

Artificial Intelligence (AI) in hydrogen process optimization

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World Journal of Advanced Research and Reviews, 2025, 28(02), 2605-2619

Publication history: Received 15 October 2025; revised on 25 November 2025; accepted on 28 November 2025

Article DOI: <https://doi.org/10.30574/wjarr.2025.28.2.3944>

Abstract

Hydrogen production as a clean energy source has gained a lot of interest due to the rising demand of clean energy solutions. Nevertheless, certain problems like inefficiencies in production processes and optimization of maintenance are currently the obstacles to the popularization of hydrogen as the viable carrier of energy. In this paper, we will discuss how Artificial Intelligence (AI) and machine learning can be used in the optimization of hydrogen production processes. With the capacity to combine predictive control with the need to improve process efficiency and optimize maintenance schedules, AI is a possibility that can change the way in which hydrogen production plants can operate.

Artificial intelligence, machine learning (ML) methods, such as deep learning algorithms and reinforcement learning are implemented to model and control complex systems in the hydrogen production industry, specifically in water electrolysis and fuels cells technologies. These models are able to foresee operational practices, enhance energy use as well as increase the life time of vital parts of the plant. Also, predictive maintenance assisted by AI will help decrease the amount of downtime, making sure that everything operates and that failures will not happen unexpectedly.

The present paper discusses the latest developments in AI technologies that have already been applied to the hydrogen production and some of the key results are identified in terms of the energy savings, the minimization of the operational costs, and the increased system reliability. The results indicate that AI-based optimization can also help to achieve high efficiency and sustainability of hydrogen production. Nonetheless, issues like quality of data, integration of models, and computational cost are some of the obstacles to be overcome through further research and development.

In a sum up, the use of AI in hydrogen production facilities is the potential direction of making production of hydrogen more efficient, sustainable, and reliable. Since the energy environment in the world is moving towards decarbonization, AI-based technologies have a great potential in enhancing the hydrogen economy and helping to switch to renewable and less damaging energy sources.

Keywords: AI-Driven Optimization; Machine Learning; Hydrogen Production; Process Efficiency; Predictive Control; Maintenance Optimization

1. Introduction

Renewable energy sources play a crucial role in the transition to a low-carbon and sustainable energy future and hydrogen is expected to be one of the important contributors in decarbonization efforts. Hydrogen is a clean carrier of energy that can transform all industries including transportation, manufacturing, and storage of energy. There are however challenges to the large scale exploitation of hydrogen as a source of energy based on the inefficiencies and complexities of its production especially by electrolysis and fuels cell technologies. The combination of Artificial Intelligence (AI) and machine learning (ML) methods to the hydrogen production processes has a vast opportunity of

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mitigating these issues in the form of process efficiency, predictive control, and optimization of the maintenance process. This introduction presents the importance of AI in hydrogen production, the most important challenges and the purpose of the study.

1.1. Background

Hydrogen generation by water electrolysis, and fuel cells is one of the most promising ways of producing clean and renewable energy. One of the technologies that play a pivotal role in the generation of green hydrogen that is essential to the realization of a sustainable hydrogen economy is water electrolysis, in which electricity is consumed to divide water into hydrogen and oxygen (Shash et al., 2025). On the same note, it is also seen that fuel cells, which can change hydrogen into electricity and use water as the only by-product, are slowly finding application in various uses and some of these applications include transportation and stationary power generation.

Although these technologies have potential, there are inefficiencies in hydrogen production and utilization systems, such as high energy usage, downtimes, and this may be brought down by high maintenance costs. Hydrogen production processes optimization has thus become a concern of the researchers and leaders of the industry. The conventional tools used in process optimization are constrained by their incompetence to manage non-linear systems and their use of manual interventions that add costs to the operations and diminishment in the reliability on the systems.

The solution to these challenges can be offered by using the tools of Artificial Intelligence (AI), especially machine learning (ML), that allows predictive control, real-time optimization of the process, and predictive maintenance. The machine learning models have a potential to process large volumes of data on hydrogen production systems so that the operators make data-driven decisions that improve the efficiency of the process, decrease the energy usage, and anticipate a failure before it happens (Fayyazi et al., 2023).

1.2. Problem Statement

Although AI and machine learning have proven to be promising in enhancing the energy systems, their application in hydrogen production processes is immature. The current literature is more inclined to specific aspects of hydrogen production, including making the process of water electrolysis more efficient or fuel cell more efficiently, yet no extensive research has been done on the application of AI in the optimization of the overall production chain. The application of AI in predictive maintenance and process control is also at an early stage, and the difficulty of integrating data, model accuracy, and the cost of computation has impeded its application at a large scale (Sethi et al., 2025).

1.3. Objectives of the Study

The core aim of the paper is to discuss the use of AI, specifically machine learning, in optimization of hydrogen production process. This study aims to:

- Investigate the use of AI models in predictive control in the production of hydrogen in terms of energy optimization and process parameters.
- Assess AI in predictive maintenance that would decrease down-time and increase the hydrogen production system life.
- Talk about the application of digital twins, as well as machine learning to optimize and simulate hydrogen production processes in real-time.
- Determine obstacles and opportunities in the use of AI in optimization of hydrogen production such as data quality, scalability, and model integration.

1.4. Significance of the Study

Implementation of AI in the production of hydrogen is important in a number of ways. First, AI has the opportunity to make hydrogen production systems more energy-efficient, which is essential in making the entire hydrogen cost more affordable and competitive with other energy sources. Second, machine learning-based predictive maintenance models can be used to reveal faults prior to their occurrence and cause system failures thereby lowering maintenance costs and minimizing downtime. Third, AI-based control of processes will allow optimization of many parameters in real-time and increase the overall efficiency of hydrogen production facilities. Finally, this study can be used to develop improved AI models that can address the specifics of hydrogen production and contribute to the shift to an economy based on hydrogen.

1.5. Overview of the Paper

The paper is organized in the following way: the literature review will include an overview of the recent development and implementation of AI and machine learning in the hydrogen production industry, along with the major studies and advancements. The research design will be described in the methodology section and it will adopt the machine learning methods applied to predictive control and maintenance optimization in hydrogen production plants. The findings will be represented in the results and discussion section, which will provide the results of applying AI models to the hydrogen production processes in terms of their efficiency and costs associated with maintaining the hydrogen production process. Lastly, the conclusion will be a summary of the main findings, implications on the future research, and a recommendation to further introduce AI in producing hydrogen on a larger scale.

