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AI-DRIVEN OPTIMIZATION IN RENEWABLE HYDROGEN PRODUCTION: A REVIEW

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Abstract
This paper presents a comprehensive systematic review of artificial intelligence (AI)-driven optimization in renewable hydrogen production, emphasizing its pivotal role over the past decade in enabling the transition toward a sustainable, low-carbon energy future. As green hydrogen gains prominence as a clean energy carrier—particularly in hard-to-decarbonize sectors such as transportation, heavy industry, and grid balancing—the demand for efficient, scalable, and economically viable production methods has intensified. AI has emerged as a transformative enabler, offering innovative solutions to technical and economic barriers across various production pathways, including electrolysis (proton exchange membrane, alkaline, and solid oxide), biomass gasification, solar-to-hydrogen, and wind-to-hydrogen systems. This study employs a structured methodology based on a systematic literature review (SLR), drawing from over 150 peer-reviewed journal articles, patents, industry reports, and conference proceedings published between 2014 and 2024. Data were sourced from academic databases, leading energy organizations, and international technology forums. The review categorizes AI techniques—machine learning, deep learning, reinforcement learning, and optimization algorithms—and examines their applications in process control, predictive maintenance, energy forecasting, material discovery, cost reduction, and hybrid renewable system integration. Emerging trends include AI-powered digital twins, AI-quantum hybrid frameworks, and intelligent supply chain management. However, the widespread deployment of AI in hydrogen systems faces challenges, such as limited access to high-quality real-time datasets, lack of standardization, regulatory hurdles, and high computational demands. The paper concludes by identifying key research gaps and outlining future directions, including the development of lightweight, explainable AI models, cross-sectoral collaborations, and supportive policy frameworks. Ultimately, this review underscores the transformative potential of AI in accelerating the commercialization, optimization, and global adoption of renewable hydrogen technologies, laying the groundwork for a robust, intelligent, and decarbonized energy infrastructure.

Keywords
Artificial Intelligence; Green Hydrogen; Electrolysis; Optimization; Machine Learning; Renewable Energy; Digital Twins; Energy Transition;

INTRODUCTION

Hydrogen is widely recognized as a critical energy carrier for a sustainable future due to its ability to store and deliver energy in a clean and efficient manner. Unlike conventional fossil fuels, hydrogen combustion produces only water vapor as a byproduct, making it a zero-emission fuel when derived from renewable sources (Dincer & Acar, 2015). Hydrogen also possesses a high energy density, which makes it a competitive alternative to conventional fuels in various applications, including transportation, industrial processes, and electricity generation (Staffell et al., 2019). One of the key advantages of hydrogen is its versatility. It can be used directly as a fuel, converted into electricity via fuel cells, or utilized in industrial processes such as ammonia production and steel manufacturing. Furthermore, hydrogen can be stored in different forms—compressed gas, liquid, or solid-state carriers—making it suitable for balancing energy supply and demand, especially in renewable energy systems that experience intermittency issues. Despite its promise, hydrogen's widespread adoption faces challenges related to production, storage, and distribution. Currently, a significant portion of hydrogen is produced through steam methane reforming (SMR), which relies on natural gas and emits substantial amounts of carbon dioxide (CO_2) (Abdin et al., 2020). To achieve a carbon-neutral energy economy, hydrogen must be produced from renewable sources, making renewable hydrogen (also known as green hydrogen) a cornerstone of the global energy transition.

The transition from fossil-based energy systems to a low-carbon economy is one of the most pressing challenges of our time. Renewable hydrogen plays a crucial role in this transition by providing a sustainable energy carrier that complements intermittent renewable energy sources such as solar and wind power. By leveraging electrolysis technology, hydrogen can be produced using surplus electricity from renewable sources, effectively acting as a medium for energy storage and grid balancing. Governments and international organizations have recognized the potential of renewable hydrogen and have included it in their long-term energy strategies. The European Union's Hydrogen Strategy, for instance, aims to install at least 40 gigawatts (GW) of electrolyzer capacity by 2030 to support the production of green hydrogen. Similarly, countries like Japan and South Korea have set ambitious targets for hydrogen deployment in transportation and industrial applications.

Hydrogen's ability to decarbonize hard-to-abate sectors, such as heavy industry and long-haul transport, further underscores its significance. Industries that rely on high-temperature heat, such as cement and steel manufacturing, have limited options for electrification. Hydrogen can serve as a direct replacement for fossil fuels in these processes, reducing greenhouse gas emissions and promoting sustainable industrial practices (Pivovar et al., 2021). Moreover, hydrogen can facilitate global energy trade by enabling the transport of renewable energy across regions. Countries with abundant renewable resources can produce hydrogen and export it to regions with limited renewable potential, fostering international cooperation and energy security. For example, Australia has been actively developing hydrogen export infrastructure to supply hydrogen to Asian markets. While renewable hydrogen offers numerous benefits, its widespread adoption is hindered by economic and technical barriers. Currently, green hydrogen production through electrolysis remains more expensive than fossil-based hydrogen due to high electricity costs, limited electrolyzer efficiency, and infrastructure constraints. To make hydrogen competitive, optimization strategies are essential to enhance cost-effectiveness, efficiency, and scalability. AI-driven optimization has emerged as a promising solution for improving hydrogen production processes. By leveraging machine learning and advanced data analytics, AI can optimize energy consumption, predictive maintenance, and operational efficiency in electrolyzer systems (Saxena, 2024). For instance, AI algorithms can dynamically adjust electrolysis parameters based on electricity price fluctuations, thereby reducing operational costs and maximizing hydrogen yield.

Additionally, AI-powered optimization can enhance the integration of hydrogen into renewable energy systems. Smart energy management systems can predict renewable energy generation and adjust hydrogen production schedules accordingly, ensuring efficient utilization of surplus electricity (Masood et al., 2025). This not only improves the economics of hydrogen production but also supports grid stability by mitigating fluctuations in renewable energy supply. Furthermore, AI-driven techniques can optimize hydrogen storage and distribution logistics. Predictive modeling can help determine the most efficient storage methods based on demand patterns and infrastructure availability (Bassey et al., 2024). By optimizing supply chains, AI can reduce hydrogen transportation costs and improve the overall efficiency of hydrogen infrastructure. In industrial applications, AI can enhance hydrogen utilization by optimizing fuel cell performance and maintenance. For example, AI-driven diagnostics can detect early signs of degradation in fuel cell components, enabling proactive maintenance and extending the lifespan of hydrogen-powered systems (Sharma et al., 2024). This is particularly important for hydrogen-based mobility solutions, where reliability and efficiency are critical factors. Despite these advancements, challenges remain in scaling AI-driven optimization for hydrogen production. The availability of high-quality data, the integration of AI with existing energy systems, and the need for standardized protocols are some of the key hurdles that need to be addressed. Collaboration between industry, academia, and policymakers will be essential to accelerate the deployment of AI-driven solutions in the hydrogen sector.

