Hydrogen Supply Chain Optimization

Summary

This report presents a comparative analysis of two control strategies—Model Predictive Control (MPC) and Rule-Based Control (RBC)—for optimizing the operation of a solar-powered hydrogen supply chain. The supply chain consists of renewable electricity input, battery energy storage, hydrogen production via electrolysis, and hydrogen storage and sales. Using a Python-based simulation framework, both strategies are evaluated under identical time-varying conditions of solar availability, electricity pricing, and hydrogen demand.

The MPC strategy leverages forecasted disturbances and rolling-horizon optimization to allocate energy resources in a cost-effective manner while satisfying system constraints. In contrast, the RBC approach applies fixed, heuristic rules and operates reactively without predictive capabilities. Results show that MPC achieves significantly higher cost-efficiency by avoiding expensive grid electricity, aligning production with demand, and maximizing hydrogen utilization. The RBC system, although simpler, suffers from overproduction, high energy waste, and severe financial losses due to excessive grid usage. Both strategies show limited battery engagement, indicating a potential area for system design improvement.

Overall, the study highlights the advantages of predictive, optimization-based control for managing hydrogen systems under uncertainty, and lays the foundation for future research in adaptive, data-driven methods such as reinforcement learning.

Introduction

A **supply chain** refers to the interconnected flow of materials, energy, and information across various stages of production, storage, and delivery. It encompasses the coordination of suppliers, manufacturing processes, and logistics to ensure that goods or services move efficiently from their origin to the final consumer. In modern energy systems, supply chains must be designed not only for cost-effectiveness but also for adaptability, resilience, and sustainability.

The **hydrogen supply chain** represents a complex subset of this broader system. It begins with energy inputs—either from renewable sources like solar and wind, or from fossil-based sources with carbon capture. These are used in various hydrogen production technologies such as water electrolysis or steam methane reforming. Once produced, hydrogen must be efficiently stored, transported, and distributed to meet demand in sectors like industry, transport, and power generation. Some supply chains also involve conversion to hydrogen carriers (e.g., ammonia or methanol) for long-distance export.

Optimizing the hydrogen supply chain is essential due to several challenges. First, hydrogen production and storage are capital- and energy-intensive. Second, renewable electricity, key to green hydrogen, is inherently variable and uncertain. Third, hydrogen demand fluctuates across time and sectors, requiring systems that can dynamically adapt. Without optimization, the system risks inefficiencies, high emissions, and supply unreliability.

By employing advanced optimization and control strategies, it becomes possible to enhance efficiency, reduce operational costs and emissions, and ensure a more reliable hydrogen delivery system. This is particularly crucial for enabling hydrogen to play a central role in future decarbonized energy systems.

Literature Review: Solution Strategies for Hydrogen Supply Chain Optimization

Optimizing the hydrogen supply chain (HSC) is critical for enabling hydrogen's role in a low-carbon future. Due to its complexity, various solution strategies have been developed to address the challenges posed by fluctuating renewable energy supply, high storage costs, and dynamic demand. These strategies can be broadly categorized into rule-based controls, heuristic methods, and optimization-based techniques.

1. Overview of Solution Strategies

- **Rule-Based Approaches** use predefined logic or threshold rules to govern system operation. While these methods are intuitive and simple to implement, they are inherently reactive and lack adaptability to future uncertainties. They are often applied in early-stage feasibility studies or in systems with limited computational resources [1].
- **Heuristic Methods** rely on empirical knowledge, simplified rules, or learning from historical trends. Though faster and computationally cheaper than full optimization, they generally offer lower accuracy and may fail to respect critical system constraints [2].
- **Optimization-Based Methods** formulate the HSC problem as a mathematical program, seeking to minimize objectives such as cost or emissions under

operational, technical, and policy constraints. This family of methods is highly adaptable and can be applied to both short-term operations and long-term planning. A recent review by Sadeghi et al. [3] emphasizes the growing role of mathematical programming, particularly Mixed Integer Linear Programming (MILP), in hydrogen system design and operations.

