Journal of Applied Business and Technology

AI-Based Digital Twin Development for Optimizing Hydrogen Production, Distribution, and Business Profitability

Article History
Received
31 July 2025
Received in revised form
11 November 2025
Accepted
9 January 2026
Published Online
31 January 2026

Nicholas Renaldo [a*], Jaswar Koto [b], M. Dalil [c], Dodi Sofyan Arief [c], Sulaiman Musa [d], Nindy Daviny [e], Cecilia Cecilia [f], Kristy Veronica [a]

[a] Faculty of Business, Institut Bisnis dan Teknologi Pelita Indonesia, Indonesia
[b] Ocean and Aerospace Research Institute, Japan
[c] Faculty of Engineering, Universitas Riau, Indonesia
[d] Faculty of Economics and Management Sciences, Bayero University, Nigeria
[e] Faculty of Environmental Study, Universitas Riau, Indonesia
[f] International College of Chinese Studies, East China Normal University, China

*Corresponding author
nicholasrenaldo@lecturer.pelitaindonesia.ac.id

Abstract
The transition toward a low-carbon energy system has increased interest in green hydrogen as an energy carrier for renewable energy integration, industrial applications, and sustainable transportation. However, the economic competitiveness of hydrogen remains constrained by the complexity of coordinating renewable-energy availability, electrolyzer operation, hydrogen storage, distribution, market demand, and profitability. This study proposes an AI-Based Hydrogen Business Digital Twin (HBDT) to optimize hydrogen production, distribution, and business profitability through an integrated digital decision-making framework. The research employs a simulation-based development approach that combines Digital Twin technology, Artificial Intelligence, predictive analytics, multi-objective optimization, and techno-economic analysis. Several machine-learning models, including Random Forest, Support Vector Regression, XGBoost, Artificial Neural Network, and Long Short-Term Memory (LSTM), are evaluated for predictive performance. The simulation results indicate that LSTM provides the strongest performance, achieving an MAE of 0.041, RMSE of 0.068, and R^2 of 0.981. Scenario analysis demonstrates that profitability increases from 12.5% under fixed production and distribution to 32.4% under the integrated AI, Digital Twin, and optimization scenario. The techno-economic simulation further indicates reductions in hydrogen production cost, levelized cost of hydrogen, and distribution costs, accompanied by improvements in renewable-energy utilization, revenue, ROI, and payback period. These findings demonstrate that the proposed HBDT can transform hydrogen management from a static and reactive process into a predictive, prescriptive, and potentially autonomous business ecosystem. The study contributes to the emerging concept of Hydrogen Business 4.0, in which technical operations and economic decisions are continuously optimized through AI and Digital Twin technologies.

Keywords: Artificial Intelligence; Digital Twin; Green Hydrogen; Hydrogen Business; Techno-Economic Optimization
DOI: https://doi.org/10.35145/s04p2v22
SDGs: Affordable and Clean Energy (7); Industry, Innovation and Infrastructure (9); Climate Action (13); Decent Work and Economic Growth (8); Sustainable Cities and Communities (11)

1.0 INTRODUCTION

The global energy transition is shifting from conventional fossil-fuel systems toward intelligent, low-carbon, and highly adaptive energy ecosystems (Yang et al., 2024). Hydrogen has emerged as a strategic energy carrier because it can connect renewable electricity, industrial processes, energy storage, and transportation. However, the development of a hydrogen economy faces a fundamental challenge: hydrogen is not merely a production problem, but a complex business system involving production efficiency, energy availability, storage, distribution, demand uncertainty, operational risk, and profitability.

Conventional hydrogen business planning generally evaluates production capacity, investment costs, distribution infrastructure, and market demand as relatively separate components (Riera et al., 2023). This fragmented approach creates a significant gap between technical optimization and business decision-making. A hydrogen facility may be technically efficient but economically uncompetitive, while a profitable distribution strategy may generate operational inefficiencies or underutilize production capacity.

This research proposes an AI-Based Digital Twin for Hydrogen Business, transforming hydrogen infrastructure from a static physical asset into a dynamic, intelligent, and continuously optimized business ecosystem. The Digital Twin will digitally replicate critical components of the hydrogen value chain, including renewable energy input, electrolyzer performance, hydrogen production, storage, transportation, distribution, demand, operating costs, and revenue.

Artificial Intelligence will be integrated into the Digital Twin to analyze real-time and historical data, predict hydrogen demand and production capacity, identify operational risks, optimize distribution routes, and simulate alternative business scenarios. The system will enable decision-makers to ask not only *“How much hydrogen can we produce?”*, but also “What should we produce, when should we produce it, where should we distribute it, and which strategy generates the highest sustainable profit?”

The proposed concept therefore moves beyond conventional hydrogen management toward autonomous, predictive, and economically intelligent hydrogen infrastructure. By integrating engineering data with market and financial variables, the research seeks to establish a new paradigm in which hydrogen facilities can continuously adapt their operations according to energy availability, market demand, logistics conditions, and profitability.

Novelty

The primary novelty of this research lies in developing a business-oriented Digital Twin architecture for the entire hydrogen value chain, rather than using Digital Twin technology only for monitoring or maintenance of individual equipment.

1. From Digital Monitoring to Digital Business Intelligence

Existing Digital Twin applications predominantly focus on equipment monitoring, predictive maintenance, or production optimization. This research extends the concept into **Business Digital Twin**, where technical, operational, market, and financial variables are integrated into a single decision-making environment (Sudarno et al., 2022).

The Digital Twin will connect:

Renewable Energy → Electrolysis → Hydrogen Production → Storage → Distribution → Market Demand → Revenue → Profitability

Thus, every technical decision can be evaluated against its **economic consequences**.

2. AI-Driven Predictive Hydrogen Economy

The system will not simply display current hydrogen production. AI will be used to predict:

- hydrogen production capacity;
- renewable energy availability;
- hydrogen demand;
- storage requirements;
- distribution requirements;
- operational costs;
- market opportunities;
- potential bottlenecks; and
- expected profitability.

This creates a transition from:

Reactive → Predictive → Prescriptive → Autonomous Decision-Making

3. Profitability as an Optimization Variable

A major disruptive element is the integration of **profitability directly into the optimization engine**.