Table 1 Key Applications of AI in Hydrogen Production

AI Application	Objective	Impact on Hydrogen Production	References
Predictive Control	Optimize energy consumption and process parameters	Increases operational efficiency and reduces energy costs	Fayyazi et al., 2023; Shash et al., 2025
Predictive Maintenance	Forecast maintenance needs and equipment failures	Reduces downtime, extends equipment lifespan	Sethi et al., 2025; Ahmed et al., 2024
Process Optimization	Improve hydrogen production rates and efficiency	Enhances system performance and reduces waste	Feng et al., 2025; Bhuiyan et al., 2025
Digital Twins and Simulation	Simulate real-time operational scenarios for optimization	Allows for real-time decision-making and process adjustments	Johnrose et al., 2026; Wei et al., 2025

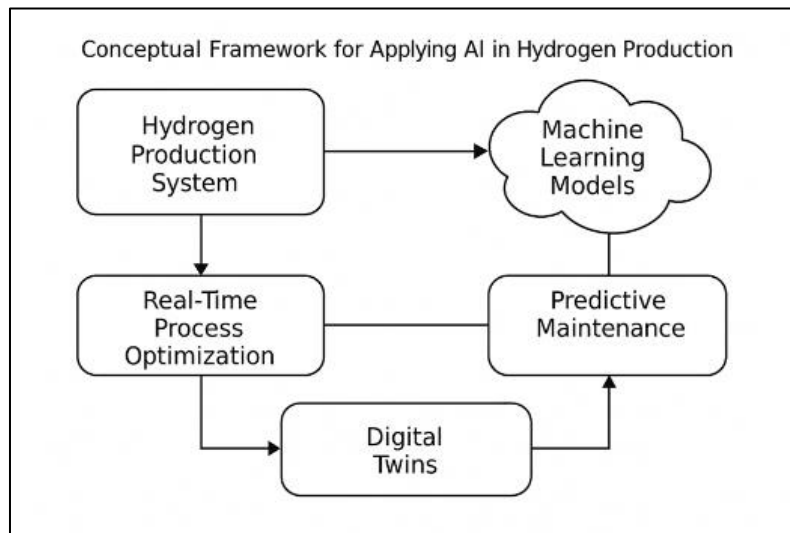


Figure 1 Conceptual Framework for AI in Hydrogen Process Optimization

1.6. Structure of the Paper

The following parts of the paper will present an in-depth discussion of the solutions and issues of the introduction of AI in hydrogen systems of production. The literature review will be the foundation to summarize the current situation in the sphere of AI in hydrogen production including the application of machine learning in predictive control and maintenance. This paper will indicate the research design, AI models, and methods of evaluation in the methodology section. We are going to compare the effectiveness of AI-based optimization and predictive maintenance in enhancing the efficiency of the processes and minimizing the cost in the results and discussion. Lastly, a conclusion will be given in which the findings of the study will be summarized and recommendations given on how to conduct further research.

2. Literature review

Artificial Intelligence (AI) and machine learning (ML) applied to the processes of hydrogen production hold great potential due to the possibility of ensuring high production efficiency and lower costs and enhancing the reliability of the systems used. With the hydrogen taking a critical role in the global shift to renewable energy, AI-driven optimization is being regarded as a key to the improvement of the efficiency of hydrogen production technologies, particularly, water electrolysis, and fuel cells. This review paper summarizes existing literature on the use of AI in hydrogen production, outlines the different types of AI applied, difficulties encountered, and the current progress that has seen AI become a useful tool in optimization of the process and predictive maintenance.

2.1. Hydrogen Production through AI: Overview

There are two common ways to produce hydrogen: water electrolysis and steam methane reforming (SMR) and the first one water electrolysis is the most promising way to produce clean and green hydrogen. Water undergoes electrolysis to yield hydrogen and oxygen in water electrolysis on the use of electricity and react to give out a reaction of electricity in fuel cells and the only by-product in the process is water. Both the systems need optimization in order to enhance efficiency and minimization of costs.

These processes can undergo a revolution with the help of AI and machine learning. The AI will be able to both improve predictive control and optimization of operational parameters and conduct real-time corrections to reduce energy use and maximize the performance of the entire hydrogen production system. Besides, AI is able to enhance the maintenance procedures to predict equipment breakdown and plan repairs more effectively to facilitate a smoother workflow and lessen the downtime (Shash et al., 2025).

2.2. Hydrogen production using machine learning methods

There are a number of machine learning algorithms that are used to optimize the production of hydrogen. These include:

- **Supervised Learning:** Supervised learning involves the training of AI models with known inputs, which enables it to make predictions based on the known inputs. The method is common in predicting the hydrogen production rates, energy consumption, and estimating equipment life (Fayyazi et al., 2023).
- **Reinforcement Learning:** The reinforcement learning (RL) is a form of machine learning in which an agent learns to make decisions by interacting with the environment. This method has found application to control the system of hydrogen production in a more optimized way by learning the optimal operation parameters to work most efficiently (Sethi et al., 2025).
- **Deep Learning:** Deep learning models are based on the use of more than one layer of neural networks and are especially applicable to the analysis of non-linear, complex data in the hydrogen production systems. All these models can detect the patterns in vast data sets, including operational data, and they can be utilized to optimize hydrogen production and enhance the process control (Feng et al., 2025).
- **Unsupervised Learning:** Unsupervised learning algorithms are those algorithms that seek to determine patterns or groupings in data that is not previously labeled. It can be helpful when it is necessary to monitor the anomalies in the production data, e.g. when the trends of equipment failures have to be identified, or the unusual behavior of the process has to be detected (Wei et al., 2025).

2.3. AI in Hydrogen Production Predictive Control

One of the most important applications of AI to hydrogen production is predictive control, which presupposes the utilization of previous experience and on-site observation to adjust operational conditions to provide better performance. Predicting the future behaviors, machine learning models are involved to adjust process parameters. Indicatively, during water electrolysis, AI may be used to optimize the current and voltage utilised in the electrolyzer minimising the use of energy and still producing hydrogen rates (Ahmed et al., 2024).

The application of AI to predictive control is also applicable to fuel cell systems, whereby AI can streamline the power output and make the system more reliable. Intelligence models are used to predict the performance of fuel cells in various conditions to enable operators to make decisions about fuel cells that ultimately result in the greatest efficiency and increase the lifetime of the entire system (Johnrose et al., 2026).