2. Rule-Based Control as a Benchmark

In this study, a **rule-based control (RBC)** scheme is implemented as a benchmark. This approach operates using simple threshold logic, for example, charging batteries only when solar energy exceeds a limit or prioritizing hydrogen production when excess renewable energy is available. RBC does not incorporate forecasting or optimization and instead responds to the real-time system state. While not optimal, this approach is widely used in preliminary control schemes due to its clarity and low implementation cost [4].

3. Optimization-Based Methods: MPC and MILP

More rigorous strategies include **Model Predictive Control (MPC)** and **Mixed Integer Linear Programming (MILP)**. MPC optimizes system operation over a moving time horizon using real-time forecasts, adapting decisions to current states and predicted changes. It is particularly suited for operational control in dynamic environments [5], such as those with variable solar generation and shifting hydrogen demand. MILP, by contrast, is often used in strategic planning and design, including infrastructure investment, technology selection, and location optimization [6].

These advanced methods allow for constraint-aware, multi-timescale decision-making and have been applied to integrated energy-hydrogen systems, demonstrating substantial gains in efficiency, reliability, and cost-effectiveness.

Methods

1. Rule-Based Control (RBC) Logic

The Rule-Based Control (RBC) approach is designed as a simple, heuristic benchmark to simulate hydrogen system operation under basic control logic. It operates reactively, making real-time decisions based on current system states without any foresight or optimization. The control logic is structured around prioritizing renewable energy utilization, maintaining battery and hydrogen storage within safe bounds, and meeting hydrogen demand efficiently.

The RBC system follows these operational rules:

- **Solar Usage Priority**
  - Solar power is prioritized for direct use in the electrolyzer.
  - Any excess solar is diverted to battery charging if the state of charge (SOC) is below 70%.
- **Battery Charging**
  - The battery is charged only when SOC is below 80%.
  - Charging stops if SOC reaches or exceeds 80% or if the charging rate hits its technical limit.
- **Battery Discharging**
  - The battery discharges only when SOC exceeds 20% and solar energy is insufficient.
  - Discharging is used exclusively to help meet unmet hydrogen production demand.
- **Grid Use**
  - Grid electricity is used as a last resort, only when solar and battery energy cannot meet the power requirements of the electrolyzer.
  - Grid usage is limited to the difference between the electrolyzer's maximum input and the sum of available solar and battery power.
- **Electrolyzer Operation**
  - The electrolyzer is operated at maximum capacity using all available power, prioritizing sources in the order: solar → battery → grid.
  - Produced hydrogen is used to meet current demand first, and any excess is stored.
- **Hydrogen Storage Logic**
  - Hydrogen is stored only if the storage tank is below 90% of its maximum capacity.
  - Hydrogen is discharged from storage only when current production is insufficient to meet demand.

This logic ensures the system remains simple, interpretable, and computationally light, serving as a valuable benchmark for comparing against more sophisticated optimization-based methods.

2. Model Predictive Control (MPC)

Model Predictive Control (MPC) is a dynamic optimization-based control strategy that continuously solves a constrained optimization problem over a future prediction horizon. At each time step, it incorporates updated forecasts and system states, computes an optimal control trajectory, and implements only the first control action before re-optimizing at the next step. This makes MPC particularly suitable for systems with time-varying inputs, delays, and competing objectives — such as the hydrogen supply chain with its reliance on fluctuating solar generation and dynamic hydrogen demand.

The MPC framework integrates three core components: system modeling, variable classification, and optimization formulation. The implementation in this study is tailored to a hydrogen supply chain consisting of solar energy supply, battery storage, electrolytic hydrogen production, and hydrogen storage and distribution systems.

Process Model

The hydrogen supply chain is modeled using deterministic mass and energy balances. At each time step, the system models how energy from solar, grid, and battery sources is allocated to the electrolyzer, and how hydrogen is produced, stored, and sold. The model includes operational constraints on maximum charging/discharging rates, state-of-charge (SOC) limits, electrolyzer capacity, and hydrogen storage capacity.

