



## REVIEW OF EMERGING AI TECHNIQUES FOR GREEN HYDROGEN IN SUSTAINABLE ENERGY

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### ABSTRACT

Green hydrogen is sustainable energy and clean source that has the potential to significantly alter important industries like manufacturing, the production of electricity, and transportation. Green hydrogen has the potential to ease the transition to low-carbon energy sources because of its leading role in global decarbonization initiatives. Increasing manufacturing productivity, ensuring the stability of storage, and coordinating usage strategies with commercial scalability remain significant challenges. This review examines the application of artificial intelligence (AI) to these pressing issues throughout the green hydrogen value chain. In particular, it examines how optimization, deep learning, and machine learning (ML) can boost electrolyzer efficiency in fuel cell applications, improve energy conversion processes, forecast system performance, and optimize storage options. In addition, it is shown how AI-driven real-time monitoring systems and digital twins can be integrated into hydrogen infrastructures, showing how these tools make adaptive operational control and predictive maintenance easier. This article uses current technology advancements and a few selected case studies to critically examine how AI accelerates innovation in green hydrogen technologies in order to facilitate the development of affordable, scalable, and sustainable energy systems of the next generation.



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### I. INTRODUCTION

The greenhouse gases, like methane, nitrous oxide and carbon dioxide, with the increase of emissions, have significantly exacerbated global warming. These gases cause irregularities in climate, threatening to raise sea levels, and subjecting the world to frequent natural disasters [1], [2]. Thus, transitioning to low-carbon, sustainable energy systems has become a strategic imperative in the world's search for immediate intervention to counter the challenging effects of climate change. Of these choices, green hydrogen is receiving attention as a promising vector of decarbonization for generating power, movement, and course industries [3]. Green hydrogen is the environmentally most sustainable type of hydrogen produced by electrolysis using renewable energy and emitting no greenhouse gases. Unlike grey, blue, or brown hydrogen produced using fossil fuels, they neither cause oxygen depletion nor increase water vapour. Yellow and white hydrogen share almost the same benefits, but are less scalable or occur naturally or in the rarest forms. Pink and turquoise hydrogen offer a moderate environmental impact, depending on whether one goes for the nuclear route or carbon-handling [4]. Figure. 1 display the production of green hydrogen types.

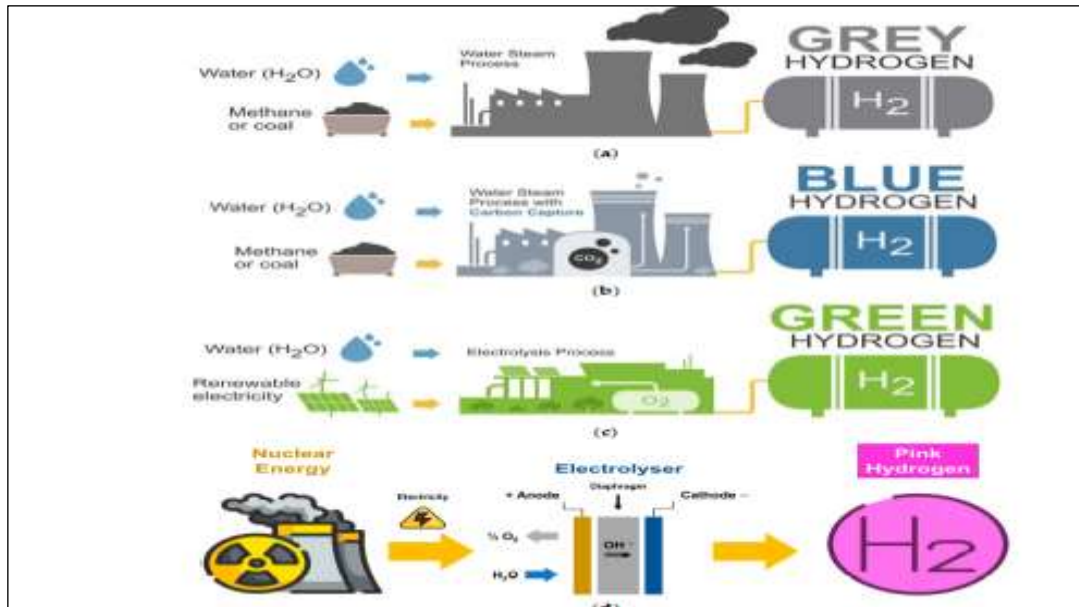


Figure 1: Production methods of hydrogen types.  
Source: [5].