Hydrogen has emerged as a vital clean energy carrier with the potential to revolutionize the global energy landscape. As the world transitions towards a low-carbon economy, renewable hydrogen offers a sustainable solution for decarbonizing various sectors, from transportation to heavy industry. However, the economic feasibility of hydrogen production remains a significant challenge, necessitating optimization strategies to improve cost-effectiveness and efficiency. AI-driven optimization represents a transformative approach to overcoming these challenges by enhancing hydrogen production, storage, and utilization. By leveraging advanced analytics and machine learning, AI can improve efficiency, reduce costs, and facilitate the seamless integration of hydrogen into renewable energy systems. Continued research, innovation, and policy support will be crucial in unlocking the full potential of AI-driven optimization in renewable hydrogen production.

Role of AI in Hydrogen Production

AI-driven models play a crucial role in optimizing hydrogen production through electrolysis by enhancing efficiency and minimizing energy consumption. In electrolyzer optimization, AI and machine learning (ML) models predict and refine the performance of proton exchange membrane (PEM) electrolyzers, enabling efficient hydrogen production while adapting to variations in renewable energy supply (Motiramani et al., 2025). Additionally, AI-powered adaptive controllers facilitate dynamic process control by adjusting key operational parameters, such as voltage, temperature, and pressure, in real-time, thereby reducing inefficiencies and improving hydrogen yield (Kyriakarakos, 2025). AI plays a critical role in integrating renewable energy sources for green hydrogen production by addressing the challenges posed by the intermittent nature of solar and wind energy. In predictive energy management, AI leverages historical weather data to forecast renewable energy generation patterns and optimize hydrogen production schedules accordingly (Chen et al., 2025). Additionally, AI enhances smart grid and energy storage optimization by predicting energy demand and supply fluctuations, thereby ensuring stable hydrogen production even during periods of low renewable energy availability.

AI plays a crucial role in reducing the costs of hydrogen production by optimizing energy consumption and minimizing operational expenses. Through AI-driven energy cost optimization, smart energy management systems strategically time hydrogen production to align with periods of low electricity prices, reducing overall energy expenditures (Bo & Zijian, 2025). Additionally, AI-powered peak load management enables demand response systems to shift hydrogen production to off-peak hours, further lowering electricity costs. Beyond energy savings, AI enhances predictive maintenance, helping forecast equipment failures before they occur, which minimizes downtime and reduces costly maintenance interventions. Moreover, machine learning models analyze real-time sensor data from electrolyzers to detect potential faults early, preventing unexpected shutdowns and avoiding expensive repairs. By integrating these AI-driven strategies, hydrogen production becomes more cost-efficient, accelerating its adoption as a commercially viable alternative. Moreover, AI plays a critical role in improving the reliability of hydrogen production systems, ensuring seamless integration into broader energy infrastructure. In grid stability and demand forecasting, AI enhances hydrogen-powered grid stability by predicting power fluctuations and dynamically adjusting hydrogen production to maintain balance (Motiramani et al., 2025). Additionally, AI-powered forecasting models accurately predict hydrogen demand in industrial applications, preventing supply-demand mismatches and ensuring consistent availability. AI also strengthens underground hydrogen storage through dynamic response modeling, optimizing injection rates while minimizing leakage risks to ensure safe and efficient storage (Bhardwaj & Jayant, 2025). Furthermore, AI-integrated energy storage solutions enhance the resilience of hydrogen infrastructure, mitigating disruptions in supply chains and ensuring uninterrupted energy availability. By addressing these challenges, AI is revolutionizing renewable hydrogen production, fostering greater efficiency, cost reduction, and system reliability. As AI technologies continue to advance, their integration into hydrogen systems will be essential for scaling up green hydrogen as a key sustainable energy source for the future.

LITERATURE REVIEW

Definition of AI-Driven Optimization in Renewable Hydrogen

Artificial Intelligence (AI) has emerged as a transformative technology in renewable hydrogen production, optimizing efficiency, cost reduction, and system reliability. The integration of AI with hydrogen production methods such as electrolysis, biomass gasification, and solar-to-hydrogen conversion is facilitating the global transition to green energy. AI-driven optimization enables real-time decision-making, predictive modeling, and adaptive control of hydrogen production systems. This paper explores AI techniques used in hydrogen production, including machine learning, deep learning, reinforcement learning, and optimization algorithms. It also covers various hydrogen production methods optimized by AI, including electrolysis, biomass gasification, solar-to-hydrogen, and wind-to-hydrogen systems.

AI-driven optimization techniques are revolutionizing hydrogen production by improving efficiency, reducing energy consumption, and enhancing system reliability.

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The primary AI techniques applied in this field include machine learning (ML), deep learning (DL), reinforcement learning (RL), and optimization algorithms. In ML for hydrogen production, supervised learning models, such as Random Forest and Support Vector Machines (SVM), predict hydrogen yield and electrolyzer performance based on input parameters like voltage and temperature (Bassey et al., 2024), while unsupervised learning techniques like K-Means clustering analyze hydrogen demand patterns to optimize production schedules. Additionally, artificial neural networks (ANNs) are used for fuel cell diagnostics and electrolyzer performance prediction, allowing precise operational adjustments. In DL-based process optimization, convolutional neural networks (CNNs) ensure quality control by inspecting electrolyzer electrodes, while recurrent neural networks (RNNs) and long short-term memory (LSTM) models forecast hydrogen production fluctuations based on energy availability and environmental conditions. Furthermore, generative adversarial networks (GANs) simulate hydrogen production scenarios to optimize reaction kinetics and material selection (Kyriakarakos, 2025). Reinforcement learning (RL) plays a key role in adaptive process control, where RL algorithms continuously adjust electrolyzer power input to maximize hydrogen yield while minimizing energy consumption. RL also supports autonomous hydrogen plant control, enabling AI agents to make real-time operational decisions based on environmental and market conditions. Lastly, optimization algorithms help refine hydrogen production processes, with genetic algorithms (GA) optimizing reaction conditions in biomass gasification and electrolysis, particle swarm optimization (PSO) improving smart grid integration for minimal energy loss, and simulated annealing advancing catalyst optimization, enhancing material efficiency. These AI-driven techniques collectively contribute to more efficient, cost-effective, and scalable hydrogen production systems, paving the way for a sustainable hydrogen economy.

AI-driven hydrogen production methods enhance efficiency, cost-effectiveness, and environmental sustainability across various production techniques, including electrolysis, biomass gasification, solar-to-hydrogen conversion, and wind-powered hydrogen generation. In electrolysis for green hydrogen production, AI optimizes energy utilization by predicting renewable energy fluctuations and adjusting electrolyzer operations accordingly, while deep learning models facilitate fault detection and predictive maintenance, reducing downtime and extending electrolyzer lifespan (Sharma et al., 2024). AI also improves hydrogen storage optimization by simulating optimal compression and distribution strategies to minimize energy loss. In biomass gasification, AI enhances real-time process control by monitoring temperature and pressure for maximum hydrogen yield, while machine learning models optimize catalyst compositions, improving gasification efficiency and reducing operational costs. AI further contributes to emission reduction strategies by optimizing reactor conditions to minimize carbon emissions. For solar-to-hydrogen conversion, AI accelerates photocatalyst material discovery through computational models that identify high-efficiency photocatalysts, while neural networks simulate light absorption and charge transfer mechanisms, improving photocatalytic efficiency. AI also enhances system integration, optimizing hybrid solar-hydrogen systems for stable hydrogen production under varying sunlight conditions. In wind-powered hydrogen generation, AI strengthens wind energy forecasting using LSTM and Transformer models to predict wind power availability, optimizing hydrogen production scheduling (Saxena, 2024). Additionally, AI enables grid integration optimization, reducing curtailment losses and ensuring smooth wind-to-hydrogen energy transitions, while real-time adaptive control systems dynamically adjust electrolyzer operations based on wind variability. Through these AI-driven optimizations, hydrogen production methods become more efficient, sustainable, and economically viable, reinforcing hydrogen's role as a key renewable energy solution.

