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MODELLING AND OPTIMIZATION OF HYDROGEN FUEL SYSTEMS IN RAILWAY VEHICLES USING DATA ANALYSIS AND MACHINE LEARNING

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Resume
Hydrogen fuel cell systems offer a zero-emission alternative to diesel-powered trains, combining high energy density with the potential for renewable energy integration. A hybrid data-driven modelling and optimization approach of improving the efficiency, reliability, and cost-effectiveness of hydrogen fuel systems for rail applications is developed in this research. Using operational and thermodynamic data from simulated and experimental sources, a predictive model of fuel cell performance based on non-linear regression and machine learning methods was developed. Results indicate that the data-driven model predicts system efficiency with a mean absolute error (MAE) of 1.9%, while the optimization framework reduces fuel consumption by up to 12.4% compared to reference operation strategies. The study proves the value of machine learning in optimizing hydrogen energy systems.

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1 Introduction

The railway transport remains among the most energy-efficient modes of terrestrial mobility. It is supposed to be the most effective and economical mode for transport of goods and it is also favorite mode of transport of passengers in many countries. It is a quite fast, comfortable and reliable transportation system, which allows movement of people for shorter (urban railway transport) to long distances [1-2]. The huge amount of goods is transported by freight railway wagons [3-4]. There are many types of freight railway wagons, which are intended to transport various types of goods [5-7]. Similarly, passengers are transported by various kind of railway vehicle, such as passenger wagons, trams, metro vehicles and others [8].

Due to relative purity of produced gas emissions mainly on electrified railway lines, it is also supposed to be one of the most environmentally friendly modes of transport [9-12]. The European continent is one of the leading regions, where the efforts and emphasis is placed on massive reduction of gas emission production by transport means [13-16].

It is necessary to ensure reliable and sufficient sources of energy to power rail vehicles. This energy is obtained by thermal conversion of fuel in internal combustion engines in the case of railway vehicles for railway lines with an independent traction system. It is considered an older traction system. Electrified railway lines have a dependent traction system, which requires a suitable infrastructure and this kind of traction is supposed to be more environmentally friendly kind of traction system [17]. In this case, trains are towed by electric locomotives powered by electric traction system equipped with modern electric motors of a high efficiency [18-20]. Although the older option still dominates the modern transport system, considerable efforts are being made to find the new, innovative and environmentally friendly energy sources as a source of

a)

b)

Figure 1 *a) A multiple unit by Alstom equipped by hydrogen fuel powertrain known as Coradia iLint, b) an illustration of a layout of the components of the hydrogen powertrain on a vehicle roof [39]*

energy for rail vehicles [21-22]. The chemical energy, which is contained in fuels with a carbon base, such as oil, is converted during the combustion process into mechanical work. Carbon dioxide (CO_2) as an associated result and the direct consequence of the combustion process is released into the air [23-24]. Therefore, continuous development of railway vehicles is aimed at the reduction of the proportion of pollutants emitted into the air. Moreover, this phenomenon is connected not only with actual operation, but with the production, distribution and storage of used fuel, as well. As a possible and perspective alternative to hydrocarbon fuels, alternative fuels, as well as power plants are currently being developed and introduced in railway vehicles in large quantities [25-26]. It is mainly in a form of electromobility, hydrogen fuel cells and other methods.

Railway transport is recently one of the most dominant sector, where the electric energy is used and consumed for powering railway vehicles. Although electrification of railway lines seems to be the most effective way to reduce a production of harmful exhaust gases, full electrification of all railway lines is not possible. Therefore, a substantial share of the world's rail lines remains non-electrified, leading to persistent reliance on diesel traction. Additionally, electrification of railway lines can be too costly and even unprofitable [27-28]. Therefore, there are rather efforts to find innovative and at the same time suitable technical solutions of sources of energy for railway vehicles with an independent traction system [29]. One of the possible options is to apply hydrogen fuel systems to the railway vehicles design as a source of energy [30-32]. In such a case, electricity is produced from hydrogen. The main advantage of this technical solution is practically zero exhaust emissions, which are released into the air during the operation of railway vehicles [33-37].

