risks across different data subsets, 5-fold cross-validation is widely adopted as a reliable technique, improving predictive stability. Comparative analyses in the literature consistently highlight the necessity of balancing model complexity with computational efficiency to achieve optimal predictions for electrolyzer systems. In the context of ANN-based electrolyzer modeling, researchers have thoroughly investigated various network architectures to identify the most effective configurations. A typical and effective ANN model structure, conceptually depicted in Fig 4 (b), often follows a multi-layered approach comprising: an input layer (four neurons representing distinct parameters like cell voltage, electrolyte concentration, water flow rate, and temperature), two hidden layers (each with 12 neurons, designed to enhance model complexity and processing capacity, with a representative subset often displayed for clarity), and a single output layer (one neuron predicting hydrogen flow rate). The selection of such an optimal ANN architecture involves systematically varying the number of hidden layers, neuron counts per layer, activation functions (e.g., ReLU, Tanh, or Sigmoid), learning rates, and batch sizes. Studies by (Tawalbeh et al. 2024) employing grid search techniques have identified configurations featuring two hidden layers and ReLU activation functions as particularly effective for electrolyzer system modeling, consistently yielding lower Mean Squared Error (MSE) values during validation. These findings underscore the critical importance of a structured and systematic hyperparameter tuning approach in achieving accurate and computationally efficient ANN models for electrolyzer applications. Overall, hyperparameter optimization remains a key factor in developing high-precision ML models. Future research should prioritize refining automated tuning strategies, integrate domain-specific constraints, and leverage hybrid ML techniques to further enhance predictive accuracy and system efficiency in hydrogen production.

ENHANCING PROCESS CONTROL AND SYSTEM DESIGN

In the realm of electrolyzer, the overall system operation fundamentally bifurcates into two interdependent phases: system design and process control. System design inherently dictates the capabilities of process control, as each physical component within the electrolyzer must be meticulously configured with appropriate communication ports and specifications to facilitate electronic control (Figure 5). This seamless integration is paramount for ensuring efficient, precise, and dynamic interaction between the physical hardware and its regulating mechanisms. Fundamentally, system design pertains to the configuration and arrangement of components within an electrolyzer to maximize performance, efficiency, and overall reliability. For advanced electrolyzer technologies such as PEMWE and AEMWE, this encompasses critical considerations including the judicious selection of materials, the intricate cell stack configuration, the design of flow fields, and the integration of essential supporting equipment such as pumps, heat exchangers, and power supplies. Each electrolyzer technology presents unique design considerations: AWE typically involves simpler designs with liquid electrolyte reservoirs and separators, often utilizing durable, lower-cost materials but requiring larger operational footprints. PEMWE, conversely features compact designs reliant on proton-conducting membranes and high-pressure operation, necessitating precious metal catalysts and advanced sealing techniques. AEMWE combines aspects of both, utilizing anion-conducting membranes, with a significant design focus on optimizing non-precious materials to reduce costs and enhance durability. Beyond component selection, ML algorithms can be rigorously employed during the design phase to analyze various combinations of equipment types, layouts, and operating procedures. By processing vast datasets, these algorithms can identify complex patterns and correlations that are difficult to discern manually, thereby leading to optimal system configurations that minimize energy consumption, improve reliability, and maximize overall hydrogen output.

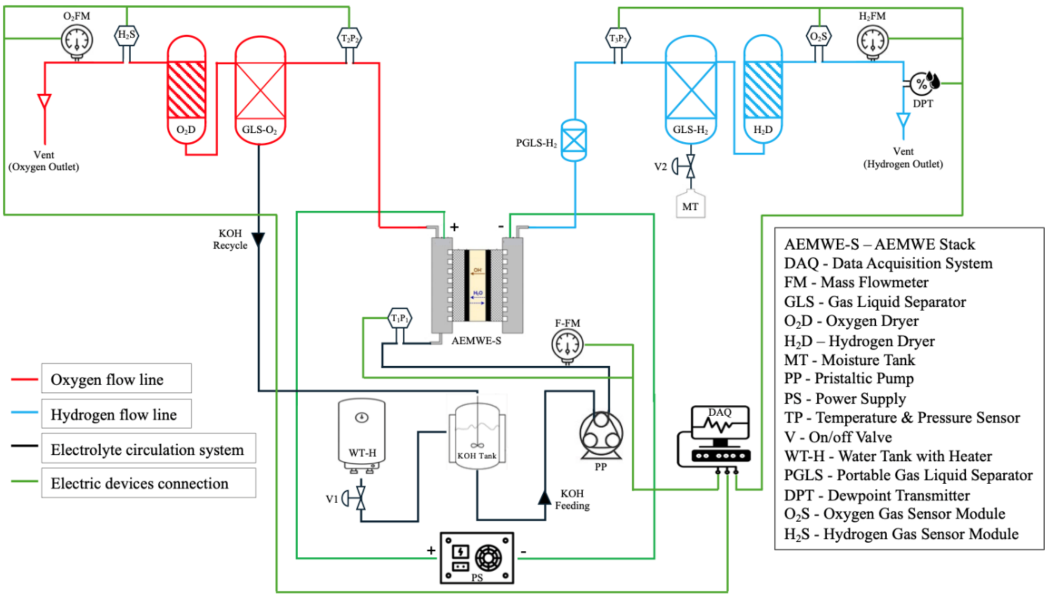

FIGURE 5. Schematic diagram of a full AEMWE system design components

Control systems are unequivocally integral to modern technology, playing a fundamental role in nearly every automated industrial process by reducing the need for continuous human intervention. The primary objective of any control system is to regulate and maintain a desired output by precisely adjusting system inputs based on real-time feedback. Control theory, a multidisciplinary field spanning mathematics and engineering, rigorously focuses on managing dynamic systems to achieve and sustain a predefined setpoint value (SV) (Dev et al. 2021). This is achieved by systematically modifying one or more input parameters that influence system behavior while continuously monitoring the system's current state. In the specific context of electrolyzers, process control entails the precise regulation of key operating parameters such as temperature, pressure, feed water flow rate, current density, and voltage. Effective control strategies are critical for ensuring stable, efficient, and safe hydrogen production, thereby enhancing hydrogen yield and energy efficiency while preserving system stability and longevity. The implementation of advanced control mechanisms, particularly those leveraging artificial intelligence-based predictive control, allows electrolyzer systems to dynamically adapt to fluctuations in operating conditions, further improving process reliability and efficiency.

