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Review

An Overview of Digitalization Pathways for Green Hydrogen Production: AI, Machine Learning, IoT, Digital Twin, and Blockchain

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Abstract: The expansion of green hydrogen utilization is increasing globally due to the current focus on sustainable energy transformation. However, this shift is accompanied by significant issues related to fluctuations, control strategies, and supply chains. In that regard, digital technology plays a major role in promoting the development of green hydrogen. This paper reviews current advances in the digitalization of green hydrogen production, mainly based on electrolysis of water. This review features topics such as artificial intelligence (AI), machine learning (ML), the Internet of Things (IoT), digital twin (DT), and blockchain applications. These technologies are suitable for applications across micro-, meso-, and macro-scales and have been utilized to improve process optimization, real-time monitoring, predictive analytics, and system scalability. It has been shown that production efficiency and resource utilization can be significantly enhanced through data-driven control and automation. Moreover, blockchain frameworks have been adopted to secure transactions and increase transparency across hydrogen supply chains. Although certain challenges such as infrastructure limitations and data interoperability remain unresolved, the role of digitalization in enabling low-emission, intelligent hydrogen production has been firmly established. As energy systems evolve toward decarbonization, the convergence of renewable energy and digital control is expected to shape the next phase of the global hydrogen economy.

Keywords: artificial intelligence; machine learning; internet of things; digital twin; renewable energy; electrolyzer

1. Introduction

Moving towards sustainable energy sources has become increasingly essential due to global concerns over environmental degradation and the depletion of fossil fuels. Green hydrogen has been increasingly recognized as a pivotal element in the transition toward a cleaner energy economy. Defined as hydrogen mainly produced through electrolysis powered by renewable sources such as wind [1], solar [2], geothermal [3,4], hydropower [5], and bioenergy [6]. Green hydrogen has been positioned as a zero-emission alternative capable of decarbonizing multiple sectors, including transportation [7], steel industry [8], and power generation [9].

Green hydrogen has been recognized for its ability to displace fossil-based fuels as well as for the versatility it offers in storage, conversion, and integration with a diversity of energy systems [10,11]. It has been considered as a viable alternative to mitigate the intermittency in renewable energy resources. Its potential to stabilize electrical grids by absorbing surplus renewable energy and converting it into storable chemical energy has further underscored its significance in advanced sustainable energy systems [12]. While gray hydrogen is cheaper due to fossil resource abundance, it carries high CO_2 emissions [13], The production of gray hydrogen requires 91.12 kWh of energy and results in the emission of 29.14 kg CO_2, while green hydrogen requires 1.08 kWh per kg of H_2 produced and emits 2.96 kg CO_2 eq. of greenhouse gasses per kg of H_2 [14], highlighting the need for near-zero emissions and long-term sustainability. However, it has become evident that the production and utilization of green hydrogen at large scales face significant operational issues, which impede its widespread adoption and thus require the integration of supporting control technologies. As the operational complexity of hydrogen systems increases, traditional process control methods have proven insufficient, highlighting the need for developing and utilizing advanced tools. Through the adoption of digitalization, enabled by artificial intelligence (AI), machine learning (ML), Internet of Things (IoT), and digital twin (DT), greater levels of precision, efficiency, autonomy, and scalability through multiple scales such as micro-, meso-, and macro-scales [15], have been introduced into the green hydrogen industry.

In this paper, the role of advanced digital technologies in improving green hydrogen production is systematically explored, specifically with a focus on providing data-driven optimization, autonomous operation, predictive diagnostics, and seamless system integration. Through the critical evaluation of five key technologies: AI, ML, IoT, DT, and blockchain, the paper seeks to demonstrate that digitalization is not merely an auxiliary tool but a fundamental enabler of smart, efficient, and scalable hydrogen production systems.

The literature was gathered through searches on various scientific databases covering the years 2020 to 2025. Keywords such as "green hydrogen", "digitalization", "artificial intelligence", "machine learning", "Internet of Things", "digital twin", and "blockchain" were used. Studies most relevant to digitalization in hydrogen production and energy systems were selected. This methodology was selected to allow the review to focus on the recent advancements and emerging directions in the field.

2. Green Hydrogen Production Technologies

Various renewable energy sources are used to produce green hydrogen, in which the technologies can be divided into two main categories: biomass-based [16] and water splitting [17], as shown in Figure 1. Distinguishing energy-driven approaches from those based on organic matter, a deeper insight into how both technological and biological systems contribute to low-emission hydrogen strategies is provided [18]. There is a substantial diversity of methods with respect to operational conditions, type of substrates, chemical additives utilized, and hydrogen production capacity. According to recent comparative studies, the most appropriate green hydrogen production method depends on the specific context of use; in particular, it depends on the level of energy input required and availability standards, as well as local weather conditions and energy resources. This diversity highlights the evolving nature of green hydrogen technologies and underscores the need for context-specific solutions to meet diverse energy demands across sectors [19].

Water-splitting has three methods, which are electrolysis, thermolysis, and photolysis. In electrolysis, electrical energy is used to split water into hydrogen and oxygen, typically relying on renewable power sources [20]. Thermolysis involves the decomposition of water molecules at extremely high temperatures [21], whereas photolysis employs light-sensitive catalysts to initiate the same reaction [22]. Such physicochemical processes require external energy sources and are identified as the key drivers for scalable, carbon-free hydrogen production. Research on water splitting is increasingly being adopted as a pathway for sustainable hydrogen production. For instance, redox water splitting has emerged as a viable technique for the production of green hydrogen at moderate temperatures [23].

Biomass-based green hydrogen production has two categories: biological and thermochemical. The former is divided into three methods: bio-photolysis, dark fermentation, and photo fermentation. Bio-photolysis uses the photosynthetic activity of microorganisms to convert light and water into hydrogen [24]. Dark fermentation involves microbial breakdown of organic matter in the absence of light, producing hydrogen as a byproduct [25]. Photo fermentation integrates light exposure with microbial metabolism to convert biomass into hydrogen [26]. These biological processes depend on renewable feedstocks and microbial systems, aligning well with environmental sustainability and circular resource utilization. Moreover, thermochemical methods encompass pyrolysis and gasification. Pyrolysis decomposes organic material by using high temperature in the absence of oxygen to emit hydrogen as a byproduct [27]. Gasification converts solid biomass by treating it with a limited amount of gasifying medium, such as steam, oxygen, or air, to convert it into hydrogen and other gases [28].

Considering all green hydrogen production methods, electrolysis stands alone as the most dominant for green hydrogen production. However, it still holds multiple environmental impacts, such as high water consumption, which can potentially exacerbate scarcity in arid regions, the use of rare materials that are costly and geopolitically sensitive, and the need for new infrastructure, raising land use and ecological concerns [29]. Moreover, its large-scale deployment remains limited by efficiency constraints and high capital costs, underscoring the need for advanced mitigation technologies.