Hydrogen fuel cell technology offers a sustainable alternative [38-39] capable of providing the high power density and long range without direct emissions of CO_2 or NO_x. Several demonstration projects, such as Alstom's Coradia iLint in Germany and HydroFLEX in the UK, have established the technical viability of hydrogen-powered rail systems. As it is known, the Alstom Coradia iLint multiple-unit was the first railway vehicle, which was equipped by hydrogen fuel-cells and presented at the International railway exhibition Innotrans in 2016. It is shown in Figure 1.

Besides that, other important manufacturers of railway vehicles, such as Siemens within the project Mireo Plus H [40], shown in Figure 2, Alstom with Eversholt Rail with the model Project Breeze and also Stadler and its model Flirt H2 [41] (Figure 3), consider application of hydrogen powertrains with fuel-cells.

A Slovak producer ZOS Vrutky, Inc. [42] also tried to reflect current trends in the field of alternative fuels for a multiple unit 862 class. It is a railway vehicle with independent traction systems, and it is shown in Figure 4. They proposed to replace an original diesel traction powertrain by a powertrain including hydrogen fuel cells.

An example of a layout of components in a multiple

Figure 2 *An illustration of multiple units Mireo Plus H produced by the Siemens company [40]*

Figure 3 *An illustration of the multiple unit by Stadler known as Flirt H2 [41]*

Figure 4 *The multiple unit 861 class produced by the ZOS company originally powered by diesel powertrain [42]*

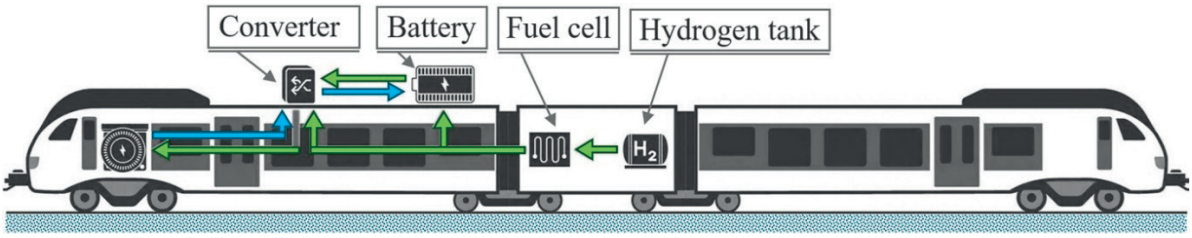

Figure 5 *A layout of hydrogen powertrain components in the Stadler Flirt H2 [41]*

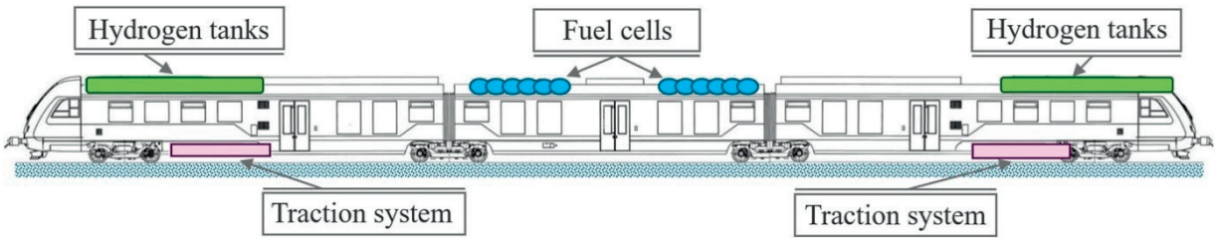

Figure 6 *A layout of hydrogen powertrain components in the multiple unit 861 class multi [42]*

unit powered by hydrogen fuel cells is illustrated in Figure 5 on an example of the Stadler Flirt H2 vehicle and a proposed layout of components of the hydrogen powertrain installed in the ZOS multiple unit 861 class is depicted in Figure 6. As it can be seen, the vehicle by Stadler, as well as the vehicle by the ZOS, include components, which need to implement hydrogen fuel cells as a source of power.

Nevertheless, optimizing system efficiency and lifetime under real-world conditions remains a major challenge.