Green hydrogen is primarily an energy carrier that needs to remain clean and flexible, produced by splitting water molecules using electrolysis powered by wind, solar, or other renewable energy sources. At least slightly, or somewhat, zero emissions at the point of use [6], [7]. Electrolytic hydrogen production methods from renewable sources are compatible with modular and scalable infrastructures for energy generation, enabling constant flux to meet supply patterns and demand a capability that traditional fossil fuels cannot match [8]. While grey hydrogen uses steam methane reforming to produce (9–12) of CO<sub>2</sub> per ton of H<sub>2</sub>, green hydrogen is carbon-free [9]. This flexibility is advantageous for ammonia production and other energy-intensive applications [10]. However, problems persist throughout the green hydrogen value chain despite these advantages. The two types (Metal hydrides and liquid organic hydrogen) carriers are storage technologies that are far behind conventional storage systems like underground caverns or compressed gas in terms of development, which results in inefficiencies and safety risks [11]. Moreover, the lack of an established distribution infrastructure and also technical challenges, such as hydrogen embrittlement and leakage caused by small molecular size, do not allow consideration of these highways to be integrated into existing natural gas grids [12]. The term Artificial Intelligence (AI) is currently popular as a method to power solutions for these varying issues. Algorithms of optimization, machine learning, deep learning, and other methods of artificial intelligence can effectively model complex, nonlinear systems and draw valuable information from voluminous data [13]. Figure 2, illustrate how artificial intelligence and machine learning are infused into the hydrogen cycle, including production, storage, safety, and distribution, to produce a worthwhile energy system that is sustainable, safe, and efficient.

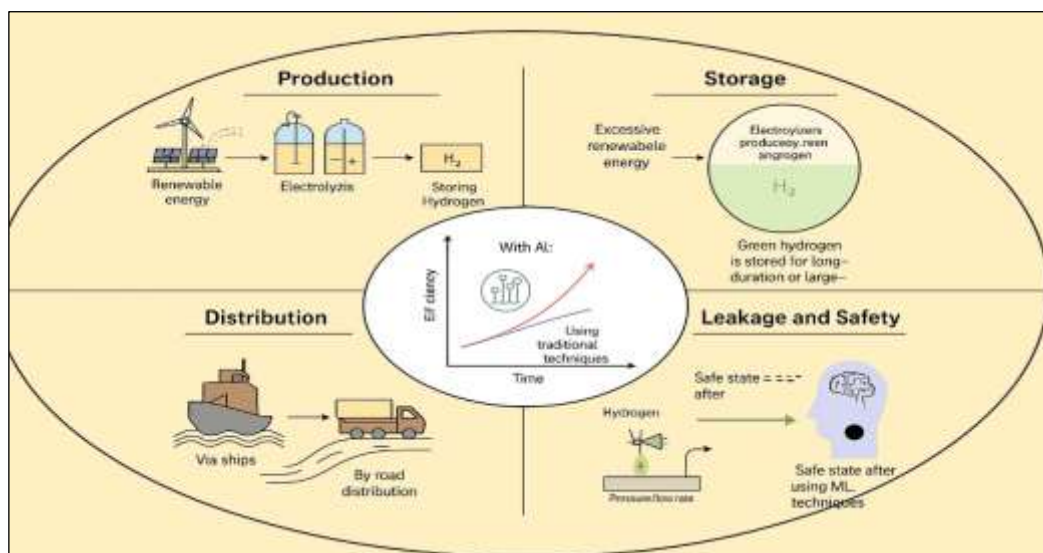


Figure 2: ProAI and ML integration across the hydrogen cycle from production to safety and distribution.  
Source: [14].