Instead of optimizing only:

kg H_2 produced/day

the system will optimize a multidimensional objective:

Maximum hydrogen production + minimum energy cost + minimum logistics cost + optimal storage utilization + maximum revenue + sustainable profitability

This changes hydrogen management from an **engineering optimization problem** into an **integrated techno-economic optimization problem**.

4. What-If Simulation Before Real-World Decisions

The Digital Twin will enable virtual experiments before decisions are implemented in the physical system.

For example:

What happens to profitability if electricity prices increase by 20%?

What happens if hydrogen demand increases by 50%?

Which distribution center should receive the available hydrogen?

Is it more profitable to sell hydrogen for mobility or industrial applications?

What is the optimal electrolyzer operating schedule under fluctuating solar power?

This creates a **“test-before-invest”** capability for hydrogen businesses.

5. Toward an Autonomous Hydrogen Business
The most disruptive vision is the development of a **self-optimizing hydrogen business system**.
The architecture can be conceptualized as:
PHYSICAL HYDROGEN SYSTEM
↓
DIGITAL TWIN
↓
REAL-TIME DATA
↓
AI PREDICTION
↓
SCENARIO SIMULATION
↓
OPTIMIZATION ENGINE
↓
BUSINESS DECISION
↓
PHYSICAL SYSTEM RESPONSE

This creates a continuous feedback loop between the physical hydrogen infrastructure and its digital representation.

Core Disruptive Proposition
The research ultimately proposes a shift:
From “producing hydrogen efficiently” to “operating an intelligent hydrogen economy profitably.”

The innovation is therefore not simply the use of AI, Digital Twin, or hydrogen technology individually. The disruption emerges from **integrating these technologies into one intelligent techno-economic ecosystem** capable of predicting, simulating, optimizing, and continuously improving hydrogen production and distribution decisions.

Proposed Novel Concept
AI-Based Hydrogen Business Digital Twin (HBDT)
A conceptual platform that integrates:
AI + Digital Twin + Renewable Energy + Electrolysis + Storage + Logistics + Market Intelligence + Financial Analytics to create a **predictive and self-optimizing hydrogen business ecosystem**.
This positions the research not merely as a study of hydrogen technology, but as a foundation for a new **“Hydrogen Business 4.0” paradigm**.

2.0 LITERATURE REVIEW

Hydrogen Economy and Green Hydrogen

Hydrogen is increasingly recognized as an important energy carrier in the global transition toward low-carbon energy systems (Algburi et al., 2025). Unlike fossil fuels, hydrogen can be produced using renewable electricity and water through electrolysis, generating green hydrogen with potentially very low lifecycle greenhouse-gas emissions when renewable electricity is used. Its versatility enables hydrogen to connect sectors that are otherwise difficult to decarbonize, including heavy transportation, industry, energy storage, and electricity generation.

However, the economic viability of hydrogen remains strongly dependent on electricity prices, electrolyzer utilization, capital expenditure, storage costs, transportation infrastructure, and market demand. Consequently, the competitiveness of hydrogen cannot be evaluated solely through production efficiency. It requires an integrated analysis of the technical, logistical, market, and financial dimensions of the hydrogen value chain.

This creates an important research opportunity for intelligent systems capable of simultaneously evaluating hydrogen production and business performance.

Hydrogen Production and Electrolyzer Optimization

Water electrolysis is a key pathway for producing green hydrogen (Amini Horri et al., 2024). The performance of an electrolyzer depends on variables such as electricity input, operating temperature, pressure, water availability, electrolyzer efficiency, degradation, and renewable-energy intermittency.

Renewable energy introduces additional complexity because solar and wind generation fluctuate over time. Operating an electrolyzer continuously may therefore result in periods of high electricity costs or insufficient renewable electricity, while operating only when renewable electricity is abundant may reduce electrolyzer utilization.

Previous research on electrolyzer optimization has therefore focused on determining optimal operating schedules, renewable-energy integration, energy consumption, and production efficiency. However, many optimization approaches remain focused primarily on the **technical performance of hydrogen production**.

For a commercial hydrogen ecosystem, technical optimization alone is insufficient. The optimal production schedule should also consider hydrogen demand, storage capacity, transportation costs, selling prices, and expected profit. This motivates the integration of production optimization with business intelligence.

Digital Twin Technology

Digital Twin technology represents a physical system through a dynamic digital model that can interact with real-world data (Abdelrahman et al., 2025). Unlike conventional simulation models, a Digital Twin is designed to maintain a continuous relationship between the physical and digital environments (Renaldo, Suhardjo, et al., 2022).

The Digital Twin concept has been widely applied in manufacturing, energy systems, transportation, predictive maintenance, and smart infrastructure. Its major advantages include real-time monitoring, anomaly detection, predictive analysis, simulation, and optimization.

In the context of hydrogen, Digital Twin technology can potentially represent the behavior of electrolyzers, hydrogen storage systems, pipelines, transportation systems, refueling stations, and renewable-energy resources. Such a system could provide a virtual representation of the hydrogen infrastructure and allow operators to test alternative operational strategies without immediately changing the physical system.

However, the application of Digital Twin technology to hydrogen has generally emphasized asset-level monitoring and engineering optimization rather than the integration of technical performance with comprehensive business profitability.

Artificial Intelligence in Energy Systems

Artificial Intelligence has increasingly been applied to energy forecasting, optimization, anomaly detection, predictive maintenance, demand forecasting, and intelligent energy management (Wigger et al., 2025). Machine learning algorithms can identify complex relationships between historical operational data and future system behavior.

For hydrogen systems, AI can be applied to predict renewable-energy generation, hydrogen demand, electrolyzer performance, equipment degradation, energy prices, and distribution requirements. These predictions can subsequently support optimization algorithms in determining when to produce, store, transport, or sell hydrogen.

The combination of AI and Digital Twin technology is particularly promising because AI can transform the Digital Twin from a descriptive digital representation into a predictive and prescriptive decision-support system.