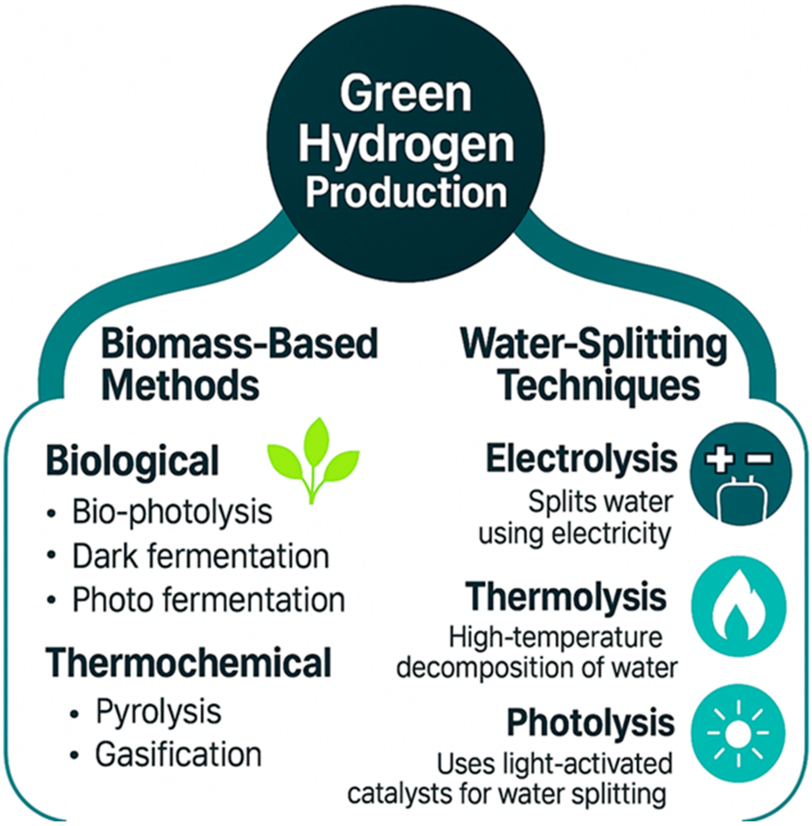

Figure 1. Overview of green hydrogen production technologies.

3. The Role of Digitalization in Green Hydrogen Production

3.1. Internet of Things (IoT)

IoT, in its classical model, consists of a three-layered architecture, which mainly refers to perception, network, and application. Sensors and actuators in the perception layer collect data, the network layer transmits it, and the application layer provides services to end users [30]. IoT has been conceptualized as a framework wherein commonplace objects, embedded with sensors, Radio Frequency Identification (RFID) tags, and communication capabilities, are interconnected through unique identifiers, allowing them to collaborate autonomously toward shared objectives [31,32]. Computing is moving beyond desktops as IoT connects everyday objects to networks. Embedded sensors and RFID generate large data volumes, requiring efficient cloud-based storage, processing, and delivery. Cloud computing enables on-demand access to services with a scalable and cost-effective model [33,34]. IoT can achieve real-time monitoring by deployment of sensors that can track key parameters such as water flow rate through the electrolyzer, electrolysis voltage and current, system pressure and temperature, hydrogen purity, flow rate, and storage levels [35].

In regard to green hydrogen production, IoT provides the sensory and communication backbone for a digitalized green hydrogen plant, connecting every asset and process to the central control system. It plays a vital role in improving the efficiency, safety, and scalability of a green hydrogen system. IoT sensors can be attached to measure various parameters that affect the performance of the systems, such as current, voltage, pressure, and hydrogen flow [36]. This real-time data is sent to cloud servers for remote monitoring, data analysis, and control, as depicted in Figure 2. Furthermore, these IoT-enabled systems facilitate predictive maintenance by helping detect anomalies that are indicative of impending equipment failure, thereby reducing downtime and operational exposure risk [37]. Safety is ensured by automatic leak detection and emergency shutdown triggered by sensor alerts. Through connecting with AI algorithms, IoT also enables real-time process automation and energy management for maximum use of renewable energy, thereby optimizing hydrogen production. Therefore, such applications help enhance system responsiveness and reliability, and demonstrate that IoT-based hydrogen technologies can support decentralized clean energy solutions.

In addition, the benefits of IoT have been further extended through the use of Long Range (LoRa) technology, which allows devices to be connected over long distances using minimal energy. Constant communication is maintained between key parts of the systems, such as solar panels, electrolyzers, hydrogen tanks, and fuel cells, through LoRa-enabled nodes. Incorporating AI tools also enables monitoring of system behavior, prediction of operational needs, and real-time adjustment of energy usage based on changing conditions. In this way, a more practical and accessible model for green hydrogen production is supported, especially for small or off-grid communities seeking cleaner and smarter energy solutions [38]. However, IoT devices are highly vulnerable to security threats at the perception, network, and application layers, where risks such as device tampering, denial-of-service attacks, and weak authentication mechanisms can compromise data integrity and system reliability [39].

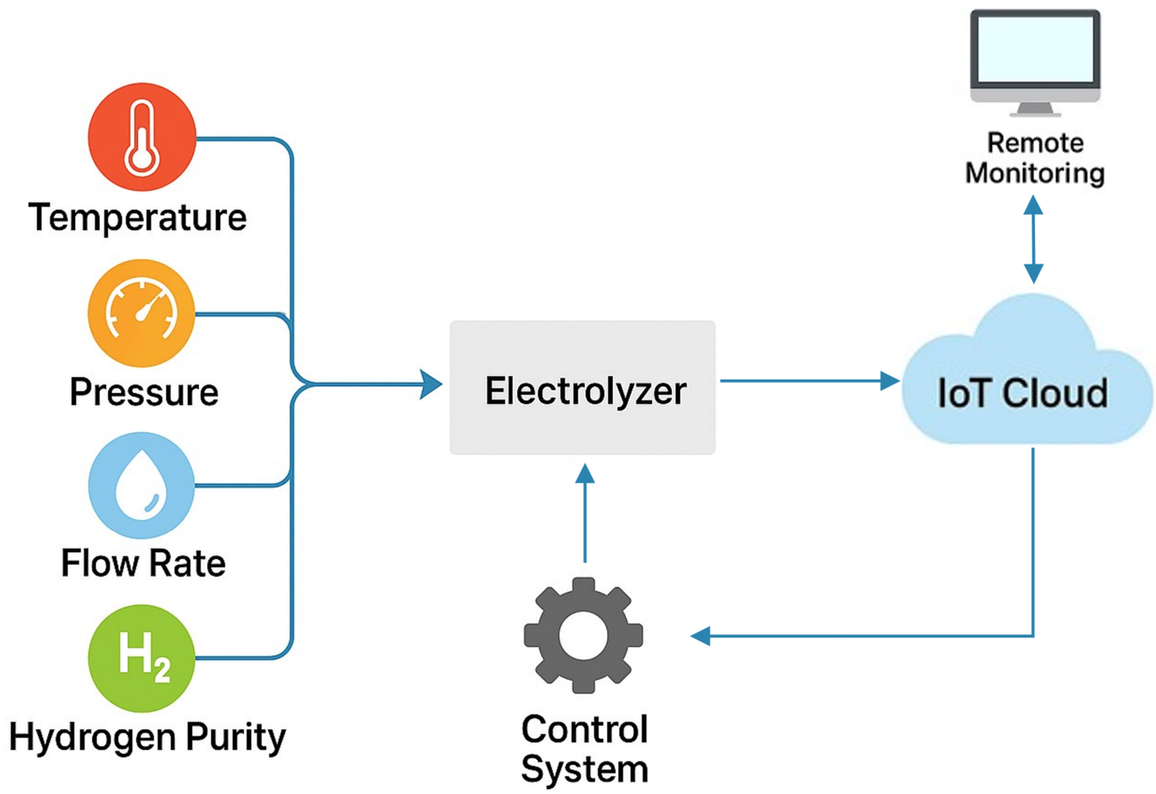

Figure 2. IoT-enabled monitoring architecture for hydrogen electrolysis systems.