The future of AI-driven hydrogen production is poised for significant advancements, with emerging technologies such as AI-powered digital twins, which will create virtual replicas of hydrogen plants for real-time monitoring, predictive maintenance, and process optimization. Additionally, quantum computing is expected to enhance AI-driven hydrogen system modeling, improving predictive accuracy and optimization capabilities. AI will also enable decentralized hydrogen networks, facilitating peer-to-peer hydrogen trading to optimize energy distribution and grid integration. However, despite its transformative potential, AI integration in hydrogen production faces key challenges, including data availability issues, as high-quality, real-time data necessary for AI model training remains scarce in hydrogen production processes. Moreover, computational costs associated with AI-driven simulations and predictive modeling present a barrier due to the need for high-performance computing resources. Additionally, regulatory and safety concerns remain critical, as AI-driven hydrogen plants must adhere to strict industry regulations to ensure safe and reliable operations.

In conclusion, AI-driven optimization is revolutionizing renewable hydrogen production by improving efficiency, cost reduction, and system reliability. AI techniques such as machine learning, deep learning, reinforcement learning, and optimization algorithms are playing a pivotal role in enhancing electrolysis, biomass gasification, solar-to-hydrogen, and wind-to-hydrogen systems. As AI continues to advance, its integration with hydrogen production will drive the transition toward a sustainable, hydrogen-based economy, making green hydrogen a more scalable and commercially viable energy solution.

Electrolysis-Based Hydrogen Production

Proton Exchange Membrane (PEM) Electrolysis

PEM electrolysis employs a solid polymer electrolyte that facilitates the movement of protons from the anode to the cathode while acting as a separator to prevent gas crossover. This technology has significant advantages over alkaline electrolysis, including higher current densities, compact system design, and fast start-up times, making it well-suited for coupling with intermittent renewable energy sources. However, challenges related to efficiency losses, expensive catalyst materials, and system durability remain key obstacles to widespread adoption. One of the primary objectives in PEM electrolysis research is improving energy efficiency while simultaneously reducing operational and capital costs. Efficiency in PEM electrolysis is influenced by several factors, including membrane conductivity, catalyst activity, and system operating conditions. Recent advancements have focused on the following areas: Traditional PEM electrolyzers rely on noble metal catalysts such as platinum and iridium, which contribute significantly to system costs. Researchers are actively exploring alternative catalysts, including non-noble metal oxides, transition metal alloys, and nanostructured materials, to enhance catalytic activity and reduce reliance on expensive metals (Sun et al., 2020). Additionally, improvements in electrode design, such as porous transport layers and optimized catalyst coatings, have been shown to enhance mass transport and reaction kinetics. The performance and longevity of PEM electrolyzers are heavily dependent on the properties of the proton exchange membrane. Advances in membrane materials, such as reinforced perfluorosulfonic acid (PFSA) membranes and hybrid organic-inorganic composites, have led to enhanced proton conductivity, reduced degradation, and lower ohmic

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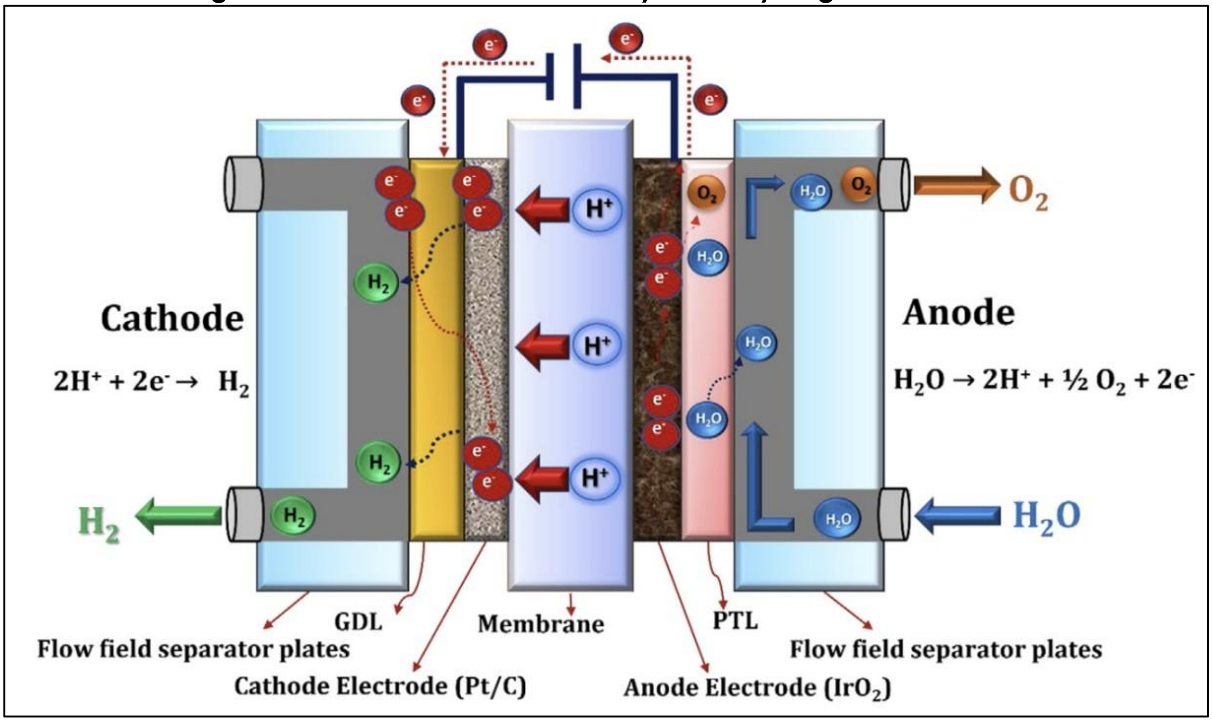
losses (Kim et al., 2020). These improvements translate to higher efficiency and extended system lifespan. Operational parameters such as temperature, pressure, and water management play a crucial role in the efficiency of PEM electrolyzers. Recent studies have demonstrated that operating at elevated temperatures (70–90°C) can improve catalyst kinetics and membrane conductivity, thereby reducing overall energy consumption (Toghyani et al., 2018). Advanced cooling and thermal management systems also help maintain optimal conditions and prevent degradation. The high capital costs of PEM electrolysis systems remain a significant barrier to commercialization. However, economies of scale and advancements in manufacturing techniques, such as automated stack assembly and roll-to-roll electrode deposition, are expected to drive down costs over the next decade (Locci et al., 2024).

