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AI-supported supervision and management of PEM electrolyzers for green hydrogen production

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Resumen

La producción de hidrógeno verde, impulsada por fuentes de energía renovable, es fundamental para la transición hacia un futuro energético sostenible. No obstante, la eficiencia y seguridad de las instalaciones de generación de hidrógeno verde dependen críticamente de sistemas de supervisión y monitorización avanzados. Este artículo explora el potencial transformador de la IA generativa en el diseño y optimización de estos sistemas. Se analizan las capacidades de la IA generativa para crear modelos predictivos, detectar anomalías, optimizar el rendimiento y mejorar la seguridad en la producción de hidrógeno verde, abordando desafíos clave y delineando futuras líneas de investigación.

Palabras clave: Inteligencia Artificial, Supervisión, Gestión, Optimización, Hidrógeno, Electrolizador.

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Abstract

Green hydrogen production, powered by renewable energy sources, is fundamental to the transition to a sustainable energy future. However, the efficiency and safety of green hydrogen generation facilities depend critically on advanced monitoring and supervision systems. This article explores the transformative potential of generative AI in the design and optimization of these systems. The paper analyzes generative AI's capabilities to create predictive models, detect faults, optimize performance, and improve safety in green hydrogen production, addressing key challenges and outlining future research directions.

Keywords: Artificial Intelligence, Supervision, Management, Optimization Hydrogen, Electrolyzer.

1. Introduction

The imminent need for energy solutions that limit the carbon footprint has positioned hydrogen as a promising alternative to fossil fuels. However, currently, much of hydrogen production is derived from fossil fuels, limiting its potential as an energy carrier.

Hydrogen is not a primary energy source but rather an energy carrier, that is, a product that requires an energy input to be obtained and that has the ability to store energy for subsequent, gradual release when required.

Depending on the raw material required and the CO_2 emissions generated to obtain it, hydrogen is generally classified into the following colors:

- Green hydrogen or renewable hydrogen: hydrogen generated from renewable electricity, using water as a raw material, through an electrolysis process. Likewise, hydrogen obtained through biogas reforming or biochemical conversion of biomass, provided that established sustainability requirements are met will be renewable.
- Gray hydrogen: Hydrogen produced from natural gas or other light hydrocarbons such as methane or liquefied petroleum gases through reforming processes.
- Blue hydrogen: hydrogen obtained in a similar way to grey hydrogen, but to which carbon capture, use and storage techniques are applied (CCUS: *Carbon Capture, Utilization and Storage*), which allows reducing up to 95% of CO_2 emissions generated during the process.

In particular, green hydrogen produced through the electrolysis of water generated by renewable energy, is the key

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to the energy transition. This one is crucial for decarbonization, acting as a clean and flexible energy carrier (IEA, 2019). Its production from renewable sources is essential for a sustainable energy future. Efficiency, cost, safety, and scalability are key challenges in green hydrogen production (IRENA, 2020).

Among the various electrolysis technologies, Proton Exchange Membrane (PEM) electrolysis stands out for its high efficiency, high current density, and ability to operate dynamically, effectively integrating with intermittent renewable energy sources such as solar and wind (Ursua *et al.*, 2012). Its rapid response has made it the most widely used technology in combination with renewable energy (Gong *et al.*, 2023), (Folgado *et al.*, 2024b). PEM electrolyzers offer a sustainable method of hydrogen production, using electricity to split water into H_2 and oxygen.

However, optimizing the performance and durability of PEM electrolyzers presents significant challenges. The complexity of the electrochemical process, the gradual degradation of components over time, and the sensitivity to operating conditions (temperature, pressure, humidity) require advanced management strategies. Robust supervision and monitoring systems are necessary to ensure the efficient, safe, and reliable operation of this equipment (Folgado *et al*., 2023). These systems have evolved with advances in automation, computing, communications, and control (Folgado *et al.*, 2024a). The latest generation derives from the confluence of Supervisory Control and Data Acquisition (SCADA) systems and the Industrial Internet of Things (IIoT) (Folgado *et al.*, 2024a).