Machine learning has emerged as a transformative tool for modelling the complex, non-linear processes in energy systems [43-44]. The application of machine learning to hydrogen fuel cell systems in the rail transport can aid in both system design and operational optimization, leveraging large datasets obtained from real-time monitoring. A systematic approach to modelling and optimizing hydrogen fuel systems for railway applications, integrating experimental data, thermodynamic modelling, and machine learning-based optimization is presented in this research. Moreover, a hybrid framework, combining a Proton Exchange Membrane Fuel Cell (PEMFC) performance predictor trained on a mixed simulated-experimental dataset, and a multi-objective genetic optimization strategy simultaneously minimizing hydrogen consumption and stack degradation under realistic hybrid train duty cycles in presented in this research. The proposed method yields route-relevant operating policies improving efficiency, while explicitly accounting for the long-term degradation risks compared to the conventional single-objective or purely physics-based approaches.

2 Background and related work

Hydrogen fuel cells convert chemical energy directly into electricity via electrochemical reactions between hydrogen and oxygen. The overall efficiency depends on multiple dynamic parameters: stack temperature, pressure, humidity, hydrogen flow rate, and load fluctuations. Conventional modelling approaches, such as equivalent circuit or empirical models, depend on simplifying assumptions that do not capture non-linear operational dynamics.

In contrast, the machine learning techniques enable data-driven inference of system relationships without explicit physical modelling. Previous research has demonstrated the use of artificial neural networks for predicting polymer electrolyte membrane fuel cell (PEMFC) performance [45-46] and genetic algorithms for optimizing fuel utilization [47]. However, these methods are rarely tailored for railway conditions, where the transient loads, regenerative braking, and hybrid power management with batteries create unique optimization challenges.

This research bridges that gap by combining the empirical data from simulated railway duty cycles with supervised machine learning models and multi-objective optimization algorithms to minimize hydrogen consumption and degradation rate simultaneously.

3 Hydrogen combustion engines and local pollutant control

Hydrogen fuelled or hydrogen blended internal combustion engines can serve as a cost effective transitional option in rail, especially through retrofits [48-49] Matlab (ML) models such as artificial neural networks, random forest, XGBoost, CatBoost, and other ensemble techniques accurately predict brake specific fuel consumption, efficiency, and emissions (CO_2, HC, particulates, NO_x), enabling optimization of injection, Exhaust Gas Recirculation (EGR), and after treatment strategies [48-49]. Studies on hydrogen enriched engines report:

- Substantial reductions in CO_2 and smoke, accompanied by NO_x increases that must be controlled via combustion tuning and after treatment [50-51].
- High fidelity ML predictors that support the real time Electronic Control Unit (ECU) optimization while highlighting risks of overfitting and data bias [50].

These methods are directly applicable to hydrogen rail engines to balance fuel efficiency with stringent NO_x and air quality targets.

4 Hydrogen production, storage, and refuelling for railway vehicles

Hydrogen production dominates the lifecycle environmental profile of hydrogen rail [52]. The ML is increasingly used to optimize both gray/blue (e.g., steam methane reforming) and green (electrolysis based) hydrogen systems [53-58]:

- Artificial Neural Network (ANN) based process models for Steam Methane Reforming (SMR) capture complex heat transfer phenomena with $R^2 \approx 0.999$ and are used to optimize nine operating variables, achieving thermal efficiencies of ~85.6% [55].
- For renewable powered electrolysis, the ML models, such as K-Nearest Neighbor (KNN), Random Forest (RF), XGBoost, Long Short-Term Memory (LSTM), Artificial Neural Network (ANN) and Lasso trained on decade scale meteorological data accurately predict green hydrogen yields and associated CO_2 savings; one study estimates nearly 400,000 kg CO_2 avoided per year for a single wind powered site [59].
- Bibliometric and technical reviews show ML widely applied to catalyst discovery, operating point

optimization, and cost/emission reduction across electrochemical, thermochemical, and biological hydrogen production routes [53-54, 56-57].

Integrated Reinforcement Learning - Internet of Things (Integrated RL-IoT) systems for hydrogen infrastructure demonstrate that combining real time sensing with Reinforcement Learning (RL) dispatch can reduce emissions up to 97.8% and costs by 40% in renewable hydrogen scenarios, with additional 30% emission reductions through the RL logistics optimization [59]. Such architectures are directly relevant to hydrogen rail refuelling corridors.

5 Methodology

This section includes a presentation of the applied methodology to the research. An overview of the of the system is presented together with collection of the data, processing of the data, a used model for machine learning and a framework for optimization.