The design of modern control systems leverages diverse methodologies, each offering distinct advantages tailored to specific applications. Figure 6 provides a comprehensive overview of control system methodologies utilized in electrolyzer processes, highlighting a rich array of strategies aimed at optimizing performance, stability, and efficiency. At the core, conventional approaches such as PID (Proportional-Integral-Derivative) control and adaptive control provide foundational techniques for maintaining system stability and responding effectively to changes in operational conditions, widely adopted for their simplicity and effectiveness in basic control tasks. Advanced methodologies, including Model Predictive Control (MPC) and observer-based controllers, offer significant improvements by incorporating predictive capabilities and real-time system monitoring. Such approaches are particularly advantageous for managing the dynamic and non-linear behaviours characteristic of electrolyzer processes, enabling precise control of parameters like current density, temperature, and reactant flow. Furthermore, fault-tolerant control ensures system resilience by identifying and mitigating potential faults, thereby enhancing the reliability of electrolyzer systems under diverse operating conditions. Innovative techniques like fuzzy logic control and AI-based controls introduce a new dimension of adaptability and autonomous decision-making. Fuzzy logic control is effective in managing uncertainties and imprecise inputs, while AI-driven methodologies leverage machine learning algorithms to optimize system performance through real-time data analysis and prediction. Collectively, these methodologies represent a holistic framework for advancing electrolyzer control systems, addressing both traditional challenges and emerging needs in sustainable energy technologies.

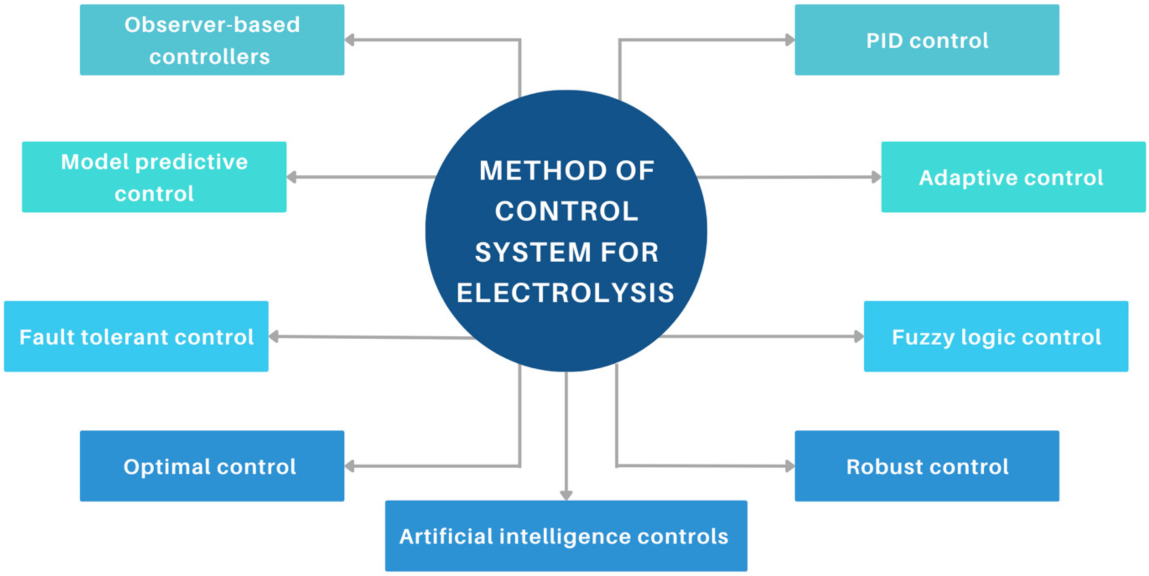

FIGURE 6. Overview of control system methodologies for electrolyzer processes

The advancement of modern control systems, particularly through the integration of microcontrollers, has significantly enhanced system interface capabilities while enabling extensive data collection on system responses to various inputs and disturbances. This high-fidelity data acquisition facilitates a deeper understanding of complex system dynamics, allowing researchers to develop sophisticated predictive models that substantially improve control strategies. The integration of ML into control systems has revolutionized process optimization by enabling advanced predictive analytics and adaptive decision-making. ML is widely employed across diverse applications, including image recognition, security systems, autonomous vehicles, predictive maintenance, robotics, and classification tasks (Libbrecht & Noble 2015; Wang & Siau 2019). As the foundational technology of Artificial Intelligence, ML has become instrumental in designing intelligent control systems, particularly critical for complex and highly nonlinear electrochemical processes such as AEMWE. Control system modeling can be represented using various mathematical frameworks, including transfer function models, state-space representations, and differential equations. However, with recent advancements in microprocessors and computational power, researchers have increasingly focused on neural network-based models for representing nonlinear dynamic systems. Neural networks, inspired by biological neurons, function as powerful computational models capable of approximating highly complex system behaviours. A typical feedforward neural network comprises an input layer, one or more hidden layers, and an output layer. A schematic simple Feed Forward 3-layer neural network representing the hierarchical structure comprising an input layer, a hidden layer, and an output layer. The model processes weighted inputs through activation functions to capture complex system dynamics, enabling nonlinear function approximation and predictive modeling. The above shown neural network has an input layer, a hidden layer and an output layer. Consider a single neuron 'H_1' in the hidden layer. Where w_{11}, w_{21} and w_{31} are the weights connecting the input layers to the 'H_1' neuron. The output this neuron is calculated as:

$$H_1 = f(x1.w_{11} + x2.w_{21} + x3.w_{31}) \tag{3}$$

Where f is the activation function of the layer which is usually a non-linear in nature The entire network can be represented in matrix form. The output of the hidden layer can be represented as:

$$H = f_1 (X.W^1) \quad (4)$$

Where f_1 is the activation function, X is the input matrix, $x1$, $x2$, $x3$ and W^1 is the weight matrix connecting the input and hidden layers. The final output of the neural network is then computed as:

$$Y = f_2 (H.W^2) \quad (5)$$

Where f_2 is the activation function of the output layer, and W^2 represents the weight matrix connecting the hidden layer to the output layer.

