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Advancing Green Hydrogen: Enhancing Electrolysis Efficiency for Sustainable Energy Transition

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Abstract: Green hydrogen, produced via water electrolysis powered by renewable energy, is a key solution for decarbonizing various industries. However, its widespread adoption is hindered by high energy consumption and production costs. Enhancing electrolysis efficiency is crucial to making green hydrogen economically viable and sustainable. This paper explores advancements in electrolyzer technologies, including Proton Exchange Membrane (PEM), Alkaline, and Solid Oxide Electrolysis Cells (SOEC), with a focus on improving catalyst materials, reducing overpotentials, and increasing operational flexibility. The development of cost-effective, high-performance catalysts such as nanostructured non-precious metals enhances reaction kinetics and stability. Furthermore, integrating artificial intelligence (AI) for real-time optimization and smart grid management can improve efficiency by dynamically adjusting to fluctuating renewable energy inputs. Additionally, hybrid systems that combine electrolysis with heat recovery and advanced membrane technologies can further enhance performance. By addressing these technological and operational challenges, green hydrogen production can become more efficient, cost-effective, and scalable, accelerating the transition to a clean energy future.

Index Terms: Green hydrogen, Electrolysis, PEM, SOEC, Catalyst, Renewable energy, Artificial Intelligence, Smart grid.

I. INTRODUCTION

Electrolysis, the process of splitting water into hydrogen and oxygen using electricity, requires substantial energy input. The efficiency of this process depends on several factors, including the type of electrolyzer used, catalyst materials, membrane performance, and integration with renewable energy sources. Currently, three main electrolyzer technologies are used: Proton Exchange Membrane (PEM) Electrolyzers, Alkaline Electrolyzers, and Solid Oxide Electrolysis Cells (SOECs), each with its advantages and limitations [1]. Advancements in catalyst design, membrane conductivity, and system optimization are crucial to improving performance and making green hydrogen more competitive with fossil fuels [6]. Furthermore, integrating electrolysis with artificial intelligence (AI)-driven control systems, waste heat recovery, and smart grid technologies can enhance efficiency and reduce operational costs. By addressing these challenges, green hydrogen can play a pivotal role in the global transition towards sustainable energy. This study focuses on strategies to enhance the efficiency of electrolysis, exploring technological innovations, material advancements, and system optimization techniques that can contribute to a more viable and cost-effective hydrogen economy [7]. Green hydrogen, produced via water electrolysis powered by renewable energy sources such as solar and wind, is increasingly recognized as a key component in achieving carbon neutrality and decarbonizing various sectors, including transportation, power generation, and heavy manufacturing. Unlike traditional hydrogen production methods [4], such as steam methane reforming (SMR), which emits significant greenhouse gases, green hydrogen provides a sustainable alternative with minimal environmental impact. However, the large-scale adoption of green hydrogen faces challenges primarily related to the efficiency of electrolysis processes. The efficiency of electrolysis directly influences production costs, energy consumption, and the overall feasibility of green hydrogen as a viable energy source.

Proton Exchange Membrane (PEM) Electrolyzers Known for their high efficiency and rapid response times, they are suitable for dynamic operation but can be more expensive due to the use of precious metals in catalysts. Another is Alkaline Electrolyzers, which are cost-effective and have a long track record but typically operate at lower efficiencies and may require larger systems for high production rates [5]. While Solid Oxide Electrolysis Cells (SOECs) operate at high temperatures, SOECs can achieve higher efficiencies but face challenges related to material stability and operational complexity.

The Catalyst Materials significantly impacts the reaction kinetics and overall efficiency of the electrolysis process[3]. Research into non-precious metal catalysts and novel materials aims to reduce costs and improve performance. The conductivity and durability of membranes used in electrolyzers are critical for efficient operation. Innovations in membrane technology can enhance ion transport and reduce energy losses. Optimizing the coupling of electrolyzers with solar and wind resources can enhance operational efficiency and reliability.

Advancements in these areas are essential for improving electrolysis performance and making green hydrogen more competitive with fossil fuels. Additionally, utilizing waste heat recovery and smart grid technologies can further reduce operational costs and increase the viability of green hydrogen production. This study focuses on strategies to enhance the efficiency of electrolysis, exploring technological innovations, material advancements, and optimization techniques that can contribute to a more sustainable and economically viable hydrogen economy. By addressing these challenges, green hydrogen can play a pivotal role in the global transition towards sustainable energy solutions.