5.1 System overview

The hydrogen fuel cell powertrain considered consists of:

- Proton Exchange Membrane Fuel Cell (PEMFC) stack: providing primary traction power.
- Lithium-Ion Battery: supplying transient and peak loads.
- Hydrogen Storage Tank: compressed at 350 bar.
- Power Management System (PMS): balancing the fuel cell and battery contributions.

The analyzed data represent a hybrid multiple-unit (HMU) rail vehicle with the gross mass of 120 tons operating over typical European regional routes.

5.2 Data collection

Data were derived from two sources:

1. Simulated Data: MATLAB/Simulink model of the hybrid multiple-unit energy system under variable duty cycles.
2. Experimental Data: Controlled PEMFC test bench including parameters such as voltage, current density, temperature, humidity, and degraded performance over time.

The combined dataset included 42,000 data points divided into training (70%), validation (15%), and testing (15%) sets.

Key variables:

- Input: Current density, hydrogen flow rate, cell temperature, pressure, and relative humidity.
- Output: Stack voltage, power output, hydrogen consumption rate, and degradation index.

The output voltage of a hydrogen fuel cell can be expressed as:

$$V = E - \eta_{act} - \eta_{ohmic} - \eta_{conc}\,, \tag{1}$$

where:
E is open-circuit voltage [V],
η_{act} are activation losses,
η_{ohmic} are ohmic losses,
η_{conc} are concentration losses.

The hydrogen consumption rate is defined as:

$$\dot{m}_{H_2} = \frac{1}{2 \cdot F} \cdot M_{H2}\,, \tag{2}$$

where:
I is electric current [A],
F equals to the value of 96,485 [kg/mol],
M_{H2} equals to the value of 2 [kg/mol],

The total environmental impact is estimated as:

$$EI = \alpha \cdot \dot{m}_{H_2} + \beta \cdot D_{stack}\,, \tag{3}$$

where:
EI is environmental impact index,
$\dot{m}_{H_2}$ is hydrogen consumption,
D_{stack} is degradation index,
α, β are weighting coefficients.

The simulated dataset was generated using a MATLAB/Simulink model of a hybrid multiple-unit (HMU) energy system operating under variable European regional duty cycles (urban, intercity, and steep gradient profiles). The Simulink model includes a PEMFC stack representation, hydrogen mass-flow dynamics, a compressor/power-management subsystem, and battery buffering to capture the transient load sharing during acceleration and regenerative braking.

The experimental data was obtained from a controlled PEMFC test-bench. Measured signals included stack voltage, current density, cell temperature, inlet hydrogen pressure, relative humidity, hydrogen flow rate, and long-term degradation indicators. The dataset covers both quasi-steady operation points and transient excitation regimes. An empirical degradation index was derived from the evolution of performance loss over time (e.g., capacity/voltage decay trends under comparable operating conditions) to support degradation-aware learning.

5.3 Data processing

The data were standardized and filtered for outliers using the Hampel identifier. Non-stationary time-series components were decomposed using Discrete Wavelet Transform (DWT) to isolate the steady-state and transient behavior. Missing data (≈1%) were imputed through K-nearest neighbor interpolation.

5.4 Machine learning models

Two supervised regression models were employed:

1. Random Forest Regression (RFR): robust against noise and capable of modelling non-linearities.
2. Support Vector Regression (SVR): optimized via radial basis function Kernel for generalization.

A Random Forest regression model was used to predict fuel cell voltage:

$$\hat{V} = f(T, j, \dot{m}_{H_2}, P), \tag{4}$$

where:
T is stack temperature,
J is current density,
P is pressure.

Hyperparameter tuning was conducted using the Bayesian optimization with 5-fold cross-validation. Performance metrics included Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Coefficient of Determination (R^2).

5.5 Optimization framework

A multi-objective genetic algorithm (MOGA) was formulated to minimize the two competing objectives:

Minimize:
f_1 = hydrogen consumption (g/s),
f_2 = stack degradation index. (5)

The formulation of minimization of the two competing objectives in Equation (5) can be written as follows:

$$f_1 = \dot{m}_{H_2}, f_2 = D_{stack}. \tag{6}$$

Further, the multi-objective optimization problem is subjected to:

$$\begin{aligned} &P_{demand} = P_{fuel\,cell} + P_{battery} \\ &SOC_{\min} \le SOC \le SOC_{\max} \end{aligned}, \tag{7}$$

at which, the decision variables are considered as follows:

- fuel cell load ratio: $x_1 \in [0\ 1]$,
- battery State of Charge (SOC) threshold: $x_2 \in [0.2, 0.9]$,
- compressor speed: x_3.