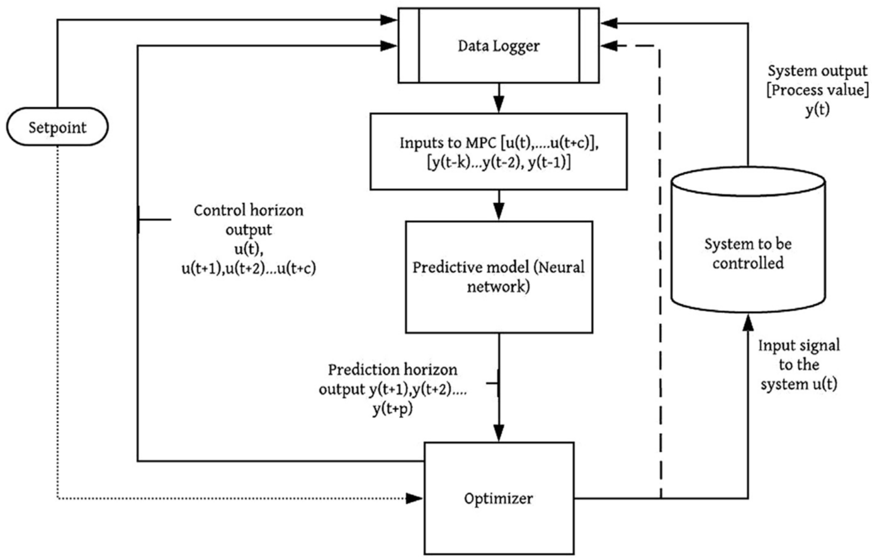

FIGURE 7. Schematic representation of the general layout of MPC.
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MPC is an advanced control strategy that utilizes a mathematical model to forecast the future states of a system, enabling the optimization of control inputs over a predictive horizon. By solving an optimization problem at each sampling interval, MPC dynamically adjusts control actions to achieve optimal system performance while maintaining stability. The effectiveness of MPC relies on an accurate predictive model capable of estimating future system outputs based on historical data. Recurrent Neural Networks (RNNs), known for their ability to model sequential dependencies, have emerged as a powerful tool for implementing MPC. As illustrated in Figure 7, the MPC framework integrates a neural network-based predictive model with an optimizer to generate control signals, ensuring precise regulation of process variables. This approach is particularly beneficial in complex, nonlinear systems such as AEMWE, where real-time adaptability and predictive accuracy are essential for optimizing hydrogen production efficiency. ML algorithms can be employed to analyze various combinations of equipment types, layouts, and operating procedures to determine the most efficient system design. By processing vast amounts of data, these algorithms can identify patterns and correlations that would be difficult to discern manually, ultimately leading to the optimal configuration for hydrogen production systems. This approach enables researcher to design systems that minimize energy consumption, improve reliability, and maximize overall output. In addition to design optimization, machine learning can contribute to the development of sophisticated process control systems for electrolyzer. These AI-driven systems continuously monitor a range of operational and environmental parameters, making real-time adjustments to ensure the electrolyzer process operates at peak efficiency. For instance, machine learning models can dynamically adjust operational conditions such as temperature, pressure, and current density based on real-time data, ensuring that hydrogen production remains stable and efficient under varying conditions. This adaptability is crucial for managing the inherent fluctuations in renewable energy sources, which often influence electrolyzer performance.

PREDICTIVE MAINTENANCE AND DEGRADATION MONITORING

Effective maintenance strategies are paramount for ensuring the sustained efficiency, reliability, and longevity of electrolyzer systems. Maintenance approaches are broadly categorized into three primary types: corrective, preventive, and predictive maintenance (Ben-Daya et al. 2016). Corrective maintenance, performed only after a fault or failure has occurred, invariably leads to unscheduled operational downtime, significant production losses, and reactive increases in repair costs. In contrast, preventive maintenance involves scheduled servicing at predetermined intervals; however, this approach frequently overlooks the actual health status of the electrolyzer, potentially resulting in unnecessary servicing, inefficient resource utilization, and suboptimal allocation of labor and spare parts. To circumvent these limitations, predictive maintenance (PdM) has emerged as an advanced, data-driven strategy. PdM leverages real-time data analysis to anticipate potential failures before they manifest, enabling maintenance activities to be precisely deployed just prior to an expected fault. This proactive methodology optimizes resource allocation, minimizes unscheduled downtime, and significantly extends the operational lifespan of the electrolyzer (Namuduri et al. 2020). The efficacy of PdM relies on continuous monitoring via embedded sensors that capture critical operational parameters such as voltage, temperature, and pressure, thereby providing invaluable data for accurate failure prediction and comprehensive health assessment.