Conceptually:

Digital Twin + AI = Predictive Digital Twin

and

Predictive Digital Twin + Optimization = Prescriptive Digital Twin

This progression provides the technological foundation for an intelligent hydrogen business ecosystem.

Hydrogen Storage and Distribution

Hydrogen storage and distribution represent major challenges in establishing a competitive hydrogen economy (Anekwe et al., 2025). Hydrogen has a low volumetric energy density under ambient conditions, requiring specialized storage and transportation technologies such as compressed hydrogen, liquefied hydrogen, pipelines, or chemical hydrogen carriers.

The selection of a distribution strategy depends on distance, hydrogen volume, infrastructure availability, demand density, transportation costs, and delivery frequency. Consequently, hydrogen distribution represents a complex optimization problem involving multiple interconnected variables.

Traditional logistics optimization may minimize transportation distance or cost. However, a commercial hydrogen system should consider broader objectives, including production cost, storage utilization, delivery reliability, customer demand, and revenue.

An AI-based Digital Twin could provide a virtual environment for evaluating alternative distribution scenarios and identifying the most economically attractive configuration.

Techno-Economic Analysis of Hydrogen

Techno-economic analysis (TEA) is commonly used to evaluate the economic feasibility of hydrogen production and infrastructure (Bahou, 2025). Typical indicators include capital expenditure (CAPEX), operational expenditure (OPEX), levelized cost of hydrogen (LCOH), revenue, net present value (NPV), internal rate of return (IRR), payback period, and profitability.

While TEA provides important information about economic feasibility, conventional approaches are often based on predefined assumptions and static scenarios. Real-world hydrogen systems, however, are dynamic. Electricity prices, renewable generation, hydrogen demand, transportation costs, and equipment performance may change continuously.

Therefore, a static financial model may not adequately represent the operational reality of a hydrogen business. The proposed research addresses this limitation by embedding financial and market variables directly into the Digital Twin. This allows profitability to be evaluated dynamically as operating conditions change.

AI-Based Optimization and Hydrogen Business Decisions

The integration of AI with optimization algorithms provides opportunities for more sophisticated hydrogen business decisions (Arsad et al., 2025). Rather than optimizing a single variable, a multi-objective framework can simultaneously consider:

- hydrogen production;
- energy consumption;
- renewable-energy utilization;
- electrolyzer efficiency;
- storage capacity;
- transportation cost;
- hydrogen demand;
- selling price;
- operational expenditure; and
- profitability.

The optimization problem can therefore be expressed conceptually as: subject to technical and business constraints such as: Such an approach enables the Digital Twin to identify not only technically feasible solutions but also economically optimal solutions.

Research Gap

Based on the existing literature, several gaps can be identified.

Research Area	Existing Focus	Remaining Gap
Green hydrogen	Production and energy efficiency	Limited integration with real-time business decisions
Electrolyzer optimization	Technical performance	Limited consideration of market profitability
Digital Twin	Monitoring and predictive maintenance	Limited integration across the entire hydrogen value chain
AI in energy	Forecasting and optimization	Often developed as isolated applications
Hydrogen logistics	Transportation and infrastructure optimization	Limited integration with production and market variables
Hydrogen TEA	Economic feasibility	Often static rather than continuously adaptive
Hydrogen business	Business models and feasibility	Limited AI-driven dynamic optimization

The central research gap is therefore the absence of a comprehensive framework that integrates **Digital Twin, Artificial Intelligence, hydrogen production, distribution, market demand, and profitability within a unified dynamic system**.

Proposed Research Position

This research addresses the identified gap through the development of an:

AI-Based Hydrogen Business Digital Twin (HBDT)

The proposed framework integrates five interconnected layers:

1. Physical Layer. Renewable energy, electrolyzer, water, storage, transportation, and distribution infrastructure.
2. Data Layer. Real-time operational, energy, market, logistics, and financial data.
3. AI Layer. Demand forecasting, renewable-energy prediction, equipment-performance prediction, anomaly detection, and price forecasting.
4. Digital Twin & Optimization Layer. Virtual simulation, scenario analysis, multi-objective optimization, and operational scheduling.
5. Business Decision Layer. Production planning, inventory decisions, distribution strategy, pricing scenarios, investment decisions, and profitability optimization.

The conceptual innovation can therefore be summarized as:

Conventional Hydrogen System → Digital Hydrogen System → Intelligent Hydrogen System → Autonomous Hydrogen Business Ecosystem

The ultimate contribution is a transition from **static feasibility analysis** toward a **dynamic, predictive, and prescriptive hydrogen business model** in which technical operations and economic performance are optimized simultaneously.

Conceptual Framework
Renewable Energy + Market Data + Operational Data
↓
AI Prediction
↓
Hydrogen Business Digital Twin
↓
Scenario Simulation
↓
Multi-Objective Optimization
↓
Production + Storage + Distribution Decisions
↓
Revenue & Cost Optimization
↓
Maximum Sustainable Hydrogen Business Profitability

This literature position establishes the research as a potential contribution to Hydrogen 4.0, where hydrogen infrastructure evolves from a conventional energy-production facility into an AI-driven, self-learning, digitally simulated, and economically optimized business ecosystem.

3.0 METHODOLOGY

Research Design

This study employs a Research and Development (R&D) approach to develop an AI-Based Hydrogen Business Digital Twin (HBDT) for optimizing hydrogen production, distribution, and business profitability. The research combines system modeling, artificial intelligence, digital twin technology, optimization, and techno-economic analysis. The proposed system will digitally represent the hydrogen business ecosystem and use real-world or simulated operational data to predict system behavior and identify optimal business decisions. The research follows the conceptual sequence:

Data Acquisition → Hydrogen System Modeling → Digital Twin Development → AI Prediction → Scenario Simulation → Multi-Objective Optimization → Techno-Economic Evaluation → Validation

Research Objectives

The methodology is designed to achieve four main objectives:

1. Develop a digital representation of an integrated hydrogen production and distribution system.
2. Develop AI models for predicting hydrogen production, renewable-energy availability, and market demand.
3. Develop an optimization mechanism for production, storage, and distribution decisions.
4. Evaluate the impact of the proposed system on hydrogen cost, operational efficiency, revenue, and profitability.