On the other hand, one of the most disruptive and promising technologies currently available is Artificial Intelligence (AI), which is making significant inroads into many sectors, most notably the energy sector (Verma *et al.*, 2024). AI is also impacting supervision and monitoring systems, providing advanced resources and functionalities. Therefore, AI is positioned as a powerful tool to address the challenges related to electrolyzer management.

Generative AI refers to a class of artificial intelligence that has multiple algorithms with the remarkable ability to generate new, realistic data that was not part of the original data. Generative AI, with models such as Generative Adversarial Networks (GANs), Variational Autoencoders (VAEs), and Transformers, can create new data, designs, and solutions (Goodfellow *et al.*, 2014).

GANs consist of a generating network and a discriminator network that are trained simultaneously through an adversarial process. The generating network aims to create realistic synthetic data, while the discriminator network attempts to distinguish between real and generated data. This process creates a competition between the two networks, ultimately resulting in the generation of highly convincing synthetic content. VAEs, on the other hand, take a probabilistic approach to generating new data. They learn the underlying distribution of the data and use it to generate new samples. Variational autoencoders are generative models used in Machine Learning (ML) to generate new data as variations of the input data they are trained on.

The term "Transformer" in AI refers to a type of neural network architecture that uses Deep learning and self-attention techniques to handle data sequences, providing significant improvement in tasks such as machine translation, text generation, and language understanding. Transformers are a type of neural network architecture that changes an input sequence into an output sequence.

This article addresses the diverse applications of AI in the monitoring and management of PEM electrolyzers, from process optimization and early fault diagnosis to lifespan prediction and the development of predictive control strategies. The various AI techniques used, such as ML, Deep learning, and expert systems, will be discussed, as well as the benefits and challenges associated with their implementation. Figure 1 aims at illustrating the interplay between AI technologies and PEM electrolyzers.

The structure of the document is as follows. After the introductory section, the fundamentals of hydrogen generation using PEM technology are described. Subsequently, generative AI applications in management and monitoring of PEM electrolyzers are expounded. The applications in the scope of predictive maintenance of PEM generators are analyzed in the fourth section. Finally, the main conclusions and future research works are outlined in the fifth section.

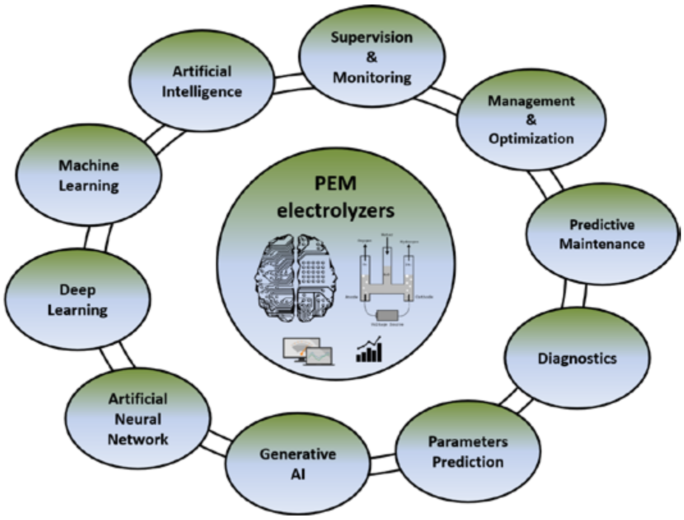

Figure 1: Interplay between AI technologies and PEM electrolyzers.

2. Operating description and working principle of PEM electrolyzers

PEM electrolyzers work by splitting water molecules into hydrogen and oxygen using a proton-conducting polymer membrane as a solid electrolyte. Water is fed to the anode, where it is oxidized to produce oxygen, protons, and electrons. The protons travel through the membrane to the cathode, where they combine with electrons to form hydrogen.

The corresponding chemical reaction is shown in (1):

$$2H_2O \rightarrow 2H_2 + O_2 \qquad (1)$$

where E denotes the amount of electrical energy needed to drive the electrolysis reaction.