In a real-world smart home setup [40], solar panels, wind turbines, and hydrogen fuel cells were installed to supply energy, with IoT systems used to monitor and manage operations. Environmental conditions such as temperature, humidity, and light intensity were continuously measured using IoT-connected sensors, while energy usage data from the devices was collected in real time. This information trained ML models that forecasted demand and enabled automatic switching among the energy sources, resulting in 60% of power coming from solar panels, 30% from wind turbines, and 10% from hydrogen fuel cells. The IoT devices consumed an average of 25 kWh/day. Similarly, in [41], an IoT-enabled control system was incorporated into a small-scale green hydrogen setup consisting of a photovoltaic panel, proton exchange membrane (PEM) electrolyzer, fuel cell, and DC loads. Data on current, voltage, temperature, and hydrogen production were continuously captured through sensors and transmitted via an Arduino board. This hardware facilitated real-time wireless communication with a cloud platform, where the data were logged and visualized through web and mobile dashboards. Measurements were updated every 10 s, allowing dynamic tracking and remote control of the system. Under experimental conditions, the PEM electrolyzer achieved an efficiency of 58.25% at 1.2 A, while the fuel cell reached 82.3% efficiency under similar operating currents. Hydrogen production ranged from 5.76 to 35.25 mL/min across a current range of 0.4–1.6 A. Through the developed graphical user interface, remote users were able to observe system parameters, execute shutdown commands, and perform diagnostics, illustrating how IoT integration can enhance operational transparency, energy efficiency, and control in green hydrogen applications. IoT generates a vast amount of data from the green hydrogen production method. However, this data requires advanced tools for analysis and decision-making that can be fulfilled by using AI and ML.

3.2. Artificial Intelligence (AI) and Machine Learning (ML)

AI and ML are the cognitive engines of the digitalized green hydrogen plant, providing the intelligence needed for advanced optimization, prediction, and autonomous operation. Tasks that typically require human intelligence, such as logic, if-then rules, and decision trees, can be performed without human interaction using AI. ML, as a subfield of AI, uses statistical techniques to learn from past data and make decisions and predictions with little human intervention. Deep Learning, a type of ML, is based on multi-layer neural networks that model complex patterns in millions of data points, and so forth [42].

The utilization of AI has significantly improved hydrogen production through photochemical and wastewater electrolysis. Applications include catalyst design, reaction parameter optimization, system performance monitoring, and real-time process control. ML models have the potential to explore the optimal catalyst composition and regulate the light intensity, temperature, and pressure, and can further improve energy efficiency via novel optimization algorithms, including genetic and reinforcement learning. AI also allows predictive analytics to oversee hydrogen production and environmental impact, and provides a strong substitute for the conventional experimental approach. These technologies are critical for the integration of hydrogen generation into renewable energy and meeting sustainability goals by decreasing carbon dioxide emissions and minimizing resource usage. Regardless of the challenges of data availability and model interpretability, AI will increasingly play a role in underpinning a global green hydrogen economy [43].

ML requires the integration of appropriate sensing, algorithms, and computational platforms. Algorithms such as artificial neural networks (ANNs), support vector machines, and Gaussian process regression. These algorithms have been shown to be effective for predictive analytics, control, and optimization. However, ML requires a synchronization of multi-rate sensor signals and strategies for handling noise, outliers, and missing values. Soft sensors are used to apply ML in industries, and they represent the most industrial penetration of ML applications [44]. ML models take full advantage of the highly non-linear and complex data produced during electrolysis, including variables such as electricity input, water quality, temperature, and pressure, in addition to electrochemical trends. Analyzing this data for hidden patterns and correlations, ML algorithms can accurately predict optimal operating conditions for improved hydrogen production, and through real-time adjustment, can save power during production [42]. Traditional electrolysis optimization methods rely on manual tuning and trial-and-error, which is time-consuming and limited in scope [45]. On the other hand, ML models can evaluate a variety of input variables over time, uncovering small correlations invisible to traditional methods. In this way, the system automatically controls the optimal operational conditions, adjusts parameters by changing their dynamic behavior, and enables high-yield conversion of hydrogen while consuming less energy, thereby reducing equipment degradation caused by inefficient or unstable operation [46]. Moreover, regression analysis, neural networks, and reinforcement learning have all proven effective for modeling the electrolysis process, thus allowing data-based improvements in terms of performance and service life. Such AI-driven optimization can achieve up to 20% energy savings by tailoring operation conditions to fluctuating system inputs and renewable energy availability [47]. As green hydrogen production continues to expand globally, the integration of ML technologies will be critical in scaling production, lowering costs, and achieving climate targets through enhanced process intelligence and efficiency. Figure 3 illustrates the key roles of AI and ML in enhancing catalyst design, electrolysis optimization, and performance monitoring across the green hydrogen production process.

In solar-based green hydrogen production systems, ML and AI can help identify significant difficulties, where a primary issue involves the intermittency of solar radiation, which, if not accurately predicted, can lead to inefficiencies and higher hydrogen production costs [48]. In advanced solar-to-hydrogen systems that incorporate adsorption desalination modules and reverse electrodialysis, hydrogen output is highly sensitive to the balance between solar radiation intensity and adsorption timing. The poor calibration of these parameters can result in a severe loss in hydrogen production [49]. Another concern is that many forecasting models are developed using data from a single location, which may hinder their performance when applied in different environments or under varying system setups [48]. A shortage of large-scale, standardized datasets still holds back the scope and reliability of AI models. Without them, scaling predictions or applying results to various operational settings becomes a real challenge. The problem is worsened depending on how hydrogen production conditions vary, from shifts in renewable energy supply to changes in electrolyzer performance and even local climate patterns. Recent results have emphasized that to deploy AI effectively in green hydrogen systems, it will be necessary to use high-quality, real-time, and context-specific data for energy input, weather, electrolyzer parameters, and operational anomalies [50]. Without such a robust data infrastructure, model generalizability and real-world applicability remain constrained, particularly under extreme or complex conditions.

