Day-ahead Optimization of a Green Hydrogen Hub Using Synthetic Hydrogen Demand Data

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Abstract— **This paper introduces a comprehensive methodology for day-ahead planning of renewable energy systems geared toward green hydrogen and ammonia production. This approach is a forecasting algorithm that uses synthetic data, which feeds a short-term load forecasting (STLF) algorithm to predict the 24-hour hydrogen demand. This capability enables the optimization of hourly system operations, with the goal of maximizing profitability while maintaining system efficiency. The case study presented includes a renewable energy source – photovoltaic power plant (PV) – and a grid connection, which supply power to an electrolyser. Essential supporting infrastructure such as the auxiliary system of the electrolyser is incorporated into the model. Additionally, an electrochemical battery - a battery energy storage system (BESS) - is incorporated, which helps to keep a high electrolyser load factor and creates smoother operating profiles. This BESS also allows the system to contribute to the energy reserves market, enhancing its economic and operational viability.**

Index Terms--**Synthetic data, Short-term load forecasting (STLF), Green Hydrogen, Battery Energy Storage System, Reserves Market.**

I. INTRODUCTION

Green hydrogen is becoming a crucial element in the shift towards a sustainable, low-carbon economy, as outlined in [1], [2]. The production of green hydrogen from renewable energy sources such as wind, solar, and hydropower is drawing considerable attention, given its potential to decarbonize multiple industries, as highlighted in [3], [4]. As green hydrogen gains importance as a clean energy carrier, it is crucial to develop an in-depth understanding of optimal plant management strategies.

Efficient operation of electrolysers is essential to maximize green hydrogen production, as demonstrated in [5], where the study finds that optimal planning can significantly reduce both overall costs and environmental impacts. Advanced control systems, predictive maintenance algorithms [6], and real-time monitoring technologies [7] contribute to improving the reliability and performance of electrolysers. Since green hydrogen production plants depend on intermittent renewable energy production [8], cutting-edge predictive management strategies are required, including advanced forecasting models [9], [10], energy storage management [11] and the coordination between electrolysers and these renewable energy sources [12]. These approaches guarantee a more stable and continuous renewable-based power supply, reducing the effects of renewables' fluctuations.

Another important aspect is the lack of historical data about green hydrogen demand. Synthetic data generation has emerged as a critical tool in energy demand modeling, particularly when historical datasets are incomplete or unavailable [13], and is a potential solution for the case of green hydrogen demand. Recent advancements utilize route-specific schedules, daily and seasonal cycles, and stochastic processes to emulate real-world variations with high accuracy. Techniques such as sinusoidal functions for capturing temporal patterns [14], Gaussian noise for introducing randomness [15], and traffic-based impact factors [16] have been widely employed to enhance the realism of synthetic datasets. Furthermore, the incorporation of rush-hour multipliers [17] and seasonal modifiers [18] has proven essential in reflecting context-specific dynamics, such as urban transit behavior [19] and seasonal shifts in energy demand [20]. These methods, supported by statistical models and computational frameworks, provide robust tools for simulating complex energy systems and optimizing resource planning.

Short-term load forecasting (STLF) is a critical task in the operation and planning of power systems, enabling utilities to predict electricity demand over short horizons ranging from one hour to one week [21]. Traditional STLF methods have predominantly relied on statistical approaches, such as time series analysis [22]. Among these, autoregressive integrated moving averages (ARIMA) stand out due to their simplicity, interpretability, and ability to model linear patterns and seasonality in time series data [23]. ARIMA is often used as a benchmark in forecasting studies, providing a solid foundation for comparing more advanced methods [24].

However, electricity and green hydrogen demand is influenced by complex, nonlinear relationships among variables such as temperature, economic activity, and consumer

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behavior [25]. To capture these nonlinearities, machine learning methods like Random Forest (RF) have been increasingly adopted [26]. Random Forest is an ensemble learning technique that constructs multiple decision trees and averages their outputs, making it robust to overfitting and well-suited for datasets with intricate patterns [27]. RF has shown significant promise in improving forecast accuracy, especially when handling datasets with a mix of numerical and categorical features [28].

