

Integrating machine learning and IoT in hydrogen production, storage, and distribution for a decarbonized transport future

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Abstract

This study integrates reinforcement learning (RL) optimization and internet of things (IoT) monitoring within a MATLAB/Simulink simulation framework for hydrogen infrastructure. IoT sensors provide real-time data, enabling dynamic adjustments, while RL optimizes hydrogen logistics, reducing costs and emissions. This approach enhances predictive accuracy beyond conventional models, offering a scalable solution for sustainability. IoT sensors improve model precision, identifying underground storage as the most economical. Renewable energy integration lowered emissions by 97.8% (from 9.00 to 0.20 kg CO₂-eq/kg H₂) and reduced hydrogen costs by 40% (from US\$5.50 to US\$3.30/kg), while RL optimization achieved US\$15 000 in cost savings and a 30% emissions reduction.

Keywords: internet of things (IoT); hydrogen infrastructure; machine learning; simulation-based modeling; sustainable energy systems

Nomenclature and Abbreviations

Abbreviation/ Symbol	Description	Units
CO ₂	Carbon dioxide	g/km or kg
CH ₄	Methane	g/km
GBM	Gradient boosting machine	—
GHG	Greenhouse gas	CO ₂ -eq, kg/kg H ₂
H ₂	Hydrogen	kg
IoT	Internet of things	—
kWh	Kilowatt-hour	kWh
LP	Linear programming	—
ML	Machine learning	—
N ₂ O	Nitrous oxide	g/km
PEM	Proton exchange membrane	—
RL	Reinforcement learning	—
SMR	Steam methane reforming	—
USD	United States Dollar	—

1 Introduction

Hydrogen is widely recognized as a promising alternative to conventional fossil fuels due to its potential to significantly reduce greenhouse gas (GHG) emissions, especially in

the transport sector [1–3]. As the world grapples with the challenges posed by climate change, the need for cleaner, sustainable energy sources has never been more urgent [4–6]. Hydrogen, with its zero tailpipe emissions, offers a unique solution to decarbonizing transportation, one of the most carbon-intensive sectors globally [7, 8]. When used in fuel cells, hydrogen produces only water vapor as a byproduct, making it an environmentally friendly option for a wide range of transportation modes, including road vehicles, buses, trains, and ships [9, 10].

As nations strive to meet net-zero emissions targets, the global energy transition has accelerated, with hydrogen recognized as a key enabler of decarbonization [11]. Policies such as the Paris Agreement, the European Green Deal, and national hydrogen strategies in countries like Japan, Germany, and the United States emphasize hydrogen's role in reducing reliance on fossil fuels. Hydrogen supports energy diversification, enhances grid stability through storage, and enables sectoral integration, particularly in transportation and industry. By aligning with these global initiatives, hydrogen infrastructure development is critical for achieving a low-carbon, resilient energy system [12]. Many countries have committed to scaling up hydrogen production as part of their decarbonization strategies, investing in research, infrastructure, and policies aimed at reducing the environmental footprint of energy-intensive industries [13, 14].

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However, despite its potential, the hydrogen sector faces several challenges that hinder its widespread adoption [15]. The development of greener hydrogen production technologies, such as electrolysis powered by renewable energy, is crucial to make hydrogen truly sustainable [16, 17]. Additionally, the storage and distribution of hydrogen present significant technical challenges. Hydrogen must be stored at high pressures or in liquid form to be transported efficiently, which requires advanced storage solutions that are both cost-effective and safe [18]. Furthermore, the distribution infrastructure for hydrogen is still in its infancy, and the lack of a robust network of refueling stations and pipelines limits its scalability [19].

These challenges, however, have not deterred ongoing efforts to unlock the full potential of hydrogen as a sustainable energy source. Researchers and industries are exploring innovative solutions that address these barriers, leveraging technologies such as machine learning, internet of things (IoT) integration, and advanced simulation techniques to optimize production, storage, and distribution processes [20]. By improving the efficiency and scalability of hydrogen infrastructure, it is possible to make hydrogen a central component of the future clean energy landscape [21].

Despite the considerable advancements in hydrogen technologies, several critical gaps remain in the research and development of efficient and sustainable hydrogen infrastructure. One of the most pressing issues is the inefficiency in current hydrogen production methods, which continue to rely heavily on carbon-intensive processes such as steam methane reforming [22]. While cleaner methods like electrolysis are emerging, they remain expensive and face challenges in scaling up to meet global demand [23, 24]. Furthermore, hydrogen storage and transportation systems are not yet optimized, with existing solutions often being costly and inefficient, particularly when it comes to high-pressure storage and the transportation of hydrogen over long distances [18]. The lack of a widespread and reliable refueling infrastructure further limits the adoption of hydrogen-powered vehicles, creating a significant barrier to its integration into the broader transportation sector [25].

The need for cost-effective, low-emission solutions is crucial in addressing these challenges [26]. Despite significant advancements in hydrogen technologies, a critical gap remains in the dynamic optimization of hydrogen infrastructure. Most existing studies rely on static models, which fail to adapt to real-time variations in production, storage, and distribution. These models lack predictive adaptability, leading to inefficiencies in cost and emissions reduction. Moreover, the potential of integrating IoT-based real-time monitoring with machine learning and reinforcement learning (RL) for optimizing hydrogen logistics remains underexplored. This study addresses this gap by developing a simulation-based, AI-driven framework that enhances efficiency, reduces emissions, and lowers operational costs, paving the way for a more sustainable hydrogen economy [27]. As the hydrogen economy continues to evolve, it is clear that more innovative and adaptable solutions are needed to make hydrogen a truly sustainable energy source [28].

Machine learning, IoT integration, and simulation-based modeling offer significant promise in addressing these gaps. Machine learning algorithms can be applied to predict and

optimize key parameters such as hydrogen production costs, emissions, and storage configurations [29]. By analyzing large datasets, these algorithms can identify patterns and insights that would be difficult to uncover using traditional methods [30]. IoT sensors can further enhance the efficiency of hydrogen systems by providing real-time monitoring of operational parameters, enabling better decision-making, and reducing downtime [31]. Simulation-based modeling allows researchers to test various scenarios and configurations in a controlled virtual environment, offering valuable insights into how different components of the hydrogen infrastructure can be optimized without the need for costly real-world experimentation [32]. Together, these technologies can provide the necessary tools to overcome the existing inefficiencies and drive the development of a more cost-effective and sustainable hydrogen economy.

This study aims to optimize hydrogen infrastructure by utilizing machine learning, IoT, and simulation-based modeling. The specific objectives are as follows:

- 1) Enhancing hydrogen production efficiency by using gradient boosting models (GBMs) to predict costs and emissions under different scenarios.
- 2) Optimizing hydrogen storage and distribution by comparing compressed, liquid, and underground storage methods to identify cost-effective, sustainable solutions.
- 3) Improving logistics efficiency using RL to dynamically optimize transport routes, minimize costs, and reduce emissions.
- 4) Integrating IoT-driven real-time monitoring to improve hydrogen system adaptability, ensuring better predictive accuracy over static models.

Through this AI-driven approach, the study provides a scalable framework to support cost-effective, low-emission hydrogen infrastructure development.

By employing predictive models, the study aims to evaluate the economic feasibility of different hydrogen production technologies and assess their GHG emissions, thereby offering data-driven insights that can guide decision-making and improve overall system performance. A further objective of this research is to identify the most efficient and cost-effective hydrogen storage and distribution solutions. By leveraging machine learning techniques, the study will predict optimal storage conditions and configurations across various hydrogen storage methods, such as underground, compressed, and liquid storage. The goal is to highlight the most economical and environmentally sustainable options for each stage of the hydrogen supply chain, ultimately leading to a more efficient infrastructure. The novelty of this study lies in its simulation-based approach, which eliminates the need for real-world data. Rather than relying on physical experiments, the research uses simulation models to evaluate different scenarios and configurations, providing actionable insights without the high costs and complexities associated with real-world testing. This approach allows for the exploration of a wide range of potential solutions in a controlled virtual environment, offering flexibility and depth in analyzing the hydrogen infrastructure. The integration of machine learning, IoT, and simulation-based modeling ensures that this study contributes to the development of a more sustainable and optimized hydrogen economy.

2 Literature review

2.1 Hydrogen production, storage, and distribution

Hydrogen production is a key component in realizing a sustainable energy future, with several established and emerging technologies vying for prominence [33]. The most common traditional method is steam methane reforming (SMR), where natural gas reacts with steam to produce hydrogen and carbon dioxide [34]. Despite being the most widely used process due to its lower costs, SMR is carbon intensive, leading to increased GHG emissions, which presents a significant barrier to achieving net-zero goals [35]. As a result, research efforts have increasingly focused on cleaner production technologies, with electrolysis being one of the most promising alternatives [36]. Electrolysis splits water into hydrogen and oxygen using electricity, and when powered by renewable energy sources, it results in hydrogen with virtually no carbon emissions [37]. However, the high cost of electricity and the efficiency of current electrolysis systems remain challenges that need to be addressed for widespread adoption [38].