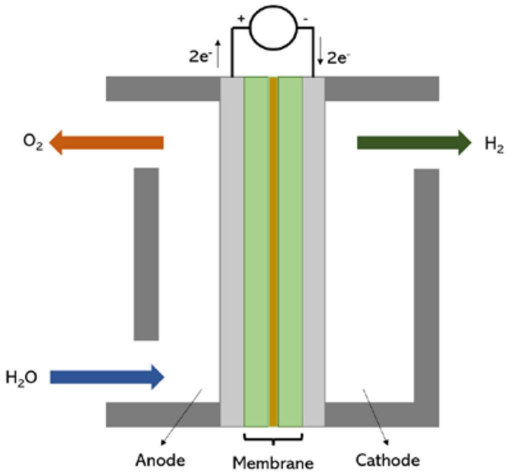

Figure 2: Schematic diagram of a PEM electrolyzer showing the anode, cathode, membrane, water supply, and hydrogen and oxygen production.

In a PEM electrolyzer, water is dissociated into H_2 and O_2 by application of an electric current. O_2 is hereby generated at the anode, while hydrogen is produced at the cathode with the reactions occurring on a catalyst layer coated on each respective electrode. Positioned in between both electrodes is the solid PEM, which serves three main purposes: it provides a gas-diffusion barrier for the generated O_2 and H_2, it functions as semi-permeable membrane allowing only H+ to cross, and it is electrically non-conductive.

When water decomposes into O_2-gas and H+ at the anodic side, O_2 exits the chamber, while H+ is drawn through the PEM by application of an electric field. After permeating the PEM, they recombine at the cathode and produce H_2-gas. There are two diffusion layers, one positioned on each side of the two electrodes, which together make up the Membrane Electrode Assembly (MEA). Their job is to facilitate efficient current distribution to and from the electrodes, supplying a homogeneous dispersion of water to the anode surface, and lastly alloying gaseous products to diffuse out of the MEA assembly and exit their respective chambers (Figure 2). Lastly, encasing the MEA are bipolar plates (BPP), which contribute to the cell's structural integrity and separate individual cells when assembled into a stack.

Figure 3 shows the general layout of a green hydrogen production plant in which hydrogen is generated from photovoltaic energy and stored in bottles for later use.

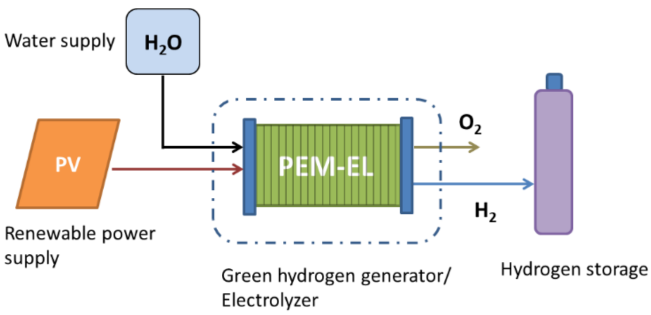

Figure 3: General layout of a green hydrogen production plant.

3. Applications of AI in the Supervision and Management of PEM Electrolyzers

In the context of hydrogen, AI can contribute to improving its production, storage, transportation and use, serving to predict different parameters, safety protocols or the management of hydrogen generation (Ramesh *et al.*, 2023).

Specifically, as noted in the Introduction, AI can be integrated with monitoring systems to provide advanced features and improve the management and control/operation capabilities of PEM electrolyzers. Furthermore, IoT and Digital Twin technologies can also contribute to these functionalities through effective real-time data transmission and virtual representation of physical equipment, respectively.

One of the biggest challenges to be solved in the application of AI to generate green hydrogen is the availability and quality of data to train the algorithms (Bassey and Ibegbulam, 2023). The scarcity of data in failure scenarios or rare events makes it difficult to train robust models. Generative AI can create synthetic data that mimics normal and abnormal plant behavior by varying pressure, temperature, flow rate, voltage, etc.

Precise control of the operating conditions of these devices to maintain optimal temperature, pressure, and humidity is crucial to ensuring system efficiency and stability. AI can be used to optimize operating parameters, such as voltage, current, and temperature, to maximize efficiency and hydrogen production.