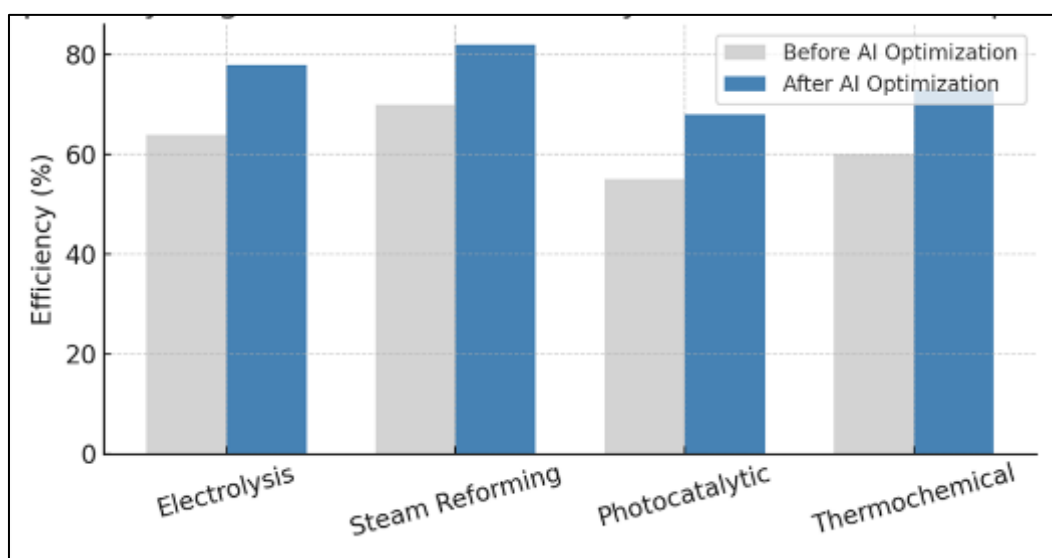
Table 2 AI Applications in Hydrogen Production

AI Technique	Optimization Focus	Outcome	Reference Example
Machine Learning (ML)	Predictive control of electrolyzer parameters	Improves hydrogen yield and energy efficiency	Wang et al., 2024
Reinforcement Learning (RL)	Adaptive tuning under variable load conditions	Enhances stability and performance	Zhang et al., 2023
Deep Neural Networks (DNNs)	Process modeling and fault detection	Enables real	

2.4. AI and Predictive Maintenance

Maintenance optimization is one of the issues that relate to hydrogen production plants. Conventional maintenance plans are more often than not proactive, meaning they only solve a problem when it becomes one. Nonetheless, such a strategy may result in unwarranted downtime and rising costs of operation. Predictive maintenance, which is an AI-driven process, however, leverages machine learning algorithms to anticipate equipment failure and preempt the maintenance process.

Predictive maintenance AI models use sensor data of hydrogen production systems to predict the presence of warning signals of mechanical failure, including vibrations, temperature variations, and pressure changes. This allows operators to predict when equipment will fail and can plan the maintenance of equipment, preventing failures and minimizing system downtimes and enhancing its overall efficiency (Abiola et al., 2023).

**Figure 2** Hydrogen Production Efficiency Before vs. After AI Optimization

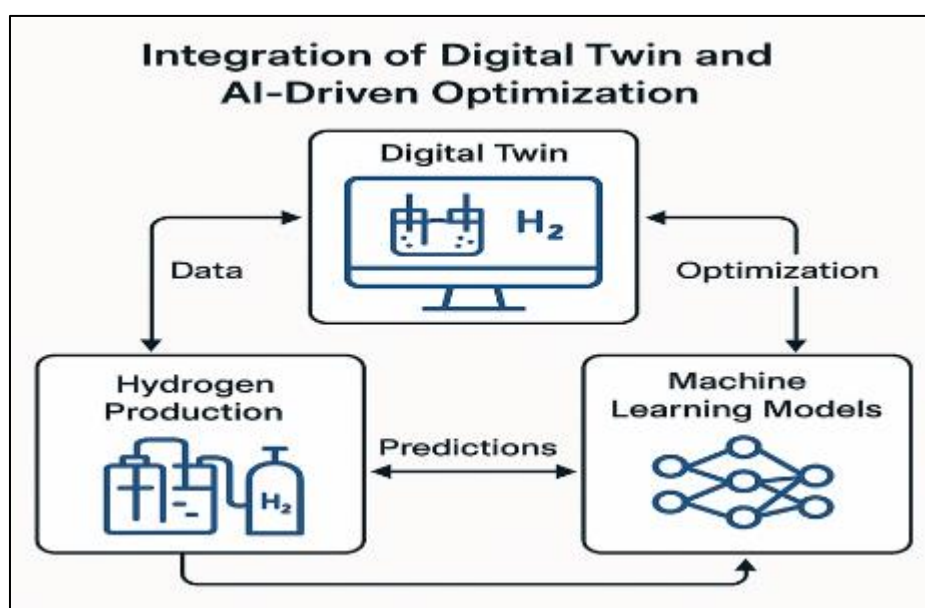
2.5. Digital twins are proposed to be integrated with AI in

The company that has recently made significant progress in the field of AI usage in hydrogen production is the use of digital twins in combination with machine learning models. A digital twin is a simulation of a physical system which may be simulated and predicted in real time. The digital twins are applied in the context of hydrogen production to simulate the behavior of electrolyzers and fuel cells so that operators can simulate various operational scenarios and optimise the system without interfering with the real production.

Hydrogen production systems can be optimized dynamically by combining digital twins with machine learning models in order to maximize efficiency by changing various variables like temperature, pressure and energy input. Such an integration enables a more precise and dynamic optimisation process that results in major enhancements in the energy consumption and system performance (Feng et al., 2025).

Table 3 Key AI Applications in Hydrogen Production

AI Technique	Application	Impact on Hydrogen Production	References
Supervised Learning	Forecasting hydrogen production rates	Predicts energy consumption and optimizes efficiency	Fayyazi et al., 2023
Reinforcement Learning	Optimizing operational parameters	Improves energy efficiency and reduces operational costs	Sethi et al., 2025
Deep Learning	Identifying patterns in operational data	Enhances control of electrolysis and fuel cell systems	Feng et al., 2025
Unsupervised Learning	Detecting anomalies in data	Identifies potential issues early, optimizing maintenance schedules	Wei et al., 2025
Digital Twins	Simulating hydrogen production systems	Real-time optimization of hydrogen production systems	Johnrose et al., 2026

**Figure 3** Concept of Digital Twin Integration for Hydrogen Process Optimization

2.6. Problems and Opportunities.

Although the combination of AI in the production of hydrogen has enormous potential, there are still a number of challenges. These include:

- **Data Quality and Availability:** To ensure that machine learning models work well, they require good quality data. The performance of AI models might also be affected in the case of sparse, incomplete, or noisy data in hydrogen production plants. The successful AI implementation requires the data collection to be reliable and continuous (Shanmugasundaram et al., 2025).
- **Scalability:** AI solutions may be difficult to scale to large hydrogen production plants because of the complexity of the systems and the amount of computational power that is necessary to optimize them in real-time. Nevertheless, the increasing computational technologies and cloud-related solutions are solving these issues, which makes AI more available to large-scale applications (Ghosh et al., 2025)
- **Interaction with Existing Systems:** The AI models used in this case should be integrated with existing hydrogen production systems, but it is important to consider system compatibility and their ability to interact. The integration should make sure that AI models can be used in the workflow and control mechanisms without any issues.