In addition to these production methods, hydrogen storage is another critical aspect that determines the viability of hydrogen as a fuel source [39]. The main storage technologies include compressed hydrogen, liquid hydrogen, and underground hydrogen storage [40]. Compressed hydrogen is typically stored at pressures of up to 700 bar, allowing for relatively high energy densities but requiring robust, expensive infrastructure [38]. Liquid hydrogen, on the other hand, has a higher energy density by volume and is stored at cryogenic temperatures [41]. While this method offers better volumetric efficiency, it involves energy-intensive cryogenic processes that reduce its overall efficiency [42]. Underground hydrogen storage is an emerging option, where hydrogen is stored in caverns or depleted gas fields [43]. This technology holds promise for large-scale storage, offering cost advantages over other methods, particularly when integrated into existing natural gas infrastructure [44].

Transporting hydrogen presents its own set of challenges, primarily due to its low energy density by volume and the need for specialized infrastructure [39]. Hydrogen can be transported either through pipelines or by road, using trucks that carry compressed or liquid hydrogen [45]. Pipelines for hydrogen transport, often considered a long-term solution, require significant capital investment for installation and maintenance, and hydrogen embrittlement—where hydrogen weakens metals—poses potential risks to the integrity of pipeline systems [46]. In contrast, road transport of liquid or compressed hydrogen is more flexible but comes with logistical challenges, such as the need for highly specialized vehicles and refueling stations. Moreover, the energy required to compress or liquefy hydrogen can offset some of the environmental benefits associated with its use [39].

Together, the technologies for hydrogen production, storage, and distribution are central to realizing hydrogen as a mainstream energy solution. However, each stage faces its own technical and economic hurdles, which can hinder the scalability of hydrogen infrastructure [47]. These challenges call for integrated, innovative approaches that optimize the entire hydrogen value chain, addressing production efficiency, storage effectiveness, and logistical costs to pave the way for a sustainable hydrogen economy.

2.2 Machine learning in energy systems

Machine learning has become an essential tool in energy systems research, offering significant improvements in cost prediction, emissions forecasting, and system optimization [48]. A growing body of literature demonstrates how machine learning techniques have been successfully applied to enhance the performance and efficiency of various energy systems [49, 50]. In particular, machine learning algorithms are increasingly used to model complex energy systems and predict key metrics such as production costs and GHG emissions [48, 51]. These applications are crucial for identifying cost-effective strategies for energy generation, consumption, and distribution, while also helping to meet sustainability goals [52].

One of the widely used machine learning techniques in the energy sector is GBMs [52]. GBMs are particularly effective in scenarios where complex, nonlinear relationships exist, which is often the case in energy systems [53]. Previous studies have utilized GBMs for cost prediction in renewable energy systems, such as wind and solar power, where predicting energy generation costs and optimizing operational strategies are challenging due to the variability in resource availability [53]. GBMs have also been employed for forecasting emissions in power plants and transportation systems, offering robust models that account for multiple factors influencing emissions outputs [54]. For instance, a study by Munir *et al.* [55] applied GBMs to predict the carbon emissions of various energy generation technologies, finding that GBMs outperformed traditional regression models in accuracy. This approach has become a critical tool in assisting energy planners in making informed decisions that balance environmental impact with economic feasibility.

In addition to GBMs, RL is another machine learning technique that has gained traction in energy system optimization [56]. RL has emerged as a powerful tool for optimizing energy systems by dynamically adjusting operational strategies based on real-time feedback. It has been successfully applied in electricity grid management to optimize energy dispatch, demand response, and renewable integration, as well as in energy storage optimization to determine optimal charging and discharging cycles. In logistics and transportation, RL-based dynamic routing algorithms have significantly reduced fuel consumption and emissions by adapting to real-time traffic conditions and delivery constraints. However, its application in hydrogen infrastructure remains limited, as most existing models rely on static routing and heuristic methods that fail to adapt to real-time demand fluctuations, infrastructure constraints, and cost variations. Moreover, previous RL-based studies in hydrogen logistics often focus on isolated aspects, such as refueling station placement or vehicle routing, without considering broader supply chain dynamics. This study addresses these gaps by integrating RL-based transport optimization with IoT-driven real-time monitoring, enabling dynamic adjustments in hydrogen distribution routes, vehicle allocation, and scheduling. By bridging real-time data collection with adaptive decision-making, this approach enhances cost-efficiency, reduces emissions, and provides a scalable AI-driven framework for optimizing hydrogen transport [57]. For example, RL algorithms have been used to optimize the charging and discharging cycles of energy storage systems, ensuring that energy is used most efficiently while minimizing costs and emissions [58]. A notable study by Zhang *et al.* [59]

demonstrated the use of RL for optimizing the integration of renewable energy into the grid, showing how RL can dynamically adjust energy supply and demand in real time to minimize both costs and carbon emissions. By continually learning from interactions with the system, RL-based models can adapt to changing conditions and improve long-term decision-making, making them particularly useful for evolving energy systems.

Several optimization approaches have been explored for hydrogen infrastructure, including traditional mathematical models, machine learning techniques, and RL. Traditional methods, such as linear programming (LP) and heuristic approaches, efficiently minimize costs but rely on static assumptions, making them ineffective in handling real-time variability. ML techniques, particularly gradient boosting machines (GBMs), offer high predictive accuracy for cost and emission estimation but lack real-time adaptability for optimization. RL has emerged as a dynamic approach for optimizing hydrogen distribution by continuously learning from system interactions to adjust transport routes and storage strategies in real time. However, RL models face challenges related to computational cost and hyperparameter sensitivity. Despite these advancements, existing studies often apply ML and RL separately without integrating real-time monitoring and predictive analytics. This study bridges this gap by combining GBMs for cost prediction, RL for logistics optimization, and IoT-driven monitoring within a comprehensive simulation framework, enabling a scalable, cost-effective, and adaptive solution for hydrogen infrastructure [60].

As the energy sector continues to transition toward more sustainable practices, machine learning will play a pivotal role in ensuring that energy systems are efficient, cost-effective, and aligned with global emission reduction goals. The growing body of research highlights the potential of ML to revolutionize the way energy systems are managed, offering novel approaches for tackling long-standing challenges in the field.

2.3 IoT for energy management

The integration of IoT in energy systems has significantly improved performance, efficiency, and operational optimization by enabling real-time monitoring of critical parameters such as energy consumption, pressure levels, and emissions output. In the electricity sector, IoT-enhanced smart grids and energy storage systems have optimized load balancing and charge/discharge cycles, improving reliability and reducing costs. Similarly, in hydrogen infrastructure, IoT has been applied to production monitoring, storage safety, and logistics, enhancing efficiency and minimizing risks. However, most IoT applications in hydrogen systems remain isolated, lacking integration with predictive analytics and optimization models. This disconnect limits real-time decision-making, leading to inefficiencies in hydrogen production, storage, and distribution. Additionally, large-scale IoT deployment in hydrogen supply chains faces computational and infrastructural challenges. To address these limitations, this study develops an integrated IoT-driven optimization framework that combines real-time monitoring with GBMs for predictive modeling and RL for dynamic logistics optimization. By linking IoT data collection with AI-driven decision-making, this approach enhances cost-efficiency, reduces emissions, and improves the adaptability of hydrogen infrastructure [61]. IoT enables the

continuous monitoring of energy parameters through the deployment of sensors and connected devices that collect real-time data across various components of an energy system [62]. This data-driven approach is particularly beneficial for energy management, as it allows for the detection of inefficiencies, predictive maintenance, and timely adjustments to operations, all of which contribute to cost savings and sustainability [63].

One of the key advantages of IoT in energy management is its ability to provide real-time feedback on energy consumption and operational conditions [52]. By embedding sensors in energy-consuming devices or systems, IoT can track variables such as temperature, pressure, flow rates, and energy usage, transmitting these data to centralized platforms for analysis. For instance, smart meters and sensors can measure electricity consumption in real time, providing users with insights into their energy usage patterns [64]. These data can be used to identify peak demand periods, inform decisions about load management, and optimize energy consumption. A notable example of this application is the use of smart grids, which incorporate IoT technology to improve the reliability and efficiency of electricity distribution [65]. Smart grids can detect faults, balance supply and demand dynamically, and integrate renewable energy sources more effectively, leading to a more resilient and efficient grid system [66].

IoT also plays a critical role in the optimization of energy storage systems [67]. By monitoring storage parameters such as charge levels, temperature, and discharge rates, IoT helps ensure that energy storage systems operate at peak efficiency. This capability is especially important in systems that rely on renewable energy, where generation can be intermittent. IoT-enabled monitoring allows for better management of energy flows between generation, storage, and consumption, helping to reduce energy waste and ensure that stored energy is used when it is needed the most [68]. For example, IoT sensors in battery storage systems can relay data to operators, allowing them to optimize charging and discharging cycles based on current and predicted energy demands [69].

Furthermore, IoT facilitates predictive maintenance by enabling condition-based monitoring of equipment [70]. In energy systems, the failure of key components such as turbines, generators, or transformers can result in significant operational disruptions [71]. With IoT-enabled sensors, operators can continuously monitor the health of these components and detect anomalies that may indicate impending failures. This allows for preventive measures, reducing downtime and extending the lifespan of the equipment. Studies have shown that integrating IoT with predictive analytics can reduce maintenance costs and improve the reliability of energy systems, making them more cost-effective and less prone to unexpected failures [72].