Furthermore, due to the intermittent nature of renewable energy, integrating electrolyzers with these renewable primary energy sources poses a considerable challenge. In fact, the dynamic operation of a PEM stack, i.e., with a variable generated flow rate, negatively affects its degradation and performance (Frensch *et al.*, 2019), (Wei *et al.*, 2019).

On the other hand, PEM electrolyzers generate large volumes of sensor data related to voltage, current, temperature, pressure, humidity, and hydrogen generation. AI can be used to analyze this data to identify patterns, trends, and correlations that would be difficult or impossible to detect manually.

3.1. Specific Applications of Machine Learning in PEM Electrolyzer Optimization

ML has become an indispensable tool for process optimization in various industries, and PEM electrolyzer management is no exception. ML algorithms can learn from historical data and adapt their models to optimize performance based on changing conditions (Schmidt *et al.*, 2019). Some of the most commonly used types of ML algorithms include:

- Classification: Used to classify data into different categories, such as the health status of the electrolyzer (good, average, poor) or the presence of specific faults. Common classification models include logistic regression, Support Vector Machines (SVMs), decision trees, and neural networks.
- Regression: Used to predict continuous variables, such as energy efficiency, hydrogen production, or membrane degradation. Common regression models include linear regression, polynomial regression, SVM, and decision trees. Support Vector Regression (SVR) is an extension of SVM.

- Clustering: Used to group similar data together, which can help identify patterns and anomalies. Common clustering algorithms include K-means, hierarchical clustering, and DBSCAN (Density-Based Spatial Clustering of Applications with Noise).
- Reinforcement Learning: Used to train an agent to make decisions that maximize reward over time. In the context of PEM electrolyzers, reinforcement learning can be used to develop optimal control strategies that minimize energy consumption and maximize hydrogen production.

Generative AI can be used to analyze operating data and simulate different configurations to identify operating parameters that maximize hydrogen production and minimize energy consumption, optimizing pressure, temperature, flow rate, and voltage in the electrolysis process. In this sense, AI can address the optimization of the performance and energy efficiency of PEM electrolyzers from different perspectives.

ML algorithms can be used to optimize voltage, current, temperature, pressure, and water flow to maximize efficiency and hydrogen production. For example, regression models can be used to predict energy efficiency based on operating parameters and then optimization algorithms can be used to find optimal values. In a similar sense, membrane degradation is one of the main factors limiting the lifespan of PEM electrolyzers. ML algorithms can be used to predict membrane degradation based on historical data and operating conditions. This enables preventive maintenance and an extension of electrolyzer lifespan. Moreover, ML algorithms can be used to enhance the design of electrolyzer components, such as the membrane, electrodes, and flow channels. This can improve the electrolyzer's efficiency, durability, and cost.

Reinforcement learning can be used to develop control strategies that allow the electrolyzer to adapt to fluctuations in energy from renewable sources. This improves system stability and reliability.

The output of a PEM generator is estimated using ML from solar radiation data in (Mert, 2021). The hydrogen flow rate and current of a laboratory-scale PEM electrolyzer are estimated through ML algorithms in (Ozdemir and Pektezel, 2024). ML is also applied to predict the hydrogen production rate in a PEM generator from photovoltaics in (Salari *et al.*, 2024). The cell voltage of an electrolyzer is estimated using ML-based models in (Bonab *et al.*, 2024).

3.2. Advanced management of PEM electrolyzers

In addition to ML and Deep learning, expert systems and AI-based predictive control play a crucial role in the advanced management of PEM electrolyzers.

Expert systems are computer programs designed to emulate the decision-making capabilities of a human expert in a specific field. In the context of PEM electrolyzers, an expert system could be used to diagnose faults, recommend corrective actions, and optimize operating parameters based on the knowledge and experience of engineers and scientists working in the field. The components of an expert system are:

- Knowledge base: Contains expert knowledge about the problem domain, including rules, facts, and heuristics.
- Inference engine: Uses knowledge from the knowledge base to reason and reach conclusions.
- User interface: Allows users to interact with the system and receive explanations and recommendations.