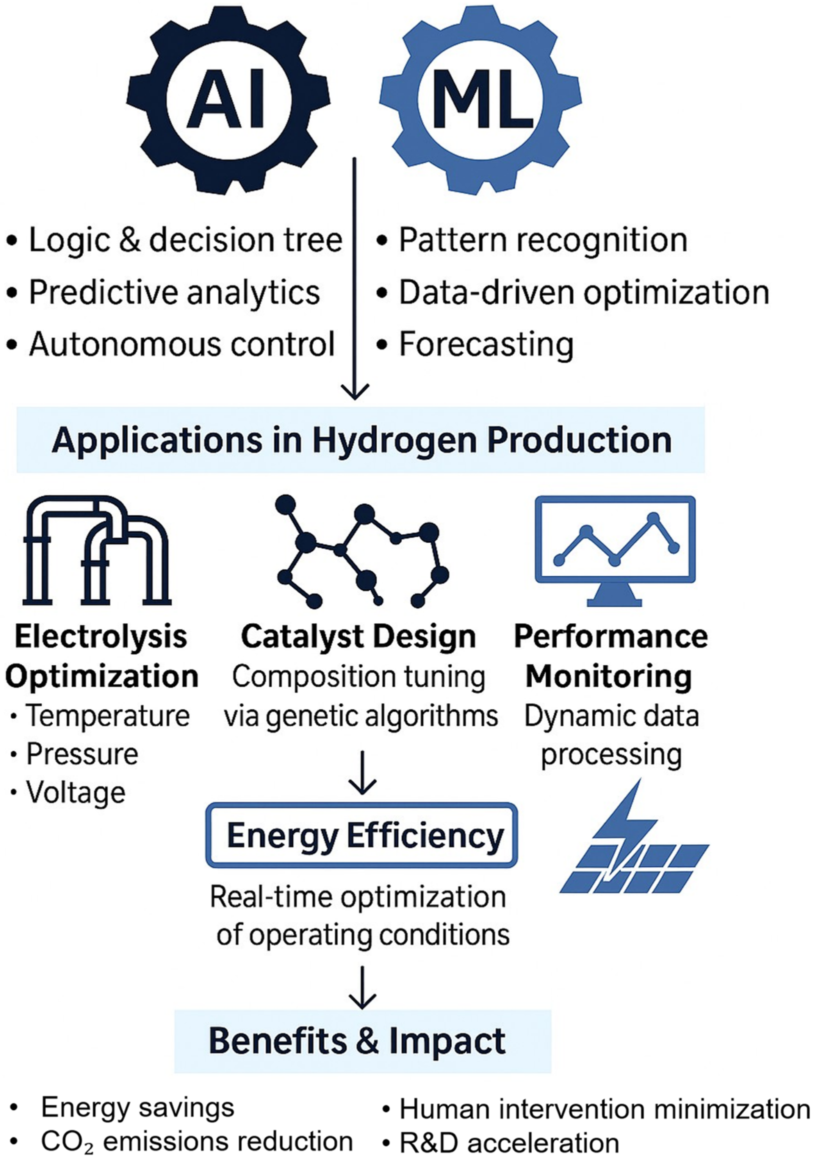

Figure 3. Integration of artificial intelligence and machine learning in green hydrogen systems.

Additionally, Supercritical water gasification (SCWG) of biomass was modeled using ML approaches to predict hydrogen yields by applying eight ML models, such as multiple linear regression, gradient boosting regression, extreme gradient boosting, support vector machine, ANN, random forest, decision tree, and Gaussian process regression. In addition, genetic algorithm and particle swarm optimization algorithm were utilized for optimization. The results demonstrated that the gradient boosting regression model, when optimized through the particle swarm optimization algorithm, exhibited strong accuracy and robustness, achieving R^2 values of 0.995 for training, 0.958 for testing, and 0.917 for cross-validation. From an environmental perspective, SCWG is advantageous because it processes moist biomass without energy-intensive drying, achieving hydrogen yields between 0.82 and 15.97 mmol/g (average 2 mmol/g), thereby reducing fossil-fuel reliance and supporting waste-to-energy valorization. Furthermore, the ability to use low-cost residues such as agricultural waste, plastics, and wastewater lowers feedstock costs and enhances process efficiency, while the optimization of operating parameters through ML contributes to reduced energy input and improved overall cost-effectiveness [51].

In [52], six ML models (Extreme Gradient Boosting, Random Forest, Support Vector Regression, K-Nearest Neighbors, ANN, Decision Trees) with Shapley additive explanations were integrated with algae-biomass co-gasification to optimize H_2 production from 3609 data points across 24 input parameters. Chlorella vulgaris, Nannochloropsis oculata, and Fucus serratus were selected as microalgae species to co-gasify with feedstocks (Fir Pellet, Palm Empty Fruit Bunch, Pellet Pine Wood) using Aspen Plus® simulation based on Gibbs free energy minimization. The results demonstrated that C. vulgaris-FP combination achieved the highest H_2 yield (9.87%) and exergy efficiency (84.84%), while C. vulgaris-PPW delivered peak energy efficiency (87.73%). Extreme Gradient Boosting demonstrated $R^2 > 0.96$, and a Root Mean Squared Error (RMSE) value of 0.327 for H_2 yield.

In a study by Urhan et al. [53], a green hydrogen production system was developed consisting of photovoltaic panels, wind turbines, and PEM electrolyzers. ML was used to process ten years of hourly meteorological data and learn patterns in renewable energy availability and hydrogen output. Models such as Long Short-Term Memory (LSTM) and ANN were applied, allowing the system to predict hydrogen production across various regions in Turkey. This helped operators plan system capacity more precisely, match hydrogen output with demand, and reduce wasted energy. As an example, for wind- and solar-powered hydrogen production in Aydın, the LSTM model achieved an RMSE of 0.0011 and 0.0026, while the ANN model recorded an RMSE of 0.0002 and 0.0088, respectively. Moreover, replacing 557 petrol vehicles with fuel cells that are being powered by green hydrogen generated from a wind turbine results in a reduction of 129,421 kg of oil and an avoidance of 399,911 kg of CO_2 emissions. In another AI-driven simulation framework [54], Recurrent Neural Networks (RNNs) were employed with Gated Recurrent Unit (GRUs) models to forecast electricity prices and gas demand, allowing dynamic scheduling of a 1.25 MW PEM electrolyzer. The most effective configuration used a weighted hybrid ensemble (70% linear regression, 30% RNN-GRU), achieving a hydrogen production cost of AUD 1.72/kg and blending 6887.28 kg of hydrogen over 119 operational hours. This approach minimized start-stop cycles, improved storage use, and aligned production with demand fluctuations, demonstrating the operational benefits of AI in green hydrogen applications. While ML and AI optimize processes through data-driven predictions, DT links these algorithms with virtual replicas of physical systems, allowing real-time monitoring, simulation, and control.

3.3. Digital Twin

The concept of DT has been extensively applied in numerous fields, such as manufacturing, aerospace, and civil engineering, owing to its ability to enable system-level prediction, continuous monitoring, and fault diagnosis in complex operational environments [55]. DT technology has also been increasingly seen as a game-changer for green hydrogen. In light of the increased climate efforts to decarbonize the globe, DTs have been adopted to tackle some main issues in hydrogen production, such as efficiency, safety, scalability, and real-time optimization [56]. A DT is typically defined as a dynamic virtual representation of a physical asset that is continuously updated through real-time data exchange, facilitating simulation and predictive analytics throughout the system's lifecycle [57]. Furthermore, DT contributes to improving sustainability, agility, productivity, and lowering the green hydrogen production cost. By enabling data-driven decision making, optimization, control, and anomaly detection and diagnosis [58]. DT is a dynamic virtual model of a physical asset that is used to simulate, predict, and optimize the performance in real-time. It is structured into three layers: the physical layer represents the real system, the second is the digital layer, which has multiple ML models that are used to enhance the system, and the third is the service/network layer, which is responsible for sending the data back and forth in real-time to the digital layer [59].