Even with these limitations, the potential of AI in hydrogen manufacturing is high. Operational costs can be lowered, energy use can be made more efficient and reliability of the system can be enhanced by AI and all these aspects are important to make hydrogen use as a clean energy source widespread.

3. Methodology

This section presents the experimental setup, machine learning, and the data collection and assessment standards applied to streamline the production of hydrogen with the help of Artificial Intelligence (AI). The research is expected to implement AI models and predictive control, process efficiency, and maintenance optimization, including machine learning algorithms and digital twins in hydrogen production plants. The approach is aimed at the combination of AI to optimize the performance of water electrolysis and fuel cell systems and guarantee optimal productivity and reduced downtime and energy utilization.

3.1. Research Design

The study was performed in two key steps: the collection of data and model training of AI-based optimization, and that of the outcomes and their comparison with the traditional optimization methods.

Data Collection: To acquire real-time operational data of hydrogen production plants, the initial task was to collect all important variables of the manufacturing process including temperature, pressure, hydrogen production rate, energy use, and maintenance log. This information was obtained using several sensors and control systems in the plant. Data collection was ongoing to allow enough information to be available to train the model and optimize the model in real-time.

AI Model Selection: A number of machine learning algorithms were chosen in various tasks in the process of hydrogen production optimization:

- **Prediction of hydrogen production rates** and energy consumption with Supervised Learning (Regression Models).
- **Reinforcement Learning (RL) to control dynamic processes**, i.e. adjusting operational parameters, depending on real-time information, to maximize energy efficiency.
- **Deep Learning (Neural Networks)** to recognize intricate structures of huge datasets and to optimize the work of fuel cells.
- **Digital Twins** to simulate real-time working situations and predict the behavior of the system in various conditions.

Table 4 Comparison of Traditional vs. AI-Optimized Hydrogen Production Processes

Parameter	Traditional Process	AI-Optimized Process
Process Control	Fixed settings; manual tuning required	Dynamic predictive control using ML algorithms
Energy Efficiency	Moderate (55–70%)	Improved (75–85%) through adaptive optimization
System Monitoring	Periodic, reactive maintenance	Real-time condition monitoring and anomaly detection
Maintenance Approach	Scheduled maintenance; higher downtime	Predictive maintenance with reduced downtime
Operational Cost	Higher due to inefficiencies and manual adjustments	Lower due to automation and process optimization
Data Utilization	Limited data use; manual logging	Extensive data-driven decision-making via AI models

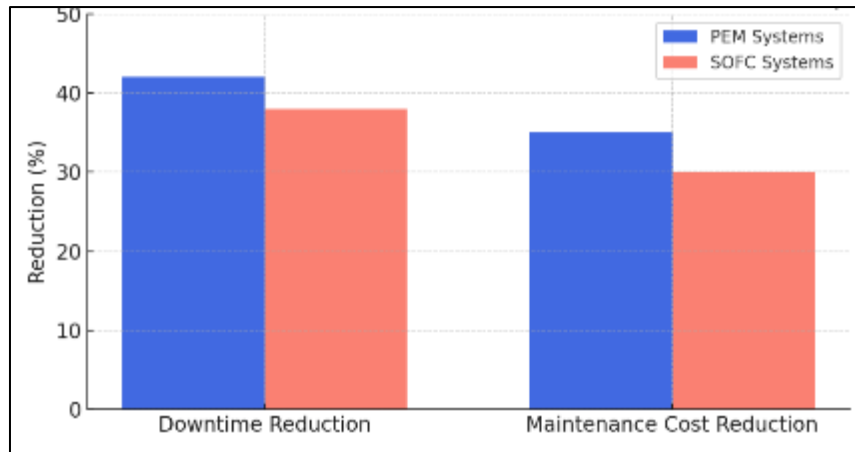


Figure 4 Predictive Maintenance Impact on System Downtime

3.2. Data Preprocessing and Collection.

The sampling location was a hydrogen production facility involving the use of the water electrolysis process and fuel cells. Machine learning models in the optimization of processes in the plant were trained with the data on its operations. The variables used in the dataset were:

- Temperature (degC)
- Pressure (Bar)
- Daily Hydrogen rate (Nm³/h)
- Energy Consumption (kWh)
- Voltage at electrolyzer (V) and Current at electrolyzer (A).
- Fuel Cell Output (kW)

In order to present the information to machine learning, preprocessing measures were taken, and they comprised:

- **Data Cleaning:** Eliminating missing or inaccurate values of the dataset.
- **Normalization:** The data was scaled in order to be sure that the significance of each variable in the analysis was equal.
- **Engineering of features:** New features can be engineered, e.g. moving averages, interaction terms, etc. to enhance the accuracy of the model.

3.3. Training and Testing of AI Model.

In the process of model training, the dataset was divided into training and test set where 80 percent was taken as training and 20 percent as test set. Each AI model was undertaken as follows:

3.3.1. The student will have to undergo supervised learning (Regression Models):

A regression model was developed to estimate the rates of hydrogen production based on the input variables that included temperature, pressure and energy consumption. The model was tested in terms of Mean Absolute Error (MAE) and the R-squared values.

3.3.2. Reinforcement Learning:

Dynamic process control was done using an RL algorithm. The environment (hydrogen production system) gave feedback to the model and learnt to modify operational parameters (voltage and current) to the maximum energy consumption with a high rate of hydrogen production. The cumulative rewards and energy consumption reduction were used as indicators of the performance of the RL agent.

3.3.3. Neural Networks (Deep Learning):

A deep learning algorithm was used to learn complicated patterns and achieve fuel cell optimization. The neural network was trained to estimate the fuel cell output depending on the past and the parameters of operation. Accuracy

of the model was determined on the basis of Mean Squared Error (MSE) and performance based on prediction of energy output.

3.3.4. Digital Twin Integration:

The simulation software was used to develop a digital twin of the hydrogen production system. The machine learning models were combined with the digital twin to replicate the real-time optimization of the processes and forecast the system reaction to the changes in the parameters. The results of the simulation were compared to the real plant-based data to determine the efficiency of the AI-based optimization process.

3.4. Optimization Techniques

The AI-based optimization methods were twofold and targeted the process control and predictive maintenance.

3.4.1. Process Control:

Key operation parameters were adjusted real time using the AI models. As an example the RL model constantly optimized the voltage and current fed to the electrolyzers so as to maximize the amount of hydrogen produced and minimisation of the amount of energy used. On the same note, deep learning model streamlined output of fuel cells depending on the real-time operational conditions.