Building on the strengths of traditional and machine learning methods, deep learning techniques like Long Short-Term Memory (LSTM) networks have further advanced STLF [29]. LSTM, a type of recurrent neural network (RNN), excels in modeling temporal dependencies and long-term patterns within sequential data [30]. This makes it highly effective for energy forecasting, where historical consumption data exhibit both short-term fluctuations and long-term trends [31]. LSTM networks have been widely recognized for their ability to manage noisy and incomplete data, making them a preferred choice for modern STLF applications [32].

In this paper, we propose a comprehensive methodology for day-ahead planning of a renewable-based energy systems for producing green hydrogen for usage by public transportation – buses.. This approach relies on a forecasting algorithm that uses synthetic data to feed a short-term load forecasting (STLF) procedure to predict the 24-hour hydrogen demand. The synthetic data generation is used due to the lack of real data to feed the forecast algorithms. This enables the hourly optimization of system operations, with the goal of maximizing profitability while maintaining system efficiency.

Next section presents a detailed description of the proposed methodology. Section III describes the synthetic data generation based on hydrogen buses routes. In section IV a comparison of forecasting models is provided, with the focus on hydrogen consumption prediction. Section V presents the results of the optimization algorithm. The main conclusions are discussed in the last section of the article.

II. METHODOLOGY

The proposed methodology is structured into three main phases: (1) Synthetic Data Generation, (2) Short-Term Load Forecasting (STLF), and (3) Day-Ahead Operational Optimization. The overall process is illustrated in Figure 1, where each step feeds into the next to enable effective day-ahead scheduling of a green hydrogen production system.

1) *Synthetic Data Generation*

Due to the absence of historical hydrogen consumption data for public transportation, synthetic datasets were developed to emulate realistic demand patterns. The data generation process is based on operational characteristics of hydrogen-powered bus fleets, including:

- Number of buses per route,
- Average daily distance traveled,
- Fuel efficiency (kg H_2/100 km),
- Hourly traffic dynamics,
- Seasonal variability.

2) *Short-Term Load Forecasting*

The synthetic dataset serves as input to a short-term load forecasting (STLF) pipeline, designed to predict the 24-hour hydrogen demand. Three models were assessed for this task:

- ARIMA (Auto-Regressive Integrated Moving Average),
- Random Forest (RF),
- Long Short-Term Memory (LSTM) neural networks.

Each model was trained and validated using one and four years of synthetic data, across the nine defined routes.

3) *Day-Ahead Optimization*

The final stage involves a day-ahead optimization of the hydrogen production system, leveraging the forecasted hydrogen demand. The optimization algorithm—based on the formulation presented in [33]—aims to determine the optimal hourly setpoints for the following components:

- Electrolyser power input,
- Battery Energy Storage System (BESS) operation,
- Participation in the secondary reserves market.

The optimization maximizes economic performance by accounting for real-time electricity prices from the Iberian Electricity Market (MIBEL), while also ensuring operational constraints are satisfied. The BESS is strategically controlled to stabilize the electrolyser's load factor and to provide grid services, enhancing both reliability and profitability.

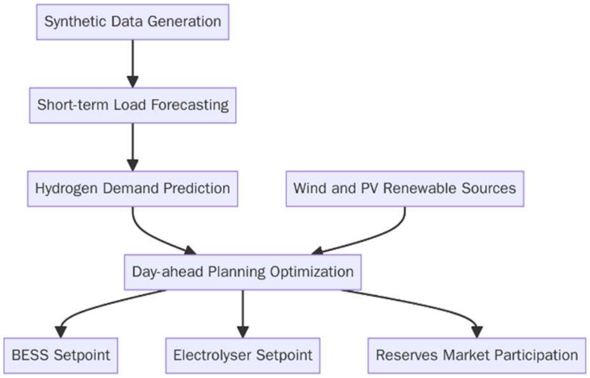

Figure 1. Algorithm flowchart for the day-ahead optimization of the system

III. SYNTHETIC DATA GENERATION

This section presents the mathematical formulation of the algorithm used to generate synthetic data for hydrogen consumption. A set of routes (9) has been defined, each characterized by attributes such as the number of buses, operating hours, and fuel efficiency. These factors determine hydrogen demand during operation.