The Pareto-optimal solutions were evaluated based on the weighted sum of normalized objectives, emphasizing the hydrogen economy. An optimal solution based on the Pareto-optimal approach is achieved using MOGA. A weighted objective function is also used:

$$F = w_1 \cdot f_1^{norm} + w_2 \cdot f_2^{norm}, \tag{8}$$

with $w_1 > w_2$.

6 Environmental impact reduction

When the baseline hydrogen consumption is assumed:

$$\dot{m}_{H_2}^{base} = 1.0\ \mathrm{g/s}, \tag{9}$$

then the optimized hydrogen consumption is as follows:

$$\dot{m}_{H_2}^{base} = 0.876\ \mathrm{g/s}, \tag{10}$$

and the reduction of hydrogen consumption is calculated by means of the following formulation:

$$\Delta H_2 = 1.0 - 0.876 = 0.124\ \mathrm{g/s}. \tag{11}$$

Annual savings of fuel (for 3000 h operation) is given:

$$0.124 \cdot 3600 \cdot 3000 = 1.34 \cdot 10^6 = 1.34\ \mathrm{tons}\ . \tag{12}$$

6.1 Emission equivalent

A calculation of emission equivalent is evaluated based on the following statement. When the hydrogen is produced via electrolysis, then the production of carbon dioxide is given as follows:

$$CO_2^{eqv} = 9\frac{\mathrm{kg}(CO_2)}{\mathrm{kg}(H_2)}. \tag{13}$$

When the value from Equation (12) is considered, then:

$$1.34 \cdot 9 = 12.06\frac{\mathrm{t}(CO_2)}{\mathrm{year}}. \tag{14}$$

7 Results and data analysis

This section includes a presentation of the obtained results based on the model performance, further the optimization results and validation of the research based on the operational scenarios.

7.1 Model performance

The Random Forest model demonstrated superior accuracy and stability. The Random Forest model outperformed SVR across all metrics, with less overfitting in transient regimes (Table 1). An important feature analysis indicated that stack temperature (37%) and current density (31%) were the most influential parameters, followed by hydrogen flow rate (18%) and pressure (9%).

The dependences of the values listed in Table 1 are shown in Figure 7. The dependence of the predicted voltage on the measured voltage is depicted. The value

Table 1 *The results of the model*

Error	Random Forest	SVR
RMSE [V]	0.045	0.057
MAE [V]	0.019	0.023
R^2	0.985	0.974

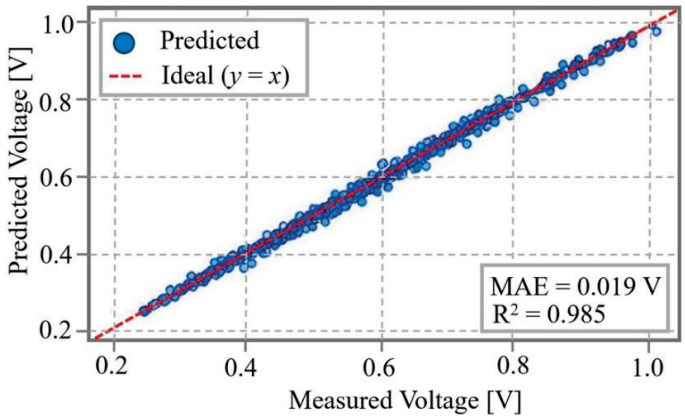

Figure 7 *The dependence of the predicted and measured voltage (on the test set)*