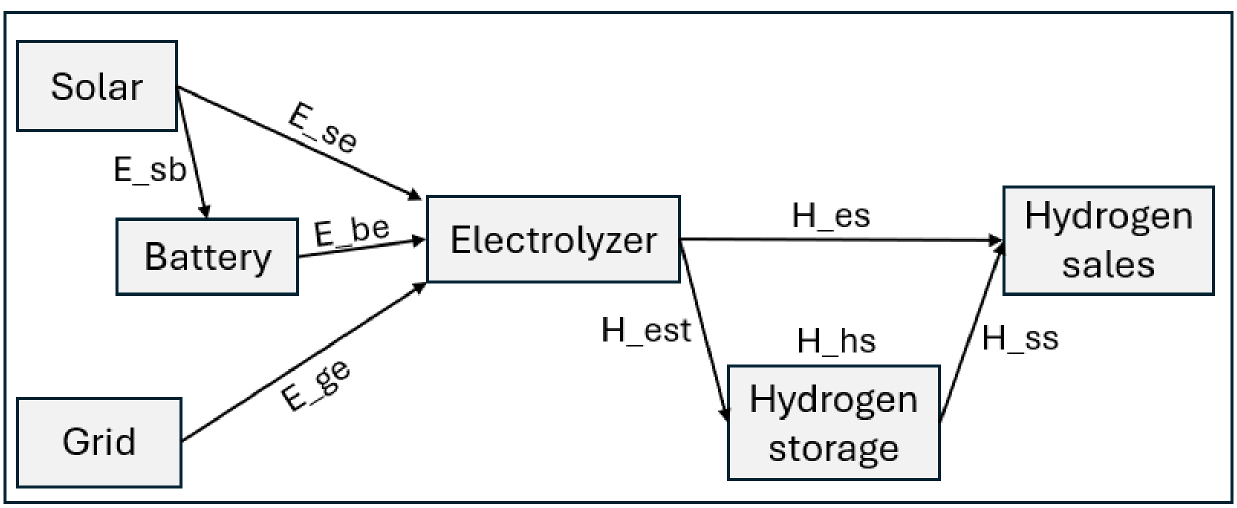

Figure 1. Process model

Mass and Energy Balance

The MPC model incorporates detailed mass and energy balances to describe the physical behavior of the hydrogen supply chain. These equations govern the interaction of solar, battery, and grid energy with hydrogen production, storage, and delivery.

1. Solar Energy Allocation

Solar energy is first used to power the electrolyzer. Excess solar can be directed to charge the battery:

$$P_{solar}[t]=E_{se}[t]+E_{sb}[t]$$

Where:

- $E_{se}[t]$: Solar to electrolyzer
- $E_{sb}[t]$: Solar to battery

2. Electricity Flow into Electrolyzer

The total power input to the electrolyzer includes solar, battery discharge, and grid supply:

$$P_{elec}[t]=P_{solar}[t]-E_{sb}[t]+E_{be}[t]+E_{ge}[t]$$

3. Hydrogen Production via Electrolysis

Hydrogen production is modeled as a function of electricity input with an electrolyzer efficiency η_{elec}:

$$H_{prod}[t]=\eta_{elec}\cdot P_{elec}[t]$$

4. Battery Energy Storage Dynamics

The battery state-of-charge (SOC) evolves based on charging and discharging activity, accounting for round-trip efficiency:

$$SOC[t]=SOC[t-1]+\eta_{ch}\cdot E_{sb}[t]-E_{be}[t]/\eta_{dch}$$

5. Hydrogen Storage Dynamics

Hydrogen storage state evolves from net hydrogen inflows and outflows:

$$Hstore[t]=Hstore[t-1]+Hest[t]-Hss[t]$$

6. Hydrogen Sales Flow

Total hydrogen sold is the sum of direct sales from production and sales from storage:

$$Hsales[t]=Hes[t]+Hss[t]$$

Feasibility and Operational Constraints

The system is subject to several physical and operational constraints to ensure feasibility:

1. Electrolyzer-to-Sales Constraint

Only hydrogen produced in the current step can be sold directly:

$$Hes[t]\leq Hprod[t]$$

2. Storage-to-Sales Constraint

Hydrogen sold from storage cannot exceed stored amount:

$$Hss[t]\leq Hstore[t]$$

3. Hydrogen Demand Constraint

Total hydrogen sold must not exceed forecasted demand:

$$Hsales[t]\leq DH2[t]$$

4. Hydrogen Storage Capacity Limit

Storage cannot exceed its physical limit:

$$Hstore[t]\leq Hstoremax$$

5. Battery Charging/Discharging and SOC Constraints

Battery operations are limited by power capacity and SOC bounds:

$$Esb[t],Ebe[t]\leq Pbatmax$$

$$0\leq SOC[t]\leq SOCmax$$

6. Electrolyzer Power Limit

Power input to the electrolyzer is limited by its maximum operating capacity:

$$Pelec[t] \leq Pelecmax$$

7. Non-Negativity Constraints

All energy and hydrogen flow variables must be non-negative:

$Esb[t], Ebe[t], Ege[t], Pelec[t] \geq 0$

$Hprod[t], Hes[t], Hest[t], Hss[t], Hstore[t] \geq 0$

Real-Time Models and Forecasts

Effective implementation of Model Predictive Control (MPC) relies on accurate real-time models and reliable forecasts of key disturbances. In this hydrogen supply chain, the main disturbances include **solar availability**, **grid electricity price**, and **hydrogen demand**. These are modeled as time-varying functions with predictable diurnal patterns.

1. Real-Time Profiles

The following functions define the real-time behavior of key inputs:

Solar Availability: Modeled as a sinusoidal profile to represent day-night cycles and variability in solar radiation:

$$\text{Solar}_{\text{real}}(t) = 100 \cdot \left(0.8 + 0.1 \cdot \sin\left(\frac{2\pi t}{24}\right)\right)$$

Grid Electricity Price

Modeled with a cosine variation to reflect daily price fluctuations:

$$C_{\text{grid, real}}(t) = 75 + 10 \cdot \cos\left(\frac{2\pi t}{24}\right)$$

Hydrogen Demand

Includes a phase shift to simulate consumption peaks at different times of day:

$$D_{\text{H2, real}}(t) = 100 + 10 \cdot \sin\left(\frac{2\pi t}{24} - \frac{\pi}{3}\right)$$

2. Forecasting with Uncertainty

At each time step, the controller forecasts future values of disturbances using a statistical model. Forecasts incorporate increasing uncertainty the further they extend into the prediction horizon. The general forecast equation is:

$$\hat{X}(t,\delta) = X_{\text{real}}(t) + \mathcal{N}\left(0,\sigma_0 \cdot \sqrt{1 + \alpha \cdot \delta}\right)$$

Where:

δ: steps into the future

σ_0 : initial standard deviation

α: controls forecast uncertainty growth

This forecasting method is applied to:

$\text{Solar}_{\text{avail}}[t]$

$C_{\text{grid}}[t]$

$D_{\text{H2}}[t]$

These predicted values are treated as fixed parameters within each optimization step, providing foresight to the MPC controller.

3. Integration into the Optimization Problem

The forecasted variables feed directly into the **objective function**, which aims to minimize cost while maximizing hydrogen sales. Forecasted grid prices $C_{\text{grid}}[t]$ and hydrogen demand $D_{\text{H2}}[t]$ influence the trade-off between energy cost and sales revenue. Forecasted solar availability $\text{Solar}_{\text{avail}}[t]$ determines how much free renewable energy can be leveraged (see equation 1 for solar allocation logic and equation 2 for electrolyzer power input).

4. Constraint Overview

The forecasted inputs are used in conjunction with a set of physical and operational constraints:

- **Hydrogen Production**: Based on electrolyzer input power (see equation 2)
- **Battery SOC Update**: Tracks charging/discharging dynamics (see equation 4)
- **Hydrogen Storage**: Captures inflow and outflow from tank (see equation 5)
- **Hydrogen Sales Logic**: Ensures hydrogen is only sold if available (see equation 6 and related constraints)

- **Demand and Capacity Limits**: Prevent overselling and overcharging (refer to constraints under section "Feasibility and Operational Constraints")

Together, these real-time models and forecasts allow MPC to anticipate future states, respond to variability, and operate the hydrogen system efficiently under uncertainty.