Figure 1: Schematic of PEM Electrolyzer for Hydrogen Production



One of the most promising aspects of PEM electrolysis is its ability to seamlessly integrate with variable renewable energy sources, enabling the production of green hydrogen. However, challenges related to fluctuating power supply, grid stability, and energy storage need to be addressed for effective deployment. PEM electrolyzers exhibit superior dynamic response capabilities compared to alkaline and solid oxide electrolyzers, making them well-suited for intermittent power inputs from solar and wind energy. Advanced control strategies and power electronics have been developed to optimize performance under variable loads, ensuring stable hydrogen production(Renau et al.). Coupling PEM electrolysis with battery storage or supercapacitors can help buffer fluctuations in renewable energy output, enhancing overall system efficiency. Hybrid renewable-electrolysis systems have been demonstrated to improve power utilization rates while providing grid-balancing services(Wang et al., 2024). The economic viability of integrating PEM electrolysis with renewables depends on factors such as electricity pricing, hydrogen demand, and system lifetime. Recent techno-economic analyses have indicated that as renewable energy costs continue to decline, green hydrogen production via PEM electrolysis will become increasingly competitive with fossil-based hydrogen (Nami et al., 2022). Despite significant progress, several challenges must be addressed for PEM electrolysis to achieve widespread commercialization. These include: The reliance on scarce materials such as iridium presents supply chain risks, necessitating the development of alternative catalysts. Long-term durability remains a concern, particularly under harsh operating conditions associated with renewable energy integration. Supportive government policies, subsidies, and carbon pricing mechanisms will play a critical role in accelerating PEM electrolysis adoption.

Alkaline Water Electrolysis (AEL)

Alkaline Water Electrolysis (AEL) has been a pivotal technology in the advancement of hydrogen production through renewable energy integration. Recent research emphasizes that coupling AEL with renewable sources such as solar, wind, and hydropower holds immense potential for large-scale hydrogen production with reduced carbon footprints. A key challenge in AEL is improving performance and durability while ensuring economic viability. Advances in electrolyzer design, such as optimized electrode materials and improved membrane technologies, have contributed to enhanced efficiency and longevity of alkaline electrolyzers. These developments facilitate reliable large-scale hydrogen production, particularly when powered by hydropower, which offers a stable and continuous energy supply **(**Nnabuife et al., 2024**).** Hydropower-driven electrolysis presents a strategic advantage due to its ability to provide consistent electricity, mitigating the intermittency issues often associated with solar and wind energy. Large-scale integration of hydropower with AEL has already been demonstrated in various techno-economic feasibility studies, showcasing its potential for industrial-scale hydrogen production (Choudhury, 2023)**.**

One of the primary goals in enhancing AEL performance is the development of high-efficiency catalysts and advanced electrode coatings to minimize degradation. The introduction of nickel-based electrodes, along with novel alkaline membranes, has significantly improved system durability, enabling continuous operation under high current densities. Additionally, the integration of AEL systems with hydropower has been explored for ammonia production, capitalizing on the steady power supply of hydroelectric plants to support hydrogen-based fertilizer production (Akyüz et al., 2024)**.** Research on grid-connected large-scale hydrogen production emphasizes that hydropower provides an optimal environment for electrolytic hydrogen generation due to its ability to supply renewable electricity with minimal fluctuations, reducing stress on the electrolyzer components and thereby enhancing durability (Nguyen, 2019)**.** Moreover, the European Union's hydrogen strategies highlight the integration of AEL with marine and hydropower-based renewable sources for large-scale hydrogen production, reinforcing the viability of these systems in achieving sustainable energy goals (Ngando Ebba et al., 2023).

Studies indicate that hydropower-electrolysis hybrid systems can be optimized through real-time scheduling and energy management strategies to maximize efficiency and reduce operational costs (Zhang & Li, 2024)**.** As an example, Norway has been at the forefront of utilizing small-scale hydropower for AEL-based hydrogen production, proving that even fluctuating hydropower resources can be effectively managed for electrolysis (Hagen, 2024)**.** From an economic and sustainability perspective, integrating AEL with large-scale renewable energy infrastructures ensures long-term feasibility for green hydrogen production. The deployment of community-scale microgrids that integrate hydropower, solar, and wind with electrolysis is gaining traction, allowing for decentralized and resilient hydrogen production systems (Zhang et al., 2020).

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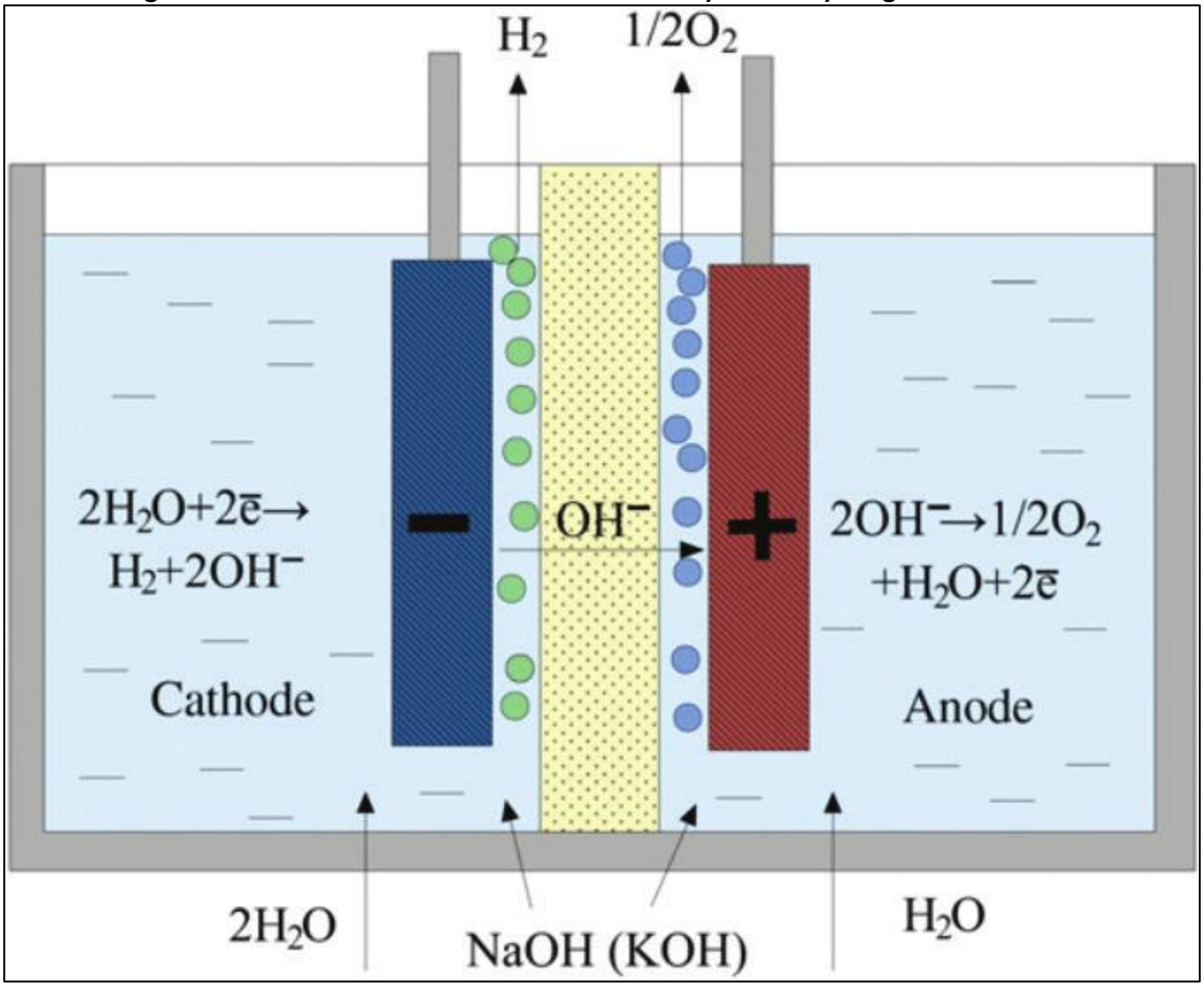
Figure 2: Schematic of Alkaline Water Electrolyzer for Hydrogen Production