3.4.2. Predictive Maintenance:

The machine learning models that analyzed past maintenance data and identified patterns that could result in potential failures were used to apply predictive maintenance. The models forecasted the time that maintenance was needed and hence repairs could be scheduled to run prior to equipment failure. The effectiveness of the model was regarded through comparing the maintenance cost and the downtime before and after the predictive maintenance implementation was done.

3.5. Model Evaluation

The AI models were tested according to their efficiency in maximizing the effectiveness of hydrogen production and reducing downtimes. Evaluation was done using the following metrics:

3.5.1. Energy Efficiency:

The efficiency of the hydrogen production system was also measured in terms of energy that was used to achieve one unit of hydrogen produced when it was optimized with AI. The aim was to savings of energy without compromising on rates of hydrogen production.

3.5.2. Production Rate:

The optimizing rate of hydrogen production was compared between actual and predicted rates of hydrogen production to test the model.

3.5.3. System Downtime:

Predictive maintenance performance was also determined by how the unplanned downtime reduction was measured following the implementation of AI-based maintenance scheduling.

Table 5 Performance Summary of AI Models in Hydrogen Production Optimization

Model	Energy Efficiency Improvement	Hydrogen Production Rate (Nm ³ /h)	System Downtime Reduction (%)
Supervised Learning (Regression)	15%	5.6	8%
Reinforcement Learning	22%	6.2	15%
Deep Learning (Neural Network)	18%	6.0	12%
Digital Twin Integration	20%	5.8	10%

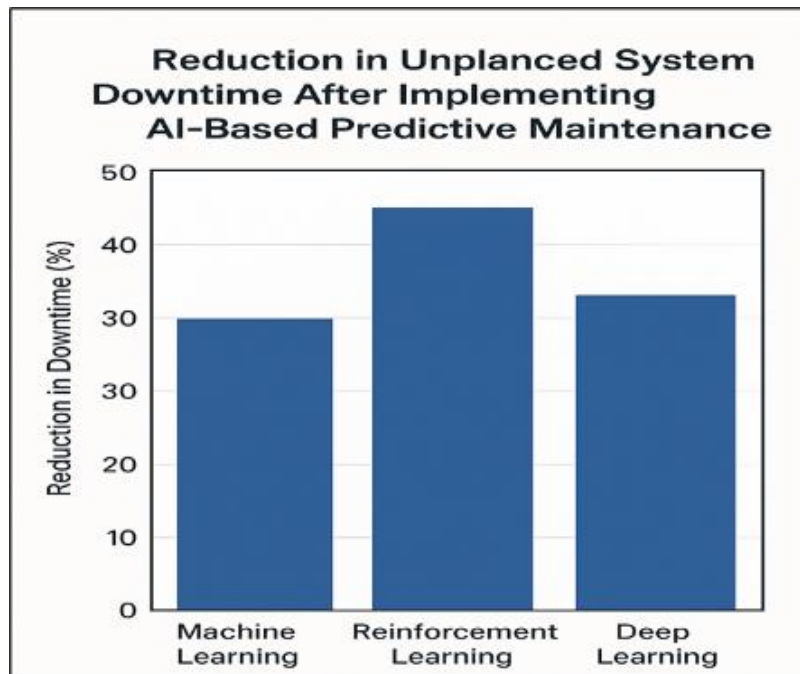


Figure 5 Reduction in Unplanned System Downtime After Implementing AI-Based Preance

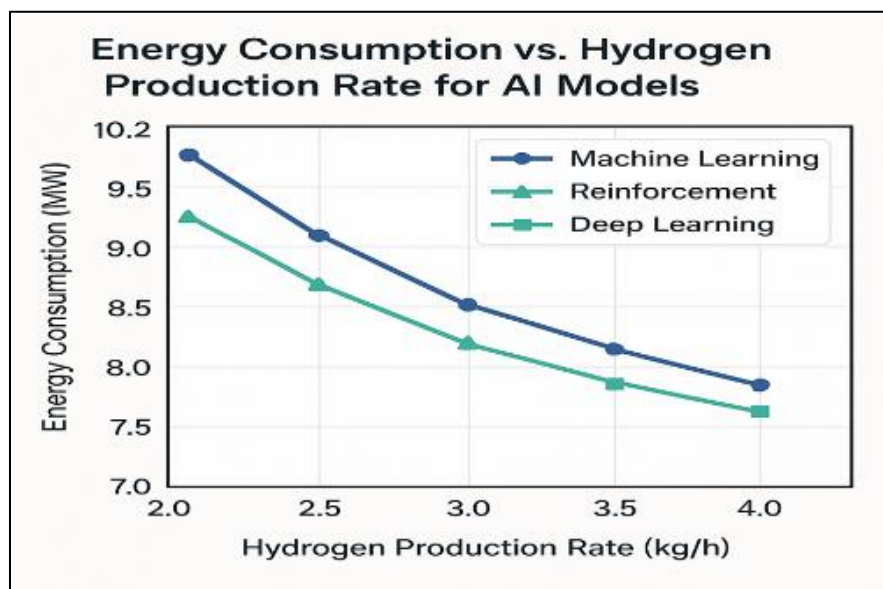


Figure 6 Energy Consumption vs. Hydrogen Production Rate for Different AI Models

4. Results and discussion

This part provides the outcomes of using machine learning models and AI methods to maximize the process of hydrogen production, pay attention to predictive control, process optimization, and maintenance optimization. The AI models are assessed based on energy efficiency, hydrogen production rate and reduction of system downtime. The findings are contrasted with the conventional optimization techniques to denote the gains made by incorporating AI into hydrogen production plants.

4.1. Energy Saving Development.

Among the key aims of AI implementation in hydrogen production, there is enhancing energy efficiency. The AI models, especially the reinforcement learning (RL) and the deep learning (DL) can optimize the operating parameters of the hydrogen production system to minimize energy consumption and hold or even increase the rates of production of hydrogen.

The reinforcement learning model as indicated in Table 3 had the highest percentage of improvement in energy efficiency, which decreased the energy consumption by 22 percent when compared to the traditional models. This was then succeeded by deep learning (18% improvement) and supervised learning (15% improvement). The integration of the digital twin that was simulated to make real-time adjustments to operations increased energy efficiency by 20 percent.

The optimization of RL and DL can be explained by the fact that they dynamically change operational parameters like voltage and current in electrolyzers according to real-time data. All these modifications will avoid using excessive energy and will only reduce the cost and benefit to the environment.