2. System Variables

- **Control Variables**
  - Esb[t]: Solar to battery
  - Ebe[t]: Battery to electrolyzer
  - Ege[t]: Grid to electrolyzer
  - Hes[t]: Hydrogen to sales
  - Hest[t]: Hydrogen to storage
  - Hss[t]: Hydrogen from storage
- **State Variables**
  - SOC[t]: Battery state-of-charge
  - Hstore[t]: Hydrogen storage level
- **Derived Variables**
  - Pelec[t]: Power input to electrolyzer
  - Hprod[t]: Hydrogen production
  - Hsales[t]=Hes[t]+Hss[t]: Hydrogen sold
- **Disturbance and Measured Outputs**
  - Real-time forecasts of:
    - Solar availability
    - Grid electricity price
    - Hydrogen demand

3. Optimization Formulation

Objective Function

The MPC minimizes net cost over the prediction horizon by optimizing the use of energy sources and maximizing hydrogen sales:

$$\min \sum_{t=0}^{T_p} \left[(C_{\text{grid}} + \text{CO}_2\text{Tax}) \cdot E_{ge}[t] + C_{\text{bat}} \cdot (E_{sb}[t] + E_{be}[t]) + C_{\text{store}} \cdot H_{\text{store}}[t] - P_{\text{H2}} \cdot H_{\text{sales}}[t] \right]$$

Constraints

The optimization is subject to:

- Power and hydrogen balance equations
- Capacity limits:

$$P_{\text{elec}}[t] \leq P_{\max}$$
$$SOC[t] \leq SOC_{\max}$$
$$H_{\text{store}}[t] \leq H_{\text{store,max}}$$
$$E_{sb}[t], E_{be}[t] \leq P_{\text{bat,max}}$$

Non-negativity and logical coupling constraints (e.g., H_2 storage only from production)

Prediction and Control Horizons

- Prediction horizon $T_p = 12$ hours
- Control horizon: Only the first hour's decision is implemented; optimization is repeated at the next step (rolling horizon strategy).

Results and Discussion

This section presents and analyzes the performance outcomes of the **Model Predictive Control (MPC)** strategy versus a **Rule-Based Control (RBC)** baseline for the hydrogen supply chain. The comparison is based on key performance indicators (KPIs), including energy usage, hydrogen production and sales, cost breakdowns, and overall profit. The goal is to evaluate the effectiveness of predictive optimization (MPC) against a reactive, fixed-logic approach (RBC).

1. **KPI Summary: MPC vs. Rule-Based Control**

Metric	**MPC**	**Rule-Based**
Solar Used (E_se)	13,434.74	13,440.00
Grid Energy Used (E_ge)	0.00	36,560.00
Battery Charge (E_sb)	0.00	0.00
Battery Discharge (E_be)	0.00	400.00
Electrolyzer Energy	13,434.74	50,400.00
Hydrogen Produced	9,404.32	35,280.00
Hydrogen Sold (Total)	9,704.32	16,800.00
↳ From Production (H_es)	9,169.02	16,800.00
↳ From Storage (H_ss)	535.30	0.00
Hydrogen Sent to Storage (H_est)	235.30	680.73
Revenue from H_2 Sales ($)	97,043.21	168,000.00
Grid Cost ($)	0.00	2,924,800.00
Battery Cost ($)	0.00	400.00
Electrolyzer Cost ($)	13,434.74	50,400.00
Storage Cost ($)	144.98	16,242.02
Total Cost ($)	**13,579.73**	**2,991,842.02**
Net Profit ($)	**83,463.48**	**−2,823,842.02**