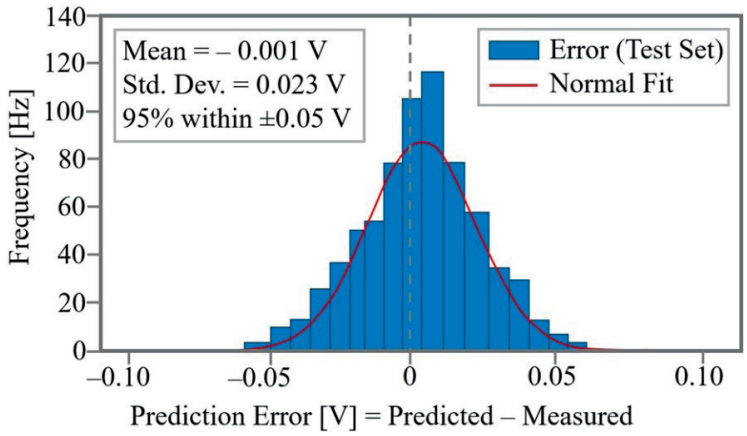

Figure 8 *The error distribution (The Error histogram)*

MAE represents the mean absolute error and R^2 is the coefficient of determination.

Then, a distribution of the predicted error of the predicted value and the measured value is depicted in Figure 8. It has a character of the centered distribution. The error distribution, i.e., the error histogram is centered near the zero value. It indicates no systematic bias.

7.2 Optimization results

MOGA produced a Pareto front illustrating the trade-off between the hydrogen efficiency and stack degradation. The optimal configuration (fuel cell load share ≈ 70%) resulted in:

- 12.4% reduction in hydrogen consumption
- 8.7% extension of projected stack lifetime
- 5.3% improvement in overall energy efficiency compared to baseline control.

The MOGA Pareto front is presented in Figure 9.

A trade-off between hydrogen consumption (a function f_1) and a degradation index (a function f_2) is depicted. The selected optimal point corresponds to a fuel cell load share of 70%.

7.3 Validation under operational scenarios

Three simulated railway duty cycles - urban, intercity, and steep gradient routes-were tested. The optimized controller demonstrated the stable SOC management, maintaining the battery levels between 35-85% and preventing voltage undershoot during acceleration peaks:

$$35\% \leq SOC \leq 85\%. \tag{15}$$

The machine learning model was further validated using experimental bench data, yielding a