Traffic follows a sinusoidal pattern, with peaks during typical rush hours (morning and evening). A random noise element adds variability to the impact of traffic. The demand is calculated for each hour of the year by summing the contributions from all routes and applying modifiers for traffic, daily cycles, and seasonal variations.

Equation 1 defines the hydrogen consumption for each hour, based on the number of buses, daily distance, and fuel consumption efficiency:

$$D_{route,h} = N_{buses} \cdot \left(\frac{d_{daily}}{24}\right) \cdot \frac{\eta}{100} \qquad (1)$$

where:

N_{buses}: Number of buses per route.

d_{daily}: Average daily distance (km).

η: Fuel efficiency (kg of hydrogen/100 km).

Equation 2 depicts the traffic impact factor and combines the effects of peak hours with a sinusoidal variation that simulates daily patterns:

$$T_h = 1 + \left(0.5 + 0.5\sin\left(2\pi\frac{h}{24}\right)\right) \cdot M \cdot \mathcal{N}(0.1{,}0.05) \qquad (2)$$

where:

h: Hour of the day.

M: Peak hour multiplier (1.5 during peak hours, 1 otherwise).

$\mathcal{N}(0.1{,}0.05)$: Gaussian noise with a mean of 0.1 and a standard deviation of 0.05.

Equation 3 mathematically represents a sinusoidal modifier that simulates daily demand patterns:

$$C_{daily,h} = \sin\left(2\pi\frac{h}{24}\right) + 1 \qquad (3)$$

Equation 4 defines a seasonal factor that adjusts demand based on the month and a sinusoidal trend:

$$S_d = \begin{cases} 0.9\ if\ summer \\ 1.1\ if\ winter\ +\ 0.1\left(2\pi\frac{day\ of\ year}{365}\right) \\ 1.0\ other\ seasons \end{cases} \qquad (4)$$

Seasonal Demand Modifier (S_d):

- Winter (1.1): Demand increases by 10% in winter due to higher energy needs for heating and transportation during the colder months.
- Summer (0.9): Demand decreases by 10% in summer, as energy consumption may drop due to lower heating needs or a reduction in the number of buses in operation due to the holiday period.
- Other Seasons (1.0): Demand remains unchanged in spring and autumn, as these are transition periods with average usage.

Equation 5 combines all the modifiers and calculations for the final hydrogen demand calculation:

$$D_h = \sum_{routes} D_{route,h} \cdot T_h \cdot C_{daily,h} \cdot S_d + \mathcal{N}(0{,}2) \qquad (5)$$

Figure 2 compares 4 weeks of the data generated. Each week represents one of the seasons (winter, spring, summer, and autumn).

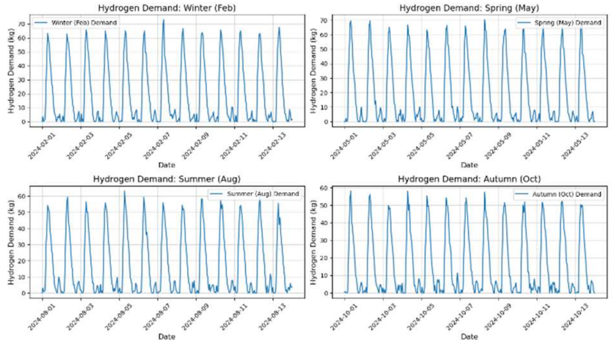

Figure 2. Four representative weeks for four seasons of hydrogen demand

IV. SHORT TERM LOAD FORECAST

Short-term load forecasting (STLF) plays a critical role in the methodology by using synthesized data to predict the hydrogen demand load for the next 24 hours. Through machine learning algorithms and time-series analysis, the STLF model learns patterns in synthetic data to provide accurate hourly demand forecasts. This forecasting process is essential for day-ahead planning, enabling the system to anticipate demand changes and optimize energy distribution from renewable sources.