Recent academic endeavors have extensively explored diverse PdM methodologies for electrolyzers. (Siracusano et al. 2018) pioneered the utilization of electrochemical techniques for diagnosing degradation mechanisms in PEMWE, successfully predicting membrane electrode assembly (MEA) longevity under authentic operating conditions. Similarly, (Li et al. 2019) identified iron contamination in feedwater as a critical factor influencing degradation, highlighting that undetected accumulation on the membrane and catalytic layer can lead to increased ohmic resistance and charge transfer losses, underscoring its importance in a reliable PdM framework. Furthermore, previous research by (Chandesris et al. 2015; Frensch et al. 2019) has consistently demonstrated the effectiveness of temperature-based monitoring as an early indicator for detecting membrane drying and its associated performance degradation. While continuous sensor-based monitoring is crucial for assessing operational parameters and detecting early indicators of potential failures, a fundamental challenge in PdM is ensuring the reliability of sensor data. Sensor degradation or outright failure can lead to erroneous predictions and subsequent unnecessary maintenance actions. To address this, advanced ML techniques have been increasingly employed to enhance the PdM framework by leveraging redundant sensor data and inferring missing or inaccurate readings from alternative system parameters, thereby significantly improving the reliability of predictive maintenance strategies.

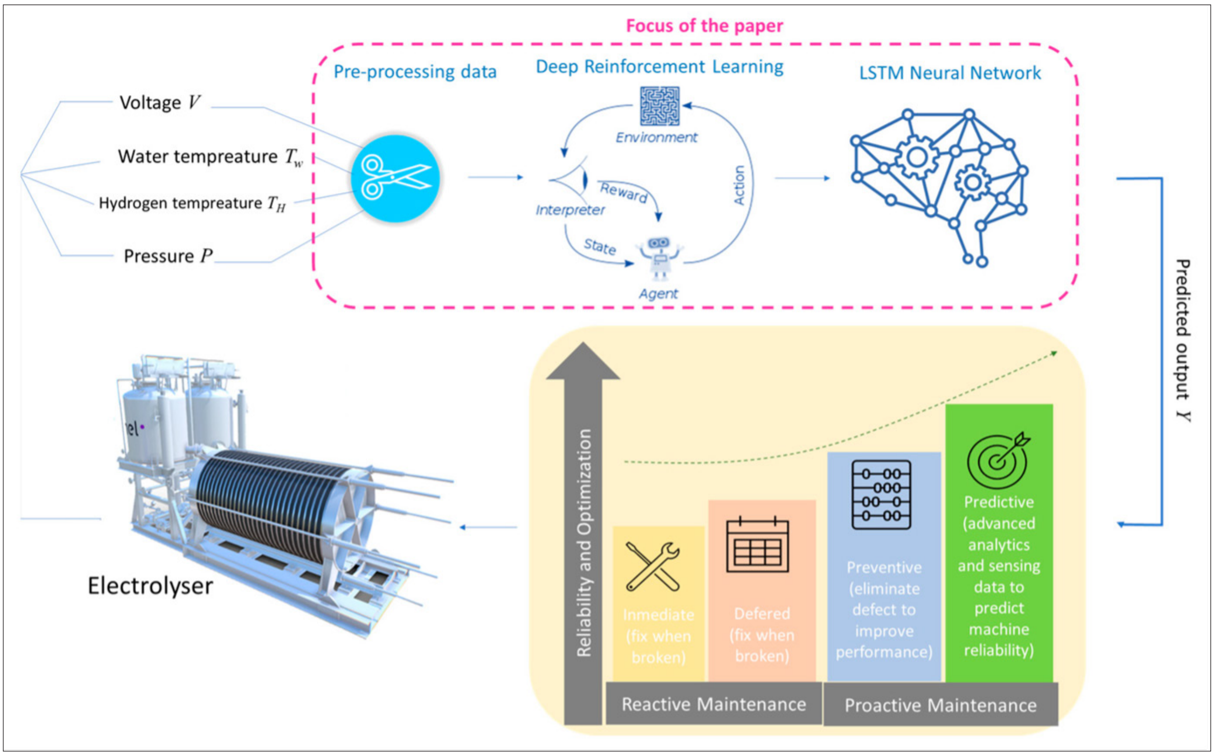

FIGURE 8. Schematic representation of a predictive maintenance framework for electrolyzers using DRL and LSTM neural networks. Reproduced with permission from Ref. (Abiola et al. 2023). Copyright 2023, Elsevier

A notable advancement in this domain is the novel predictive maintenance approach introduced by (Abiola et al. 2023), which integrates DRL with a Long Short-Term Memory (LSTM) neural network to enhance failure prediction in electrolyzers, as schematically illustrated in Figure 8. Within this framework, DRL is strategically employed to identify the most informative system parameters such as temperature, voltage, and water flow rate ensuring optimal feature selection for subsequent predictive modeling. These carefully selected features are then utilized as inputs to the LSTM network; a deep learning architecture specifically designed for reliable sequential data analysis and the capture of long-term temporal dependencies. The proposed DRL-LSTM framework demonstrated remarkably high predictive accuracy, achieving a correlation coefficient of 0.99 with experimental data and a root-mean-square error (RMSE) of 0.1351 (Abiola et al. 2023). These compelling results underscore the model's superior capability in capturing complex operational patterns and predicting maintenance requirements with significantly greater precision compared to conventional methods. The integration of DRL and LSTM within PdM offers multiple synergistic advantages for electrolyzer performance optimization: DRL effectively reduces computational complexity by intelligently selecting the most relevant features from large datasets, while LSTM models efficiently learn and model temporal dependencies crucial for accurate degradation trend analysis. This synergistic application facilitates the development of intelligent maintenance systems capable of real-time fault detection and proactive intervention, ultimately enhancing electrolyzer lifespan, reliability, and cost-effectiveness by preventing unexpected failures and optimizing maintenance schedules.

Beyond direct failure prediction, comprehensive degradation monitoring is critical for long-term electrolyzer health. According to (Chen et al. 2024), knowledge-based degradation forecasting in PEMWE can be systematically examined from three key perspectives: domain expertise, scientific methodologies, and complexity analysis. These multi-faceted strategies aim to facilitate the understanding of complex systems, identify underlying patterns, and enhance predictive, optimization, or decision-making processes by systematically decomposing system behaviors. Given the inherent intricacy of PEMWE systems, degradation mechanisms are influenced by a confluence of factors, including material properties, environmental conditions, and operational stressors (Feng et al. 2017). To systematically identify the root causes of degradation, contributing factors are commonly categorized into three primary sub-groups, enabling a structured analysis of degradation sources and aiding in the development of targeted mitigation strategies. Figure 9 provides a comprehensive overview of PEMWE degradation processes, offering valuable insights into the intricate interplay between these influencing factors and their cumulative impact on system reliability.