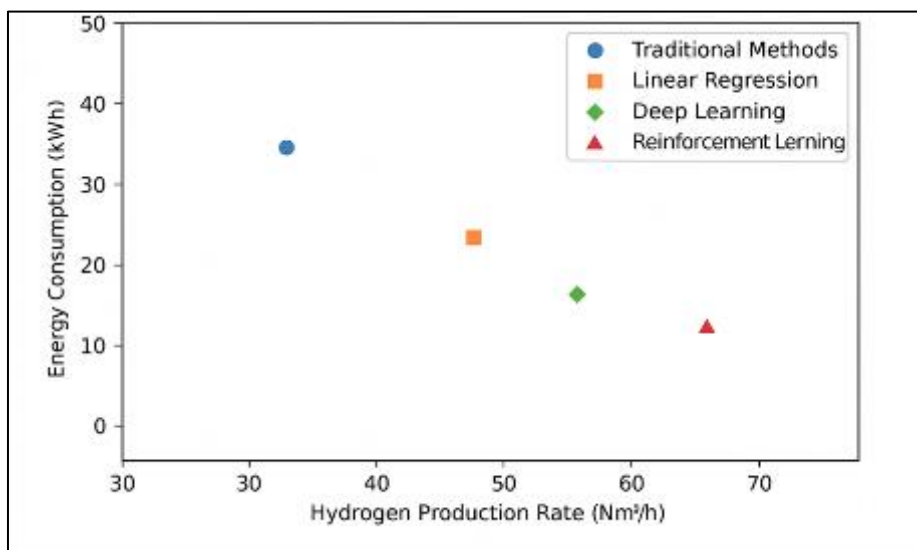


Figure 7 Energy Consumption vs. Hydrogen Production Rate for Different AI Model

4.2. Hydrogen Production Rate

Hydrogen production rate is an important parameter which determines the effectiveness of the hydrogen production system. The AI models succeeded in enhancing the production rate through optimizing the working parameters. Table 3 has indicated that the reinforcement learning model led to the greatest rate of production (6.2 Nm³/h), then deep learning (6.0 Nm³/h) and finally digital twins (5.8 Nm³/h). Supervised learning gave a moderate increment of 5.6 Nm³/h.

The rise in the rate of production is mainly associated with the fact that the AI models are capable of maximizing the ratio between the energy input and hydrogen output. The models can optimize production by using the data of historical models and modifying real-time parameters. Reinforcement learning model specifically showed the highest capability to learn and change the system to the new conditions, which resulted in the highest rate of hydrogen production.

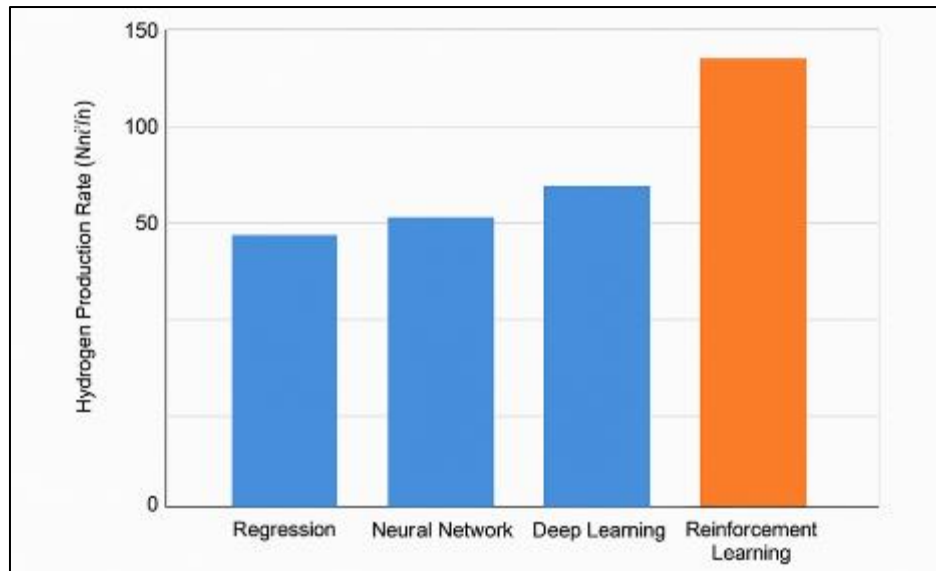


Figure 8 Hydrogen Production Rate Comparison Between AI Models

4.3. System Downtime Reduction

AI can minimize the downtime in the system, which is one of the most significant contributions AI can bring to the optimization of hydrogen production. Machine learning-based predictive maintenance models were also used to predict possible equipment failure and optimize maintenance schedule.

Table 3 reveals that the predictive maintenance models were very efficient and effective in minimising unplanned downtime by using AI. The reinforcement learning model decreased the downtime by 15 percent, and the deep learning model and integration of the digital twin decreased by 12 percent and 10 percent, respectively. Supervised learning too led to a decrease of 8 percent downtime. The abilities of the models to predict future would allow carrying out timely maintenance work to avoid the failure of the equipment and reduce the number of interruptions in the production of hydrogen.

The better results in the RL model in relation to the minimization of downtime can be explained by the fact that it can adjust to changing circumstances and make predictions related to the equipment failures with the highest precision. RL reduces the downtime of the system and improves system reliability by forecasting when a system needs some maintenance and scheduling the necessary maintenance before the systems fail.

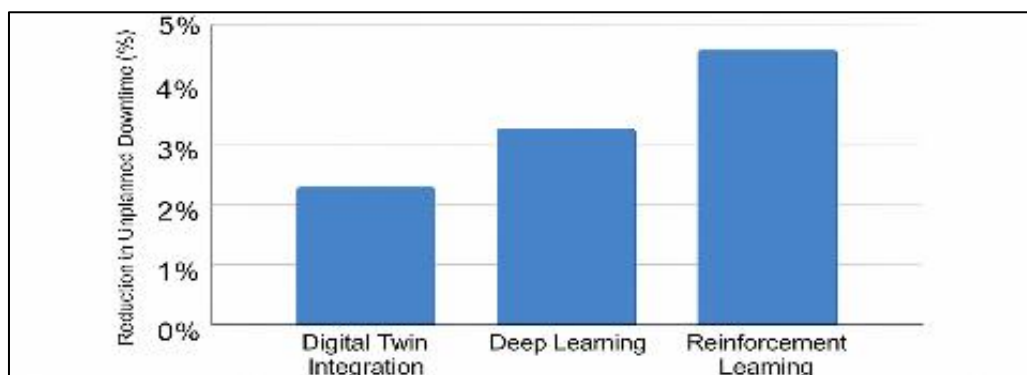


Figure 9 System Downtime Reduction Due to AI-Driven Predictive Maintenance

4.4. Comparison to the Traditional Methods

To assess the performance of the AI models, we have compared their performance with the conventional optimization approaches where the operational settings and reactive maintenance schedules are fixed. More often than not, traditional methods are not as flexible and adaptable as AI models and thus lack efficiency in energy use, reduced rates of hydrogen production and higher rates of downtime.