Process control and reduce energy consumption in green hydrogen production, potentially increasing efficiency by up to 20%. Similarly, AI enables demand forecasting, predictive maintenance, and system-level integration with renewable energy grids for storage and utilization [15]. AI offers the disruptive path to accelerate the commercialization of green hydrogen technologies in response to the growing impetus for a global energy economy based on hydrogen.

## II. GREEN HYDROGEN PRODUCTION USING RENEWABLE ENERGY SOURCES II.1 SUBTITLE

Green hydrogen production significantly reduces carbon emissions compared to conventional methods of hydrogen production by utilizing renewable energy from resources like solar, wind power and other resources to drive water electrolysis. This sustainable strategy is necessary to advance clean energy and lessen the effects of greenhouse gases [16]. Figure 3 demonstrates the integration of water electrolysis and energy storage with renewable energy sources like solar and wind energy in a grid-connected green hydrogen production facility.

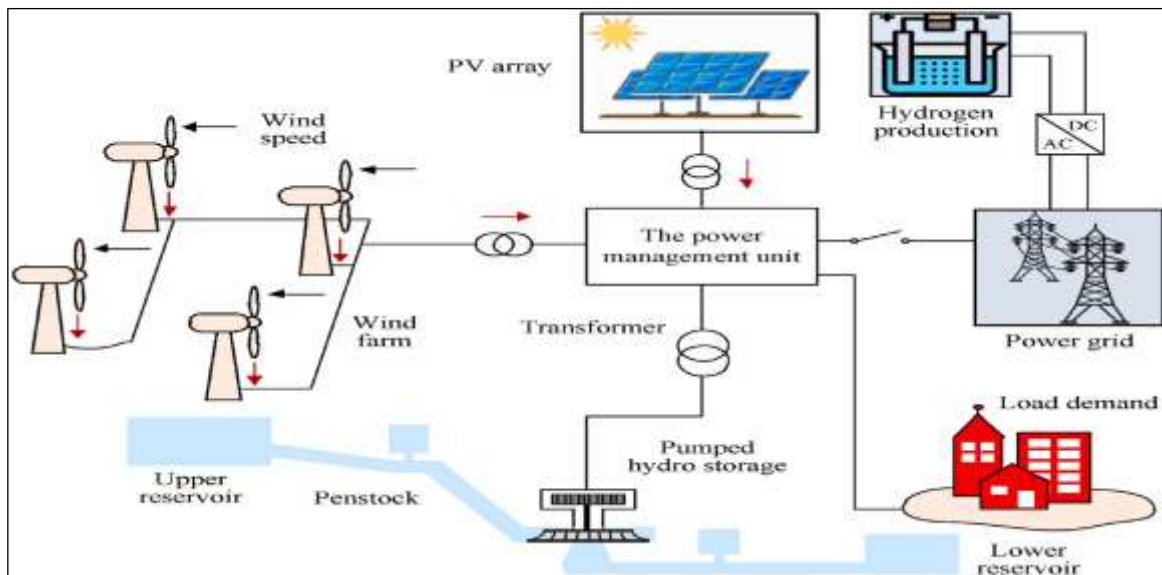


Figure 3: A diagram of a green hydrogen production system integrated into the grid using renewable resources, water electrolysis, and energy storage.

Source: [17].