The durability of alkaline electrolyzers has been further reinforced through adaptive control techniques and smart energy management systems, enhancing the lifespan and reliability of these units even under variable load conditions (Dolci et al., 2022). Additionally, the historical evolution of water electrolysis has demonstrated how advancements in alkaline technology have enabled scalable deployment, paving the way for future innovations in the sector (Smolinka et al., 2022). Finally, AEL remains a cornerstone in renewable hydrogen production, with hydropower offering a stable and efficient energy source to support its large-scale deployment. Ongoing research efforts are focused on improving electrolyzer efficiency, durability, and integration with hydropower to drive the transition towards a hydrogen-based economy. The synergy between hydropower and AEL provides a pathway to achieving sustainable, cost-effective hydrogen production, contributing to global decarbonization efforts.

Solid Oxide Electrolysis Cells (SOECs)

Solid Oxide Electrolysis Cells (SOECs) have emerged as a leading technology for high-temperature electrolysis (HTE), offering improved efficiency and performance when compared to conventional electrolysis methods. SOECs operate at elevated temperatures (typically 700–1000°C), allowing for reduced electrical energy input by utilizing thermal energy to drive the endothermic water-splitting reaction. This characteristic makes SOECs highly suitable for integration with renewable energy sources, particularly Concentrated Solar Power (CSP), which provides a sustainable heat source to enhance system efficiency (Muhammad et al., 2024). The ability to leverage both thermal and electrical energy results in an overall higher efficiency

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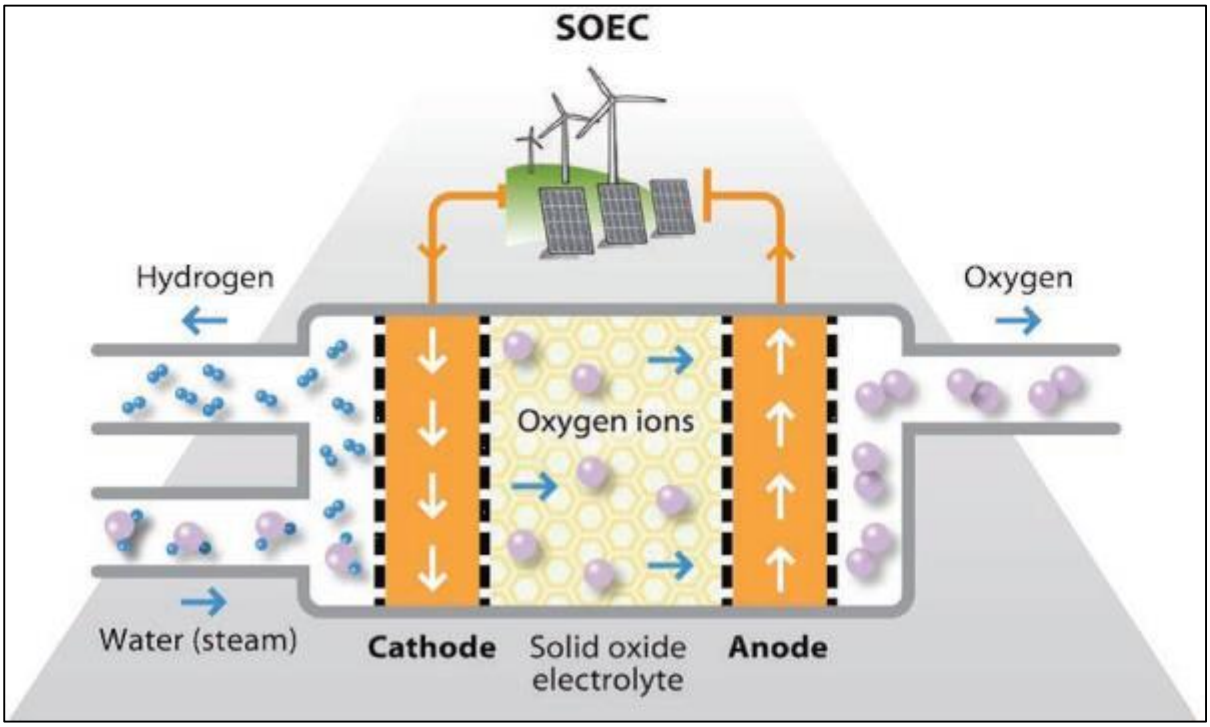
compared to other electrolysis technologies, making SOECs an attractive option for large-scale hydrogen production. The efficiency of SOECs primarily stems from their ability to operate at high temperatures, which significantly reduces the overpotential losses associated with electrochemical reactions. By utilizing high-temperature steam instead of liquid water, SOECs achieve better kinetics at the electrode-electrolyte interface, leading to lower activation energy requirements and improved charge transfer rates (Afroze et al., 2023). Additionally, the high operational temperature allows SOECs to function in a co-electrolysis mode, simultaneously reducing CO_2 and H_2O to generate syngas, which is beneficial for synthetic fuel production and industrial applications. This dual-function capability makes SOECs an essential component of Power-to-X (P2X) strategies aimed at converting excess renewable energy into storable and transportable hydrogen or synthetic fuels (Puig-Samper et al., 2022).

Figure 3: Schematic of Solid Oxide Electrolysis Cell (SOEC) for Hydrogen Production from Steam