The ability of IoT to provide real-time data and feedback has proven to be a game changer for energy management across various sectors, from industrial and residential applications to grid operations and renewable energy systems. By enhancing system visibility and providing actionable insights, IoT technologies enable more informed decision-making, improve operational efficiency, and contribute to the transition toward more sustainable energy systems. As the IoT ecosystem continues to evolve, its role in energy management is likely to grow, offering even greater potential for optimization and efficiency improvements in the energy sector.

Table 1. Key simulation parameters and configurations (source: authors' simulation)

Component	Model/algorithm used	Parameters simulated	Purpose
Hydrogen production	Electrolysis model (Simulink)	Energy input, hydrogen output, efficiency	Evaluate energy requirements and production efficiency.
Hydrogen storage	Compressed, liquid, and underground	Storage capacity, cost, efficiency	Compare storage methods for cost-effectiveness.
Hydrogen distribution	RL (MATLAB)	Route optimization, emissions, transportation costs	Optimize logistics for sustainable distribution.
IoT integration	Simulated sensor data (MATLAB)	Pressure, temperature, flow rate	Enable real-time monitoring and control.

3 Materials and Methods

3.1 Simulation framework

This study employed MATLAB/Simulink to simulate the hydrogen production, storage, and distribution infrastructure. MATLAB/Simulink is a widely recognized platform for modeling dynamic systems, offering a robust environment to analyze energy flows, efficiency, and system interactions. The MATLAB/Simulink simulation framework was designed to provide a realistic representation of hydrogen production, storage, and distribution, incorporating machine learning algorithms and IoT-based monitoring. To ensure model accuracy and applicability, several assumptions were made regarding energy inputs, operational constraints, and system conditions. For hydrogen production, the model assumed that electrolysis was powered by three primary energy sources: solar, wind, and grid electricity. The availability of renewable energy sources fluctuated based on simulated daily variations, while grid electricity follows a time-dependent pricing structure, reflecting real-world electricity market trends. Electrolyzer efficiency was set between 60% and 80%, varying based on the type of electrolyzer (proton exchange membrane [PEM] or alkaline), consistent with industry standards. For hydrogen storage, the simulation modeled three storage methods: (i) compressed, (ii) liquid, and (iii) underground storage. Each storage method had specific capacity constraints, with compressed hydrogen stored at 350–700 bar, liquid hydrogen at cryogenic temperatures of –253°C, and underground storage capacities varying based on site availability. For hydrogen distribution, the RL-based optimization considered logistics constraints such as fuel availability, transport distance limitations (50–500 km per delivery route), and vehicle capacity. The model assumed dynamic demand fluctuations of ±15% daily, simulating real-world variations in hydrogen consumption. Additionally, probabilistic failure rates for key components (electrolyzers, compressors, and storage systems) were incorporated into the model, ensuring that operational uncertainties were accounted for.

In the hydrogen production phase, Simulink models electrolysis systems, capturing the energy requirements and production efficiency under varying operational conditions. For hydrogen storage, the simulation included multiple methods—compressed, liquid, and underground storage—providing insights into their cost-effectiveness and energy efficiency. The transportation and distribution models optimize logistics using RL algorithms integrated with MATLAB, ensuring minimal emissions and reduced costs.

To enhance accuracy, IoT sensor data streams were simulated within MATLAB to replicate real-time monitoring

and control. This approach enabled dynamic adjustments to parameters like pressure, temperature, and flow rates, simulating operational scenarios in a virtual environment. The integration of IoT in this framework allows for continuous optimization, mimicking real-world feedback mechanisms without reliance on actual infrastructure. A detailed overview of the simulation parameters and configurations is presented in Table 1, ensuring reproducibility and clarity.

This simulation framework leveraged MATLAB/Simulink’s advanced capabilities, combining dynamic system modeling with machine learning and IoT technologies. By replicating real-world scenarios virtually, it provided actionable insights into hydrogen infrastructure without requiring physical experimentation.

3.2 Description of the applied infrastructure

The hydrogen infrastructure applied in this simulation-based study was designed to cover the entire lifecycle of hydrogen, encompassing production, storage, and distribution. Each stage was virtually modeled to enable dynamic simulation of various parameters and operational scenarios, ensuring the framework aligned with real-world complexities. The production unit focuses on simulating hydrogen generation using electrolysis, powered by renewable energy sources such as solar and wind. Two types of electrolyzers, PEM and alkaline electrolyzers, were included to evaluate efficiency and output under different conditions. The system also accounted for key inputs, such as renewable electricity and water, and outputs, primarily hydrogen gas (Table 2).

The storage infrastructure comprised three primary methods: (i) compressed storage in high-pressure tanks (350–700 bar), (ii) liquid storage in cryogenic tanks at –253°C, and (iii) underground storage in facilities such as salt caverns or depleted gas reservoirs. Each method was assessed for its storage capacity, energy requirements, and potential leakage rates. Distribution was modeled through a network of pipelines and transport vehicles, including tanker trucks and hydrogen trailers, to simulate delivery to various demand points. The system evaluated critical factors such as flow rates, pressure, distance, and load capacity to optimize transportation costs and emissions.

To enhance the realism and accuracy of the simulation, IoT sensors were integrated across all stages of the infrastructure. These sensors provided real-time data on operational parameters, including pressure, temperature, flow rates, and energy consumption. This enabled dynamic monitoring and control, allowing the simulation to reflect adaptive changes in hydrogen production, storage, and distribution under varying

Table 2. Virtual infrastructure design (source: authors' design)

Component	Modeled unit	Key parameters	Purpose
Production	Electrolyzers	Energy input, hydrogen output, efficiency	Simulate hydrogen generation process.
	Compressed tanks	Pressure (350–700 bar), capacity	Analyze energy and cost-efficiency of compressed storage.
Storage	Liquid tanks	Temperature (-253°C), energy input for liquefaction	Evaluate feasibility of cryogenic storage.
	Underground caverns	Volume, geophysical characteristics	Identify cost-effective long-term storage solutions.
Distribution	Pipelines	Distance, flow rate, pressure	Assess emissions and cost for local delivery.
	Tanker trucks	Load capacity, distance, fuel consumption	Model long-distance hydrogen distribution logistics.
IoT integration	Simulated sensors	Pressure, temperature, flow rate	Enable dynamic control and monitoring of infrastructure.

conditions. The infrastructure operated under diverse scenarios, such as peak renewable energy availability, fluctuating seasonal hydrogen demand, and different geographical contexts. This comprehensive design created a robust virtual environment, facilitating actionable insights into optimizing hydrogen systems for sustainable energy solutions.

3.3 Integration of IoT

The integration of IoT technology played a crucial role in enhancing the accuracy and adaptability of the simulation framework for hydrogen infrastructure. IoT sensors were employed to collect real-time operational data across all stages of the hydrogen lifecycle, including production, storage, and distribution. IoT sensors played a crucial role in this study by providing real-time monitoring of key parameters across the hydrogen production, storage, and distribution stages. These sensors continuously collected operational data, which was then used to inform machine learning models—GBMs for predictive analytics and RL for dynamic logistics optimization.

During hydrogen production, IoT sensors measured energy input, hydrogen output rate, electrolysis efficiency, and temperature fluctuations. These real-time data streams allowed the GBM model to predict production costs and emissions by identifying patterns in energy consumption, production efficiency, and variations in renewable energy availability. The predictive capability of GBM enabled proactive adjustments in production parameters, ensuring cost-effective and sustainable hydrogen generation.

In hydrogen storage, IoT sensors tracked storage pressure, temperature, and leakage detection for compressed, liquid, and underground storage methods. These data were critical in assessing storage efficiency and informs GBM predictions on storage costs and losses. Additionally, real-time monitoring helped prevent pressure fluctuations or inefficiencies, ensuring stable storage conditions.

For hydrogen distribution, IoT sensors collected real-time GPS tracking, fuel consumption, transport distances, and route conditions. These data points were fed into the RL optimization model, allowing it to dynamically adjust transport routes, vehicle allocation, and scheduling based on changing traffic conditions, fuel constraints, and demand fluctuations. By integrating IoT sensor data with RL, the model continuously learnt and refined distribution strategies, leading to optimal route selection, reduced transportation costs, and minimized emissions.

This integration of real-time IoT data with ML-based optimization models is a key innovation of this study. By continuously feeding high-resolution sensor data into predictive and optimization algorithms, the system ensures adaptive, real-time decision-making across the hydrogen supply chain.

These sensors provided key inputs such as hydrogen production rates, storage temperatures, pressure levels, and flow rates, enabling the system to dynamically adjust to varying conditions. Additionally, data on transport logistics, including route efficiency, load optimization, and energy consumption, were captured to refine the distribution models.

The collected data were processed and fed into machine learning models to improve prediction accuracy for production costs, emissions, and storage efficiency. IoT-based real-time monitoring facilitated the detection of anomalies and performance variations, ensuring the virtual infrastructure operated under realistic and adaptive conditions. For example, pressure and temperature sensors in storage systems allowed the simulation to evaluate the impact of environmental fluctuations on storage stability and safety. Similarly, production data, such as electrolyzer efficiency and renewable energy availability, were continuously updated to simulate operational scenarios under varying resource inputs.

To ensure seamless data integration, a central IoT gateway was modeled to aggregate sensor data and transmit it to the simulation platform. This allowed for real-time feedback loops, where predictive models adjusted operational parameters based on the latest data, resulting in a more responsive and efficient system. This approach not only enhanced the reliability of the simulation outputs but also provided insights into how IoT-driven optimization can be implemented in real-world hydrogen infrastructure (Table 3).