The system can regulate fluctuations in the supply of renewable energy and maintain constant hydrogen production thanks to this integration. The testbed demonstrates, through its advanced power management and conversion technologies, how electrolysis and renewables can be balanced to create a more secure and environmentally friendly energy network. Examples of these developments include novel methods like the production of hydrogen through photo-electrochemistry and biological processes, as well as technological advancements in the production of green hydrogen such as enhanced electrolyzer performance thanks to cutting-edge catalysts and materials. These strategies also increase sustainability and efficiency by utilizing wind and solar power [18]. In spite of the fact that technological advancements have proved the capability of photovoltaic (PV)-driven electrolysis systems to convert solar to hydrogen (STH) with high efficiency, there are still concerns regarding the stability of operations, safety, and storage under changing weather conditions [19]. By combining different sources like (solar, wind, and geothermal energy) not only makes the system easier to scale up but also minimizes environmental impacts in a greater extent if backed by appropriate legal and economic frameworks [20]. The national technoeconomic study has pointed that through using solar energy and various electrolysis technologies, Canada could theoretically produce more than 200 million tons of green hydrogen per year which would largely depend on regional optimization [21]. The 7 kW electrolysis system in Namibia has been successfully integrated with off-grid community wind energy and has shown that surplus wind energy can be utilized without affecting the system's load requirements to produce up to 235 kg of green hydrogen annually. This is a clean fuel substitute for the local needs that are not met like backup power and cooking [22]. In the same way, a regional study done in the Piura region estimated that yearly over 947,000 tons of green hydrogen produced through electrolysis which was majorly powered by solar PV (94.8%), with the rest wind and biomass. The study also put out that only 47.4% of hydrogen would be enough for the whole energy demand of the region and in this way there would be a significant reduction of greenhouse gas emissions [23].

## III. GREEN HYDROGEN APPLICATIONS

Green hydrogen plays the role of hydrogen source in several applications such as clean fuel for transport, energy systems and industries that do not impact the environment. The most important areas in hydrogen utilization are mainly fuel cells, ammonia production, power-to-metal technology to produce aluminum and steel anodes from water electrolysis, and synthetic fuels. They all have a pivotal role in the development of global sustainability by consuming nearly half of the global production of hydrogen [24]. Fuel cells are high-efficiency energy converters fueled by hydrogen, emitting no emissions. Adding membranes can produce additional pure water. Fuel cells make up 28% of final energy demand and are recommended by Peter Thiele of Siemens for managing electricity waste. Siemens fuel cells have an AC output of over 90%, making them an efficient option for powering various sectors globally [25]. Energy systems, conversely, would stand to benefit greatly from green hydrogen, particularly when combined with intermittent renewables such as wind and solar. The storage of excess electricity as hydrogen and conversion back into electricity during times of demand dramatically improves grid stability and flexibility, and thereby serves, as a buffer against the variable nature of renewable generation [26]. The interest in green hydrogen for industrial applications that are hard to convert to renewable electricity is high. The amount of hydrogen needed is typically rather low, but is needed for specific purposes, including hydrogen as feedstock, and hydrogen as reducing agent for metal oxides, or synthesis of more complex molecules.

The high energy consumption, the specific application and the tradition of steam methane reforming lead to much of the industrial application being found at coal sites, steel locations or refineries, as well as in ammonia production for the fertilizer market [27], [28]. The iron and steel sector is the largest industrial consumer of hydrogen used in the reduction of iron ore pellets. In this process, hydrogen reacts with the oxidized concentrate and, in combination with the carbon oxide, generates a steel result. Still used in large quantities, carbon oxide is emitted to the atmosphere and will be limited to meet climate goals. One of the ways to decarbonise the steel process is to use green hydrogen generated with zero emissions [29],[30]. The production of chemicals, such as methanol or ammonia, is another hydrogen industrial application. In the ammonia production, steam methane reforming is the traditional process and the main world source, driven by its low capital cost, high efficiency and development in the first half of the 20th century. However, the use of steam methane reforming leads to a large hydrogen carbon footprint, in one of the sectors that most contributes to the global CO<sub>2</sub> emissions [31]. Figure. 4 depicts current and future industrial applications of green hydrogen, emphasizing its importance in industries that include oil refining, ammonia, and methanol production, metalworking, and chemical processing.



Figure 4: Schematic diagram of a grid-connected green hydrogen production system consisting of renewable resources, water electrolysis, and energy storage.