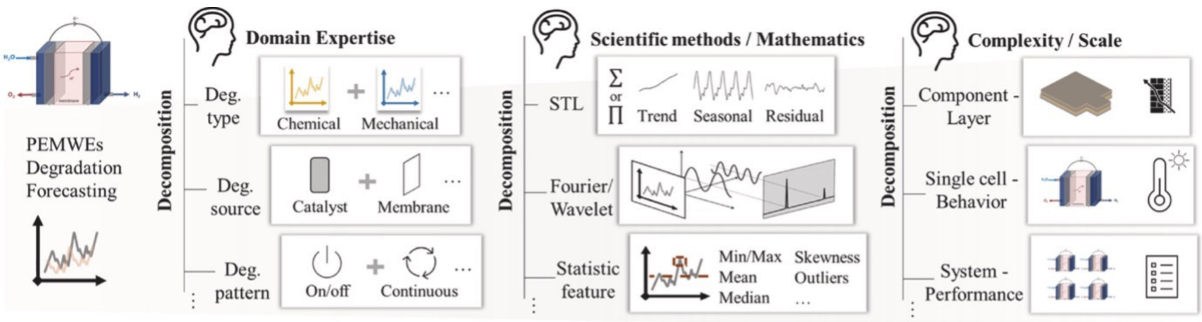

FIGURE 9. Three perspectives of knowledge-driven decomposition applied to degradation forecasting in PEMWE. This approach integrates domain expertise, scientific and mathematical methodologies, and various system complexities and scales. Key subtopics, such as degradation types and single-cell behavior, are incorporated to facilitate the decomposition of energy demand time series, enhancing insights into degradation mechanisms. Reproduced with permission from Ref (Chen et al. 2024). Copyright 2024, Elsevier

From the perspective of domain expertise, the degradation of PEMWE systems is significantly influenced by chemical and mechanical stressors. Chemical stress, often resulting from impurities in the feedwater, and mechanical stress, induced by repetitive operational cycles (start-up/shut-down), can be independently modeled using ML techniques to accurately predict their individual effects on performance deterioration (Chandesris et al. 2015). Additionally, material degradation, including catalyst deterioration and membrane wear, provides invaluable insights when analyzed under varying operating conditions, facilitating model differentiation and optimization

(Rakousky et al. 2016). The operational lifespan of PEMWEs is also closely tied to distinct operational patterns; distinguishing between continuous operation and Accelerated Stress Test (AST) phases enables a deeper understanding of long-term degradation trends, allowing for more precise assessment of their impact on system wear over time (Weiß et al. 2019). From a scientific methodology standpoint, advanced decomposition techniques are instrumental in refining the analysis of PEMWE degradation. Seasonal-Trend Decomposition (STL) is particularly valuable for segregating degradation trends, seasonal variations, and noise from time-series data, thereby enhancing ML models' ability to interpret complex degradation behaviors (Erő & Szűcs, 1974). Similarly, Wavelet Analysis and Fourier-based decomposition facilitate the identification of latent periodic or non-periodic patterns within operational data, enabling a more comprehensive understanding of time-dependent degradation signals (Duhamel & Vetterli, 1990).

Furthermore, derived statistical features such as maximum and minimum voltage, cumulative ramp cycles, mean values, and gradient slopes serve as effective degradation proxies, providing critical indicators for predictive modeling. These statistical approaches have demonstrated considerable efficacy in analogous applications, such as battery aging studies (Zhang et al. 2022). Addressing degradation from a complexity perspective necessitates a multi-scale analysis, encompassing insights from the component level, cell level, and system-wide assessments. At the component level, detailed ex-situ testing of catalysts and membranes, alongside controlled ASTs, provides foundational data crucial for higher-level system analysis and customized predictive modeling (Geu et al. 2023). On a broader scale, cell-level degradation pathways are assessed through comprehensive evaluations of individual components in conjunction with localized environmental conditions, enabling a refined understanding of degradation mechanisms unique to specific PEMWE cells (Kang et al. 2020). When scaled to the stack level, segmented cell measurements and system-wide performance data allow for the identification of degradation hotspots, thereby significantly improving the predictive accuracy of degradation trends and optimizing overall system longevity (Bazarah et al. 2022).

In conclusion, ML has significantly advanced predictive maintenance strategies for electrolyzers, offering a demonstrably more efficient and effective alternative to traditional corrective and preventive approaches. By continuously analyzing real-time operational data, ML models can identify subtle early signs of degradation, facilitating timely interventions that minimize downtime and extend the operational lifespan of the system. Recent studies have robustly demonstrated the effectiveness of ML-based techniques, such as the DRL-LSTM networks, in accurately predicting failures and optimizing maintenance schedules. These advanced methods enhance system reliability not only by accurately forecasting issues but also by compensating for sensor inaccuracies and refining predictive models based on both historical and real-time operational data. However, ongoing challenges remain in ensuring data quality, particularly from diverse sensor arrays, and in seamlessly integrating complex ML frameworks with existing industrial monitoring and control systems. Future research should thus strategically focus on improving reliable data fusion techniques, developing more computationally efficient and interpretable ML models, and rigorously validating these systems under diverse real-world operating conditions to further enhance predictive maintenance accuracy and overall electrolyzer performance.