The application of expert systems offers several advantages that make them highly suitable for advanced electrolyzer management. On the one hand, it makes expert knowledge available to operators and technicians without the need for a human expert. Furthermore, due to the consistency and objectivity of decision-making, the risk of human error is reduced. On the other hand, it allows for handling complex situations that require the integration of multiple sources of information.

Model Predictive Control (MPC) is an advanced control technique that uses a system model to predict its future behavior and optimize control variables to achieve a desired objective (Camacho and Bordons, 2007). In the context of PEM electrolyzers, MPC can be used to optimize operating parameters, such as voltage, current, and temperature, to maximize efficiency and hydrogen production while minimizing component degradation (Calderón *et al*., 2020).

AI-based predictive control can manage constraints on control variables and state variables, ensuring the electrolyzer operates within safe and efficient limits. It also compensates for disturbances, such as fluctuations in power from renewable sources, improving system stability and reliability. Furthermore, it enables real-time optimization of operating parameters, adapting to changing conditions.

The combination of ML, Deep learning, expert systems, and AI-based predictive control can create a holistic management system for PEM electrolyzers.

The integration of AI into a holistic management system enables real-time monitoring through the collection and analysis of sensor data. Operating parameters can also be optimized using ML algorithms. AI-based predictive control can optimize the performance and durability of the electrolyzer. Furthermore, it can provide recommendations and explanations to operators and technicians through an expert system to assist with decision-making.

4. Applications of Generative AI in Predictive Maintenance of PEM Electrolyzers

Degradation and a gradual loss in efficiency of PEM electrolyzer assemblies is a common issue. Reasons may involve poisoning of the electrode catalysts, clogging of the diffusion layer mesh, decomposition of the humidified perfluorosulfonated polymer membrane, leaching and migration of aggressive F--ions toward the anode, as well as corrosion of the BPP due to the presence of water and working voltage of +1.8-2.0 V at the anodic side. Particularly the latter poses a big concern for the lifetime and ultimately commercialization of PEM-cells, since BPPs are not only responsible for separating single cells and channeling reagents within the electrolyzer assembly. Instead, they are also responsible for assuring structural integrity of the stack, and for conducting heat and electrical current.

Also, the lifespan of PEM electrolyzers and their performance decrease as they are used. Various electrochemical phenomena occur, such as ohmic losses, corrosion, overvoltages, and membrane thinning, among others (Feng *et al.*, 2017), (Scheepers *et al.*, 2020). AI can predict electrolyzer behavior under different operating conditions, enabling proactive management and predictive control.

Generative AI can create predictive models of plant performance under different operating conditions, predicting hydrogen production, energy consumption, equipment wear, and maintenance needs. Different sensor configurations and their optimal placement can even be simulated to maximize coverage and accuracy, while considering costs, redundancy, and sensitivity.

Moreover, generative AI can be used to predict equipment wear and proactively schedule maintenance, reducing downtime and maintenance costs by optimizing maintenance scheduling based on equipment criticality and resource availability. This enables early fault diagnosis, allowing anomalies to be detected and potential failures to be predicted, thus avoiding unplanned downtime and reducing maintenance costs.

Generative AI offers a set of tools to address these challenges, as it can learn normal plant behavior and detect subtle deviations that could indicate impending failures, such as anomalous changes in temperature patterns, energy consumption, or hydrogen production (Patil *et al.*, 2024).

4.1. Fault Diagnosis and Prediction Using Deep Learning

Deep learning has proven particularly effective for diagnosing and predicting faults in complex systems. Deep neural networks' ability to extract complex features and learn abstract representations of data makes them ideal for health monitoring of PEM electrolyzers (Goodfellow *et al.*, 2016).