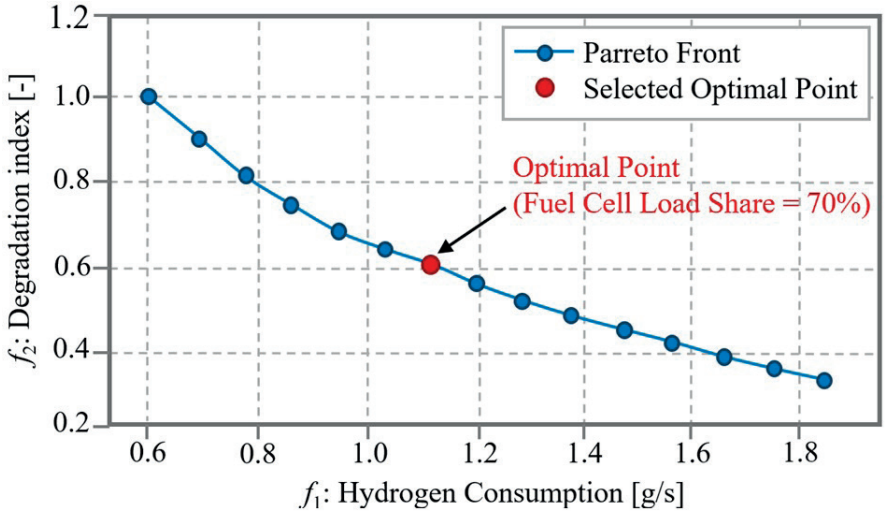

Figure 9 *An illustration of the Pareto front (MOGA) waveform*

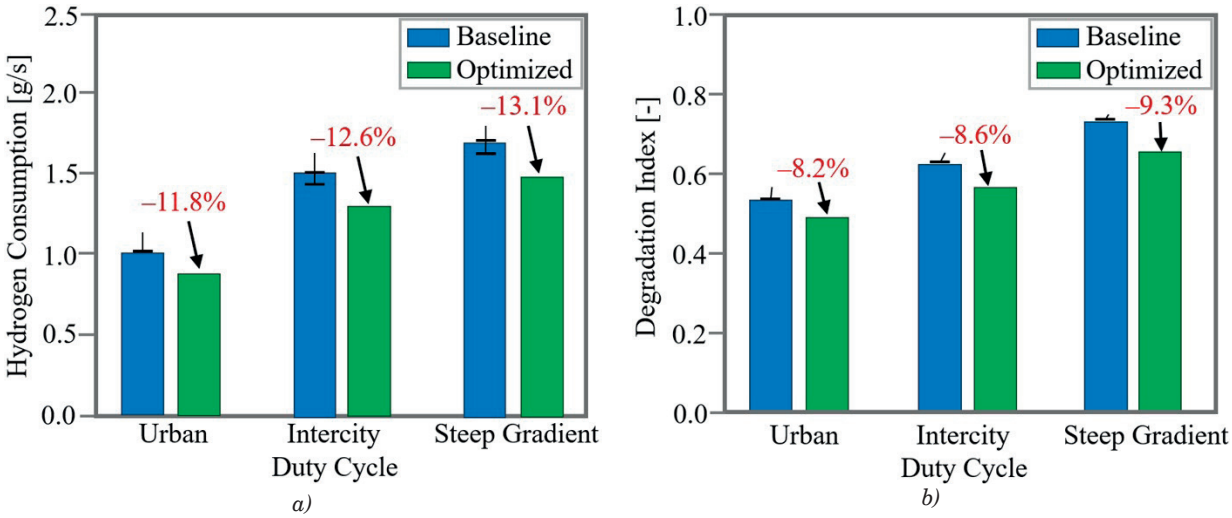

Figure 10 *Duty-cycle comparison: baseline vs. optimized: a) hydrogen consumption [g·s-1], b) the degradation index*

prediction error below 2% under dynamic load cycles, confirming the generalization capability of the proposed framework.

Figure 10 includes a comparison of duty-cycle for the baseline and optimized strategy. The optimized strategy reduces both hydrogen consumption and degradation index across all duty cycles, i.e. urban, intercity and steep gradient.

8 Discussion

The results highlight three main insights:

1. Data-driven modelling complements physical models. Traditional thermodynamic approaches often struggle with parameter uncertainty; the ML provides reliable performance prediction with minimal explicit modelling effort.
2. Hybrid optimization improves lifetime and efficiency. The multi-objective approach balances immediate fuel economy against long-term degradation, providing a framework adaptable to route-specific requirements.
3. Practical implementation requires online adaptability. Integrating the model into the real-time PMS would enable adaptive operation based on continuous feedback from onboard sensors.

In a real practical application, the proposed ML predictor would be embedded into the on-board Power Management System (PMS) to estimate the stack voltage and hydrogen consumption rate from sensor measurements (current density, temperature, pressure, humidity, hydrogen flow). The optimization module would generate updated references for the fuel-cell load share and battery SOC threshold at a fixed control interval (e.g., every few seconds/minutes), while the battery remains the fast-acting buffer for transient power peaks. Safety constraints, such as SOC limits,

compressor operating bounds, and stack temperature thresholds should be enforced as hard constraints in the optimization problem to prevent unsafe operating points.

Since the railway conditions are variables in time (ambient temperature, altitude, humidity, aging state), continuous monitoring is required. Model monitoring can include tracking prediction residuals and triggering a re-calibration/re-training step when the concept drift or data distribution shift is detected. For reliability assurance, a fallback strategy (e.g., conservative baseline controller) should be activated if the model confidence drops below a predefined threshold.

The main limitation is dependency on hydrogen production pathways. Challenges remain in ensuring robustness to unmodeled conditions, long-term data drift, and environmental variability (temperature, humidity, altitude). Future efforts should integrate reinforcement learning for adaptive control and consider digital twin architectures for real-time health monitoring.

9 Conclusion

A comprehensive data-driven methodology for modelling and optimization of hydrogen fuel systems in railway transport is presented in this research. Combining machine learning with multi-objective optimization leads to significant gains in hydrogen efficiency and fuel cell durability. The Random Forest-based predictive model achieved high accuracy (R^2 = 0.985), while optimization reduced hydrogen consumption by 12.4%. Moving forward, coupling the ML models with the real-time control architectures will be key to realizing intelligent zero-emission railway propulsion. The results confirm that:

- Machine learning improves system predictability,
- Optimization reduces both fuel use and degradation,
- Environmental impact is significantly reduced.

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Conflicts of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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