System Architecture

The proposed Hydrogen Business Digital Twin (HBDT) consists of five major layers.

Layer 1 — Physical Hydrogen System

The physical system will be represented through the following components:

- Renewable energy source, particularly solar PV;
- Water supply;
- Electrolyzer;
- Hydrogen compression/storage;
- Transportation/distribution;
- Hydrogen demand/customer;
- Refueling or delivery infrastructure.

Layer 2 — Data Acquisition

The system will collect or generate data related to:

- Solar irradiance;
- Renewable electricity generation;
- Electricity price;
- Electrolyzer efficiency;
- Electrolyzer capacity;
- Hydrogen production;
- Hydrogen storage level;
- Transportation distance;
- Distribution cost;
- Hydrogen demand;
- Hydrogen selling price;
- CAPEX;
- OPEX.

Data can be obtained from secondary datasets, technical specifications, industry data, public energy databases, and simulation data where real-time operational data are unavailable.

Layer 3 — Artificial Intelligence

AI models will be developed to predict important variables, including:

$$\widehat{H}_{2,t+1} = f(Et, Rt, Dt, Pt)$$

where:

- H_2 = hydrogen demand/production;
- E = energy availability;
- R = renewable-energy generation;
- D = demand;
- P = relevant price variables.

Candidate algorithms include:

- Random Forest;
- XGBoost;
- Support Vector Regression;
- Artificial Neural Network;
- Long Short-Term Memory (LSTM).

The best model will be selected based on predictive performance.

Digital Twin Development

The Digital Twin will replicate the behavior of the hydrogen production and distribution system in a virtual environment.

The Digital Twin will contain four interconnected models:

A. Energy Model

Represents renewable electricity availability and electricity consumption.

$$E_{available} = f(\text{Solar Irradiance, PV Capacity, Weather})$$

B. Hydrogen Production Model

Hydrogen production will be modeled according to electrolyzer capacity and energy consumption:

$$H_{2,t} = E_{electrolyzer,t} \times \eta_{electrolyzer} / SEC$$

where:

- $H_{2,t}$ = hydrogen production;
- $E_{electrolyzer,t}$ = electricity supplied;
- $\eta_{electrolyzer}$ = electrolyzer efficiency;
- SEC = specific energy consumption.

C. Storage and Distribution Model

The model will simulate hydrogen inventory:

$$S_t = S_{t-1} + H_{production,t} - H_{demand,t} - H_{distribution,t}$$

subject to storage-capacity constraints.

Distribution will consider:

- transportation distance;
- transportation capacity;
- delivery frequency;

- logistics cost;
- customer demand.

D. Business Model

The business model will integrate:

$$Revenue = H_{sold} \times P_{H2}$$

and:

$$Profit = Revenue - (CAPEX + OPEX + Energy\ Cost + Storage\ Cost + Distribution\ Cost)$$

This enables the Digital Twin to simultaneously evaluate technical and financial performance.

AI Prediction Model

The AI component will be developed using historical and simulated data.

Prediction Targets

The study will focus on predicting:

1. Renewable energy availability;
2. Hydrogen production;
3. Hydrogen demand;
4. Hydrogen selling price;
5. Potential distribution requirements.

The dataset will be divided into:

- Training set: 70%
- Validation set: 15%
- Testing set: 15%

Model performance will be evaluated using:

$$MAE = 1/n \sum |yi - yi\hat{}|$$

$$RMSE = (1/n \sum (yi - yi\hat{})^2)^{1/2}$$

and:

$$R^2 = 1 - (\sum (yi - yi\hat{})^2 / \sum (yi - \bar{y})^2)$$

The model with the best predictive performance will be integrated into the Digital Twin.

Multi-Objective Optimization

The most disruptive component of the research is the integration of AI prediction with business optimization. Instead of optimizing hydrogen production alone, the system will optimize multiple objectives simultaneously.

Objective 1 — Maximize Profitability

$$Maximize\ Z_1 = Revenue - Total\ Cost$$

Objective 2 — Minimize Hydrogen Production Cost

$$Minimize\ Z_2 = LCOH$$

Objective 3 — Maximize Renewable Energy Utilization

$$Maximize\ Z_3 = Renewable\ Energy\ Used / Renewable\ Energy\ Available$$

Objective 4 — Minimize Distribution Cost

$$Minimize\ Z_4 = Transportation + Storage + Delivery\ Cost$$

These objectives can be solved using optimization techniques such as:

- Genetic Algorithm;
- Particle Swarm Optimization;
- NSGA-II;
- Mixed-Integer Linear Programming; or
- hybrid AI-optimization approaches.

A Pareto-optimal solution can subsequently be selected to balance profitability, efficiency, and sustainability (Renaldo, Hafni, et al., 2022).

Scenario Simulation

The Digital Twin will be used to simulate different hydrogen business scenarios.

Scenario 1 — Baseline

Conventional production and distribution strategy.

Scenario 2 — Renewable Energy Optimization

Hydrogen production is adjusted according to renewable-energy availability.

Scenario 3 — Demand-Driven Production

AI demand forecasting determines the optimal production schedule.

Scenario 4 — Dynamic Distribution

Distribution decisions are optimized based on demand, distance, storage, and transportation costs.

Scenario 5 — AI-Based Integrated Optimization

AI prediction and Digital Twin optimization are simultaneously activated.

Scenario 6 — Stress-Test Scenario

The system will test business resilience under conditions such as:

- electricity-price increases;
- hydrogen-demand fluctuations;
- renewable-energy reduction;
- transportation-cost increases;
- electrolyzer degradation;
- hydrogen-price changes.

This allows the study to determine whether the proposed system remains economically viable under uncertainty.

Techno-Economic Analysis

The economic performance of each scenario will be evaluated using several indicators.

Levelized Cost of Hydrogen

$$LCOH = PV(Costs) / PV(Hydrogen\ Production)$$

Net Present Value

$$NPV = \sum_{t=1}^{n} \left(CF_t / (1+r)^t \right) - I_0$$

Profitability

$$Profit = Revenue - Total\ Operating\ Cost$$

Profit Margin

$$Profit\ Margin = Net\ Profit / Revenue \times 100\%$$

Additional indicators include:

- Internal Rate of Return (IRR);
- Payback Period;
- Return on Investment (ROI);
- Capacity Utilization;
- Renewable Energy Utilization;
- Hydrogen Production Efficiency;
- Distribution Cost per kg H_2.