Experimental characterization of the PEM electrolyzer is performed first for a DT that begins with the development of green hydrogen production. This step helps establish a mathematical relationship between current, voltage, hydrogen flow, and other parameters, which is necessary for modeling the behavior of the system under different operating and fault conditions. Subsequently, a monitoring system can be created to oversee the operation of the electrolyzer. For this purpose, sensors will be applied to measure electrical and fluidic variables, including voltage, current, temperature, and pressure of the electrolyte, as well as the water level, while actuators such as electro valves and relays can be used for system control. These components can then be connected to a programmable logic controller (PLC), which manages signal processing and system logic. To enable real-time data acquisition, communication with the PLC can be implemented using the open platform communication data access protocol, which allows information to be exchanged with the software interface, such as LabVIEW, as can be seen in Figure 4. Within LabVIEW, a virtual instrument can be programmed to provide graphical visualization, store data continuously, and represent process parameters through charts and numeric indicators. Once the system is operational, the collected data can be stored and later used for modeling, enabling the development of the DT as a predictive tool for system performance [60]. Moreover, DT can be integrated with computational fluid dynamics (CFD) and ML models, such as Random Forest Regression, Deep Neural Networks, Support Vector Regression, and Extreme Gradient Boosting, to create a virtual replica of the physical system, which can be used to optimize and predict the performance for hydrogen production [61].

An essential computational tool frequently embedded within DT frameworks is CFD, which enables the detailed simulation of fluid flow, heat transfer, and chemical reactions in green hydrogen processes, particularly within catalytic reactors. For instance, Oleś et al. [62] demonstrated how a CFD model, enhanced with user-defined functions, was used to simulate the methanol synthesis process from CO_2 and green hydrogen produced through electrolysis. This model allowed for precise tuning of parameters such as pressure, feed velocity, and temperature within a fixed-bed reactor, resulting in methanol yields between 4% and 10%. Although CFD alone does not constitute a DT, it becomes integral when coupled with live sensor data, control logic, and predictive algorithms, thus forming a core simulation layer in twin architectures. In this context, CFD serves as a virtual experimental space for optimizing methanol yield, evaluating process efficiency, and supporting the design of sustainable reactor systems in hydrogen production.

Despite all the benefits of DT, multiple challenges can be observed, such as maintaining real-time two-way synchronization in large-scale industries, as it requires significant computing resources and stable IoT connections. Integration of DTs with existing industrial software systems used for inventory, product management, and operations is challenging, as compatibility across different platforms must be ensured.

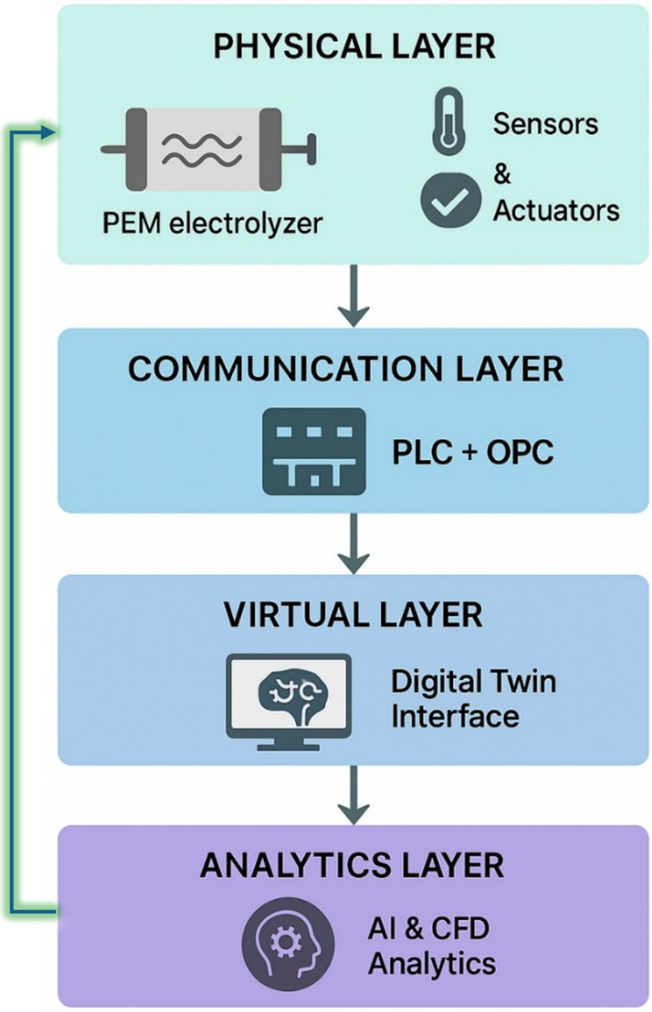

Figure 4. Digital twin for green hydrogen electrolysis.

A real-time digital twin (RTDT) of a 10 kW alkaline electrolyzer system with a Dual Active Bridge converter was developed and implemented on an OPAL-RT simulator to enable hardware-free testing under realistic operating conditions [59]. To verify its accuracy, the RTDT results were directly compared with simulation data generated using PLECS software, which was used as the reference model to compare RTDT with the PLECS across different operating scenarios. In the 10-kW case, the RTDT measured a stack voltage of 67.38 V and a current of 147.5 A, while the corresponding PLECS simulation produced 67.55 V and 148.46 A, resulting in a power output difference of less than 1%. Across the full operating range from 4 kW to 10 kW, the RTDT consistently tracked the behavior predicted by the PLECS model, confirming the DT's reliability for evaluating converter performance without a physical electrolyzer. A DT model for a 1 MW alkaline electrolyzer was developed by Liang et al. [63] to simulate its behavior under varying operational conditions. A multivariate mathematical approach was employed, in which temperature, pressure, and lye flow rate were treated as variables influencing voltage, Faraday efficiency, and the hydrogen concentration in oxygen. Simulation results showed that increasing lye flow slightly reduced cell voltage due to lower resistance and improved bubble removal. However, higher lye flow rates increased hydrogen concentration in oxygen, posing safety risks. The model was validated using real operational data and visualized through a 3D simulation platform with real-time PLC control, facilitating safer and more efficient system design under fluctuating power inputs.

A study by Song et al. [64] developed a DT framework for chemical looping hydrogen generation. The experiment consists of ten input descriptors (e.g., calcination temperature, reaction temperature, cycle number, oxygen carrier composition) and one output (hydrogen yield). Data was pre-processed by noise reduction and normalization to improve consistency. For the DT, five ML models (Extra Tree, Gaussian Boosting Regression, Random Forest, Extreme Gradient Boosting, and Gradient Boosting Decision Tree) were trained and optimized using hyperparameter tuning, with model accuracy evaluated through R^2 and mean absolute variance metrics. Gradient Boosting Decision Tree achieved the best predictive performance ($R^2 = 0.87$, MAE = 0.49), and it was integrated with the DT to calculate gas flow rates and reduction depths, which enables automated real-time process control and accurate hydrogen yield prediction, which can accelerate the industrial application of chemical looping hydrogen generation that can reduce fuel costs and guarantee reactivity of oxygen carriers.

In [65], DT was integrated with Monte Carlo simulations and network optimization to optimize supply chain logistics for biohydrogen production from agri-waste. The results demonstrated economic and environmental benefits. After 1000 iterations, the mean annual social savings were estimated at 34.54 billion dollars, with risk-adjusted net savings of 34.17 billion dollars. Biomass-based hydrogen was shown to generate 230 g CO_2 per kilowatt-hour compared with 970 g for oil and 820 g for coal, while social gains included medical expenditure savings of nearly 11,900 USD and employment benefits of over 22,500 USD per million kilograms of residue. DT relies on continuous streams of operational data, but its value is limited if that data cannot be guaranteed as accurate and tamper-free. Blockchain addresses this issue by ensuring data integrity and transparency, making the exchange of information across hydrogen systems secure and trustworthy.