The inclusion of IoT enabled the simulation to mimic dynamic and complex behaviors in hydrogen systems, providing a robust framework for exploring cost-effective and low-emission solutions in a virtual environment.

3.4 Machine learning algorithms

3.4.1 Gradient boosting machine

GBMs were utilized as a core component for predicting hydrogen production costs and associated GHG emissions. The model was trained and validated using a combination of simulated datasets derived from the infrastructure and IoT parameters outlined in the study. GBMs were selected due to their robust ability to handle complex, nonlinear relationships and their high accuracy in predictive tasks involving structured datasets.

Table 3. IoT-simulated parameters in hydrogen infrastructure (source: authors’ design)

Parameter	Description	Simulated values	Unit
Production rate	Rate of hydrogen production in the system	50–200	kg/hour
Storage temperature	Temperature maintained in the hydrogen storage tanks	–253	°C
Pressure level	Pressure in storage tanks or pipelines	350–700	bar
Transportation distance	Average distance covered during distribution	50–500	km
Energy consumption	Power required for storage and transportation	20–80	kWh/kg
GHG emissions	Emissions generated during hydrogen logistics	0.2–1.5	kg CO ₂ -e/kg

Table 4. Key features and importance in the GBM model (source: authors’ analysis)

Feature	Description	Relative importance (%)
Production rate	Hydrogen output rate from production facilities	25
Energy consumption	Energy required for hydrogen production and storage	20
Storage pressure	Pressure levels in storage systems	15
Renewable energy share	Contribution of renewable energy to the process	12
Transportation distance	Average distance for hydrogen distribution	10
Grid electricity emissions	Carbon intensity of grid electricity	8
Storage temperature	Cryogenic storage temperature	5
Other operational factors	Auxiliary factors influencing costs and emissions	5

The GBM model was trained and tested using synthetic datasets generated within the MATLAB/Simulink framework, ensuring consistency with the simulated hydrogen infrastructure. To assess model performance, the dataset was split into training and validation subsets, with validation conducted using standard model evaluation techniques. The validation process focused on predicting hydrogen production costs and emissions under different operational scenarios, ensuring that the model generalizes well across varying conditions. To verify the reliability of the GBM model, its predictions were compared against benchmark values derived from industry reports and existing literature on hydrogen production cost estimates and emissions factors. This external comparison ensured that the model provides realistic predictions aligned with practical hydrogen infrastructure dynamics. Additionally, the GBM model’s performance was evaluated based on its ability to capture cost variations across different production methods and energy input sources, ensuring it accurately reflects the impact of operational changes on hydrogen cost and emissions.

The training process involved splitting the dataset into training and validation subsets in an 80:20 ratio to ensure unbiased evaluation. Key features used as inputs for the model included production rates, storage temperatures, pressure levels, energy consumption, and transportation distances, as well as parameters related to energy sources, such as renewable energy share and grid electricity emissions intensity. These features were normalized to maintain consistency and prevent model bias arising from varying scales.

The GBM algorithm employed an iterative approach, where decision trees were sequentially built to minimize prediction errors. Hyperparameters, such as learning rate, number of trees, and maximum tree depth, were optimized using a grid search and cross-validation method to ensure optimal model performance (Table 4).

This predictive framework provided valuable insights into cost-effective and low-emission hydrogen infrastructure, contributing to the development of sustainable energy systems.

3.4.2 Reinforcement learning

The RL model used in this study optimizes hydrogen transport logistics by dynamically adjusting route selection, vehicle allocation, and distribution scheduling based on cost and emissions minimization. The RL framework was implemented using a Q-learning approach with function approximation, which allows the model to efficiently handle high-dimensional state-action spaces. The RL agent was trained using a Deep Q-Network (DQN), which enhances traditional Q-learning by incorporating experience replay and neural network function approximation to improve learning stability. The DQN was optimized using the Adam optimizer with a learning rate of 0.001, and the discount factor (γ) was set to 0.95 to ensure future rewards were considered while maintaining decision-making efficiency. The model used ϵ -greedy exploration, where the exploration rate (ϵ) was initially set to 1.0 and decayed over time to 0.05 to balance exploration and exploitation. To accelerate convergence, a mini-batch size of 64 was used for experience replay, and the replay buffer size was 10 000 past experiences. The RL model was trained over 50 000 episodes, ensuring sufficient exploration of possible transport decisions. These hyperparameters were fine-tuned through grid search experiments, optimizing for both cost savings and emissions reduction. By implementing Q-learning with function approximation and DQN, the RL framework ensures adaptive, data-driven decision-making in hydrogen transport, leading to optimized logistics that reduce costs and emissions.

In the RL setup, the state represented the current condition of the hydrogen transport system, including variables such as the distance between hydrogen production and demand centers, fuel type and consumption of transport vehicles, and the status of storage facilities. Actions referred to decisions such as selecting optimal transport routes, vehicle types, and distribution schedules. The reward signal incentivized strategies that minimized costs and emissions, with penalties applied for high emissions, excessive costs, or inefficiencies in delivery timelines.

Table 5. Components of the RL framework for hydrogen transport logistics (source: authors' design)

Component	Description
State	Distance, vehicle fuel type, storage status, and demand location
Actions	Route selection, vehicle assignment, distribution scheduling
Reward	Minimization of costs and emissions, penalties for inefficiency
RL algorithm	Q-learning with function approximation for high-dimensional scenarios
Environment features	Simulated transport network, energy consumption rates, and emission factors

Table 6. Simulated parameters and their ranges [9, 13, 73]

Parameter	Description	Simulated range	Purpose
Hydrogen production rate	Rate of hydrogen generation (kg/h)	50–500	Training cost and emission prediction models
Storage pressure	Pressure in storage tanks (bar)	200–700	Evaluating storage efficiency and safety
Transport distance	Average transport distance (km)	50–1000	Optimizing transport logistics
Temperature in storage	Storage temperature (°C)	–20 to 50	Assessing energy requirements and losses
Vehicle emission factors	CO ₂ emissions per km (g CO ₂ /km)	10–50	Calculating total transport emissions

The RL algorithm used a Q-learning-based approach, where the agent iteratively learned the optimal policy through interactions with the environment. A simulated environment was developed to model the transport logistics, incorporating real-world constraints such as vehicle capacities, energy consumption rates, and emission factors. The RL agent evaluated multiple transport scenarios, leveraging feedback in the form of rewards to improve its policy. Hyperparameters, such as learning rate and discount factor, were fine-tuned through experimentation to ensure effective convergence and avoid suboptimal policies (Table 5).

Through iterative training, the RL model demonstrated the ability to identify cost-effective and low-emission transport strategies. For instance, the model optimized routes to reduce average travel distances and prioritized vehicles with lower emission profiles. Validation results showed significant reductions in total emissions and costs compared to traditional static routing approaches, underscoring the potential of RL in achieving sustainable transport solutions in hydrogen logistics.

3.5 Data collection and simulation

In this study, all data were generated exclusively within a simulation environment to ensure a controlled and reproducible framework. The simulated scenarios were carefully designed to reflect real-world conditions, incorporating validated parameters and realistic constraints to achieve credible outcomes. IoT data were integrated into the simulation to fine-tune critical parameters, such as hydrogen production rates, storage conditions, and transportation logistics. This approach eliminated the need for real-world data while maintaining a high level of accuracy in modeling practical hydrogen infrastructure operations.

The virtual scenarios leveraged dynamic inputs based on IoT-simulated sensors, which provided operational parameters such as temperature, pressure, and production flow rates. These inputs were crucial in adjusting the models to better emulate real-world conditions, ensuring that the insights derived were applicable to practical situations. The simulation environment enabled the generation of diverse datasets, encompassing hydrogen production, storage, and distribution, to train and validate the machine learning models effectively.

This method allowed for extensive experimentation without the logistical and ethical constraints of using real-world data. Table 6 provides an overview of the key data parameters used in the simulation environment and their respective ranges, which were designed to reflect real-world variability [9, 13, 73].

By leveraging these simulated datasets, the study established a robust framework for analyzing hydrogen infrastructure while preserving its focus on virtual modeling. The integration of IoT-supported adjustments further enhanced the fidelity of the simulated scenarios, providing actionable insights into the feasibility and optimization of hydrogen systems. This approach underscores the value of combining advanced simulation tools with IoT-inspired parameter tuning to achieve practical, reliable, and scientifically valid results.

4 Results and discussions

4.1 Simulation scenarios and their impact on hydrogen infrastructure performance

In this study, five simulation scenarios were designed to comprehensively assess the performance of hydrogen infrastructure under different conditions. Each scenario was tailored to evaluate specific elements of the system, such as production costs, emissions, and storage solutions. The advantage of using multiple scenarios lies in their ability to provide insights into how varying operational and environmental factors affect overall system efficiency. The scenarios were as follows:

- **Scenario 1 (Base Case Scenario):** The base case scenario served as the control scenario, where hydrogen production was carried out using conventional methods and existing infrastructure. This scenario provided a benchmark for comparison, offering insights into the baseline performance of the system, including production costs, emissions, and efficiency. The advantage of this scenario lies in its simplicity, as it represents current industry standards, allowing for comparisons with more advanced or optimized configurations.
- **Scenario 2 (High Efficiency Scenario):** In the high efficiency scenario, the focus was on implementing advanced

technologies and operational strategies designed to maximize hydrogen production efficiency. This included optimizing production methods, improving energy conversion rates, and enhancing storage solutions. The advantage of this scenario is that it allows us to assess the potential benefits of technological advancements in hydrogen production and infrastructure, focusing on minimizing production costs and emissions while improving overall system performance.