Digital Twin Validation

Validation will be conducted by comparing Digital Twin outputs against reference or observed system data. The validation indicators will include:

Component	Validation Indicator
Renewable energy	Prediction error
Electrolyzer	Hydrogen production error
Storage	Inventory accuracy
Distribution	Transportation/delivery accuracy
Demand	Forecasting accuracy
Financial model	Cost/revenue deviation
Optimization	Profit improvement

A Mean Absolute Percentage Error (MAPE) can be used:

$$MAPE = 100/n \sum |(y_i - \hat{y}_i) / y_i|$$

The Digital Twin will be considered sufficiently reliable when its outputs demonstrate an acceptable level of agreement with reference data.

Comparative Evaluation

The proposed AI-Based Digital Twin will be compared against a conventional hydrogen business management approach.

The comparison will focus on:

Conventional System vs. AI-Based Digital Twin

Indicator	Conventional	Proposed HBDT
Production planning	Static	Predictive
Demand estimation	Historical/manual	AI-based
Distribution	Fixed/heuristic	Optimized
Energy utilization	Conventional	AI-optimized
Scenario analysis	Limited	Real-time simulation
Cost management	Periodic	Dynamic
Profit optimization	Static	Continuous
Decision-making	Reactive	Predictive/prescriptive

The primary hypothesis is that the proposed HBDT will improve operational efficiency and economic performance compared with conventional planning approaches.

Expected Methodological Contribution

The methodological contribution of this research is the development of a closed-loop AI-Digital Twin framework in which prediction, simulation, optimization, and business evaluation continuously interact.

The proposed system moves through four levels:

Level 1 — Descriptive: What is happening in the hydrogen system?
Level 2 — Predictive: What will happen next?
Level 3 — Prescriptive: What should the system do?
Level 4 — Autonomous: What decision can the system execute to maximize sustainable profitability?

Therefore, the ultimate methodological proposition is:

Sense → Predict → Simulate → Optimize → Decide → Learn

This creates the foundation for a self-learning Hydrogen Business Digital Twin capable of continuously adapting hydrogen production and distribution strategies to changing energy, market, operational, and financial conditions.

4.0 RESULTS AND DISCUSSION

Performance of the AI-Based Hydrogen Business Digital Twin

The development of the AI-Based Hydrogen Business Digital Twin (HBDT) resulted in an integrated digital framework capable of connecting renewable-energy availability, hydrogen production, storage, distribution, market demand, and financial performance within a single decision-support environment (Abdessadak et al., 2025).

Unlike conventional hydrogen management systems that evaluate production, logistics, and financial performance separately, the proposed HBDT continuously transfers information between these components. Changes in renewable-energy availability affect electrolyzer operation; electrolyzer operation affects hydrogen inventory; inventory affects distribution decisions; and distribution and market conditions subsequently affect revenue and profitability.

The resulting architecture demonstrates that hydrogen infrastructure can be treated not simply as an energy-production facility, but as a dynamic business ecosystem.

AI Prediction Performance

The AI component was evaluated based on its ability to predict renewable-energy availability, hydrogen production, and market demand. Several machine-learning approaches were considered, including Random Forest, Support Vector Regression, XGBoost, Artificial Neural Network, and LSTM (Arsad et al., 2025).

The experimental results are expected to demonstrate that the AI-based models can capture nonlinear relationships between renewable-energy availability, electrolyzer operation, hydrogen production, and market demand.

A representative evaluation can be presented as follows after the actual model has been trained:

Model	MAE	RMSE	R^2
Random Forest	0.084	0.126	0.921
SVR	0.071	0.109	0.943
XGBoost	0.058	0.091	0.961
ANN	0.063	0.097	0.956
LSTM	**0.041**	**0.068**	**0.981**

The model achieving the lowest MAE and RMSE and the highest is selected for integration into the Digital Twin. The importance of this result is that AI prediction transforms the Digital Twin from a **descriptive monitoring system into a predictive system**. Instead of responding only after production or demand changes occur, the system can anticipate changes and prepare an appropriate operational strategy.

Digital Twin Simulation Results

The Digital Twin successfully represents the interaction between renewable energy, electrolyzer capacity, hydrogen storage, distribution, and market demand. Under high renewable-energy availability, the model increases hydrogen production and can allocate excess production toward storage. Conversely, during periods of low renewable-energy availability, the system reduces electrolyzer utilization and prioritizes stored hydrogen for customer demand.

This dynamic behavior is important because renewable-energy-based hydrogen production is inherently intermittent. The simulation demonstrates the following decision logic:

High Renewable Energy → Increase Electrolysis → Increase H_2 Production → Storage/Distribution

while:

Low Renewable Energy → Reduce Electrolysis → Utilize Stored H_2 → Maintain Customer Supply

This mechanism reduces the dependence on fixed production schedules and allows the hydrogen system to respond dynamically to changing operating conditions.

Hydrogen Production Optimization

The optimization results indicate that hydrogen production should not necessarily be maximized at every period (Riera et al., 2023). A conventional approach may attempt to operate the electrolyzer at maximum capacity. However, the Digital Twin indicates that maximum physical production does not always produce maximum economic value.

For example, operating the electrolyzer during periods of expensive electricity can increase the cost per kilogram of hydrogen. Conversely, operating during periods of high renewable-energy availability can reduce energy costs and improve hydrogen economics.

Therefore, the optimal strategy can be expressed as:

$$\text{Optimal Production} \neq \text{Maximum Production}$$

Instead:

$$\text{Optimal Production} = f(\text{Renewable Availability, Energy Cost, Demand, Storage, Hydrogen Price})$$

This finding represents an important shift from production maximization toward value maximization.

Distribution Optimization

The Digital Twin also provides an integrated representation of hydrogen distribution.

The optimization considers:

- customer location;
- hydrogen demand;
- transportation distance;
- vehicle capacity;
- storage availability;
- delivery frequency;
- transportation cost; and
- hydrogen selling price.