COMPARATIVE ENGINEERING ASSESSMENT OF ML ALGORITHMS FOR ELECTROLYZER SYSTEMS

Although numerous machine learning algorithms have been applied to electrolyzer systems, their suitability varies significantly depending on the operational objective, computational complexity, interpretability, and deployment requirements. Therefore, a comparative engineering assessment is essential to identify the strengths, limitations, and industrial applicability of different ML techniques for hydrogen production systems. TABLE 3 demonstrates that different machine learning algorithms exhibit distinct advantages depending on the operational objectives and electrochemical complexity of the electrolyzer system. ANN and LSTM architectures generally provide superior capability in capturing nonlinear and transient electrochemical behavior, particularly under dynamic operating conditions involving fluctuating current density and temperature. In contrast, SVM models achieve strong predictive accuracy when limited datasets are available due to their strong generalization capability.

TABLE 3. Comparative Engineering Assessment of Machine Learning Algorithms for Electrolyzer Systems

ML Algorithm	Typical Electrolyzer Application	Key Input Parameters	Prediction / Control Target	Performance Metric	Strengths	Technical Limitations	Computational Complexity	Interpretability	Real-Time Deployment Suitability	Industrial Readiness	Ref.
ANN	Hydrogen production prediction	Voltage, current density, temperature, water flow rate	Hydrogen flow rate, efficiency	$R^2 = 0.9093$	Excellent nonlinear mapping capability; effective for electrochemical behavior prediction	Overfitting risk; requires large datasets and hyperparameter tuning	Moderate–High	Low	High	Moderate	(Tawalbeh et al. 2024)
SVM	PEM electrolyzer performance prediction	Cell voltage, temperature, torque, flow rate	Current density and hydrogen production	MAE = 0.0317	High prediction accuracy with limited datasets; strong generalization capability	Poor scalability for large datasets; kernel selection sensitivity	Moderate	Moderate	Moderate	Moderate	(Ozdemir & Pektezel, 2024)
RF	Fault detection and operational classification	Catalyst parameters, operational variables	Fault diagnosis and classification	Accuracy = 83%	Robust against noisy datasets; low overfitting tendency	Weak extrapolation for unseen operating conditions	Low–Moderate	High	High	High	(Arjmandi et al. 2023)
DRL	Predictive maintenance and adaptive optimization	Voltage, temperature, degradation indicators	Failure prediction and maintenance scheduling	RMSE = 0.1351	Adaptive autonomous learning under dynamic conditions	Computationally intensive; training instability	Very High	Low	Moderate	Emerging	(Abiola et al. 2023)
PINN	Physics-constrained electrolyzer modeling	Temperature, electrochemical parameters	Dynamic thermal prediction	RMSE = 0.1232	Integrates electrochemical physics with ML; improved physical consistency	Complex model development and training process	High	High	Moderate	Emerging	(Zerrougui et al. 2025)
MPC integrated with ML	Real-time process control	Current density, voltage, temperature	Dynamic operating optimization	Improved control stability	Strong predictive control under transient operation	Requires accurate system model and high computational resources	High	Moderate	High	Moderate–High	(Dev et al. 2021)
Hybrid ANN–Genetic Algorithm (ANN–GA)	System optimization	Operational and electrochemical variables	Energy efficiency optimization	MAE = 0.04691	Improved optimization accuracy through hybrid learning	Increased optimization complexity and computational time	High	Moderate	Moderate	Moderate	(Boekfah et al. 2025)

Random Forest algorithms exhibit high robustness against noisy operational data and are therefore suitable for fault diagnosis and classification tasks. Meanwhile, advanced approaches such as DRL and PINN show significant promise for autonomous control and physics-consistent prediction, respectively, although their industrial deployment remains constrained by computational requirements and implementation complexity. ANN, SVM, LSTM networks, and PINN are among the most widely adopted approaches for electrolyzer modeling and optimization. Among these algorithms, SVM exhibited one of the lowest prediction errors for PEM electrolyzer performance prediction, achieving a MAE of 0.0317 for current density prediction under varying voltage, temperature, torque, and water flow conditions (Ozdemir & Pektezel, 2024). The strong performance of SVM under relatively limited datasets is primarily attributed to its superior generalization capability and ability to construct optimal hyperplanes for nonlinear regression tasks. Nevertheless, SVM scalability becomes increasingly limited for large-scale industrial datasets due to computational growth associated with kernel-based optimization.

In contrast, ANN-based approaches demonstrated superior capability in modeling highly nonlinear electrochemical relationships involving hydrogen production rate, current density, and thermal effects. (Tawalbeh et al. 2024) reported an ANN R^2 of 0.9093 for hydrogen production forecasting in PEM water electrolysis systems under dynamic operating conditions. The strong nonlinear learning capability of ANN architectures is particularly suitable for electrolyzer systems because electrochemical reactions inherently involve nonlinear activation overpotentials, ohmic resistance variations, gas bubble transport phenomena, and transient thermal interactions. These nonlinear electrochemical dependencies are difficult to capture using conventional empirical or linear models but can be effectively approximated through deep neural learning structures. Temporal prediction models such as LSTM further extend this capability by incorporating sequential operational memory into degradation forecasting and predictive maintenance frameworks. Abiola et al. (2023) demonstrated that the integration of DRL with LSTM achieved a correlation coefficient approaching 0.99 and RMSE of 0.1351 for electrolyzer degradation prediction. The superior temporal learning capability of LSTM architectures enables effective tracking of gradual electrochemical degradation phenomena such as membrane thinning, catalyst poisoning, and increasing ohmic resistance under long-term operation. However, these models require significantly larger datasets and higher computational resources compared to simpler regression-based approaches.

Advanced approaches such as PINN represent an emerging direction for intelligent electrolyzer modeling by integrating electrochemical governing equations directly into neural network training. (Zerrougui et al. 2025) demonstrated that PINN models achieved RMSE values of 0.1232 for dynamic temperature prediction in PEM electrolyzers while maintaining improved physical consistency compared to purely data-driven methods. Unlike conventional ANN models, PINN architectures constrain model predictions using electrochemical and thermodynamic principles, thereby improving extrapolation capability and reducing physically unrealistic outputs. This characteristic is particularly important for industrial electrolyzer deployment, where operational reliability and physical interpretability remain critical requirements. From a computational perspective, simpler algorithms such as RF and SVM exhibit lower computational demand and faster training time, making them more suitable for fault classification and rapid operational diagnostics. Conversely, DRL, LSTM, and PINN architectures require substantially higher computational resources due to iterative optimization, sequential learning, and physics-constrained training processes. Although these advanced architectures provide superior predictive capability and adaptive control performance, their industrial deployment remains limited by hardware requirements, real-time processing constraints, and integration complexity within existing control infrastructures.