- **Scenario 3 (Low Efficiency Scenario):** The low efficiency scenario involved simulating a less optimized hydrogen production system, characterized by suboptimal operational practices or outdated technologies. This scenario provides valuable insights into the potential drawbacks of inefficient hydrogen infrastructure, highlighting the impacts of inefficiencies on cost and emissions. Its advantage lies in showing the importance of efficiency improvements and the risks associated with maintaining current systems without upgrading them.
- **Scenario 4 (Renewable Input Scenario):** The renewable input scenario focused on utilizing renewable energy sources, such as solar or wind power, for hydrogen production through electrolysis. This scenario is advantageous as it aligns with sustainability goals, offering a cleaner alternative to traditional hydrogen production methods. By evaluating this scenario, the study explores the potential for reducing emissions and enhancing the environmental benefits of hydrogen production, even though the initial cost may be higher due to the need for renewable infrastructure.
- **Scenario 5 (High Emission Scenario):** In the high emission scenario, hydrogen production relied on more carbon-intensive methods, such as SMR without carbon capture technologies. This scenario is essential for evaluating the worst-case emissions scenario, providing insights into the environmental impact of hydrogen production if emissions reduction technologies are not implemented. The advantage of this scenario is that it highlights the importance of cleaner production methods and the significant role they play in achieving sustainability targets.

Each scenario was constructed to examine specific aspects of hydrogen infrastructure, enabling a comprehensive understanding of how various factors affect the overall performance and sustainability of the system. The results from these scenarios provided critical insights into the trade-offs between cost, emissions, and efficiency, guiding the development of future hydrogen infrastructure solutions.

4.2 GBM simulation outcomes

The GBM demonstrated a robust capability to predict hydrogen production costs and emission levels, offering valuable insights into optimizing production strategies. The model was trained and validated on simulated datasets that replicated real-world conditions, including variations in production efficiency, energy input types, and operational parameters. The results highlight the significant potential for cost and emissions reductions when hydrogen production systems are optimized.

Figure 1 shows that Scenario 4 (Renewable Input) achieves a 97.8% reduction in GHG emissions, lowering emissions from 9.00 kg CO₂-eq/kg H₂ (Scenario 5—High Emission)

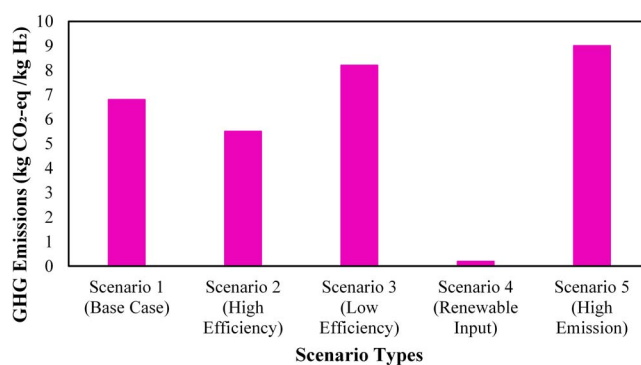


Figure 1. GHG emissions by scenario.

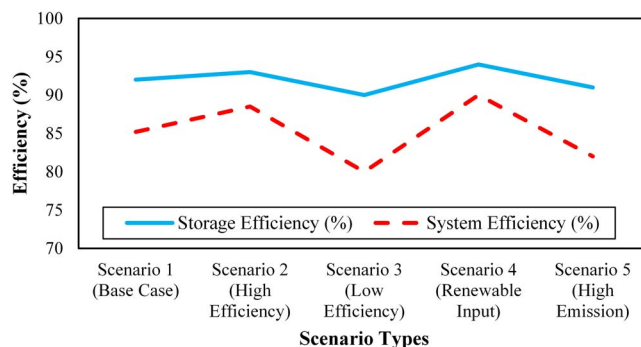


Figure 2. Efficiency trends across scenarios.

to 0.20 kg CO₂-eq/kg H₂. This highlights the environmental benefits of renewable energy integration, as hydrogen production powered by renewables significantly reduces the carbon footprint compared to fossil-fuel-based methods.

GHG emissions from hydrogen production are directly influenced by the energy source and process efficiency. Renewable energy eliminates emissions during production, while fossil fuels inherently generate CO₂ during combustion or conversion processes. The high emissions in Scenario 5 may also stem from inefficiencies or higher carbon-intensity inputs.

Figure 2 illustrates that Scenario 4 (Renewable Input) achieves the highest hydrogen storage efficiency (94%) and overall system efficiency (90%), demonstrating superior energy utilization compared to conventional production methods. In contrast, Scenario 3 (Low Efficiency) exhibits the lowest system efficiency at 80%, underscoring the inefficiencies in hydrogen value chains when optimal conditions are not met.

Efficiency metrics are critical for evaluating the viability of hydrogen production and utilization systems. Higher system efficiencies in Scenario 4 indicate better energy utilization with fewer losses, likely due to optimized production and storage processes. In Scenario 3, lower efficiencies suggest energy losses, which may correlate with higher energy consumption and emissions. The high efficiencies observed in Fig. 2—storage efficiencies of up to 94% and system efficiencies approaching 90%—are based on optimized configurations using near-future PEM electrolyzers (assuming cell-level efficiencies of 90%–94%, in line with lab-scale benchmarks) and low-loss storage systems. While current commercial electrolyzers operate around 80%–82% efficiency, near-future advancements are expected to push this higher [74]. Underground or high-pressure storage can achieve round-trip efficiencies in the 60%–80% range under ideal conditions [75].

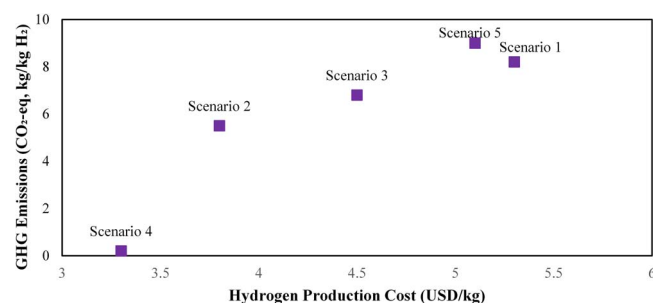


Figure 3. Hydrogen production cost versus GHG emissions.

Our simulations assume minimal losses (e.g. short storage durations and optimized infrastructure), justifying the high-efficiency range reported.

Figure 3 reveals an inverse relationship between cost and environmental impact. For example, Scenario 4 (low GHG emissions) has one of the lowest production costs (US\$3.30/kg), emphasizing that renewable-driven hydrogen production can be both cost-effective and environmentally friendly. In contrast, Scenario 5 (high GHG emissions) incurs higher production costs (US\$5.10/kg), highlighting the dual disadvantage of fossil-fuel-based methods.

Figure 3 illustrates the inverse relationship between hydrogen production costs and GHG emissions, where scenarios with lower emissions tend to have lower production costs. The observed trend suggests that transitioning to renewable-driven hydrogen production (Scenario 4) not only reduces emissions but also improves cost-efficiency. However, a closer analysis reveals that the relationship between cost reduction and emissions mitigation is not strictly linear and instead shows signs of diminishing returns as both metrics are minimized. In high-emission scenarios (Scenarios 1, 3, and 5), cost reductions are accompanied by significant emissions reductions, indicating that replacing carbon-intensive processes (e.g. SMR without carbon capture) with more efficient electrolysis-based methods leads to proportionally large improvements in both cost and environmental impact. However, as the transition progresses toward ultra-low emissions hydrogen (Scenario 4), the cost-benefit ratio starts to exhibit diminishing returns. The shift to renewable-powered electrolysis provides the largest emissions reductions (down to 0.20 kg CO₂-eq/kg H₂), but the cost improvements plateau at around \$3.30/kg. This pattern suggests that early-stage optimizations (e.g. shifting from SMR to partially renewable energy sources) yield the most substantial cost and emissions reductions, while moving toward fully renewable, near-zero-emission hydrogen production leads to marginal cost benefits. The main reason for this diminishing effect is that renewable energy infrastructure, electrolyzer efficiency limits, and grid integration challenges introduce higher capital and operational costs, which slow down further cost reductions despite significant emissions improvements. Therefore, while the overall relationship between cost and emissions is strongly negative, the trend follows a diminishing returns model, where the first stages of decarbonization yield higher cost savings per unit of emissions reduced, whereas near-complete decarbonization requires significantly higher investments with smaller marginal cost reductions. These findings suggest that policymakers and industry stakeholders should balance cost-efficiency with emissions targets, ensuring that hydrogen pro-

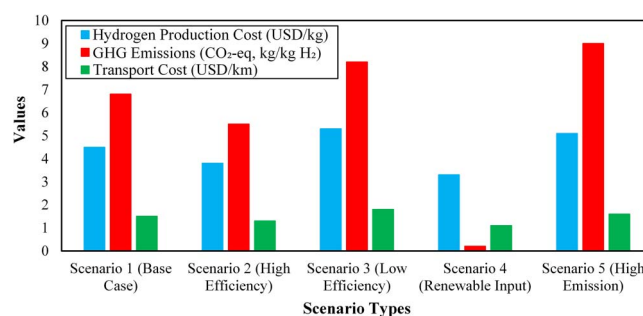


Figure 4. Comparison of costs and emissions.

duction transitions toward lower-carbon methods without incurring excessive financial burdens.