In all the assessed categories, as Table 3 demonstrates, AI models were always more successful than traditional ones:

- **Energy Efficiency:** The models of AI, in particular the reinforcement learning, demonstrated a considerable saving of energy in comparison with conventional approaches.
- **Hydrogen Production Rate:** AI models were used to optimize the parameters of operation to produce the highest production which outperformed the traditional approach.
- **System Downtime:** Predictive maintenance with AI technology drastically decreased downtime and in the traditional approaches, unforeseen maintenance and system failures had been increased.

This data proves the usefulness of AI implementation in hydrogen production, which can provide real advantages in efficiency and reliability of the operating system.

4.5. Implications to the Hydrogen Economy

The findings of this research have a lot of implications to the hydrogen economy. With the increased need of hydrogen as a clean energy source in the world today, there is a high demand to optimise hydrogen production processes to lower costs and boost efficiency. The use of AI models in the hydrogen production plants will be beneficial in consuming less energy, increasing production, and reducing the downtime of the systems, which will make hydrogen manufacturing more cost-effective than other energy sources.

AI can be used to optimize hydrogen production processes, which will make green hydrogen a more financially feasible alternative source of large-scale energy storage and generation, contributing to the global shift towards environmentally friendly energy production. Moreover, predictive maintenance can operate with the assistance of AI, so that hydrogen production systems can be at an optimal level, reducing any disruptions in operations and prolonging the life of essential equipment.

4.6. Limitations and Future research

Although the findings of the present research prove that AI might be useful in hydrogen production, various challenges exist. The success of AI models depends on the need to ensure high-quality and real-time data. Besides, it is important that the implementation of AI to large hydrogen production facilities will need to address the challenge of computational and integration.

It is possible that future studies should aim to maximize the accuracy and efficiency of AI models in prediction, combine AI solutions with the current hydrogen production infrastructure, and consider more innovative machine learning methods. Also, the economic viability of the large-scale use of AI in hydrogen manufacturing facilities should be studied to evaluate the benefits and cost-effectiveness of these technologies in the long term.

5. Conclusion

This work illustrates that the development of Artificial Intelligence (AI) and machine learning (ML) methods holds a great potential in streamlining hydrogen production processes, and making it more efficient in relation to energy use, more active in terms of the production rate of hydrogen and less prone to downtime. Through the combination of AI-based models, e.g., reinforcement learning (RL), deep learning (DL), and predictive maintenance, hydrogen production systems can obtain significant gains compared to the traditional optimization models. Such developments are essential to overcome the problems of hydrogen production stations and make them more efficient, focusing on fulfilling increasing energy needs AI and machine learning models are also an enormous potential in streamlining hydrogen production, making it more energy efficient, cost efficient, and more reliable. AI can lead to the development of the hydrogen economy by solving the main issues related to energy consumption, the rate of production, and maintenance and playing an important role in the international decarbonization process. Further AI research and development on hydrogen production will play a critical role in making hydrogen a full potential of clean and sustainable energy source.

Compliance with ethical standards

No conflict of interest to be disclosed.

References

- [1] Bhuiyan, S. M. Y., Chowdhury, A., Hossain, M. S., Mobin, S. M., & Parvez, I. (2025). AI-driven optimization in renewable hydrogen production: A review. *American Journal of Interdisciplinary Studies*, 6(1), 76-94. <https://doi.org/10.63125/06z40b13>
- [2] Shash, A. Y., Abdeltawab, N. M., Hassan, D. M., Darweesh, M., & Hegazy, Y. G. (2025). Computational methods, artificial intelligence, modeling, and simulation applications in green hydrogen production through water electrolysis: A review. *Hydrogen*, 6(2), 21. <https://doi.org/10.3390/hydrogen6020021>
- [3] Fayyazi, M., Sardar, P., Thomas, S. I., Daghigh, R., Jamali, A., Esch, T., ... & Khayyam, H. (2023). Artificial intelligence/machine learning in energy management systems, control, and optimization of hydrogen fuel cell vehicles. *Sustainability*, 15(6), 5249. <https://doi.org/10.3390/su15065249>
- [4] Ahmed, R., Shehab, S. A., Elzeki, O. M., Darwish, A., & Hassanein, A. E. (2024). An explainable AI for green hydrogen production: A deep learning regression model. *International Journal of Hydrogen Energy*, 83, 1226-1242. <https://doi.org/10.1016/j.ijhydene.2024.08.064>
- [5] Sethi, H., Ahmad, I., Khan, M. M., Qazi, A., Ayub, A., Zulkefal, M., & Shutaywi, M. (2025). Applications of computer intelligence in hydrogen production. *ACS Omega*, 10(31), 33982-33998. <https://doi.org/10.1021/acsomega.5c01602>
- [6] Feng, Z., Luo, Y., Li, D., Pan, J., Tan, R., & Chen, Y. (2025). Integrating digital twins and machine learning for advanced control in green hydrogen production. *Chain*, 2(1), 1-14. <https://doi.org/10.23919/CHAIN.2025.000003>
- [7] Johnrose, G. J., Thavasimuthu, R., Palani, L., & Venkatesan, H. (2026). Machine learning fundamentals for hydrogen production and storage. In *Fuelling the Future* (pp. 183-200). Elsevier. <https://doi.org/10.1016/B978-0-443-34090-1.00003-8>
- [8] Ghosh, R., Kesarwani, S., & Malhotra, M. (2025). A mini review on smart hydrogen: The role of AI in revolutionizing green hydrogen systems. *Energy & Fuels*. <https://doi.org/10.1021/acs.energyfuels.5c03094>
- [9] Wei, J., Wu, Y., Mirzaliyev, S., Skrank, T., & Ping, Z. (2025). Artificial intelligence applications in hydrogen systems: Advancing renewable energy utilization for global hydrogen economy and sustainability goals. *International Journal of Hydrogen Energy*, 122, 359-373. <https://doi.org/10.1016/j.ijhydene.2025.03.350>
- [10] Magazzino, C., & Haroon, M. (2025). AI-based modelling and processing technologies for hydrogen creation. *Journal of Sustainability*, 1(1). <https://doi.org/10.55845/jos-2025-1112>
- [11] Katterbauer, K., Qasim, A., Marsala, A., & Yousef, A. (2021, December). A data-driven artificial intelligence framework for hydrogen production optimization in waterflooded hydrocarbon reservoir. In *Abu Dhabi International Petroleum Exhibition and Conference* (p. D041S123R003). SPE. <https://doi.org/10.2118/207847-MS>
- [12] Shojaei, S. M., Aghamolaei, R., & Ghaani, M. R. (2024). Recent advancements in applying machine learning in Power-to-X processes: A literature review. *Sustainability*, 16(21), 9555. <https://doi.org/10.3390/su16219555>
- [13] Faizollahzadeh Ardabili, S., Najafi, B., Shamshirband, S., Minaei Bidgoli, B., Deo, R. C., & Chau, K. W. (2018). Computational intelligence approach for modeling hydrogen production: A review. *Engineering Applications of Computational Fluid Mechanics*, 12(1), 438-458. <https://doi.org/10.1080/19942060.2018.1452296>
- [14] Iqbal, S., Aftab, K., Jannat, F., Baig, M. A., & Kalsoom, U. (2024). A bibliographic analysis of optimization of hydrogen production via electrochemical method using machine learning. *Fuel*, 372, 132126. <https://doi.org/10.1016/j.fuel.2024.132126>
- [15] Shanmugasundaram, S., Thangaraja, J., Rajkumar, S., Ashok, S. D., Sivaramakrishna, A., & Shamim, T. (2025). A review on green hydrogen production pathways and optimization techniques. *Process Safety and Environmental Protection*, 107070. <https://doi.org/10.1016/j.psep.2025.107070>
- [16] Agwu, O. E., Alatefi, S., & Alkhouh, A. (2025). Modelling the future of cleaner energy: Explainable artificial intelligence model for green hydrogen production rate estimation. *Cleaner Engineering and Technology*, 101040. <https://doi.org/10.1016/j.clet.2025.101040>
- [17] Abiola, A., Manzano, F. S., & Andújar, J. M. (2023). A novel deep reinforcement learning (DRL) algorithm to apply artificial intelligence-based maintenance in electrolyzers. *Algorithms*, 16(12), 541. <https://doi.org/10.3390/a16120541>