The scalability of ML algorithms also differs considerably across electrolyzer applications. ANN and SVM models are generally effective for stack-level performance prediction under controlled laboratory conditions, whereas DRL and PINN approaches exhibit stronger potential for large-scale autonomous hydrogen production systems integrated with fluctuating renewable energy sources. Reinforcement learning algorithms are particularly attractive for adaptive process control because they continuously optimize operating parameters such as voltage, current density, and water flow rate in response to changing environmental conditions. Nevertheless, training instability and safety concerns remain major barriers for real-time industrial implementation.

APPROACH AND IMPACT OF ML IN HYDROGEN PRODUCTION

The integration of ML into hydrogen production processes represents a revolutionary advancement, fundamentally enhancing the efficiency, reliability, and sustainability of hydrogen generation (Ghailane et al. 2025). As global efforts intensify to transition toward cleaner energy sources, ML-driven techniques offer advanced capabilities for process optimization, predictive control, and real-time decision-making (Bogireddy 2024). Key areas where ML has demonstrated significant impact, as conceptually illustrated in Figure 10, include sophisticated modeling and simulation, precise catalyst performance optimization, and seamless integration with inherently variable renewable energy sources such as solar and wind. Furthermore, recent advancements in explainable AI (XAI) models address critical challenges related to system transparency and decision-making reliability. These developments collectively underscore ML's transformative potential in hydrogen production, paving the way for enhanced energy efficiency, reduced operational timelines, and improved environmental sustainability. domains through distinct methodological approaches. One of the primary applications lies in modeling and simulation, where ML techniques are employed to develop highly accurate metamodels for analyzing complex industrial hydrogen reaction systems. Techniques such as linear regression, kriging, and Gaussian processes facilitate real-time prediction of system behavior, enable advanced process control, and support early fault detection, thereby significantly improving operational efficiency and sustainability (Lima Silva et al. 2023). Furthermore, sophisticated ML algorithms, including k-nearest neighbors (KNN), Extreme Gradient Boosting (XGBoost), Least Absolute Shrinkage and Selection Operator (Lasso), ANN, LSTM networks, and RF, are extensively utilized to predict green hydrogen production by integrating and interpreting data from diverse renewable energy sources like photovoltaic panels, wind turbines, and hybrid renewable systems (Urhan et al. 2025).