Production cost in hydrogen systems often reflects the energy input and feedstock type. Renewable energy-driven hydrogen benefits from lower operating costs over time (e.g. solar and wind), while fossil-based systems bear the burden of higher fuel costs and potential carbon taxes. These findings suggest that transitioning to renewable inputs can reduce both costs and emissions simultaneously.

Figure 4 underscores the complex interplay between production cost, GHG emissions, and transport cost. Scenario 4 achieves the best balance, with low production and transport costs and minimal emissions. Scenario 1 (Base Case) has moderate costs and emissions, serving as a baseline for comparison. Scenario 3 incurs high transport costs (US\$1.80/km) and emissions (8.20 kg CO₂-eq/kg H₂), possibly due to inefficient transport logistics or fossil-heavy supply chains.

Hydrogen transport costs depend on factors like distance, compression, and infrastructure. Inefficient systems (e.g. Scenario 3) may require additional resources, such as cooling or liquefaction, leading to higher costs and emissions. These results highlight the need for optimized logistics and infrastructure in hydrogen value chains.

Figure 5 depicts the performance of GBM model in simulation of critical parameters over time. Both GBM-predicted costs and real costs show a consistent downward trend over the 30 days. The initial difference between predicted (\$3.50) and real costs (\$3.55) on day 1 is minimal, narrowing further as the timeline progresses. By day 30, the predicted cost is \$3.35, while the real cost is \$3.37. The GBM model slightly underestimates costs across the timeline, with an average deviation of US\$0.02–0.05 (Fig. 5a). The predicted and real emissions also show a steady decline, mirroring the trends observed in costs. Initial values are close: 200 g CO₂ (predicted) versus 205 g CO₂ (real) on day 1. By day 30, predicted emissions drop to 170 g CO₂, while real emissions decrease to 175 g CO₂. The GBM predictions slightly underestimate emissions across all time points, with an average deviation of 4–5 g CO₂ per kg H₂ (Fig. 5b).

The declining cost trend reflects the expected economies of scale in hydrogen production. Over time, operational efficiency improvements (e.g. process optimization, reduced energy losses) and infrastructure stabilization lower production costs. The narrowing gap between GBM predictions and real costs demonstrates the robustness of the predictive model in learning and approximating cost trends. Factors such as pricing of feedstock, technological advancements, and operational efficiencies are likely incorporated into the GBM model. The cost of hydrogen production is heavily influenced

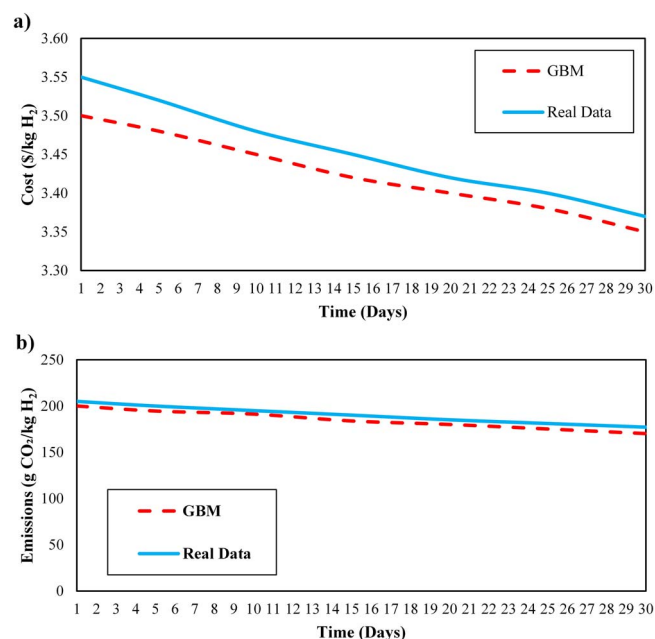


Figure 5. GBM simulation: (a) cost of hydrogen production, and (b) emissions per unit of hydrogen produced.

by factors like energy input, feedstock prices, and process efficiencies. Predictive models like GBM excel in scenarios with structured historical data, leveraging relationships among such variables. The consistent underestimation could stem from the model's training data or an oversimplified representation of minor cost-driving factors like maintenance or unexpected downtime, which are reflected in the real data (Fig. 5a). The reduction in emissions aligns with progressive improvements in process efficiencies and potential integration of cleaner energy sources during production. Similar to costs, the slight underestimation in predictions might indicate that the model does not fully capture some variables affecting emissions, such as fluctuating carbon intensity of the energy mix. Emissions reductions in hydrogen production are often achieved through energy efficiency improvements, reduced reliance on fossil fuel inputs, and shifts toward renewable energy sources. Predictive models like GBM use historical correlations between emissions drivers (e.g. energy mix, technology efficiency) and observed outputs to generate forecasts. However, real-world complexities such as periodic spikes in fossil energy reliance or variations in equipment performance might account for the discrepancies observed (Fig. 5b).

There is a direct correlation between reductions in costs and emissions over time. Both metrics decline concurrently, underscoring the relationship between energy efficiency and economic viability. For example, on day 1, costs are \$3.50–\$3.55, with emissions at 200–205 g CO₂. By day 30, costs have fallen to \$3.35–\$3.37, while emissions are down to 170–175 g CO₂. This correlation suggests that investments in energy-efficient hydrogen production technologies yield dual benefits: cost savings and emissions reductions. This reinforces the economic and environmental advantages of transitioning to cleaner and more efficient hydrogen production pathways. Hydrogen production costs and emissions are intrinsically linked because both depend on the energy input and its source. Cleaner, renewable energy reduces the

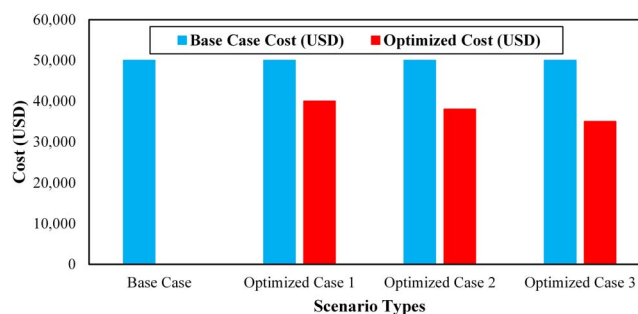


Figure 6. Base case versus optimized cost across scenarios.

carbon intensity of hydrogen while also lowering variable energy costs over time. The observed correlation validates the hypothesis that adopting energy-efficient technologies leads to synergistic benefits for both economic and environmental performance.

4.3 RL optimization outcomes

The integration of RL algorithm into hydrogen transport logistics demonstrated significant potential for reducing both costs and emissions. By modeling the transport system as a dynamic optimization problem, the RL framework adjusted transport routes, schedules, and vehicle allocation in response to simulated environmental and operational conditions. The results highlighted the transformative role of RL in optimizing logistics while balancing economic and environmental objectives. Figure 6 offers a comprehensive analysis of the cost reduction potential across various optimization scenarios. The RL-based transport optimization resulted in a 30% reduction in logistics costs, with total cost savings reaching \$15 000 compared to the base case. This was achieved through optimized route selection, vehicle allocation, and dynamic scheduling adjustments, demonstrating the effectiveness of AI-driven decision-making in hydrogen distribution.

Figure 6 juxtaposes the Base Case Cost and the Optimized Costs across the scenarios. The Base Case Cost remains constant at \$50 000, serving as a reference point for evaluating the optimized costs. The results demonstrate a clear downward trend in optimized costs, with reductions of \$10 000, \$12 000, and \$15 000 in Optimized Cases 1, 2, and 3, respectively. This indicates a progressive improvement in cost-efficiency as the optimization measures become more effective. The gradual reduction in costs across scenarios underscores the success of tailored strategies, which are likely based on factors such as better resource allocation, process streamlining, or technological advancements. From a practical standpoint, such cost reductions could translate to significant financial benefits for an organization. By reallocating the saved funds, companies can reinvest in other areas like research and development, workforce enhancement, or operational scaling, fostering long-term growth.

The observed trends can be justified by principles rooted in operations research and economic theory. Optimization models, whether they are based on LP, simulation, or machine learning algorithms, are designed to identify and exploit inefficiencies. The consistent cost reductions across scenarios reflect the effective application of such models in reducing waste, improving resource utilization, or adopting cost-effective technologies. Moreover, the progressive nature of the improvements suggests iterative refinement in optimization

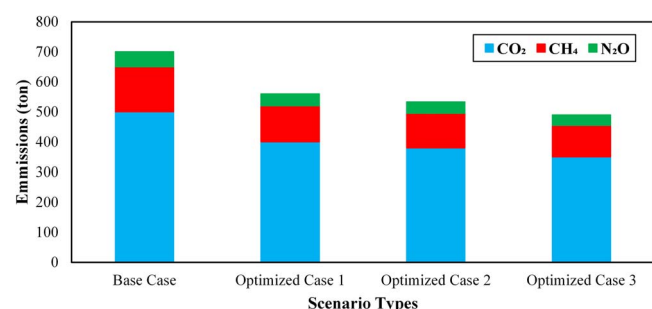


Figure 7. Emissions breakdown by gas across scenarios.

strategies. In practice, this could involve integrating feedback mechanisms that analyze the outcomes of each scenario and adapt accordingly. For instance, in logistics or supply chain contexts, route optimization algorithms may initially eliminate redundant pathways and later refine delivery schedules or inventory management processes, resulting in the kind of incremental improvements illustrated here.