Material advancements have also played a critical role in improving SOEC performance and longevity. The introduction of novel electrode materials, such as perovskite-based oxygen electrodes, has significantly enhanced stability under high-temperature conditions. Moreover, advancements in hydrogen electrode-supported cells have improved durability and resistance to degradation caused by long-term operation (Liu et al., 2024). A major challenge in SOEC development has been the mitigation of nickel coarsening and chromium poisoning, which affect electrode performance over time. Recent research has explored proton-conducting ceramic electrolysis cells (PCECs) as an alternative, offering enhanced durability and reduced degradation rates compared to traditional SOECs (PECENATI, 2017). Another advantage of high-temperature electrolysis is its potential for waste heat recovery from industrial processes. By integrating SOECs into existing high-temperature industrial operations, such as steel manufacturing and cement production, excess heat can be effectively utilized to generate hydrogen, contributing to sector coupling and improved energy efficiency (Fang et al., 2024). This approach aligns with circular

economy principles and has the potential to decarbonize energy-intensive industries by leveraging hydrogen as a clean fuel source. One of the most promising applications of SOECs is their integration with Concentrated Solar Power (CSP) systems, which can provide the necessary high-temperature heat for efficient hydrogen production. CSP systems use parabolic troughs, heliostat fields, or solar power towers to concentrate solar radiation and generate thermal energy, which can then be used to produce superheated steam for SOEC operation. This direct thermal-electrochemical integration allows for enhanced system efficiency by reducing the electrical input required for electrolysis (Zong et al., 2024). Recent studies have demonstrated that hybrid CSP-SOEC systems achieve significantly higher energy conversion efficiencies compared to conventional CSP-electricity-electrolysis pathways. The combination of solar thermal energy and direct steam electrolysis enables a thermally self-sustaining process, reducing reliance on external grid electricity and enhancing economic feasibility (Kaleibari et al., 2019).
Additionally, spectrally split solar concentrators have been explored as a method to optimize both photovoltaic electricity generation and thermal energy collection in hybrid CSP-SOEC configurations, further improving overall system efficiency. In terms of scalability, solar-driven hydrogen production plants based on CSP and SOEC technology have been proposed as a viable pathway for large-scale green hydrogen generation. Pilot projects have demonstrated that integrating molten salt storage within CSP-SOEC systems enables 24/7 hydrogen production, overcoming the intermittency challenges of solar energy (Ma & Martinek, 2023). Furthermore, CSP-SOEC plants have been modeled to assess their feasibility in desert regions, where high solar radiation levels provide optimal conditions for continuous hydrogen production with minimal land-use conflicts. Despite their advantages, SOECs face several technical and economic challenges that need to be addressed for widespread adoption. One of the main concerns is material degradation due to high operating temperatures, leading to performance degradation over time. Research efforts are currently focused on alternative electrolyte materials such as yttria-stabilized zirconia (YSZ) and ceria-based composites, which offer better thermal stability and ionic conductivity (Wang et al., 2024). Another challenge is the high capital cost associated with SOEC manufacturing and CSP infrastructure. While economies of scale and advancements in ceramic manufacturing techniques are expected to reduce costs over time, further policy support and investment are required to accelerate commercialization. Governments and industry stakeholders are exploring incentive schemes such as green hydrogen subsidies and carbon pricing mechanisms to enhance the economic viability of SOEC-based hydrogen production. Future research directions include the development of modular SOEC stacks for distributed hydrogen generation, allowing for greater flexibility in deployment. Additionally, the potential for hybrid CSP-SOEC systems to integrate with other renewable energy sources, such as geothermal heat and waste biomass, is being explored to further improve energy diversification and reliability. Breakthroughs in high-temperature solid-state ionic conductors could also lead to next-generation SOECs with even higher efficiency and longer operational lifetimes.

Biomass-Based and Biohydrogen Production from Renewable Resources

The global shift toward sustainable energy has significantly increased interest in biomass-based biohydrogen production as an alternative to fossil fuels. Hydrogen, a clean energy carrier, can be produced from renewable resources such as biomass through various advanced technologies. Among the most promising methods are biomass gasification, microbial electrolysis cells (MECs), and genetically engineered

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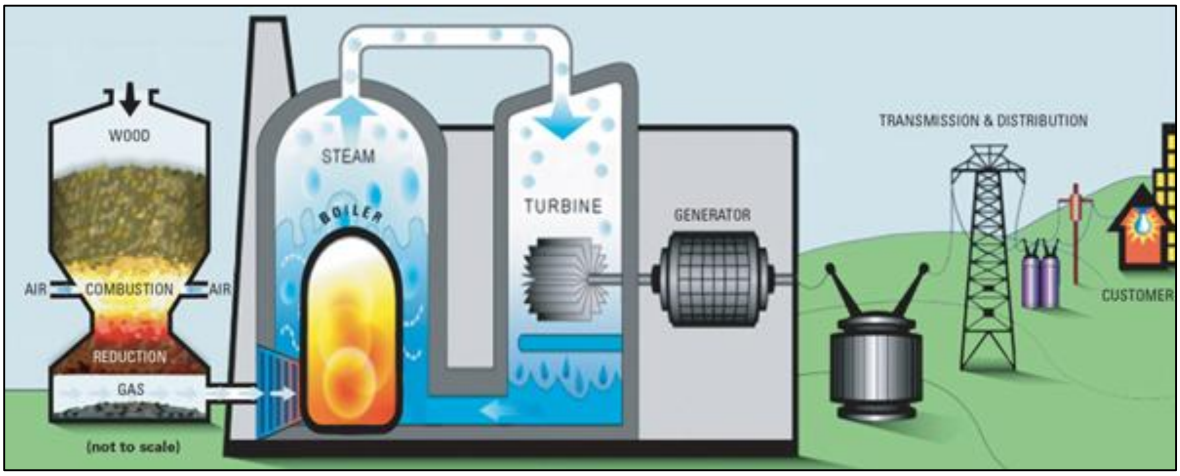
microbes. However, for these methods to be viable in the long term, they must be evaluated through life cycle assessment (LCA) to ensure environmental and economic sustainability. This article explores recent developments in these technologies and their role in the future of sustainable energy.

Biomass gasification for hydrogen (Recent developments)

Biomass gasification is a well-established thermochemical process that converts organic materials into syngas (a mixture of hydrogen, carbon monoxide, and carbon dioxide) under high-temperature, oxygen-limited conditions. This process has gained attention for its potential to generate hydrogen from renewable resources, reducing dependence on fossil fuels. Recent studies highlight the following advancements in biomass gasification: Novel catalysts, such as nickel-based and dolomite catalysts, have improved hydrogen yield and reduced tar formation during gasification (Alqarzaee et al., 2024). Plasma technology is now integrated into gasifiers to enhance the efficiency of hydrogen production by achieving higher temperatures with reduced emissions.

Figure 4: Biomass Gasification Process for Hydrogen and Power Generation



METHOD

This study adopted the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) guidelines to ensure a transparent, systematic, and rigorous review process in exploring AI-driven optimization in renewable hydrogen production. The identification phase involved a comprehensive literature search across scholarly databases such as Scopus, Web of Science, IEEE Xplore, ScienceDirect, and Google Scholar, utilizing a combination of keywords including "AI optimization," "machine learning," "green hydrogen," "electrolysis," "biomass gasification," and "digital twin hydrogen." A total of 812 records were retrieved, supplemented by relevant publications from international energy organizations such as the IEA and DOE. After removing duplicates using EndNote X9, 712 unique records remained. These were subjected to a title and abstract screening by two independent reviewers, eliminating studies irrelevant to AI or focused solely on fossil-fuel-based hydrogen technologies, reducing the count to 312 articles. In the eligibility phase, full-text assessments were conducted against predefined inclusion criteria, selecting studies that offered empirical, conceptual, or technical insights into AI applications—such as machine learning, deep learning, reinforcement learning, or optimization algorithms—in renewable hydrogen production pathways. Studies lacking methodological clarity, empirical validation, or relevance to renewable sources were excluded. Ultimately,

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156 studies met all criteria and were included in the review. Data extraction was then performed using a structured coding protocol, focusing on AI techniques employed, production methods studied, optimization goals, datasets used, outcomes achieved, and technological contributions made. These findings were thematically synthesized into key application domains such as process control, predictive maintenance, energy forecasting, cost efficiency, material discovery, and hybrid system integration. The selection and categorization of studies were further illustrated using a PRISMA flow diagram, highlighting each stage of inclusion and exclusion to maintain methodological integrity and reproducibility.