In this study it is explored three different forecasting models, result of the study of STLF in the first chapter of this paper, with the objective to perceive the more suitable one, according to three indicators; root mean square error (RMSE), mean absolute error (MAE) and coefficient of determination (R^2). The three models are the ARIMA, the Random Forest and LSTM. The study compares the models for 9 routes over 1 year of synthetic data and for 9 routes over 4 years of synthetic data. The data is sorted by periods of 1 hour.

The Random Forest model is created using scikit-learn's *RandomForestRegressor*, with GridSearchCV and *TimeSeriesSplit* optimizing hyperparameters like the number of trees and tree depth. For the LSTM neural network, Keras (from TensorFlow) is used to build a Bidirectional LSTM model, which captures sequential dependencies in both forward and backward directions. The architecture includes multiple LSTM layers with *Dropout* for regularization, and the *Adam* optimizer is used for efficient training. Data is preprocessed using *MinMaxScaler* from scikit-learn to normalize the input, enhancing the neural network's performance.

A. *9 routes over 1 year*

1) *ARIMA*

The ARIMA model has the lowest RMSE (2.35) and MAE (1.78), indicating that this model has the smallest average error, both absolute and quadratic. R^2 (0.9872) is the highest, showing that the model explains approximately 98.7% of the variance in the demand data.

2) *Random Forest*

The Random Forest model shows indicators slightly higher than those of ARIMA, RMSE (2.41) and MAE (1.76), but still close, suggesting that the model performs well. R^2 (0.9846) is slightly lower than ARIMA, indicating the model explains about 98.5% of the variance.

3) LSTM

The LSTM has the highest RMSE (2.85) and MAE (2.10), showing that this model struggles more to minimize errors. R² (0.9785) is the lowest but still explains about 97.8% of the variance, which is a reasonable overall fit.

TABLE I. FORECAST MODELS COMPARISON FOR 1 YEAR OF DATA GENERATION FOR 3 ROUTES

Performance Indicators	**Forecast Models**		
	ARIMA	***Random Forest***	***LSTM***
RMSE	2.352603728809	2.412727129661	2.8481307013
MAE	1.784056103918	1.763541715442	2.1024319514
R^2	0.987201972532	0.984565623282	0.9784923722

B. 9 routes over 4 years

1) ARIMA

The ARIMA model struggled in maintaining consistency through the various rolls. ARIMA models can exhibit high memory usage and produce inconsistent values, especially with large, high-frequency datasets like hourly hydrogen demand over several years. The high memory consumption stems from the complex optimization required to estimate the autoregressive (AR), differencing (I), and moving average (MA) components, particularly when dealing with large datasets or high AR and MA orders.

2) Random Forest

The Random Forest model delivered exceptional performance, achieving a Mean Squared Error of 16.53 kg² and a Mean Absolute Error of 2.54 kg. These metrics indicate that the model's predictions were consistently close to the actual hydrogen demand values, with only minor deviations. The R² score of 0.9955 shows that the model explains 99.55% of the variance in the data, highlighting its strong ability to capture temporal patterns and fluctuations in hydrogen consumption.

3) LSTM

The LSTM model also demonstrated strong predictive capabilities, achieving an MSE of 20.10 kg² and an MAE of 2.84 kg. These values show that the LSTM model performed slightly below the Random Forest but still delivered highly accurate forecasts. The R² score of 0.9945 confirms that the model explains 99.45% of the variance in the data, highlighting its ability to learn complex temporal dependencies inherent in hydrogen consumption patterns.