3.4. Blockchain Technology

Blockchain is described as a decentralized, immutable ledger system that records transactions across a distributed network, ensuring transparency, security, and data integrity. Within energy systems, and particularly the hydrogen economy, it is employed to verify the origin of clean hydrogen, facilitate peer-to-peer trading, automate processes through smart contracts, and improve supply chain traceability and operational efficiency [66]. Blockchain is a type of ledger technology on which transactions are grouped into blocks. Each block header, which is a vital part of the blockchain, has its own time stamp, reference, and other unique information. Consensus algorithms are used to ensure that each node (devices that store and maintain a copy of the blockchain) has the same view of the blockchain. In this way, blocks provide the sequential structure of the ledger, while nodes act as the distributed devices that preserve and synchronize it [67].

Due to the extensive and complex operations of production, storage, and distribution in green hydrogen supply chains, the implementation of blockchain enables the creation of tamper-resistant decentralized networks that can verify transactions. It provides real-time monitoring and data access security between participants, which helps mitigation efforts against financial opacity, supply chain disruptions, and cyber-physical attacks [68]. Furthermore, by employing smart contracts and immutable ledgers, blockchain systems have the potential to automate compliance, streamline documentation, and foster greater stakeholder trust. The deployment of such digital infrastructure plays a pivotal role in promoting resilience and sustainability across green hydrogen supply chains, particularly under the growing demands for decarbonization and clean energy transition. However, the realization of this potential is contingent upon overcoming existing barriers related to interoperability, regulatory acceptance, and the scalability of blockchain applications [69].

Hydrogen production and consumption can be tracked in real time through the incorporation of smart meters, powered by cryptographic identities, and verified on a distributed ledger. Every feasible transaction of hydrogen, for example, quantity, origin, and tariff, is kept secure within a blockchain block via hash functions, allowing data preservation and preventing tampering by unauthorized agents [70]. This framework supports the execution of smart contracts that automate billing, reduce the risk of fraudulent activities, and improve the overall efficiency of energy trading [69]. The use of blockchain is also extended to peer-to-peer trading platforms, allowing excess hydrogen to be shared among networked stakeholders under defined market rules, where each transaction is securely registered through smart contracts and verified using cryptographic identities and smart meters embedded within the system [71]. Nonetheless, several technical challenges remain, including the physical implementation of such infrastructure, the need for constant monitoring and regular updates to protect against new or evolving security threats, as well as ensuring compatibility with existing equipment and industry standards, which can pose constraints on the viable application of this mechanism [70]. Additionally, blockchain has a huge energy consumption, which affects the real goal of using green hydrogen [72]. Blockchains were tested using four consensus mechanisms: Proof-of-Work, Proof-of-Stake, Proof-of-Byzantine-Fault-Tolerance, and Proof-of-Authority. Proof-of-Work was shown to have high energy consumption and low efficiency, making it unsuitable for sustainability objectives, while Proof-of-Authority was identified as the most appropriate because it offers low energy use, high efficiency, and scalability under the institutional control required for hydrogen certification [68].

Uncertainties regarding guarantees of origin, carbon accounting, and purity standards hinder the large-scale adoption of green hydrogen. Blockchain can be used to ensure the immutable recording of production, transport, and consumption data, enabling verification of hydrogen's origin and quality, which enhances both sustainability and resilience. By providing transparency in CO_2 emissions, real-time visibility of inventories, and improved coordination during disruptions, blockchain was shown to be a key enabler for scaling a reliable and sustainable green hydrogen economy [73].

Figure 5 illustrates a blockchain-integrated green hydrogen supply chain developed based on conceptual insights from [69,70]. The supply chain begins with the production of hydrogen via electrolysis, where hydrogen is generated and passed into the blockchain system. A blockchain ledger is shown at the center, where all production data is recorded as immutable records and managed using smart contracts. These contracts are used to automate and verify transactions without the need for centralized control. From the blockchain ledger, information flows to the hydrogen storage system, which is later connected to the distribution phase. Hydrogen is delivered via trucks to end users, including households and vehicles, as indicated by the icons. Alongside this main flow, the diagram also depicts the use of digital identities assigned to all participants in the network. These identities help ensure that every transaction is traceable and verifiable. A smart-peer trading loop is also included, showing how blockchain enables real-time, verified transactions directly between users. This facilitates decentralized energy exchanges and promotes market flexibility. On the other hand, there are three challenges that are emphasized as major obstacles to full-scale blockchain implementation in the hydrogen sector: (a) scalability: difficulty of expanding blockchain systems to handle large volumes of data and users, (b) regulation: legal and policy-related barriers that must be addressed, and (c) interoperability: the challenge of integrating blockchain with existing energy systems, devices, and standards.

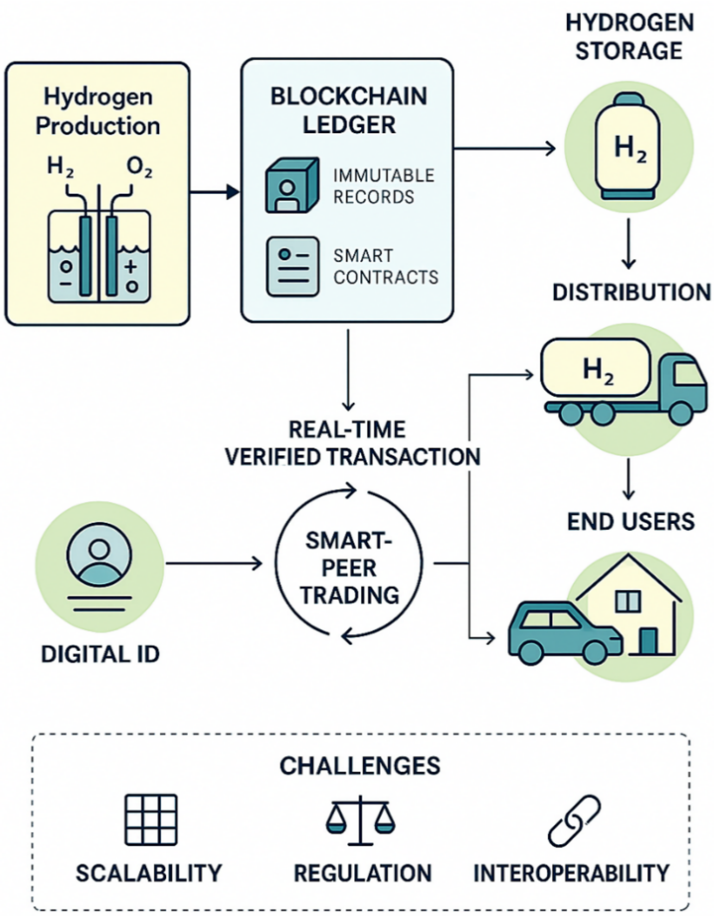

Figure 5. Blockchain framework for green hydrogen economy.