Source: [32].

#### IV. ARTIFICIAL INTELLIGENCE ROLE IN GREEN HYDROGEN PRODUCTION TECHNOLOGIES

Artificial Intelligence plays a key role in driving green hydrogen production by making it more efficient and cost-effective. The use of machine learning on large datasets makes it possible to modify the operational settings of electrocatalysts making them perform better, produce more hydrogen, and consume less energy [33]. These artificial intelligence-based tools quickly match material compositions with desirable properties, powering the discovery of low-cost, high-performance electrode materials for water electrolysis. Load balancing, by storing the excess of possible solar and wind energy, is made easier through AI technologies because AI allows for dynamic adjustment of operations so that electrolyzers operate during peak generation only [34]. Refining demand-supply forecasting is a significant avenue of AI, which improves forecasts for renewable energy outturns and energy demand estimations, leading to better operation and innovation in green hydrogen systems [35]. Supported by data-driven screening and optimization, AI accelerates the design process of catalysts, which can be time-consuming and costly through traditional experiments, and enables pinpointing highly potent ones. With the help of a data-driven screening and optimization process, AI speeds up the design of catalysts, reduces experimental times and costs, and ensures the accurate discovery of high-performing materials [36]. Together, these advances highlight the importance of AI as a key enabler in the (sustainable, cheaper) development of green hydrogen technology. AI and automation are widely used in renewable energy, including solar and wind energy AI is the mainstay in the green hydrogen production process as it regulates the electrolyzer performance with the aid of cybernetic control [37].

The system has the ability to utilize weather forecasting to predict the renewable energy delivery and thus, to maintain the operation at the required level [38]. AI has, in fact, become the key factor in the production of hydrogen and the co-generation of solar and wind power, both of which are working together to provide a more sustainable and energy-efficient system for the future. Energy was wisely handled and hence a significant reduction in carbon emissions was achieved which, in turn, is going to power a grid of the future that is going to be not only more reliable but also more sustainable [39]. Besides these, the AI application to predictive maintenance and the hydrogen production equipment life cycle extension was an advantage. AI will be deployed to analyze the data from sensors mounted on the trucks and simultaneously, an artificial intelligence system will be used to monitor, predict, and control the maintenance in a modern, efficient, and effective way. ITM Power has released a case study on its stage 2 and claimed an availability percentage that is up to 12% greater. This also worked out well for the equipment's lifespan as it increased by twice and operating costs got cut. These results indicate that AI can greatly improve hydrogen production industry wide in terms of both productivity and stability [40]. A new hybrid system for energy dangers and hydrogen generation has been named Zink-Zwischenschritt-Elektrolyseur (ZZE) in German. The model utilized several machine-learning models to predict the state of charge (SOC). The LSTM neural network achieved the lowest error in its forecasting (MAE = 3.21%). The precise SOC estimation is vital for the optimization of future ZZE management software.

The findings highlighted the support of data-driven AI methods in next-generation hydrogen storage technologies development [41]. Table 1 explain the summary of the key AI-centered works intended to enhance the range of green hydrogen production processes via electrolysis. It highlights that the new method can beat the traditional ones not only in terms of efficiency but also in accuracy of prediction and performance of systems in applications of Green Hydrogen Technologies.

Table 1: The AI-Driven Enhancement of Electrolysis-Based Green Hydrogen Production.