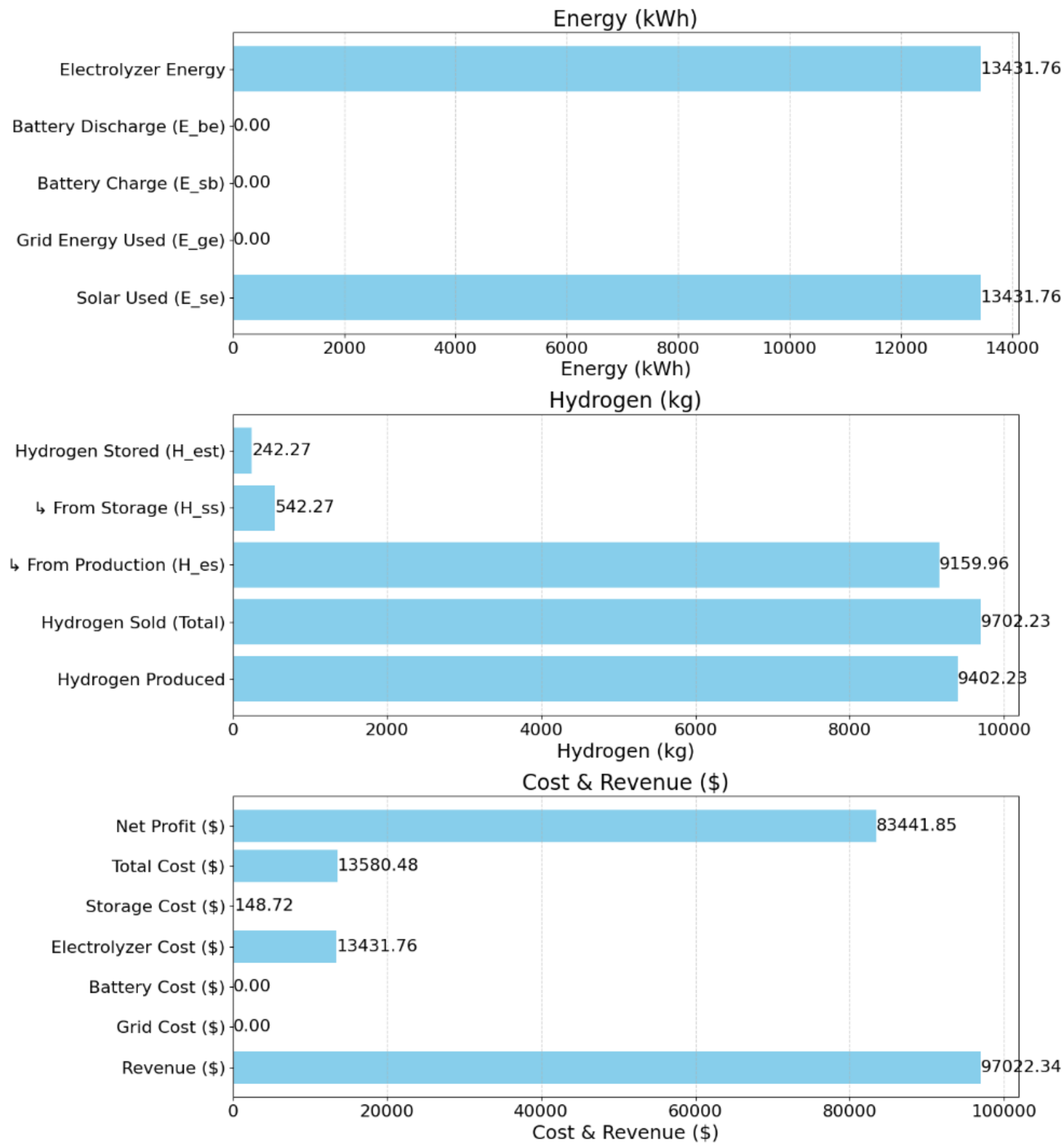

Figure 2. MPC KPIs

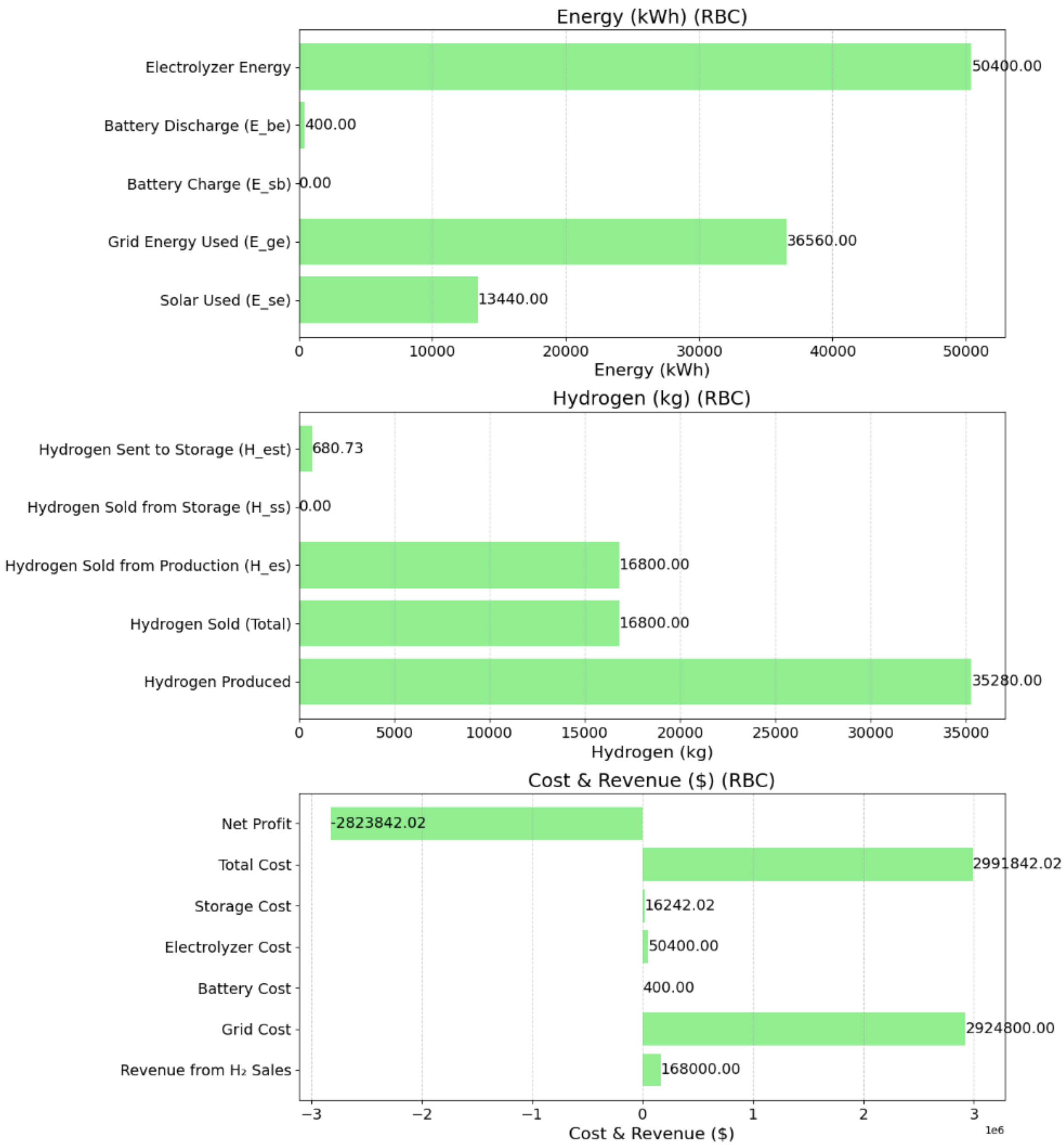

Figure 3. Rule-based control KPIs

Analysis and Interpretation of Results

The MPC strategy demonstrates a markedly superior performance over the rule-based approach across nearly all key metrics. Both strategies make full use of the available solar energy, as evidenced by nearly identical values for solar usage—13,434.74 kWh for MPC versus 13,440.00 kWh for RBC. However, the real divergence begins in how each strategy handles the energy shortfall and fluctuating hydrogen demand beyond what solar can cover.