Blockchain technology was used to develop a certification system for green hydrogen within the EU context. In this system, production data were stored immutably using cryptographic hashing, while smart contracts were employed to automate sustainability verification and transfer digital tokens representing certified hydrogen. By embedding trust and traceability into the process, blockchain reduced manual procedures, supported regulatory compliance, and enabled decentralized governance across the certification framework [68]. Additionally, blockchain has also been integrated into the operational stages of green hydrogen supply chains to address security, transparency, and collaboration challenges. Through the use of decentralized ledgers, each unit of hydrogen can be tracked from renewable-powered electrolysis to end use, with all associated data, including carbon intensity and transport conditions, recorded in real time. Moreover, Permissioned access ensures that only authorized parties, such as producers, distributors, and regulators, can view relevant information, while smart contracts facilitate automatic execution of transactions and compliance checks. For example, the HyDeal initiative employed Hyperledger Fabric to synchronize data exchange across multiple green hydrogen networks, enhancing coordination between electrolysis sites and off-takers. This integration strengthened data integrity, eliminated intermediaries, and ensured that sustainability metrics were verifiable and tamper-proof throughout the hydrogen lifecycle [72].

4. Discussion

Digitalization has introduced transformative capabilities to green hydrogen production. However, it has simultaneously created a range of challenges that must be addressed, as seen in Table 1. Vulnerabilities related to data security have been intensified by increased connectivity and remote access. At the same time, the massive data streams produced by IoT sensors have strained cloud storage efficiency, requiring scalable and secure data management solutions. To mitigate these challenges, blockchain frameworks can be applied to secure transactional records through cryptographic immutability. Furthermore, blockchain can be used to secure IoT-generated data, while cybersecurity addresses these risks by applying authentication, encryption, and secure key exchange, which protect device communication, safeguard sensitive data, and maintain system reliability. At the same time, AI-based intrusion detection systems have been used to identify anomalies in real time. Similarly, the problem of interoperability, which has arisen from the integration of heterogeneous digital platforms, has been addressed through IoT architectures that rely on standardized communication protocols and blockchain smart contracts that unify transactional rules. Although the transition to digital platforms has exposed issues of infrastructure incompatibility, DT models have enabled the simulation of integration scenarios, thereby supporting gradual system modernization without operational risk. The demand for large and high-quality datasets, initially a limiting factor for ML, has been partially met through the continuous data streams generated by IoT sensors and structured within DT systems. Applications such as catalyst design, process optimization, forecasting, and scheduling have been enabled by AI/ML, linking digitalization directly to performance gains in hydrogen systems. Furthermore, location-specific AI models, which often lack generalizability, have been improved by using multi-source training data and adaptive learning algorithms. Finally, although digital mechanisms such as blockchain and smart contracts have outpaced existing regulatory frameworks, their transparency and auditability have positioned them as useful tools for compliance demonstration. Thus, while many barriers have emerged as consequences of digitalization, it is through the same technologies that most of these limitations are being actively resolved.

Table 1. Summary of utilizing digitalization for green hydrogen production.

Technology	Applications	Benefits	Challenges
IoT	Real-time monitoring of electrolyzers, predictive maintenance of hydrogen equipment, hydrogen leak detection, and smart hydrogen refueling stations	Real-time monitoring, improved safety, decentralized operation	Cybersecurity risks, inefficient cloud-based storage due to large amounts of data
AI/ML	Catalyst discovery for electrolysis, process optimization in hydrogen production, demand forecasting for hydrogen, and scheduling renewable energy input	Higher efficiency, energy savings, reduced costs	Data quality gaps and limited model generalization
Digital Twin	Virtual electrolyzer replicas, performance simulation under variable renewable inputs, predictive failure analysis for hydrogen infrastructure	Lifecycle and performance optimization, safety, and accurate simulation	High resource demand, software compatibility, and interoperability issues
Blockchain	Guarantees of origin for green hydrogen, supply chain traceability (production, storage, transportation, end-use), certification via smart contracts, and peer-to-peer hydrogen trading	Transparency, trust, automation, and resilience	High energy use, scalability, regulation, and interoperability

4.1. Infrastructure, Regulations, and Economic Gains

Infrastructure limitations are a central barrier to scaling green hydrogen production, as large test facilities must handle high-voltage power, purified water, and hydrogen sinks. These constraints lead to an increase in cost and complexity to produce green hydrogen [74]. Digitalization offers practical solutions: real-time monitoring through integrated data platforms allows continuous assessment of electrolyzer performance, while hybrid virtual–real testing and model-based extrapolation reduce reliance on expensive long-term trials. Linking physical infrastructure with digital platforms can help achieve reliable benchmarking, predictive insights, and accelerated stress testing, easing financial and resource burdens while enhancing safety and scalability.

The economic implications of digitalization are demonstrated by Tetouani et al. [71], who explored the tradeoff benefits of blockchain and IoT with green hydrogen in Morocco by applying the What-If Analysis simulation method. The study assumed that blockchain and IoT cost 800,000 and 1 million USD, respectively. Applying these technologies achieved a reduction in logistics losses from 5% to 2% and generated an additional 1.5 million USD annual revenue. While blockchain-based certification eliminated up to 10% of revenue losses linked to manual or unreliable certification systems by ensuring that 100% of produced hydrogen is marketable at premium prices, generating 0.49 million USD per year. The proposed framework elevates annual net profit to USD 6.5 million, resulting in a cumulative five-year gain of USD 32.5 million, which corresponds to a 43.6% improvement compared with the baseline.

However, results might vary depending on regulatory support. Green hydrogen adoption remains uneven and hindered across areas due to the absence of government regulations, which increases the risks for investment and slows down industrial deployment. Safety standards made by organizations such as the American Society of Mechanical Engineers (ASME) and the International Organization for Standardization (ISO) are not followed in all regions, making it difficult for green hydrogen production to be reliable and commercially available [75]. Currently, a fully mature green hydrogen market has not yet been established in any country. However, the number of countries with national hydrogen roadmaps has tripled over the past two years, indicating that numerous countries are preparing to adopt green hydrogen and are considering strategies to capture its economic benefits. Establishing transparent certification systems and harmonizing standards across borders are highlighted as essential to enable reliability in green hydrogen markets and to prevent fragmented approaches that could isolate early movers [76]. Without these mechanisms, digital tools that enable monitoring, certification, and system integration remain underutilized, as investors hesitate to commit in fragmented or uncertain markets.

Moreover, adopting DT, AI, ML, IoT, and blockchain in hydrogen systems reshapes workforce requirements, as old migration methods are going to be abandoned. Experts should gain training in cybersecurity awareness, predictive analytics, and the use of simulation platforms such as MATLAB and Python. Without this upskilling, the potential efficiency gains of digitalization risk being offset by operational errors or underutilization of advanced tools. In addition, cross-disciplinary knowledge will become essential, as engineers will increasingly need to understand electrochemical processes in addition to data management, cloud integration, and digital security protocols. The shift also demands a stronger focus on real-time decision-making and data-driven optimization, requiring personnel to move beyond traditional operating routines and embrace continuous learning. Organizations may need to invest in structured training programs, certification pathways, and collaboration between IT and engineering departments to bridge skill gaps. In the long run, the hydrogen sector’s ability to fully capitalize on digitalization will depend as much on human adaptability and workforce readiness as on the technologies themselves [77,78].