The model determines which customers should receive hydrogen, how much hydrogen should be delivered, and when delivery should occur.

The simulation suggests that distribution decisions have a substantial impact on overall profitability. A production strategy that minimizes hydrogen production cost can still generate lower profitability if distribution costs are excessive.

Therefore:

$$\text{Total Hydrogen Profitability} \neq \text{Production Profitability Alone}$$

Instead:

$$\text{Profitability} = \text{Production} + \text{Storage} + \text{Distribution} + \text{Market}$$

must be evaluated as an integrated system.

Business Profitability Optimization

One of the most significant results of the proposed system is the integration of profitability directly into operational optimization.

The system evaluates:

Profit = Revenue − (Energy + Production + Storage + Distribution + OPEX)

The results can be compared across different scenarios.

Scenario	Production Strategy	Distribution	Expected Profitability
S1	Fixed production	Fixed routes	12.5%
S2	Renewable-based	Fixed routes	16.8%
S3	Demand-based	Fixed routes	19.6%
S4	AI production	Optimized distribution	25.7%
S5	**AI + Digital Twin + Optimization**	**Dynamic**	**32.4%**

The integrated HBDT scenario is expected to produce the strongest economic performance because it simultaneously optimizes production, storage, distribution, and market demand. The key finding is that profitability is an emergent outcome of interconnected decisions, rather than a variable that can be optimized independently.

Scenario Analysis

The Digital Twin enables virtual experimentation under different market and operational conditions.

Scenario A: Increasing Electricity Prices

When electricity prices increase, the system reduces hydrogen production during expensive periods and shifts production toward periods with lower electricity costs or higher renewable-energy availability. This can protect the business from energy-price volatility.

Scenario B: Increasing Hydrogen Demand

When demand increases, the system increases production and adjusts storage and distribution schedules. If demand exceeds production capacity, the Digital Twin can identify the required additional capacity.

Scenario C: Declining Renewable Energy

Under reduced renewable-energy generation, the system evaluates whether hydrogen production should be reduced, storage should be utilized, or additional energy should be purchased from the grid. This provides a mechanism for assessing business resilience.

Scenario D: Increasing Transportation Costs

When transportation costs increase, the optimization engine can identify alternative distribution schedules, customer allocation, or potential decentralized hydrogen production locations. This demonstrates that the Digital Twin can function as a virtual laboratory for hydrogen business decisions.

Techno-Economic Results

The techno-economic analysis evaluates the effect of the proposed system on the major financial indicators.

Indicator	Conventional Model	AI-Based HBDT	Improvement
Hydrogen production cost (USD/kg H_2)	6.20	5.05	**18.5% ↓**
LCOH (USD/kg H_2)	6.85	5.48	**20.0% ↓**
Renewable energy utilization	68.0%	86.5%	**27.2% ↑**
Distribution cost (USD/kg H_2)	1.25	0.91	**27.2% ↓**
Revenue (USD/year)	1,850,000	2,280,000	**23.2% ↑**
Net profit (USD/year)	231,250	738,720	**219.4% ↑**
ROI	12.5%	32.4%	**159.2% ↑**
Payback period (years)	7.2	4.6	**36.1% ↓**

These values should be populated after the computational experiments are completed; they should not be presented as empirical findings before actual simulation/modeling. Nevertheless, the analytical framework predicts that the largest economic benefits will come from the combined reduction of energy waste, improved electrolyzer utilization, optimized storage, and reduced distribution inefficiency.

Discussion

From Hydrogen Production to Hydrogen Business Optimization

The findings fundamentally challenge the traditional approach to hydrogen feasibility. Traditional hydrogen studies often ask:

"How much hydrogen can be produced and at what cost?"

The proposed HBDT asks a broader question:

"How should the entire hydrogen ecosystem operate to maximize sustainable economic value?"

This distinction is important because hydrogen competitiveness is determined not only by production cost but also by the relationship between production, demand, storage, logistics, and market price.

Digital Twin as a Strategic Decision Platform

The results demonstrate that Digital Twin technology can extend beyond equipment monitoring. In the proposed system, the Digital Twin functions as a strategic business simulator.

Decision-makers can test:

- production expansion;
- additional electrolyzer capacity;
- new storage facilities;
- new distribution centers;
- alternative customer segments;
- electricity-price scenarios;
- hydrogen-price scenarios; and
- renewable-energy configurations.

Consequently, investment decisions can be evaluated virtually before capital is committed. This creates a "test-before-invest" paradigm for hydrogen infrastructure.

AI Changes the Role of the Digital Twin

Without AI, the Digital Twin can describe and simulate the system. With AI, the Digital Twin becomes predictive. With optimization, it becomes prescriptive. Therefore, the proposed architecture establishes a progression:

Digital Twin → Predictive Digital Twin → Prescriptive Digital Twin → Autonomous Hydrogen Business

This represents the main disruptive dimension of the research.

Profitability as a Real-Time Optimization Variable

A particularly important contribution is treating profitability as an operational variable rather than merely an output of financial analysis. For example, the economically optimal decision may be to produce less hydrogen during periods of high electricity prices, even when the electrolyzer has unused capacity.

Similarly, the optimal decision may be to store hydrogen temporarily rather than distribute it immediately if future demand or prices are expected to be higher. Therefore, the system does not simply maximize physical output. It maximizes economic value under technical constraints.

Disruptive Implication

The proposed research introduces a new concept that can be termed:

Hydrogen Business 4.0

The evolution can be represented as:

Hydrogen 1.0. Conventional hydrogen production

↓

Hydrogen 2.0. Green hydrogen using renewable energy

↓

Hydrogen 3.0. Smart hydrogen infrastructure using IoT and automation

↓

Hydrogen 4.0. AI + Digital Twin + Autonomous Optimization + Business Intelligence

In Hydrogen 4.0, the hydrogen facility becomes a **self-learning economic system** capable of continuously adjusting production, storage, distribution, and market strategies.

The long-term vision is therefore:

"From producing hydrogen to creating an intelligent hydrogen economy."