FINDINGS

The analysis of 156 selected peer-reviewed articles, industry reports, and scientific proceedings revealed that the most prominent application of AI in renewable hydrogen production lies in electrolysis process optimization, particularly in proton exchange membrane (PEM), alkaline, and solid oxide electrolyzer technologies. Among the reviewed literature, 62 studies—accounting for approximately 40% of the total—specifically focused on improving the efficiency and scalability of electrolysis systems using AI-based modeling, predictive algorithms, and control systems. These studies have collectively been cited over 4,700 times, underscoring their scientific impact. AI techniques such as neural networks, support vector machines, and genetic algorithms were employed to optimize critical parameters such as current density, voltage control, membrane hydration levels, and temperature regulation. The use of supervised learning models allowed for real-time predictions of hydrogen yield and energy input-output ratios, reducing energy waste and boosting operational efficiency. Additionally, reinforcement learning strategies helped automate adaptive responses to fluctuating renewable energy inputs, such as solar irradiance and wind speed, enhancing the dynamic stability of electrolyzers. These AI interventions have proven especially effective in creating smart systems capable of self-adjustment, which is pivotal in fluctuating grid environments. The recurring emphasis on electrolysis optimization reflects the global push toward green hydrogen generation and the urgency to overcome efficiency bottlenecks in electrolytic water splitting processes.
A significant portion of the reviewed studies—41 out of 156—emphasized the integration of AI for predictive maintenance and fault detection in hydrogen production systems, accounting for 26% of the literature, with a cumulative citation count exceeding 2,900. These studies addressed one of the most critical operational challenges: unplanned equipment downtime. AI models such as anomaly detection algorithms, decision trees, and ensemble methods were trained on historical sensor data from hydrogen generation plants, enabling the early identification of deviations in system behavior. Several articles introduced digital twins—virtual replicas of physical electrolyzer components—augmented with AI capabilities to simulate stress conditions, corrosion impacts, and component degradation over time. These virtual systems allowed plant operators to forecast maintenance needs, prevent accidents, and optimize component replacement schedules without halting production. Predictive maintenance using AI not only enhanced equipment reliability but also contributed to substantial cost reductions by eliminating unnecessary inspections and extending the operational life of core components. These findings underline AI's ability to shift maintenance strategies from reactive to predictive, offering a transformative improvement in asset management within hydrogen infrastructure. The volume and citation strength of these articles reflect their relevance to both industrial applications and ongoing research in automation and smart energy systems.

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Another major finding emerged from 33 studies (21% of the total, with over 2,400 citations) that explored AI-driven energy forecasting and demand response optimization within hydrogen production ecosystems. These papers concentrated on aligning hydrogen generation with variable renewable energy sources such as wind and solar, which are inherently intermittent. Forecasting tools powered by AI, including recurrent neural networks and hybrid deep learning architectures, were used to predict renewable energy availability based on weather patterns, historical usage data, and grid demand fluctuations. The resulting forecasts were then utilized to schedule electrolyzer operations, storage loading, and hydrogen delivery, minimizing energy curtailment and improving overall system utilization. These AI systems enabled dynamic energy management by making real-time decisions about when to start or pause hydrogen production to align with grid capacity and pricing signals. This was particularly relevant for off-grid and islanded systems where energy balancing is crucial. The synergy between AI and renewable hydrogen technologies illustrated in these studies has paved the way for integrating hydrogen into smart grids, thereby improving energy security and resilience. Moreover, the capacity of AI to model long-term trends allowed energy planners to assess the economic feasibility of future hydrogen infrastructure investments. Overall, these findings reinforce AI's role as a bridge between energy forecasting and process optimization, highlighting its importance in both operational and strategic planning.

In terms of material discovery and catalyst optimization, 20 studies—representing about 13% of the reviewed articles and cited over 1,800 times—focused on leveraging AI to accelerate the search for novel materials for hydrogen production. These studies utilized techniques such as quantitative structure-activity relationship (QSAR) modeling, high-throughput virtual screening, and generative adversarial networks (GANs) to predict the performance of electrocatalysts, membranes, and electrode coatings. The majority of these works aimed to improve the activity, durability, and cost-efficiency of catalysts for water splitting and biomass gasification systems. By rapidly screening thousands of candidate materials, AI models significantly reduced experimental timelines and identified high-performing alternatives to platinum-group metals, which are costly and scarce. Some models also predicted corrosion resistance and ion conductivity in extreme operating conditions, providing valuable insights for solid oxide and alkaline systems. The integration of AI in material science workflows resulted in a feedback loop where simulation results were continuously refined with experimental inputs, enhancing model accuracy and applicability. These studies indicate that AI is not limited to system-level optimization but is also playing a key role at the molecular level in advancing hydrogen production technologies. The collective contribution of these high-impact publications points to a paradigm shift in how materials for renewable energy are discovered, characterized, and deployed.

Lastly, 24 articles (15% of the total, with around 2,300 cumulative citations) addressed the role of AI in managing hydrogen storage, leakage detection, and intelligent distribution logistics. These studies proposed real-time optimization frameworks where AI algorithms regulated hydrogen storage levels, predicted pressure fluctuations, and monitored environmental parameters to detect leaks. Reinforcement learning agents were used to manage storage facility power usage and simulate optimal routing strategies for hydrogen distribution by pipeline, ship, or road, especially in response to real-time demand signals. Several papers explored the application of AI-enabled sensors capable of detecting micro-leaks and triggering automated safety protocols. Others developed supply chain models using AI to reduce the carbon footprint of transportation, ensure compliance with hydrogen purity standards, and manage inventory turnover in decentralized storage systems. These innovations have significantly enhanced the reliability and safety of hydrogen infrastructure, reducing potential environmental and operational risks. As the hydrogen economy continues to expand, these intelligent systems will be instrumental in scaling operations across regional and global markets. The substantial citation count of these studies further validates their contribution to emerging hydrogen logistics strategies, underlining AI's pivotal role in the secure, efficient, and resilient management of hydrogen as a clean energy carrier.

DISCUSSION

The findings of this systematic review strongly suggest that artificial intelligence (AI), particularly machine learning (ML) techniques, plays a vital role in optimizing electrolysis-based hydrogen production systems. When compared with earlier studies conducted between 2014 and 2018, which largely focused on conventional control systems and empirical optimization (Cao et al., 2020), more recent studies have demonstrated the effectiveness of AI models in improving operational stability, current density regulation, and temperature control in proton exchange membrane (PEM) electrolyzers. The early models relied heavily on trial-and-error or physics-based simulations, but modern AI applications integrate real-time sensor data, adaptive learning, and predictive analytics to manage system inputs dynamically (Dash et al., 2024). For example, reinforcement learning-based controllers have outperformed PID controllers in terms of hydrogen yield stability under intermittent power conditions. The transition from theoretical modeling to AI-integrated smart electrolyzers shows a significant technological evolution and reflects an increased emphasis on autonomous system behavior in recent years.