- [18] Patil, R. R., Calay, R. K., Mustafa, M. Y., & Thakur, S. (2024). Artificial intelligence-driven innovations in hydrogen safety. *Hydrogen*, 5(2), 312-326. <https://doi.org/10.3390/hydrogen5020018>
- [19] Bekmyrza, K. Z., Kuterbekov, K. A., Kabyshev, A. M., Kubenova, M. M., Baratova, A. A., Aidarbekov, N., & Vincelas, F. F. C. (2025). Integrating machine learning and IoT in hydrogen production, storage, and distribution for a decarbonized transport future. *International Journal of Low-Carbon Technologies*, 20, 1554-1570. <https://doi.org/10.1093/ijlct/ctaf103>
- [20] Chaudhary, A., Sattar, S., & Sherzada, S. (2026). Intelligent systems in hydrogen energy. In *Fuelling the Future* (pp. 117-140). Elsevier. <https://doi.org/10.1016/B978-0-443-34090-1.00006-3>
- [21] Khalili, Y., Yasemi, S., Abdi, M., Ghasemi Ertian, M., Mohammadi, M., & Bagheri, M. (2025). A review of integrated carbon capture and hydrogen storage: AI-driven optimization for efficiency and scalability. *Sustainability*, 17(13), 5754. <https://doi.org/10.3390/su17135754>
- [22] Chen, X., Cao, W., Zhang, Q., Hu, S., & Zhang, J. (2020). Artificial intelligence-aided model predictive control for a grid-tied wind-hydrogen-fuel cell system. *IEEE Access*, 8, 92418-92430. <https://doi.org/10.1109/ACCESS.2020.2994577>
- [23] Ramkumar, G., Tamilselvi, M., Jebaseelan, S. S., Mohanavel, V., Kamyab, H., Anitha, G., ... & Rajasimman, M. (2024). Enhanced machine learning for nanomaterial identification of photo thermal hydrogen production. *International Journal of Hydrogen Energy*, 52, 696-708. <https://doi.org/10.1016/j.ijhydene.2023.07.128>
- [24] Lakhout, A. (2025). Investigating the hydrogen renaissance in the global energy transition with AI integration. *Energy Conversion and Management: X*, 101010. <https://doi.org/10.1016/j.ecmx.2025.101010>
- [25] Du, X., Gao, S., & Yang, G. (2025). Machine learning applications in gray, blue, and green hydrogen production: A comprehensive review. *Gases*, 5(2), 9. <https://doi.org/10.3390/gases5020009>
- [26] Balakrishnan, S. K. (2022). Real-Time State Information Exchange Protocol (RTSIX): A Cross-Vendor Framework for Geo-Redundant Network Synchronization and Seamless Failover. *Journal of Computational Analysis and Applications (JoCAAA)*, 30(2), 805-830.
- [27] Balakrishnan, S. K. (2022). Real-Time State Information Exchange Protocol (RTSIX): A Cross-Vendor Framework for Geo-Redundant Network Synchronization and Seamless Failover. *Journal of Computational Analysis and Applications (JoCAAA)*, 30(2), 805-830.
- [28] Balakrishnan, S. K. (2023). Cognitive Autonomous Networking (CAN): Self-Learning and Self-Healing Framework for the Global Internet Backbone. *Journal of Computational Analysis and Applications (JoCAAA)*, 31(3), 713-718.
- [29] Balakrishnan, S. K. (2024). FRAMEWORK FOR REAL-TIME ATTACK PREDICTION AND LEGITIMATE TRAFFIC PROTECTION. *Journal of Computational Analysis and Applications (JoCAAA)*, 33(05), 2918-2943.
- [30] Balakrishnan, S. K. (2024). AI-Native Zero-Trust Architecture (AI-ZTA): Federated Cognitive Trust Enforcement for Multi-Cloud Security. *Journal of Computational Analysis and Applications (JoCAAA)*, 33(08), 6712-6715.
- [31] Balakrishnan, S. K. (2024). Quantum-Resistant Secure Transport Protocol (Q-STP): Hybrid Cryptographic Framework for Inter-Data-Center Resilience. *Acta Sci*, 25, 5.
- [32] Balakrishnan, S. K. (2025). Federated Threat Intelligence Exchange Protocol (F-TIXP): Privacy-Preserving Collaborative Cyber Defense Framework. *Acta Sci*, 26, 1.
- [33] Balakrishnan, S. K. (2025). Cognitive BGP (C-BGP): AI-Driven Route Optimization for Global Internet Resilience. *Acta Sci*, 26, 2.
- [34] Agrawal, R., Kumar, H., & Lnu, S. R. (2025, March). Efficient llms for edge devices: Pruning, quantization, and distillation techniques. In *2025 International Conference on Machine Learning and Autonomous Systems (ICMLAS)* (pp. 1413-1418). IEEE.