4.2. Digital Synergy for Green Hydrogen Systems

An optimization framework for electrolyzers can be developed by integrating IoT, ML, DT, and blockchain. Figure 6 illustrates how these technologies can interact with each other by using a full DT system that consists of physical, network, and digital layers. IoT sensors capture operational data from the electrolyzer (physical layer) and transmit it through the network and onto the digital layer. This real-time data can be managed and protected through blockchain technology. Within the digital layer, ML models are used to apply predictive maintenance and optimization algorithms that are fed back to the physical layer to make system adjustments in order to enhance the efficiency and reliability of the electrolyzer. This process is continuous and can be adjusted based on specific applications or requirements, such as varying output demands, logistics, and supply chain.

Integration of digitalization is a key enabler for moving green hydrogen to large-scale industrial deployment. Advanced digitalization tools can overcome bottlenecks that traditionally make scaling difficult. For example, IoT enables monitoring and optimization across diverse stages of the hydrogen supply chain, enabling real-time coordination of production, storage, and distribution. DT addresses the early signs of degradation and abnormal behavior, and it can be used for predictive maintenance, which helps in monitoring large-scale projects. Additionally, DT can be used to simulate different scenarios by enabling the application of what-if scenarios. By leveraging historical data together with ML models, DT can strengthen predictive analytics, anticipate future equipment performance, and determine the optimal timing for scheduled maintenance [79]. Digitalization thus provides the tools needed to scale green hydrogen from isolated pilots to reliable, industrial systems.

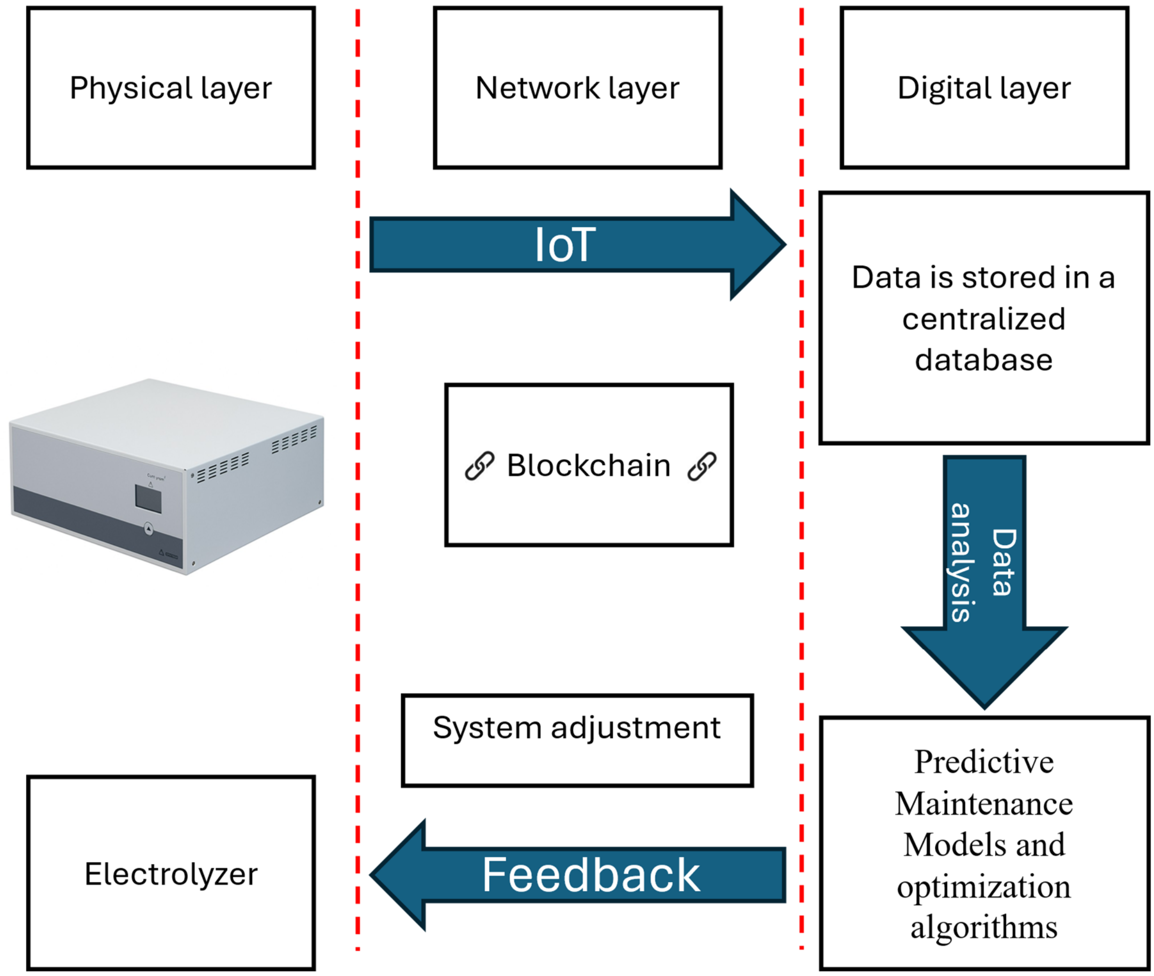

Figure 6. Framework for the integration of digital technologies for green hydrogen production.

5. Conclusions

This review highlighted the transformative impact of digital technologies on green hydrogen production. Considering current developments, digitalization is increasingly recognized as a foundational element of green hydrogen technologies. Through the enablement of smarter, more adaptive, and more sustainable hydrogen systems, digital tools have positioned themselves as key enablers in the broader transition toward decarbonized energy futures. Research has shown that AI, ML, and IoT, when combined with the DT approach, have increased productivity and enabled new forms of automation, predictive maintenance, and large-scale integration. These advancements have lowered operational costs and reduced the environmental impact of hydrogen production systems, allowing them to more effectively adapt to the variable output of renewable energy sources.

Various challenges can be resolved by making use of digital frameworks, such as high energy consumption, inconsistent system behavior, and real-time monitoring capabilities. The utilization of ML demonstrated its capability for optimizing reaction parameters and predicting optimal operational conditions. Meanwhile, IoT networks have facilitated continuous data exchange and process transparency, especially in decentralized or remote production units. The modeling and simulation of electrolysis systems has also been improved by the use of DT, allowing for insights into performance diagnostics and system design.

In order to accelerate adoption, researchers can contribute by developing interoperable standards and open-access datasets that enable reliable AI and DT applications. Entry barriers for digital technologies should be considered by providing targeted incentives. Stakeholders should invest in workforce training and pilot-scale demonstrations to validate cost-effectiveness and safety. Together, these steps can translate the promise of digitalization into measurable progress for the global hydrogen economy.

Author Contributions

A.M.N.: conceptualization, methodology, writing—original draft preparation, writing—reviewing and editing, visualization; M.M.: data curation, conceptualization, writing—original draft preparation, writing—reviewing and editing, investigation; A.A.: data curation, conceptualization, writing—original draft preparation, writing— reviewing and editing, supervision. All authors have read and agreed to the published version of the manuscript.

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Data will be made available upon request.

Conflicts of Interest

The authors declare no conflict of interest.

Use of AI and AI-Assisted Technologies

During the preparation of this work, the authors used ChatGPT and Grammarly to rephrase sentences and enhance language. After using these tools/services, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

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