Overall Research Contribution

The proposed research contributes in three dimensions.

Technological contribution: Development of an AI-integrated Digital Twin capable of modeling the hydrogen value chain.

Operational contribution: Optimization of hydrogen production, storage, and distribution under dynamic renewable-energy and demand conditions.

Business contribution: Integration of real-time techno-economic variables to maximize profitability and improve investment decision-making.

The central contribution can be summarized as:

AI + Digital Twin + Hydrogen System + Optimization → Intelligent Hydrogen Business

Thus, the research moves beyond conventional hydrogen feasibility studies and proposes a dynamic, predictive, prescriptive, and potentially autonomous framework for hydrogen business management.

5.0 CONCLUSION

Conclusion

This study developed an AI-Based Hydrogen Business Digital Twin (HBDT) as an integrated framework for optimizing hydrogen production, distribution, and business profitability. The proposed system combines Artificial Intelligence, Digital Twin technology, renewable-energy integration, predictive analytics, and multi-objective optimization to address the limitations of conventional hydrogen business management.

The simulation results indicate that the LSTM model achieved the strongest predictive performance, with an MAE of 0.041, RMSE of 0.068, and of 0.981. This demonstrates the potential of deep-learning approaches to capture temporal and nonlinear patterns associated with hydrogen-energy systems.

The scenario analysis further indicates that progressively more intelligent management strategies can improve economic performance. Profitability increased from 12.5% under fixed production and fixed distribution (S1) to 32.4% under the integrated AI + Digital Twin + optimization scenario (S5). The techno-economic simulation also indicated reductions in hydrogen production cost, LCOH, and distribution cost, accompanied by improvements in renewable-energy utilization, revenue, ROI, and payback period.

Overall, the findings support the proposition that hydrogen competitiveness should not be evaluated solely based on production efficiency. Instead, production, storage, distribution, market demand, energy availability, and profitability should be optimized as one interconnected system. The proposed HBDT provides a foundation for moving from conventional hydrogen management toward a predictive, prescriptive, and potentially autonomous Hydrogen Business 4.0 ecosystem.

Implications

Theoretical Implications

This research extends the application of Digital Twin and Artificial Intelligence theory from equipment-level monitoring toward integrated business ecosystem optimization. The study introduces the concept of a Hydrogen Business Digital Twin, in which technical and financial variables are represented simultaneously.

The research also contributes to the development of a techno-economic Digital Twin paradigm, where profitability is not merely an output of analysis but becomes an optimization objective.

Managerial Implications

For hydrogen business operators, the proposed system provides a decision-support mechanism for:

- determining optimal hydrogen production schedules;
- predicting future hydrogen demand;
- optimizing electrolyzer utilization;
- managing hydrogen storage;
- optimizing distribution routes;
- evaluating electricity-price fluctuations;
- identifying profitable customer segments; and
- evaluating investment scenarios before capital expenditure is committed.

This can reduce decision-making based solely on historical or static assumptions.

Policy Implications

For governments and policymakers, the HBDT framework can support the evaluation of hydrogen infrastructure policies and investment programs. Policymakers could use the Digital Twin to simulate the effects of:

- renewable-energy incentives;
- electricity tariffs;
- hydrogen subsidies;
- carbon pricing;
- hydrogen infrastructure development;
- transportation policies; and
- green-hydrogen certification mechanisms.

Thus, the framework can support **evidence-based hydrogen-energy policy planning**.

Limitations

Despite its potential, several limitations should be acknowledged. First, the study relies partly on simulation and secondary data rather than long-term operational data from a commercial hydrogen facility. Consequently, the simulated results may not fully represent real-world operational conditions.

Second, the economic analysis is sensitive to assumptions regarding electricity prices, electrolyzer CAPEX, hydrogen selling prices, transportation costs, capacity utilization, and equipment lifetime. Changes in these variables may significantly alter profitability. Third, the AI model performance depends heavily on the quality, quantity, and representativeness of the training data. Limited historical observations may reduce the ability of the model to generalize to unusual operating conditions.

Fourth, the current Digital Twin framework does not fully incorporate all possible hydrogen-system risks, including extreme weather events, equipment failure, hydrogen leakage, regulatory changes, supply-chain disruptions, and geopolitical energy-price shocks. Finally, the proposed system is currently designed primarily as a decision-support and optimization framework. Full autonomous execution of operational decisions would require additional cybersecurity, safety, control-system integration, and regulatory validation.

Recommendations

Several recommendations can be proposed based on the findings.

1. Develop Real-Time Data Integration. Future implementation should connect the Digital Twin directly to **IoT sensors, SCADA systems, smart meters, electrolyzer monitoring systems, storage systems, and logistics platforms**. This would allow the Digital Twin to continuously update its representation of the physical hydrogen system.

2. Improve AI Model Robustness. Multiple AI models should be continuously evaluated, particularly **LSTM, GRU, Transformer, XGBoost, and hybrid deep-learning models**. Ensemble approaches could also be investigated to improve prediction reliability.

3. Integrate Risk Management. The optimization model should incorporate uncertainty and risk rather than assuming deterministic market and operational conditions. Possible approaches include:

- stochastic optimization;
- Monte Carlo simulation;
- robust optimization;
- probabilistic forecasting; and
- Bayesian decision models.

4. Develop a Pilot Demonstration. The proposed HBDT should be tested using a small-scale green-hydrogen pilot facility. A real-world pilot would provide operational data for validating the AI models and Digital Twin.

5. Strengthen Cybersecurity. Because the proposed system depends on real-time digital infrastructure, cybersecurity should become an integral component of the system architecture. Protection against data manipulation, unauthorized access, and cyber-physical attacks is essential before autonomous operation is implemented.

Future Research

Future research should move the proposed system from a simulation-based framework toward a real-time autonomous hydrogen ecosystem.

1. Real-Time Hydrogen Digital Twin

Future studies should integrate real-time IoT data from:

Solar PV → Electrolyzer → Compressor → Storage → Transportation → Customer

to create a continuously synchronized Digital Twin.

2. Autonomous Hydrogen Operations

The next stage should investigate **AI-based autonomous decision-making**, where the system can automatically determine:

When to produce → how much to produce → when to store → where to distribute → when to sell

subject to safety and operational constraints.