Study	Key focus	Model used	Key finding
[42]	AI in Electrolysis – Optimal Operational Prediction	Support Vector Machine (SVM), XGBoost, and Random Forest (RF) trained on electrolysis variables (electricity input, temperature, pressure, water quality). Dataset: experimental data from electrolysis processes	AI models predicted optimal electrolysis conditions, enhancing electrocatalyst performance and reducing energy loss. Outperformed manual tuning by ensuring consistent hydrogen output under varying inputs
[43]	Parametric Modeling of Alkaline Electrolyzers	MATLAB/Simulink parametric model using inputs like temperature, KOH concentration, and pressure. Not AI-based, serves as a traditional comparison baseline.	Higher temperatures and a 30 wt% KOH solution reduced cell voltage, thereby boosting system efficiency. Provides a baseline to compare improvements from AI-enhanced models
[44]	PEM(Proton Exchange Membrane) Electrolyzer Design Optimization via ML (Machine Learning)	Polynomial and Logistic Regression trained on 148 experimental samples to predict 11 PEM design parameters (e.g., electrode area, hydrogen production rate).	Achieved MAE of 0.615 and 83.6% classification accuracy. Enabled faster and more precise PEM cell design than conventional iterative approaches
[45]	Hybrid Modeling of Electrocatalysts	Adaptive Neuro-Fuzzy Inference System (ANFIS) + Pelican Optimization Algorithm (POA) using catalyst property datasets	A hybrid AI model improved hydrogen output by 1.7% vs traditional methods by optimizing catalyst behavior under electrolysis conditions.
[46]	DRL (Deep Reinforcement Learning) for Predictive Maintenance of Electrolysers	Deep Reinforcement Learning (DRL) with Long Short-Term Memory (LSTM) and feature selection. Dataset: sensor time-series data from electrolyser systems	DRL model identified sensor faults with 0.99 correlation and RMSE of 0.1351, enhancing maintenance efficiency and reducing downtime compared to manual diagnostics

Source: Authors, (2026).

## V.ARTIFICIAL INTELLIGENCE TECHNIQUES FOR GREEN HYDROGEN STORAGE OPTIMIZATION

AI is a great help for green hydrogen storage. It helps to identify and control the production easily, monitor the status of storage, and predict the demand. It uses the same data analytics and optimization algorithms for efficiency and reliability thus solving the hydrogen storage and power supply cycle problem in a sustainable manner [47]. A smart system using neural networks can measure the non-linear dynamics of PEM (Proton Exchange Membrane) with a small average absolute prediction error of 0.05179. This makes the TITAN (Technology Intelligent Testbed for Advanced Networks) system more efficient and reliable for hydrogen generation and storage control compared to conventional methods of data collection. It is a revolution that not only accelerates the clean energy technology developments but also allows energy sustainability by supporting hydrogen energy developments through such innovations [48]. A MATLAB/Simulink model of the hydrogen subsystem was developed, employing a regression model to estimate hydrogen flow rates in response to input electrolyzer currents. A dynamic simulation of hydrogen storage is also developed, providing a reference for the high-pressure and compression pressures required and their effect on performance, as well as the evaluation of hydrogen storage, low energy density, and high pressure. This increases momentum for policy and regulatory support, as well as investment facilitation, for sustainable energy technologies. For this purpose, this work aims to integrate renewable-based energy storage solutions, enhance system reliability, and implement regulatory policies for sustainable energy solutions [49]. An AIoT-HES is developed based on a knowledge engineering model. With real-time analytics and predictive maintenance, hydrogen production, storage, and distribution costs are minimized while output is optimized. As a result, the AIoT ensures the operational security of the system by promptly identifying risks and determining intelligent storage conditions, which will be connected to other types of renewable energy. Maintenance or risk management of machine learning models can further enhance predictive capacity. The articles are also promoting sustainable energy alternatives, regulations, and a durable H2 infrastructure no information loss is incurred [50].