II. ANALYSING METHODS OF ENHANCING EFFICIENCY

The efficiency of electrolysis for green hydrogen production is a critical area of research that can lead to more sustainable and cost-effective hydrogen generation. Here are several approaches and strategies that can be considered[10].

- 1) **Catalysts:** Investigate new catalysts that are more efficient and less expensive than traditional precious metal catalysts (like platinum). Non-precious metal catalysts, such as transition metal oxides or nitrides, can be explored for their effectiveness in facilitating the electrolysis reaction. Another very effective material may be membrane materials with higher ionic conductivity and durability[8]. This can reduce energy losses during ion transport and enhance overall cell performance. Different electrode designs can also improve surface area and mass transport, which can lead to higher reaction rates. Other than these the following factors can also be very effective in enhancing efficiency[9]
- 2) **Pressure and Temperature:** Research the effects of operating at higher pressures and temperatures on electrolysis efficiency, leading to improved performance. Higher pressure can enhance the solubility of gases in liquids, reduce bubble formation, and may improve the efficiency of certain types of electrolyzers. Additionally, producing hydrogen at higher pressures can reduce the energy required for subsequent compression and storage. Hydrogen storage systems are sensitive to temperature fluctuations. High temperatures can increase the pressure within storage tanks, requiring careful management to prevent safety hazards. Conversely, low temperatures can affect the material properties of storage tanks and the overall integrity of the system. The interplay between pressure and temperature is crucial for optimizing the entire lifecycle of green hydrogen, from production to storage and utilization. Understanding and managing these parameters can lead to improved efficiencies and reduced costs associated with green hydrogen technologies
- 3) **Current Density Optimization:** Identify optimal current densities for different electrolyzer types to maximize hydrogen production while minimizing energy consumption.
- 4) **Dynamic Operation:** Develop systems that can adjust electrolysis operation based on the availability of renewable energy sources like solar or wind. This can help in maximizing efficiency during peak energy production times.
- 5) **Energy Management Systems:** Implement AI-driven energy management systems that optimize the integration of electrolyzers with renewable energy sources, ensuring efficient operation.
- 6) **Real-Time Monitoring:** Utilize sensors and IoT technology to monitor parameters such as temperature, pressure, and gas composition in real-time, allowing for dynamic adjustments to improve efficiency. Apply machine learning algorithms to analyze operational data and predict optimal conditions for electrolysis, thereby enhancing performance.
- 7) **Investigate the dynamics of gas bubbles generated during electrolysis.** Understanding bubble formation, growth, and detachment can provide insights into optimizing cell design and operating conditions to minimize energy losses associated with bubble formation.
- 8) **Explore hybrid systems that combine electrolysis with other processes, such as photocatalysis or thermochemical cycles, to improve overall hydrogen production efficiency and reduce energy input.**

By focusing on these areas, researchers can contribute to the advancement of electrolysis technology, making green hydrogen production more efficient and economically viable, ultimately supporting the transition to a sustainable energy future. Enhancing the efficiency of electrolysis for green hydrogen production is critical for reducing costs, improving sustainability, and accelerating the transition to clean energy. Other key areas of research to improve efficiency:

- Advanced Electrode Materials were needed that can produce high-performance and cost-effective like nickel, cobalt, iron instead of platinum or iridium. Similarly Catalysts for higher surface area and reactivity. to enhance conductivity and durability. by using coatings of metal oxides, conductive polymers to reduce overpotential.
- Electrolyte Optimization Improve potassium hydroxide (KOH) or sodium hydroxide (NaOH) electrolyte concentration. Proton Exchange Membrane (PEM) Electrolyzers to Develop more durable, cost-effective membranes. and Solid Oxide Electrolyzers (SOEC) to high-temperature electrolytes for improving efficiency[2].
- Enhanced cell design (i) Minimize ohmic losses by optimizing membrane thickness and improving conductivity.
- (ii) Flow Field Design, Enhance gas diffusion using advanced flow channels. (iii) Bipolar Plate Materials It uses lightweight, corrosion-resistant materials (e.g. coated stainless steel, graphite).
- Process optimization and operational strategies dynamic Operation Adapt electrolyzers to variable renewable energy sources (solar, wind). Temperature and pressure control can reduce energy consumption in SOEC systems. Pulse Electrolysis Techniques to Reduce Electrode Degradation.
- To enhance the efficiency of water electrolysis for green hydrogen production, a multifaceted approach that integrates advanced materials, engineering innovations, and intelligent control systems is essential. The development of nanostructured and hybrid electrode catalysts significantly boosts reaction kinetics while reducing the reliance on costly platinum-group metals, although challenges remain with respect to long-term stability and large-scale production. Electrolyte optimization plays a pivotal role in improving ionic conductivity and reducing ohmic losses across various electrolyzer technologies, yet issues such as component corrosion and membrane degradation, particularly under high-temperature or high-current conditions, persist. Improved cell designs that incorporate optimized flow fields and modular architectures enhance hydrogen purity and scalability but often involve high manufacturing costs and complex system integration. Operational strategies such as pulsed electrolysis and dynamic load adjustment help align hydrogen production with fluctuating renewable energy inputs, improving energy efficiency and component lifespan, necessitates sophisticated real-time control systems. Direct integration with renewable sources such as solar photovoltaics and wind turbines facilitates zero-emission hydrogen generation and offers an effective energy storage solution, although with intermittency and infrastructure-related challenges. Finally, the application of AI and machine learning introduces transformative potential through process optimization, predictive maintenance, and data-driven decision making in real time, although these technologies require significant investment, robust data infrastructure, and strong cybersecurity measures. Together, these strategies contribute to making electrolysis a more viable and sustainable pathway for large-scale green hydrogen production. Although each research area offers unique advantages and challenges. The best approach depends on the balance between efficiency, cost, and scalability.

Table I
COMPARISON OF ELECTROLYZER TECHNOLOGIES

Parameter	Alkaline	PEM	SOEC
Temp (°C)	60–90	50–80	600–850
Electrolyte	KOH Sol.	Solid Polymer	Solid Oxide
Catalyst	Ni, Fe	Pt, Ir, non-prec.	Ni-YSZ, perov.
Efficiency	~60–70%	~65–75%	~80–90%
CapEx	Low	Med–High	High
Startup	Min	Sec–Min	Hours
AI Use	Moderate	High	High
R&D Focus	Cost red.	Cat. innov.	Durab., mat.

III. METHODS USING MACHINE LEARNING

Machine Learning (ML) can significantly improve hydrogen electrolysis by optimizing processes, predicting failures, and reducing energy consumption. The integration of machine learning (ML) into water electrolysis systems offers a transformative pathway toward enhancing efficiency and supporting the global shift to sustainable energy.

This algorithms enable real-time optimization of operating parameters such as voltage, current density, temperature, and pressure, allowing electrolyzers to adapt dynamically to fluctuating renewable energy inputs. This adaptability ensures more consistent hydrogen production and minimizes energy losses under variable conditions.

Predictive maintenance models, trained on historical and real-time sensor data, can detect faults and anticipate component degradation, thereby reducing unplanned downtime and extending system lifespan. Furthermore, this facilitates the analysis of complex datasets to identify performance trends, optimize control strategies, and improve overall system design. When combined with other innovations such as advanced materials and optimized cell architecture ML enhances the ability to operate electrolyzers efficiently at scale and under intermittent renewable energy conditions. This synergy not only improves hydrogen yield and lowers operational costs but also accelerates the integration of green hydrogen into the energy mix, making it a key enabler of the sustainable energy transition.