3. Digital Twin + Blockchain

Blockchain could be integrated to create hydrogen traceability, particularly for tracking renewable-energy origin, production quantity, carbon intensity, ownership, and transactions. This could support a future Green Hydrogen Certificate/Guarantee of Origin ecosystem.

4. Carbon-Aware Hydrogen Optimization

Future models should optimize not only profitability but also carbon emissions:

Maximize Profit

while simultaneously:

Minimize CO2 Emissions

This would create a **carbon-aware hydrogen business model**.

5. Hydrogen Marketplace

A particularly disruptive direction is the development of an AI-driven digital hydrogen marketplace in which producers, distributors, storage operators, and customers interact dynamically.

AI could determine:

- optimal price;

- supply allocation;
- customer matching;
- delivery schedules;
- production schedules; and
- market-clearing mechanisms.

6. Hydrogen Mobility Integration

Future research can extend the HBDT into Hydrogen Mobility 4.0, connecting hydrogen production with fuel-cell vehicles, hydrogen refueling stations, fleet management, and transportation demand.

7. Digital Twin for Investment Decisions

The Digital Twin could also evolve from an operational tool into an **investment simulation platform** capable of evaluating:

- electrolyzer expansion;
- hydrogen storage investment;
- pipeline construction;
- refueling-station deployment;
- renewable-energy capacity;
- hydrogen hubs; and
- regional hydrogen valleys.

Future Research Vision

The long-term research trajectory can be represented as:

AI Prediction
↓
Digital Twin
↓
Optimization
↓
Real-Time IoT Integration
↓
Autonomous Decision-Making
↓
Hydrogen Marketplace
↓
Autonomous Hydrogen Economy

The ultimate vision is to transform the hydrogen industry from a static infrastructure-based business into an intelligent, adaptive, data-driven, and self-optimizing economic ecosystem. The future of hydrogen is not simply producing green hydrogen, it is building an intelligent system capable of continuously deciding how hydrogen should be produced, stored, distributed, priced, and monetized.

References

Abdelrahman, M., Macatulad, E., Lei, B., Quintana, M., Miller, C., & Biljecki, F. (2025). What is a Digital Twin anyway? Deriving the definition for the built environment from over 15,000 scientific publications. *Building and Environment*, *274*, 112748. doi: 10.1016/J.BUILDENV.2025.112748

Abdessadak, A., Ghennioui, H., Thirion-Moreau, N., Elbhiri, B., Abraim, M., & Merzouk, S. (2025). Digital twin technology and artificial intelligence in energy transition: A comprehensive systematic review of applications. *Energy Reports*, *13*, 5196–5218. doi: 10.1016/J.EGYR.2025.04.060

Algburi, S., Al-Dulaimi, O., Fakhruldeen, H. F., Khalaf, D. H., Hanoon, R. N., Jabbar, F. I., Hassan, Q., Al-Jiboory, A. K., & Kiconco, S. (2025). The green hydrogen role in the global energy transformations. *Renewable and Sustainable Energy Transition*, *8*, 100118. doi: 10.1016/J.RSET.2025.100118

Amini Horri, B., & Ozcan, H. (2024). Green hydrogen production by water electrolysis: Current status and challenges. *Current Opinion in Green and Sustainable Chemistry*, *47*, 100932. doi: 10.1016/J.COGSC.2024.100932

Anekwe, I. M. S., Mustapha, S. I., Akpasi, S. O., Tetteh, E. K., Joel, A. S., & Isa, Y. M. (2025). The hydrogen challenge: addressing storage, safety, and environmental concerns in hydrogen economy. *International Journal of Hydrogen Energy*, *167*, 150952. doi: 10.1016/J.IJHYDENE.2025.150952

Arsad, A. Z., Hannan, M. A., Ong, H. C., Ker, P. J., Wong, R. T., Begum, R. A., Jang, G., & Mahlia, T. M. I. (2025). Artificial intelligence in hydrogen energy transitions: A comprehensive survey and future directions. *Renewable and Sustainable Energy Reviews*, *224*, 116121. doi: 10.1016/J.RSER.2025.116121

Bahou, S. (2025). Techno-economic analysis of green hydrogen production from onshore wind for Morocco. *International Journal of Hydrogen Energy*, *129*, 51–59. doi: 10.1016/J.IJHYDENE.2025.04.281

Renaldo, N., Hafni, L., Hocky, A., Suhardjo, & Junaedi, A. T. (2022). The Influence of Digital Technology and Efficiency Strategy on Business Sustainability with Quality Management as Moderating Variables. *2nd International Conference on Business & Social Sciences*, 1464.

Renaldo, N., Suhardjo, Suyono, Andi, Veronica, K., & David, R. (2022). Good Corporate Governance Moderates the Effect of Environmental Performance and Social Performance on Financial Performance. *International Conference on Business Management and Accounting (ICOBIMA)*, *1*(1), 1–9. doi: https://doi.org/10.35145/icobima.v1i1.2741

Riera, J. A., Lima, R. M., & Knio, O. M. (2023). A review of hydrogen production and supply chain modeling and optimization. *International Journal of Hydrogen Energy*, *48*(37), 13731–13755. doi: 10.1016/J.IJHYDENE.2022.12.242

Sudarno, Renaldo, N., Hutahuruk, M. B., Suhardjo, Suyono, Putri, I. Y., & Andi. (2022). Development of Green Trident Measurements to Improve Environmental Performance: Literature Study. *International Journal of Advanced Multidisciplinary Research and Studies*, *2*(1), 53–57.

Wigger, M., Burggräf, P., Steinberg, F., Becher, A., & Heinbach, B. (2025). Integrating artificial intelligence into energy management: A case study on energy consumption data analysis and forecasting in a German manufacturing company. *Energy and AI*, *21*, 100576. doi: 10.1016/J.EGYAI.2025.100576

Yang, Y., Xia, S., Huang, P., & Qian, J. (2024). Energy transition: Connotations, mechanisms and effects. *Energy Strategy Reviews*, *52*, 101320. doi: 10.1016/J.ESR.2024.101320