## VI.APPLICATIONS OF AI IN GREEN HYDROGEN DEVELOPMENT ACROSS KEY COUNTRIES

Artificial Intelligence plays a crucial role in fronting the development of green hydrogen technologies, including production, storage, distribution, and utilization. Recent comprehensive reviews showing that AI techniques—such as Artificial Neural Networks (ANNs)—are largely employed in making electrolyzer technologies more efficient, forecasting inputs of renewable energy, optimizing storage procedures, and facilitating integration with a smart grid and GIS-based site selection [36]. In India, a deep learning-based forecasting model for solar-powered green hydrogen production was introduced. The model works through four phases, including solar irradiance forecasting, electrolyzer scheduling, and cost-effective production of hydrogen through photovoltaic sources [51]. In Turkey, hybrid artificial intelligence modeling combining CEEMDAN and GRU neural networks for hourly hydrogen production prediction was developed for optimal scheduling and integration of hydrogen production within renewable energy mechanisms [52]. For both Saudi Arabia and Germany, AI modeling frameworks were developed for the estimation of green hydrogen generation by PtX systems. Those models consider data-driven forecasting and optimise the techno-economical feasibility of hydrogen generation from renewable sources. In Saudi Arabia, the high solar irradiance is used with AI to maximize electrolyzer performance and cost efficiency. In Germany, AI tools are used to manage intermittent wind and solar inputs while optimizing grid integration. The comparative analysis helps define strategies for the installation of green hydrogen infrastructure based on ambient and economic real-time parameters [53].

In the U.S., more than 500\$ million in funding has been approved by the Department of Energy toward AI-assisted decarbonization and infrastructure development for hydrogen. According to the U.S. Energy Information Administration (EIA), AI applications optimizing electrolyzer performance and predictive maintenance would likely bring green hydrogen costs down by 20% or more in the next 10 years, further enhanced by heuristic algorithms optimizing operational parameters, yielding 15%-30% efficiency improvements in pilot projects by startups such as H2Pro. The mentioned optimization tools, besides various other AI applications such as predictive analytics, computer vision for leak detection, and AI-assisted planning, get federal tax credits and demonstration funds, which make hydrogen technologies near to commercialization [54].

## VII. CONCLUSION

AI has an influential position to play in the full green hydrogen value chain transformation which means enhancing its efficiency, reliability, and scalability. All the way through production, storage, and use, AI is gradually taking over the solutions especially those which rely on machine learning, by modeling complex systems, optimizing performance, and interpreting high-dimensional data in a manner more superior than traditional physical modeling techniques. At the very start of the hydrogen production, the AI has shown its ability by synchronizing renewable electricity disruption with the hydrogen demand variations; thus the operation became more flexible and stable. The world's energy market is still moving to a point where hydrogen can be produced and used as a primary renewable source and, therefore, the traditional models will be unable to portray the complex and dynamic workflows of the new hydrogen economy. All these considered, the future of AI in this sector looks bright but at the same time, issues such as cybersecurity and system integrity are the major obstacles to widespread acceptance. In securing the digital infrastructure that is both safe and resilient, one should not forget that this has to happen in parallel with the technical advancements in the integration of AI in hydrogen systems. In spite of the extensive progress achieved in green hydrogen technologies, the world still has to deal with some economic and technical obstacles that are upholding the large-scale use of hydrogen all over the world. The main issues are the installation of pipelines and other necessary infrastructures that are very costly, the hard task of managing energy supply and demand because of the fluctuating nature of renewable sources, and the long-standing dependence on few and expensive catalyst materials. On top of that, a lack of technically skilled labor and the absence of detailed government laws and policies are making it even harder for the green hydrogen industry to expand gradually. Therefore, it can take to a long time for that to happen unless a well-coordinated approach is adopted consisting of combining technology development, policy intervention, and very long lasting investment plans to finally secure the transition to a low-carbon energy system that is equitable and mainly supported by green hydrogen.

## VIII. AUTHOR'S CONTRIBUTION

**Conceptualization:** Hiba Abdulkareem Saleh , Rana Khalid Sabri , Omar Ibrahim Alsaif.

**Methodology:** Author One , Author Two and Author Three .

**Investigation:** Author One and Author Two.

**Discussion of results:** Author One, Author Two and Author Three.

**Writing – Original Draft:** Author One.

**Writing – Review and Editing:** Author One ,Author Two.

**Resources:** Author Two.

**Supervision:** Author Two and Author Three.

**Approval of the final text:** Author One, Author Two and Author Three.

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