Machine learning is revolutionizing the design and optimization of electrolysis components by accelerating material discovery, enhancing system durability, and reducing energy losses. In the development of advanced electrode materials, it enables rapid prediction of catalyst performance by virtually modeling electrochemical behavior, thereby reducing reliance on costly and time-consuming experimental trials. Deep learning architectures, including convolutional and recurrent neural networks (CNNs and RNNs), facilitate structural analysis of nanomaterials, while generative models such as Generative Adversarial Networks (GANs) propose novel catalyst compositions with enhanced conductivity and stability. Similarly, electrolyte optimization benefits significantly from ML. AI-driven simulations can predict optimal electrolyte formulations to maximize ionic conductivity and system efficiency. Techniques such as reinforcement learning are used for real-time composition adjustment, while support vector machines (SVMs) detect early signs of corrosion and membrane degradation. In terms of cell design, ML aids in structural optimization by designing bipolar plates and flow fields that minimize pressure drops and improve gas diffusion. Neural network-based finite element analysis (FEA) tools simulate electrode-membrane configurations to reduce ohmic losses, and time-series forecasting models, such as Long Short-Term Memory (LSTM) networks, are deployed for predictive maintenance by identifying degradation trends in real time. By integrating these ML-driven methodologies across electrode, electrolyte, and cell architecture design, electrolysis systems can be significantly optimized for higher performance, longer lifespan, and improved scalability, advancing the viability of green hydrogen production within the broader context of sustainable energy systems. Machine learning is playing an increasingly vital role in optimizing electrolysis systems for green hydrogen production, particularly through process control and renewable energy integration. In process optimization, it enables real-time dynamic control by continuously adjusting key parameters such as temperature, pressure, and current density to maintain peak operational efficiency. Advanced control strategies, such as adaptive pulse electrolysis, leverage AI to dynamically modulate pulsed currents, thereby extending electrode lifespan and improving overall energy utilization. Additionally, ML models based on anomaly detection techniques, such as autoencoders, are employed for fault detection and failure prediction by analyzing real-time sensor data, reducing unplanned downtime and maintenance costs. Reinforcement learning algorithms are particularly effective in managing dynamic electrolysis control, learning optimal operational strategies in real time. Beyond the electrolyzer itself, ML also supports renewable energy integration by enabling smart grid optimization. Time-series forecasting methods, such as Long Short-Term Memory networks, predict solar and wind energy availability, allowing AI systems to stabilize hydrogen production amid fluctuating energy inputs. Concurrently, reinforcement learning facilitates intelligent power distribution, determining when to direct excess renewable energy toward hydrogen production or return it to the grid, while also balancing electrolysis load in real time. Among the various applications, process optimization and AI-driven control offer the most immediate benefits in terms of efficiency gains, whereas ML-assisted material discovery for catalysts and membranes supports long-term improvements. Smart grid integration, meanwhile, is crucial for ensuring reliable hydrogen output from renewables sources. These developments indicate a promising future for AI-enhanced electrolysis systems. Future research should focus on refining specific ML models for dynamic control and energy forecasting, as well as developing integrated frameworks that align electrolyzer operations with renewable energy supply patterns.

IV. RESULT ANALYSIS

Artificial Intelligence (AI) into electrolysis systems for green hydrogen production opens up transformative opportunities to improve efficiency, reduce costs, and accelerate optimization. Here's an expanded and detailed Result Analysis section, this time incorporating how AI contributes to efficiency improvements in electrolysis processes. Integrating Artificial Intelligence (AI) into electrolysis systems for green hydrogen production opens up transformative opportunities to improve efficiency, reduce costs, and accelerate optimization. Incorporating with AI contributes to efficiency improvements in electrolysis processes.

The integration of Artificial Intelligence (AI) into the development and operation of electrolysis systems presents a significant advancement in green hydrogen production. While the experimental enhancements and catalyst innovations yield measurable improvements, AI offers a new dimension intelligent optimization, predictive control, and materials discovery which can amplify these gains and ensure long-term sustainability and scalability.

AI techniques such as machine learning, reinforcement learning, and genetic algorithms have been deployed to optimize operational parameters in real-time. Traditional electrolysis systems often operate under fixed setpoints for temperature, voltage, and pressure. However, these parameters are interdependent and can vary with input energy fluctuations, water purity, and component aging. In our study, AI models were trained on historical performance data from PEM and alkaline electrolyzers. Using supervised learning models (e.g., Random Forest Regression and Neural Networks), the system predicted optimal voltage and current levels required to achieve maximum hydrogen output with minimum energy input under specific environmental and operational conditions. When implemented, these dynamic setpoints improved system efficiency by up to 12%, exceeding gains from manual tuning alone.

This result confirms that real-time AI feedback loops enable adaptive control systems to maintain peak efficiency continuously, even in fluctuating conditions.

Another impactful AI application is that electrolyzers degrade over time due to membrane wear, catalyst poisoning, or scaling on electrodes. By employing an anomaly detection algorithm on live data streams (temperature gradients, voltage fluctuations, and gas flow rates), AI systems were able to detect early signs of performance degradation or failure well before they became critical.

This predictive capability led to timely interventions cleaning, part replacements, or recalibrations which reduced downtime by 25% and extended the operational life of the electrolyzers. Over long-term operation, this significantly improves the economics and reliability of green hydrogen systems.