Under MPC, the system intelligently manages its operation to avoid using any grid electricity, instead relying solely on forecasted solar power to supply the electrolyzer. In contrast, the RBC strategy consumes a staggering 36,560 kWh of grid electricity. Given the grid's cost, calculated at $80 per MWh including a $40 base and a $40 CO_2 tax, this results in an immense energy bill of $2.92 million. The stark difference stems from the fact that MPC is capable of predicting future solar availability and hydrogen demand, enabling it to avoid costly, reactive decisions. In contrast, the rule-based system, operating without any forecasting, falls back on the grid to meet its production targets, even when demand does not justify it.

This inefficiency is further evident in the hydrogen production and utilization metrics. The RBC model produces over 35,000 kg of hydrogen, yet it only manages to sell 16,800 kg. This indicates a major mismatch between production and actual demand—an overproduction problem stemming from the system's inability to anticipate future hydrogen consumption patterns. Meanwhile, MPC produces just over 9,400 kg of hydrogen and remarkably sells over 9,700 kg, partly through strategic use of stored hydrogen. This efficient matching of supply and demand illustrates MPC's ability to balance production with consumption over time, using forecasts and system feedback to adjust decisions continuously.

Despite selling less total hydrogen, the MPC strategy yields significantly better economic results. It incurs only $13,579 in total operating costs—mostly from electrolyzer usage and minimal storage—while generating $97,043 in revenue, leading to a net profit of $83,463. The RBC model, on the other hand, faces total costs nearing $3 million, largely due to grid electricity usage, and ends up with a dramatic financial loss of $2.82 million—even though it achieves higher revenue on paper. This stark loss occurs because the cost of grid electricity ($80/MWh) is eight times higher than the revenue obtained from selling the hydrogen it helps produce ($10/kg). In other words, every unit of grid electricity used results in a net economic deficit.

Notably, neither control strategy engages the battery meaningfully—battery charge and discharge values remain near zero. This implies that the system's sizing or thresholds could be revisited to better utilize storage flexibility in future implementations.

These findings underscore the importance of predictive, optimization-based control in managing complex energy systems. MPC's anticipatory planning and constraint-aware decisions lead to significant economic and operational benefits compared to the reactive, rigid approach used by rule-based control.

Conclusion

This study demonstrates the superiority of Model Predictive Control (MPC) over Rule-Based Control (RBC) in managing the operations of a hydrogen supply chain powered primarily by solar energy. The MPC strategy delivers significant economic advantages by optimizing energy allocation, strictly avoiding the use of costly grid electricity, and strategically aligning hydrogen production with forecasted demand. In contrast, the RBC approach—driven by heuristic rules and lacking predictive capability—suffers from overproduction, inefficient energy use, and substantial financial losses due to excessive reliance on grid power.

While both methods make full use of solar availability, only MPC ensures high hydrogen utilization and cost-efficiency by leveraging forecasting and rolling-horizon optimization. The RBC system, unable to anticipate future demand, produces far more hydrogen than it can sell, resulting in high storage losses and wasted energy. Interestingly, battery usage remains low in both approaches, suggesting potential underutilization of this asset and room for design improvement. Overall, MPC proves to be an economically sustainable control strategy that adapts to time-varying conditions while minimizing operational waste.

Future Work

Building upon these findings, future research could explore the integration of **reinforcement learning (RL)** for hydrogen supply chain optimization. Unlike MPC, which depends on explicit forecasts and model parameters, RL offers a **model-free, adaptive approach** that learns optimal control policies directly from system interactions. This can be especially valuable in highly uncertain environments or where system dynamics are partially known. Furthermore, **multi-agent reinforcement learning (MARL)** presents a promising direction for distributed hydrogen supply chains, where various agents—such as production units, storage facilities, and end-users—can coordinate decisions autonomously. Such decentralized frameworks could enhance scalability, resilience, and flexibility in large, complex energy networks, offering a next-generation alternative to centralized, rule- or model-based controllers.

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