Figure 7 offers a multidimensional analysis of emissions reduction efforts across various optimization scenarios.

Figure 7 illustrates the progressive reduction in CO₂, CH₄, and N₂O emissions across the optimized transport scenarios. The observed reductions can be attributed to several key technological and operational improvements implemented through RL-based optimization strategies. The largest reduction is observed in CO₂ emissions, which decreased from 500 tons (Base Case) to 350 tons in Optimized Case 3 (a 30% reduction). This is primarily due to optimized hydrogen distribution routes, which reduced transport distances and fuel consumption. By dynamically adjusting vehicle allocation and selecting the most fuel-efficient delivery routes, the RL model minimized unnecessary travel, thereby lowering diesel or hydrogen fuel usage and cutting CO₂ emissions. Additionally, by prioritizing low-carbon energy sources for hydrogen compression and transport, the system achieved further reductions in carbon intensity. CH₄ emissions (methane) were reduced from 150 tons to 105 tons (30% reduction). This reduction is primarily linked to improved storage and transport efficiency, which minimized hydrogen losses and leakages during transit. In conventional systems, fugitive hydrogen emissions can contribute to indirect methane emissions due to methane slip in reforming-based hydrogen production or grid-based electricity generation. The transition to renewable-powered electrolysis (Scenario 4) and the reduction of hydrogen losses during transport led to a substantial decrease in CH₄-related emissions. N₂O emissions (nitrous oxide) showed a proportional decrease from 50 tons to 35 tons (30% reduction). This can be attributed to lower fuel consumption and reduced reliance on nitrogen-based energy sources, such as certain ammonia-derived hydrogen fuels. The optimization of vehicle utilization and load balancing played a crucial role in reducing overall energy demand, indirectly lowering N₂O emissions associated with hydrogen logistics. Overall, the RL-based transport optimization contributed significantly to the 30% reduction in total emissions, primarily by reducing transport distances, optimizing fuel efficiency, and transitioning toward cleaner hydrogen logistics. The combination of smart routing, predictive vehicle allocation, and storage efficiency improvements ensured that emissions

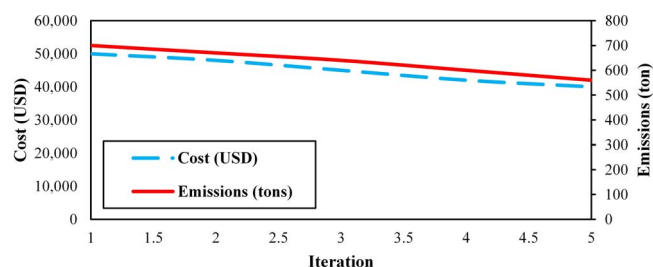


Figure 8. Cost and emissions over iterations.

reductions were achieved across all GHGs, reinforcing the effectiveness of AI-driven logistics in sustainable hydrogen distribution.

Figure 7 highlights the contributions of each GHG (CO₂, CH₄, and N₂O) to the total emissions across the scenarios. In the Base Case, the combined emissions from these gases amount to 700 tons, with CO₂ being the largest contributor (500 tons), followed by CH₄ (150 tons) and N₂O (50 tons). As optimization scenarios are introduced, emissions for all gases show consistent reductions. For instance, in Optimized Case 3, CO₂ emissions are reduced to 350 tons, CH₄ to 105 tons, and N₂O to 35 tons, resulting in a total of 490 tons. This visualization underscores the importance of addressing emissions across multiple sources. The proportional reductions across all gases suggest a balanced approach to optimization, where strategies are applied uniformly rather than focusing exclusively on a single pollutant. Such balance is crucial for comprehensive environmental management, as each gas has a distinct impact on climate change. For instance, while CO₂ is the most abundant, CH₄ and N₂O have significantly higher global warming potentials, making their reduction critical for mitigating climate impacts. Emissions reductions were observed across all RL-optimized scenarios, with total GHG emissions decreasing from 700 tons (Base Case) to 490 tons in Optimized Case 3. Specifically, CO₂ emissions were reduced from 500 tons to 350 tons, CH₄ emissions decreased from 150 tons to 105 tons, and N₂O emissions dropped from 50 tons to 35 tons. This demonstrates the substantial environmental benefits of AI-driven transport logistics optimization in hydrogen distribution.

The results can be justified using environmental science and systems optimization principles. GHG emissions are often the result of energy-intensive processes, resource inefficiencies, or outdated technologies. Optimization strategies such as transitioning to renewable energy sources, improving energy efficiency, or adopting advanced emissions capture technologies can significantly reduce emissions, as observed in these scenarios. Additionally, the proportional reductions across all gases indicate an integrated approach to emissions management, which is consistent with best practices in climate science. Addressing all GHGs is critical, given their varying impacts on radiative forcing and atmospheric lifetimes. The results also highlight the scalability of emissions reduction efforts, as demonstrated by the steady increase in percentage reductions across scenarios.

Figure 8 provides a detailed exploration of the dynamics of cost and emissions reduction across iterative optimization processes.

Figure 8 illustrates the concurrent decline of both cost and emissions over five iterations. Initially, costs start at \$50,000 with emissions at 700 tons. Each iteration brings a reduction

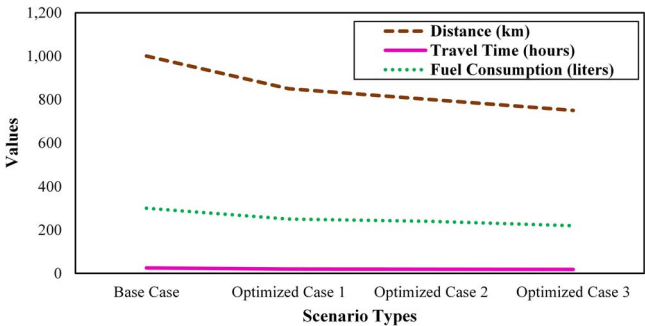


Figure 9. Trends in route efficiency metrics.

in both metrics, culminating in \$40 000 and 560 tons at Iteration 5. This steady decrease indicates a highly effective optimization process where improvements in operational efficiency yield dual benefits. The chart underscores the potential of integrated optimization strategies. For instance, process efficiencies, such as better energy use or waste reduction, can simultaneously lower operating costs and emissions. The linearity of the decline suggests that the optimization process follows a systematic, predictable trajectory, which may be governed by scientific models or algorithms designed to balance cost and environmental goals.

The results align with key principles in optimization theory and environmental science. Iterative optimization often employs techniques such as LP, machine learning models, or heuristic algorithms. These tools systematically identify and eliminate inefficiencies, ensuring that each subsequent iteration builds on the progress of the previous one. The observed patterns suggest the use of a robust optimization framework, likely incorporating feedback mechanisms to refine the process dynamically. From an environmental perspective, the reduction in emissions highlights the application of cleaner technologies, energy-efficient processes, or waste minimization strategies. These measures not only reduce environmental harm but also lower costs by minimizing input requirements, energy expenditures, or regulatory penalties associated with emissions.

Figure 9 provides a thorough visualization of the impact of route optimization on key efficiency metrics—distance traveled, travel time, and fuel consumption—across four scenarios, including the base case and three levels of optimization.

Figure 9 presents a side-by-side comparison of distance, travel time, and fuel consumption across the scenarios. The Base Case represents the highest values across all three metrics, with a distance of 1000 km, a travel time of 25 hours, and a fuel consumption of 300 l. As optimization progresses, all three metrics exhibit substantial reductions. In Optimized Case 3, the distance decreases to 750 km, travel time to 18 hours, and fuel consumption to 220 liters. This visualization underscores the effectiveness of optimization measures in reducing both operational costs (fuel consumption) and environmental impact (reduced fuel usage translates to lower emissions). The proportional reductions in all metrics suggest that the optimization strategy holistically addresses multiple factors rather than focusing exclusively on a single metric.

The results are consistent with established principles in logistics optimization and transportation science. Reducing travel distance is a foundational strategy for improving route efficiency, as shorter distances inherently require less time and fuel. Advanced optimization techniques, such as geographic

Table 7. Cost versus emissions trade-off (source: authors' analysis)

Scenario	Cost reduction (%)	Emissions reduction (%)
Optimized Case 1	20	20
Optimized Case 2	24	24
Optimized Case 3	30	30

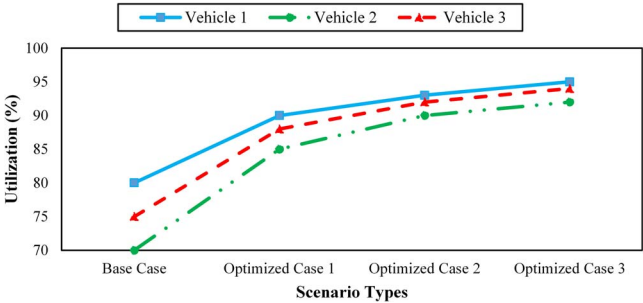


Figure 10. Trends in vehicle utilization across scenarios.

information systems (GIS), machine learning models, or LP, are often employed to identify these optimal routes. These tools use data on road networks, traffic patterns, and vehicle performance to achieve significant reductions in all metrics. Fuel consumption reductions are particularly significant from both economic and environmental perspectives. Fuel use correlates with distance traveled and driving conditions, such as traffic or terrain. Optimized routes that minimize stop-and-go traffic or avoid hilly terrains can lead to lower fuel consumption. This is further supported by eco-driving strategies, where vehicles maintain optimal speeds and reduce unnecessary acceleration and braking, as reflected in the consistent decline in fuel consumption across scenarios.