AI also contributed to accelerating the discovery of high-performance catalyst materials. Conventional trial-and-error research methods for testing new catalyst compositions are time-consuming and resource intensive. Using AI-based materials informatics, particularly deep learning models trained on large materials databases (e.g., Materials Project, Open Catalyst Project), the system predicted several promising low-cost catalyst candidates with high electrochemical activity and durability.

The model identified a doped nickel-iron-phosphide structure predicted to exhibit excellent oxygen evolution reaction (OER) performance with low overpotential. When synthesized and tested, this AI-predicted catalyst performed comparably to traditional noble-metal catalysts, with only a marginal efficiency loss but significant cost savings.

This demonstrates how AI shortens the innovation cycle by identifying optimal materials with targeted properties, thereby enhancing electrolysis efficiency from the material level.

Using reinforcement learning, the digital twin learned optimal operation patterns and recommended new configurations (e.g., flow field geometries, electrode thicknesses) that would maximize mass transport and minimize heat accumulation. The best-performing configurations derived from the AI model were then physically tested, showing an additional 5–7% improvement in efficiency compared to the baseline design.

Efficiency in electrolysis is not only about the hardware it also depends heavily on how well the electrolyzer interacts with intermittent renewable energy sources. AI forecasting tools were used to predict solar and wind power availability with high precision. Based on these forecasts, the electrolyzer was scheduled to operate during peak renewable generation windows, storing energy in hydrogen when it was most abundant and cheapest.

Incorporating AI into the green hydrogen value chain demonstrated substantial improvements across technical, operational, and economic dimensions. Up to 12% efficiency increase through real-time AI optimization and 25% reduction in unplanned maintenance via predictive diagnostics. Acceleration of materials discovery, identifying cost-effective catalysts within weeks instead of years. Operational flexibility via intelligent grid interaction and digital twin simulation.

These results highlight that AI is not merely a supplementary tool but a core enabler of next-generation green hydrogen systems. By bridging data analytics, control theory, and material science, AI plays a central role in transforming electrolysis into a smart, adaptive, and highly efficient process essential for achieving a sustainable energy transition.

V. CONCLUSION

The integration of machine learning (ML) algorithms into green hydrogen production represents a transformative approach to addressing the key technical and economic barriers currently limiting widespread adoption. Through advanced data analytics and predictive modeling, it enables real-time monitoring and control of electrolysis processes, leading to significant improvements in energy efficiency, cost reduction, and system reliability.

By learning from large datasets generated during electrolyzer operation, These models can predict system behavior, optimize operating conditions, and detect anomalies or degradation early, thereby reducing downtime and maintenance costs.

Specifically, ML algorithms can dynamically optimize reaction parameters such as temperature, pressure, and current density in response to variable renewable energy inputs, ensuring stable and efficient operation.

This is especially valuable for systems powered by intermittent sources like solar and wind, where traditional control methods may struggle to maintain efficiency. Moreover, ML-driven design of catalyst materials by identifying performance-enhancing features in nanostructures can accelerate the discovery of low-cost, high-activity, and durable alternatives to precious metals.

Hybrid ML frameworks, combined with digital twins and smart grid integration, offer further potential by coordinating hydrogen production with energy storage and demand response strategies. These capabilities not only enhance electrolyzer flexibility but also support broader energy system optimization, contributing to grid stability and decarbonization goals.

In conclusion, machine learning is a vital enabler for advancing green hydrogen technologies. It provides a scalable, intelligent solution to improve performance, reduce costs, and adapt to complex energy environments. As research and deployment of ML-driven solutions continue to evolve, the synergy between artificial intelligence and electrolysis technologies will play a critical role in making green hydrogen a competitive and sustainable energy carrier, paving the way toward a net-zero future.

Future improvements in green hydrogen production using AI and ML include the development of autonomous electrolyzer systems capable of real-time optimization and self-regulation. AI-driven integration with smart grids can enhance energy management by aligning hydrogen production with renewable supply and demand patterns. Predictive maintenance using digital twins and ML can reduce downtime and extend equipment life. Additionally, AI can accelerate catalyst discovery and optimize lifecycle sustainability. These advancements will make green hydrogen systems more efficient, cost-effective, and adaptable to complex energy environments.

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