Deep neural networks can automatically learn relevant features from data, eliminating the need for manual, often costly and time-consuming feature engineering. Furthermore, Deep learning can handle unstructured data, such as images and audio, which can be relevant for monitoring the health of PEM electrolyzers. For example, thermal images can be used to detect hot spots, which may indicate potential faults. Furthermore, in many cases, Deep learning models outperform traditional ML models in diagnostic and predictive tasks. The most commonly used types of deep neural networks are:

- Convolutional Neural Networks (CNN): These are especially useful for image processing and can be used to analyze thermographic images or scanning electron microscopy images to detect defects in the membrane or electrodes.
- Recurrent Neural Networks (RNNs): These are well-suited to processing time-series data and can be used to analyze sensor data over time to detect patterns that indicate potential failures. LSTM (Long Short-Term Memory) and GRU (Gated Recurrent Unit) variants are particularly popular due to their ability to remember long-term dependencies.
- Autoencoders: These are used to learn compact representations of data and can be used to detect anomalies. An autoencoder is trained to reconstruct input data, and any significant deviation between the input and output may indicate an anomaly.

4.2. Specific Applications of Deep Learning in Failure Diagnosis and Prediction

Deep learning models can be used to detect anomalies in sensor data, which may indicate potential faults. For example, a sudden increase in voltage or a decrease in hydrogen production could indicate a membrane or electrode failure.

These models can also be trained to identify specific faults based on sensor data. For example, a CNN can be trained to detect membrane defects from thermographic images.

Finally, these models can be used to predict the remaining lifespan of the electrolyzer based on historical data and operating conditions. This enables preventive maintenance and optimization of the replacement strategy.

5. Conclusions and future work

While the application of AI in PEM electrolyzer supervision and management offers significant potential, there are challenges that must be addressed for its successful implementation (Figure 3). Data quality and quantity are crucial to the success of AI models. Collecting relevant and reliable data can be costly and time-consuming. On the other hand, it is important to validate AI models in real-world environments to ensure their performance and reliability.

Some AI models, especially deep neural networks, can be difficult to interpret. This can make it difficult to understand how the model makes its decisions and to identify the underlying causes of failures. AI models must be robust and able to generalize well new operating conditions. This requires careful validation and testing of the models. Implementing AI systems can be expensive, especially if it requires the purchase of new hardware and software. AI systems can be vulnerable to cyberattacks. It is important to implement appropriate security measures to protect data and models.

In (Bassey and Ibegbulam, 2023) it is asserted that the full potential of AI in the production of green hydrogen needs to be explored through research on its integration with technologies such as IoT, advanced models and its application in real-world installations to demonstrate its effectiveness and scalability. Integrating AI with other technologies, such as the IoT and cloud computing, can improve the efficiency and reliability of PEM electrolyzer management systems.

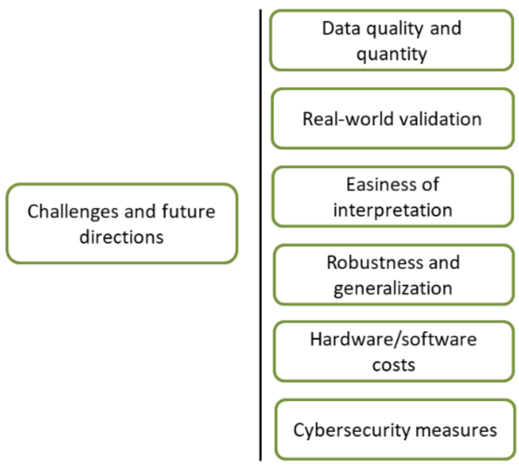

Figure 3: Scheme of challenges and future work directions.

As it has been expounded in the paper, AI offers a set of powerful tools to improve PEM electrolyzer supervision and management. From process optimization and early fault diagnosis to lifetime prediction and the development of predictive control strategies, AI has the potential to significantly improve the efficiency, durability, and cost-effectiveness of green hydrogen production. While there are challenges that need to be addressed, future research and development directions promise to further unlock AI's potential in this crucial field. As demand for green hydrogen continues to grow, the adoption of AI in PEM electrolyzer management and supervision will be critical to ensuring sustainable and efficient hydrogen production. Investment in research and development, as well as collaboration between academia, industry, and government agencies, will be key to accelerating AI implementation and making green hydrogen a global energy reality.

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