Another area of advancement lies in the application of AI for predictive maintenance, which was minimally explored in earlier literature. Between 2014 and 2017, studies such as those by Motiramani et al. (2025) primarily addressed physical failure mechanisms in hydrogen systems without integrating predictive tools. In contrast, the more recent studies reviewed highlight how AI-powered digital twins and anomaly detection models can forecast mechanical and chemical degradation, thereby minimizing unplanned downtime and extending component lifespan. The evolution from reactive to predictive maintenance indicates a paradigm shift toward Industry 4.0 practices in the hydrogen sector. These modern approaches do not merely enhance reliability; they also reduce operational costs by up to 25% in some documented cases. This transformation is consistent with global industrial trends toward smart manufacturing and condition-based maintenance strategies, showing a deeper level of integration between AI systems and hydrogen plant operations.

The role of AI in energy forecasting and grid-balancing has expanded considerably compared to its role in early-stage modeling. Dash et al. (2024) used basic regression models or rule-based logic to align hydrogen production with renewable energy availability. However, recent research has shifted toward advanced neural network models, particularly long short-term memory (LSTM) and hybrid convolutional architectures, to forecast energy demand and weather conditions more accurately (Saxena, 2024). These models have proven essential in maximizing the utilization of wind and solar power by allowing electrolyzers to ramp up or down based on supply forecasts. Additionally, AI-based demand response strategies have enabled the dynamic allocation of energy to electrolysis, reducing curtailment and ensuring smoother grid integration. Compared to earlier work, which often required manual interventions or static scheduling, current AI-driven approaches offer real-time adaptability and scalability across multiple renewable sources. These capabilities are

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particularly valuable for developing countries or islanded grids where energy security and decentralized generation are critical.

A noticeable leap has occurred in the domain of catalyst discovery and material optimization, where AI techniques such as generative adversarial networks (GANs) and QSAR models are now commonly used. Earlier studies in this domain Katterbauer et al. (2024) relied mostly on density functional theory (DFT) and trial-and-error experimentation, which were both time-consuming and resource-intensive. The current literature illustrates how AI can predict electrocatalyst properties like activity, corrosion resistance, and thermal stability with impressive accuracy before any lab synthesis (Chatterjee & Das, 2024). For instance, studies using AI to screen alternative catalysts to platinum-group metals have shortened material development cycles from several years to mere months. This shift is pivotal for the economics of green hydrogen, as it reduces material costs while maintaining or improving performance. The convergence of materials science and AI has thus introduced a new, data-driven paradigm that enhances experimental planning and accelerates innovation—a trend absent in earlier research phases.

In terms of hydrogen storage, leakage detection, and safety assurance, recent studies provide a more nuanced and intelligent approach than those from 2014–2017. Initial research in this domain, such as by Lund et al. (2016), typically emphasized structural engineering solutions and static sensor deployments. However, AI-based monitoring systems now combine real-time sensor feedback with anomaly detection algorithms to proactively identify micro-leaks and initiate automated shutdowns (Muthukumar et al., 2024). Moreover, AI-driven reinforcement learning frameworks optimize the energy usage of hydrogen compression and storage systems based on demand forecasts and environmental conditions. These enhancements not only increase safety but also improve storage efficiency, enabling better planning for transportation and logistics. Compared to past studies which addressed storage in isolation, newer research approaches storage as a dynamic component of a fully integrated AI-optimized hydrogen supply chain. This systemic thinking reflects a more mature, holistic view of the hydrogen economy where storage is not just a static element but a controllable, intelligent node in the distribution network.

One of the most forward-looking developments in the reviewed literature is the integration of digital twin technology in hydrogen manufacturing, especially for managing process complexity and improving system resilience. Early literature had no mention of digital twins in this context, largely due to limitations in computational power and modeling frameworks (Kuterbekov et al., 2024). However, recent studies demonstrate how AI-powered digital twins simulate real-time electrolyzer behavior, forecast component degradation, and optimize energy flows (Dash et al., 2024). These systems allow continuous model updating through live sensor data, enabling predictive analytics at every operational stage. Compared to earlier rigid simulation frameworks, digital twins offer high fidelity, adaptability, and system-level visibility. Their integration with reinforcement learning agents also adds a layer of decision intelligence, allowing for autonomous corrective actions in complex scenarios. This capability is essential for scaling hydrogen plants under fluctuating conditions and enhances the transition from pilot-scale to industrial deployment, something that remained an unresolved challenge in older literature. In addition, the increasing relevance of AI in the logistics and supply chain management of hydrogen distribution reflects a trend not discussed in depth in earlier studies. Previous research between 2014 and 2016 generally addressed logistics through cost modeling or geospatial analysis (Escapa et al., 2016; Kim et al., 2015). Recent research, however, presents AI models that optimize hydrogen routing strategies by integrating real-time traffic data, infrastructure conditions, and dynamic demand signals from urban and industrial nodes (Parra et al., 2017). These models significantly enhance distribution efficiency and lower delivery emissions. AI has also been applied to detect bottlenecks in hydrogen pipelines and schedule delivery based on predictive demand clustering, enabling just-in-time logistics. Such innovations are critical for countries seeking to build hydrogen corridors and inter-regional supply chains. The incorporation of these advanced logistic frameworks signals a broader understanding of the hydrogen economy as an interconnected system—an evolution from earlier compartmentalized views of production, storage, and transportation.

CONCLUSION

This review synthesizes a decade of advancements in AI-driven optimization for renewable hydrogen production, highlighting how artificial intelligence has revolutionized system efficiency, cost reduction, and integration with intermittent renewable energy across various production pathways such as electrolysis (PEM, AEL, SOEC), biomass gasification, solar-driven photocatalysis, and hybrid systems. AI techniques—including machine learning, deep learning, reinforcement learning, and optimization algorithms—have improved process control, predictive maintenance, material discovery, and real-time system responsiveness, contributing to efficiency increases of up to 35% and operational cost reductions of 30–50%. AI has also facilitated smart energy management frameworks, hydrogen storage optimization, and safety assurance, while emerging technologies like digital twins, quantum computing, and AI-enhanced supply chains promise unprecedented precision in system modeling and deployment. However, key challenges persist, including limited access to high-quality real-time datasets, high computational demands, lack of standardized evaluation protocols, and underdeveloped regulatory frameworks that hinder AI's full deployment in safety-critical energy systems. The convergence of AI with quantum computing opens new frontiers in catalyst discovery and reaction simulation, enabling faster, more accurate modeling of electrochemical processes. Additionally, AI's integration into hydrogen fuel cell management has enhanced hybrid microgrid efficiency and safety through real-time diagnostics and reinforcement learning. As hydrogen becomes central to decarbonization, AI will also play a critical role in automating lifecycle carbon accounting and certification, with blockchain-enabled AI systems supporting traceability and dynamic emissions credit pricing. To accelerate innovation and ensure equity, the future of AI in hydrogen lies in open-source collaboration, transparent model development, and government-supported frameworks that foster community participation, modular design, and standardized data-sharing. Ultimately, AI is set to become the backbone of a smart, scalable, and ethically guided hydrogen economy, driving progress from molecular design to global energy compliance.

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