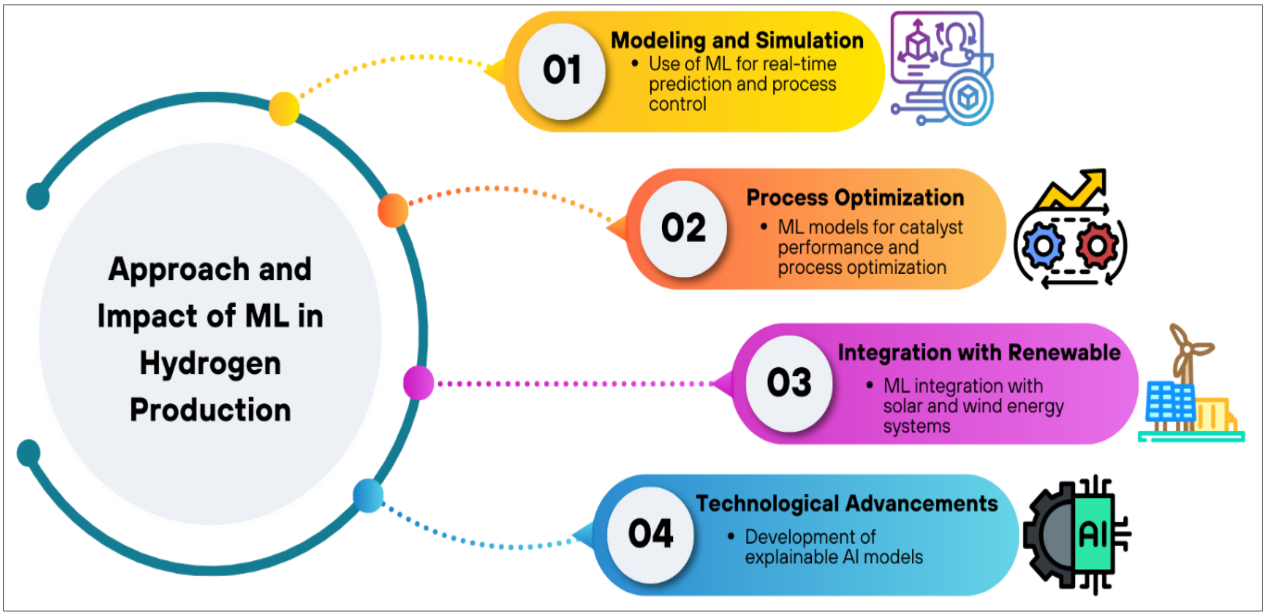

FIGURE 10. Overview of ML approaches and their impact on hydrogen production

ML APPROACHES IN HYDROGEN PRODUCTION

ML has emerged as a transformative tool in hydrogen production, enhancing efficiency, prediction accuracy, and process optimization across various. Beyond fundamental modeling, ML plays a pivotal role in process optimization, particularly in the critical areas of catalyst performance prediction and the optimization of hydrogen production pathways. Traditional kinetic-based approaches are often constrained by the limitations of experimental setups and the time-consuming nature of empirical studies. In contrast, ML-based models can predict catalyst efficiency and reaction dynamics with significantly greater accuracy, leading to substantial improvements in economic and energy efficiency (Kim et al. 2022). The predictive capabilities have been further enhanced by the development of hybrid ML models that combine ensemble and averaging techniques, notably demonstrated in biomass gasification for hydrogen production, resulting in more reliable and efficient process designs (Ukwuoma et al. 2024). Moreover, the synergistic application of ML with computational modeling has profoundly facilitated the accelerated design and synthesis of Hydrogen Evolution Reaction (HER) catalysts, leading to improved electrochemical performance and rapid advancements in hydrogen production technologies (Salehmin et al. 2024). Another crucial approach involves ML in enabling the effective integration with renewable energy sources. The inherent variability of renewable energy sources such as solar and wind power presents significant challenges for stable hydrogen generation. ML-driven optimization strategies are instrumental in mitigating these fluctuations, ensuring better system efficiency and production stability by predicting energy availability and optimizing electrolyzer operations accordingly (Bassey & Ibegbulam, 2023). Finally, recent advancements have focused on Explainable AI (XAI) models, which are becoming increasingly crucial in bridging the gap between complex ML model accuracy and interpretability (Patra 2025). These models provide a clearer, more transparent understanding of the underlying mechanisms involved in hydrogen production decisions, thereby significantly increasing their reliability for industrial applications and facilitating regulatory compliance (Ahmed et al. 2024).

IMPACT OF ML IN HYDROGEN PRODUCTION

The widespread adoption of ML has had a profound and multifaceted impact on hydrogen production, enhancing efficiency, sustainability, and economic viability, as further summarized in Table 4. From an efficiency and sustainability perspective, ML-driven approaches contribute significantly to more efficient hydrogen generation by optimizing operational parameters and dynamically reducing energy consumption. This optimization ensures minimal resource wastage and maximizes overall system performance (Huang et al. 2025; Kim et al. 2022). Crucially, the integration of ML with renewable energy systems, such as solar and wind, plays a pivotal role in accelerating the transition to green hydrogen. By improving predictive capabilities and ensuring stable production rates despite energy intermittency, this integration directly aligns with global sustainability goals and is instrumental in reducing carbon dioxide (CO<2>) emissions associated with conventional, fossil-fuel-based hydrogen production pathways (Li et al. 2024; Urhan et al. 2025). Economically, ML significantly enhances the commercial viability of hydrogen production. By improving prediction accuracy and optimizing process workflows, these advancements lead to substantial cost reductions, making hydrogen more commercially competitive and facilitating its large-scale adoption (Kim et al. 2022; Salehmin et al. 2024b). The ability to optimize process parameters in real-time allows industries to adopt highly cost-effective methods, concurrently reducing their dependence on fossil fuel-based hydrogen production (Sofian et al. 2024). In terms of technological advancements and deeper insights, ML has driven substantial progress by providing an unprecedented understanding into the complex interactions governing reaction mechanisms, material properties, and process efficiencies within electrolyzer systems. ML-based models enable superior decision-making by precisely identifying key influencing factors in hydrogen evolution, electrolyzer performance, and catalyst efficienc (Chen et al. 2024; Pandey et al. 2024). This deepened understanding, coupled with the development of explainable AI models, allows for not only highly accurate predictions but also transparent insights into the underlying processes, thereby building greater confidence in ML applications for crucial industrial processes. The overall impact of ML on hydrogen production is thus profound, offering significant advancements across its entire value chain.

TABLE 4. Summary of approaches of hydrogen production

Approach	ML Application	Impact	Ref
Modeling and Simulation	Use of ML for real-time prediction and process control	Enhanced operational efficiency and sustainability	(Urhan et al. 2025)
Process Optimization	ML models for catalyst performance and process optimization	Improved economic and energy efficiency	(Ukwuoma et al. 2024)
Integration with Renewable	ML integration with solar and wind energy systems	Better prediction and system efficiency	(Costa et al. 2024)
Technological Advancements	Development of explainable AI models	Better decision-making and process control	(Chen et al. 2024)

CONCLUSIONS

Machine learning has emerged as a powerful tool for enhancing the performance, reliability, and efficiency of modern electrolyzer systems. This review demonstrates that data-driven techniques significantly improve prediction accuracy, enable adaptive process control, and support predictive maintenance strategies across various electrolyzer technologies, including PEMWE and AEMWE. The quantitative synthesis of the reviewed literature indicates that Artificial Neural Networks, Support Vector Machines, and Reinforcement Learning are the most widely applied algorithms for performance prediction, system optimization, and fault detection in hydrogen production systems. Several major technological trends were identified in the reviewed studies. First, machine learning models are increasingly integrated with real-time monitoring systems to enable intelligent process control and operational optimization. Second, hybrid modeling approaches combining physics-based models and machine learning techniques are gaining attention for improving prediction reliability and system stability. Third, the adoption of digital twin frameworks and AI-based control strategies is emerging as a promising direction for next-generation electrolyzer systems.

Despite these advancements, several critical challenges remain. Limited availability of high-quality operational data, model interpretability issues, and difficulties in integrating machine learning models into industrial control systems continue to constrain large-scale deployment. In addition, the lack of standardized evaluation metrics and long-term experimental validation remains a significant barrier to practical implementation. The findings of this review have important implications for the development of intelligent hydrogen production systems. The integration of machine learning into electrolyzer operation enables real-time optimization of energy consumption, improved system reliability, and reduced operational costs. These capabilities are essential for supporting the transition toward sustainable and scalable green hydrogen technologies. Future research should focus on the development of robust hybrid modeling frameworks, real-time deployment of machine learning-based control systems, and systematic validation using experimental and industrial datasets. In particular, the integration of machine learning with digital twin technologies, advanced sensor networks, and intelligent control strategies represents a critical pathway for achieving reliable and efficient hydrogen production systems in industrial environments.

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DECLARATION OF COMPETING INTEREST

None.

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