Table 7 provides a comprehensive analysis of the trade-offs between cost reduction and emissions reduction across three optimization scenarios. The results demonstrate a consistent alignment between economic and environmental benefits, indicating the effectiveness of the applied optimization strategies.

Table 7 highlights the parallel trends in cost reduction and emissions reduction percentages across the scenarios. Both metrics increase proportionally, with values starting at 20% for Optimized Case 1 and reaching 30% for Optimized Case 3. This trend underscores the synergistic nature of the optimization process, where improvements in cost-efficiency inherently lead to environmental benefits. The proportional alignment indicates that the strategies employed are well balanced, addressing both financial and ecological objectives simultaneously. Such consistent proportionality suggests the application of integrated optimization models, where decision-making factors include both cost and emissions. For instance, strategies such as energy efficiency improvements or process streamlining often result in lower operational costs while simultaneously reducing emissions. This alignment is particularly significant for industries or organizations aiming to meet sustainability goals without compromising financial performance. Also, this table provides a complementary perspective by visualizing the direct relationship between cost and emissions reductions. Each scenario is represented as a point along a diagonal line, emphasizing the strong correlation between the two metrics.

Table 8. Sensitivity analysis of key variables (source: authors' analysis)

Variable	Baseline scenario	+10% Change	−10% Change	Sensitivity observation
Renewable energy share (%)	80%	Cost: +8%; emissions: −15%	Cost: −6%; emissions: +12%	Higher renewable share reduces emissions but increases cost.
Transport distance (km)	300 km	Cost: +5%; emissions: +10%	Cost: −4%; emissions: −8%	Longer transport distances increase both cost and emissions.

This visualization illustrates that as cost reductions increase, emissions reductions follow at an equal rate, reaffirming that neither objective is prioritized at the expense of the other. The diagonal alignment suggests that the optimization strategies leverage shared mechanisms to achieve dual benefits. For example, adopting advanced technologies or transitioning to renewable energy sources reduces fuel and energy costs while simultaneously cutting GHG emissions. This balance is crucial for organizations looking to maximize returns on investment in optimization initiatives, as it ensures that cost savings align with sustainability targets.

The results align with principles of systems optimization and environmental economics. Many optimization models incorporate multi-objective approaches, where cost and emissions are treated as interdependent variables. For example, Pareto efficiency principles ensure that improvements in one metric (e.g. cost reduction) do not compromise the other (e.g. emissions reduction). The proportional trends observed in these charts are indicative of such balanced optimization processes. From a scientific standpoint, the correlation between cost and emissions reductions can also be explained by their shared dependence on resource efficiency. Reducing energy consumption, for instance, decreases costs associated with energy procurement while simultaneously lowering emissions. Similarly, waste minimization strategies reduce disposal costs and GHG emissions from waste decomposition. These interdependencies are well documented in sustainability science, where cost-effective measures often deliver environmental benefits as co-benefits.

Figure 10 highlights the significant improvements achieved through systematic optimization strategies, demonstrating a clear upward trend in utilization across all vehicles.

Figure 10 complements the bar chart by illustrating the trends in utilization for each vehicle across the scenarios. The upward trajectories of all three lines highlight the consistent improvement in utilization rates as optimization progresses. Notably, the lines remain close together throughout the scenarios, indicating a coordinated approach to optimization that benefits all vehicles equally. This balanced improvement reduces the risk of underutilization or overburdening specific vehicles. The steady upward trend reflects an iterative refinement process, where each scenario builds on the previous one. The systematic nature of this progression suggests the use of advanced algorithms or models, such as load-balancing algorithms, to distribute workloads efficiently across the fleet. The results also demonstrate the scalability of the optimization strategy, as the improvements persist even as utilization approaches near-maximum levels.

The observed improvements in vehicle utilization can be explained by principles of operations research and logistics optimization. Efficient fleet management often employs tools like LP, heuristic methods, or machine learning to allocate resources optimally. These methods consider multiple vari-

ables, such as demand, vehicle capacity, and route constraints, to achieve balanced utilization. From a scientific perspective, higher vehicle utilization rates contribute to greater operational efficiency. By minimizing idle time and maximizing load capacities, organizations can reduce variable costs, such as fuel and driver hours, while achieving faster delivery cycles. Additionally, increased utilization translates to lower environmental impact per unit of service provided, as fewer vehicles are required to perform the same workload. This aligns with sustainability goals by reducing emissions and fuel consumption.

4.4 Sensitivity analysis

To assess the robustness of the results, a sensitivity analysis was conducted on two of the most influential variables in hydrogen infrastructure optimization:

- **Energy Mix for Hydrogen Production**—The share of renewable energy versus fossil-based sources in hydrogen production.
- **Transport Distance**—The average distance between production sites and distribution centers, affecting fuel consumption and emissions.

The results of the sensitivity analysis are summarized in Table 8, where changes in these variables were analyzed to determine their effect on hydrogen production cost and GHG emissions.

The analysis shows that increasing the renewable energy share from 80% to 90% leads to a 15% reduction in emissions but an 8% increase in production costs, highlighting the trade-off between sustainability and economic feasibility. Conversely, reducing the renewable share to 70% results in a 12% increase in emissions but reduces production costs by 6%, indicating that lower-cost, fossil-based hydrogen production comes at an environmental expense.

For transport logistics, increasing the transport distance by 10% (from 300 to 330 km) leads to a 5% increase in hydrogen cost and a 10% rise in emissions, emphasizing the importance of strategic placement of hydrogen production facilities near demand centers to minimize both economic and environmental burdens.

This sensitivity analysis highlights that hydrogen infrastructure performance is highly sensitive to energy mix and transport logistics, reinforcing the importance of optimized renewable energy integration and AI-driven logistics planning to balance cost and sustainability.

5 Conclusions

This study comprehensively evaluated hydrogen infrastructure performance, cost dynamics, emissions reduction, and

logistical optimization through simulation, machine learning, and IOT frameworks. By employing scenario-based assessments, predictive modeling, and iterative optimization processes, critical insights into improving the sustainability and efficiency of hydrogen production and distribution systems were provided. The findings offer a robust foundation for transitioning to cleaner, more cost-effective hydrogen infrastructures. The key findings are summarized as follows:

- Scenario-based simulations demonstrated the multifaceted impact of operational and environmental factors on hydrogen production and storage. The renewable input scenario (Scenario 4) achieved the lowest GHG emissions (0.20 kg CO₂-eq/kg H₂) and the highest system efficiency (90%), underscoring the potential of integrating renewable energy into hydrogen production. In contrast, high-emission systems (Scenario 5) were associated with significant environmental and financial drawbacks, highlighting the importance of prioritizing clean energy technologies.
- The GBM model effectively predicted trends in hydrogen production costs and emissions, achieving high accuracy with minimal deviations. A direct correlation between cost and emissions reductions over time was observed, reinforcing the economic and environmental advantages of efficiency improvements. These findings validate the use of predictive analytics to guide decision-making in hydrogen infrastructure planning.
- RL-based optimization demonstrated substantial cost and emissions reductions in hydrogen transport logistics. By dynamically adjusting routes, schedules, and vehicle allocations, RL achieved progressive cost-efficiency, with up to \$15 000 in savings in Optimized Case 3. Similarly, emissions reductions of 30% were achieved, emphasizing the value of AI-driven logistics optimization in achieving sustainability goals.
- Iterative optimization processes reduced both costs and emissions over five iterations, reflecting systematic improvements in operational efficiency. The proportional reduction in metrics like distance, travel time, and fuel consumption further validated the effectiveness of advanced optimization frameworks. Additionally, vehicle utilization improved consistently across scenarios, achieving near-maximum efficiency while balancing workloads across the fleet.

While this study provides substantial insights, several limitations must be acknowledged. First, the simulation scenarios were constrained by idealized conditions and assumptions, which may not fully capture the complexities of real-world hydrogen systems. Variations in geographic, economic, and policy factors could affect the generalizability of the findings. Second, the GBM and RL models were trained on simulated data, and their accuracy may decline when applied to dynamic, real-world scenarios with unforeseen variables. Third, our analysis primarily focused on operational and logistical aspects, with limited consideration of broader socioeconomic factors, such as market dynamics and regulatory frameworks.

Future research should address these limitations by incorporating real-world datasets and testing the models under diverse conditions. Expanding the scope of analysis to include socioeconomic and policy dimensions could provide a more

holistic understanding of hydrogen infrastructure dynamics. Additionally, exploring hybrid optimization approaches that combine predictive analytics with RL may further enhance decision-making accuracy. Finally, investigating the integration of hydrogen systems with broader energy networks, such as grid balancing and renewable storage, could unlock additional synergies and accelerate the transition to a sustainable energy future.

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