TABLE II. FORECAST MODELS COMPARISON FOR 4 YEARS OF DATA GENERATION FOR 9 ROUTES

Performance Indicators	**Forecast Models**		
	ARIMA	***Random Forest***	***LSTM***
RMSE	-	16.52710550593	20.101265474
MAE	-	2.537423152746	2.8409304417
R^2	-	0.995501906746	0.9945306423

V. DAY-AHEAD OPTIMIZATION

The algorithm used is based on previous research described in [33] and [34]. This optimization is adapted to produce green hydrogen to feed buses, and the remaining hydrogen production is fed to a natural gas grid. The battery energy storage system is integrated into the overall system, participating in the secondary reserves market and a bilateral electricity contract. The analysis is based on MIBEL data, with forecasted electricity prices informing the decision-making process, as illustrated in Figure 3.

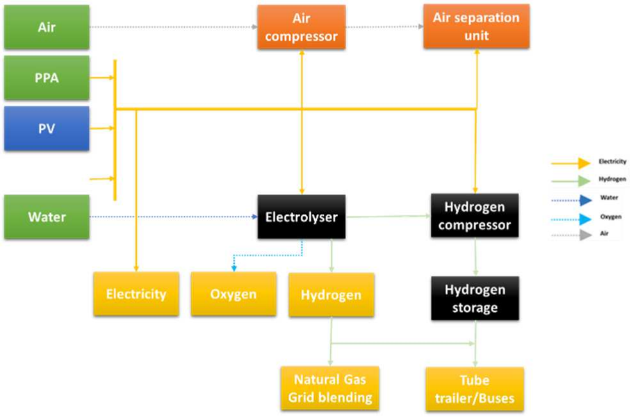

Figure 3. Renewable hydrogen production system case study

A. Results – Set points for a day (24h)

Figure 4 and Figure 5, represents two days of the optimized system setpoints for one day in the winter and the other for the summer.

The setpoints are related to the electrolyser power and the BESS power at each hour. Additionally, it is illustrated the hourly participation in the reserves market on the activated upward and downward energy as well as the SoC of the battery at each hour.

Figure 4. Day-Ahead Optimized setpoints (winter day)

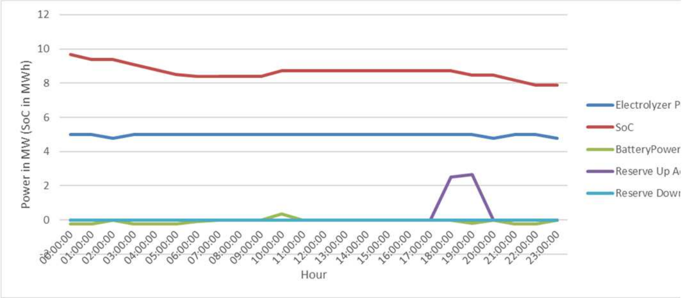

Figure 5. Day-Ahead Optimized setpoints (summer day)

VI. CONCLUSION

This study presents a comprehensive methodology for the day-ahead optimization of green hydrogen production systems, by integrating synthetic data generation, short-term load forecasting, and optimization algorithms, this approach offers a robust framework to enhance the efficiency and profitability of renewable-bases energy systems for the production of green hydrogen.

The synthetic data generation method effectively simulates hydrogen demand based on four factors, traffic patterns, seasonal variations, fuel efficiency and average daily distance. This data serves as the foundation for evaluating different forecasting models. Among the models assessed—ARIMA, Random Forest, and LSTM—the Random Forest model demonstrated superior performance, particularly in handling larger datasets over extended periods. Its high accuracy and ability to capture complex temporal patterns make it an ideal choice for forecasting hydrogen demand in dynamic environments.

The day-ahead optimization algorithm, fed by the forecasted hydrogen demand, successfully optimizes the operation of the electrolyser and the battery energy storage system (BESS). The inclusion of BESS not only stabilizes the electrolyser's load factor but also enables participation in the reserves market, further enhancing the economic viability of the system.

Future research will focus on the application of generative AI techniques to improve synthetic data generation, enhancing the realism and reliability of hydrogen consumption forecasts. This approach aims to refine forecasting accuracy by providing high-quality, data-driven inputs for optimization and decision-making processes.

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