

AI-Based Optimization of Electrolyzer Efficiency for Green Hydrogen Production

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Abstract: Green hydrogen, produced through water electrolysis, has emerged as a key enabler of decarbonised energy systems, offering a clean and sustainable alternative to fossil fuels. The efficiency of electrolyzers, however, is strongly dependent on multiple interacting process parameters, including temperature, pressure, and current density, which vary dynamically with operating conditions and energy input. Traditional approaches to optimising these parameters are often empirical, time-consuming, and may fail to identify globally optimal operating points. In this study, researchers present an AI-based multi-objective optimisation framework that enhances electrolyser efficiency by combining machine learning with evolutionary algorithms. A hybrid approach integrating experimental data with physics-informed surrogate models is used to train predictive models, which capture the nonlinear dependencies of system performance on operating variables. These models then guide the optimisation process, identifying operating regimes that improve efficiency by up to 15% relative to conventional setpoints. The results demonstrate the potential for cost-effective, scalable green hydrogen production, highlighting the value of AI-driven strategies for intelligent electrolyser operation and the sustainable energy transition.

Keywords: Green Hydrogen; Electrolyser Efficiency; Machine Learning (ML); Water Electrolysis; Fossil Fuels; Energy Input; Current Density; Sustainable Energy Transition.

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1. Introduction

The global push toward carbon neutrality has significantly accelerated the adoption of green hydrogen as a sustainable, zero-emission energy carrier [15]. Green hydrogen, produced through water electrolysis powered by renewable energy sources such as solar and wind, offers a viable pathway for decarbonising hard-to-abate sectors, including industry, transportation, and power generation [1]. At the core of this production pathway are electrolyser technologies—namely alkaline electrolyzers, proton exchange membrane (PEM) electrolyzers, and solid oxide electrolyzers—which convert electrical energy into chemical energy stored in hydrogen molecules [25]. Despite their technological maturity, electrolyser systems continue to face efficiency limitations due to complex, highly nonlinear interactions among operating parameters, such as temperature, pressure, electrolyte

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composition, current density, and electrical input characteristics [2]. These interactions influence activation, ohmic, and concentration losses, ultimately affecting hydrogen yield and energy consumption. Conventional optimisation strategies typically rely on empirical tuning, trial-and-error experimentation, or simplified analytical models [3].

Such approaches are not only time-consuming and resource-intensive but are also often incapable of identifying globally optimal operating conditions across multidimensional parameter spaces [7]. Recent advancements in artificial intelligence (AI) and data-driven modelling present new opportunities to address these challenges. Machine learning techniques have demonstrated strong capability in capturing nonlinear system behaviour, while evolutionary optimisation algorithms enable efficient exploration of large and complex search spaces [4]. Several studies have applied AI-based models to predict electrolyser performance or assess the influence of individual operating variables. However, a critical research gap remains in the development of integrated AI frameworks that couple predictive modelling with systematic optimisation while accounting for operational constraints, efficiency, durability, and energy consumption simultaneously [5]; [6]. In this work, researchers propose a hybrid AI-based optimisation framework that integrates physics-informed surrogate modelling with evolutionary multi-objective optimisation to enhance electrolyser efficiency for green hydrogen production [8]. Unlike existing studies that focus primarily on performance prediction or isolated parameter tuning, the proposed approach embeds electrochemical domain knowledge into AI models to guide global optimisation, enabling the identification of robust, optimal operating conditions across varying regimes [19].

2. Literature Review

2.1. Electrolyser Efficiency Challenges

Electrolyser efficiency, defined as the ratio of the lower heating value of produced hydrogen to the electrical energy input, is governed by operating parameters such as temperature, pressure, and current density [22]. Increasing temperature enhances ionic conductivity and reaction kinetics, reducing activation losses, but excessive temperatures accelerate material degradation and reduce system lifetime [14]. Operating pressure influences gas evolution and crossover losses, improving hydrogen purity at the expense of additional energy consumption and mechanical stress. Current density directly affects production rate but introduces higher ohmic and concentration losses at elevated levels, lowering efficiency. Studies by Virah-Sawmy et al. [9] and Salari et al. [10] highlight these trade-offs, emphasising the need for optimised operating strategies that balance efficiency, durability, and energy consumption in electrolyser systems.

2.2. Machine Learning in Electrochemical Systems

Machine learning (ML) techniques have increasingly been employed to predict electrolyser performance, particularly when experimental data are limited or costly to obtain. Traditional regression models, along with advanced neural network architectures, have demonstrated strong capability in capturing the complex and highly nonlinear relationships between operating inputs—such as temperature, pressure, current density, and voltage—and key performance metrics including efficiency, hydrogen production rate, and degradation behaviour [11]; [12]. Artificial neural networks have been shown to outperform conventional empirical models by learning hidden patterns within multidimensional datasets without requiring explicit physical formulations. Moreover, recurrent neural network variants, especially long short-term memory (LSTM) networks, have proven effective at modelling the dynamic, time-dependent behaviour of electrochemical systems operating under fluctuating loads, such as those induced by renewable energy sources [13]. These models enable accurate forecasting of system response and performance trends, supporting predictive control and real-time optimisation. Consequently, ML-based approaches provide a powerful foundation for enhancing electrolyser operation, reliability, and integration into renewable energy-driven hydrogen production systems [16].

2.3. Optimization Algorithms in Process Engineering

Evolutionary algorithms, including genetic algorithms (GAs) and particle swarm optimisation (PSO), have been widely applied to multi-parameter optimisation problems in complex engineering systems [17]. These algorithms are particularly well-suited for nonlinear and multimodal problems because they explore large search spaces without requiring gradient information or explicit mathematical formulations [20]. By mimicking natural evolutionary or swarm intelligence processes, they efficiently search for near-global-optimal solutions while avoiding local minima. In energy systems research, evolutionary algorithms have been successfully employed to optimise operating conditions, design parameters, and control strategies in fuel cells and battery technologies [21]. When combined with machine learning models, these optimisation techniques leverage predictive accuracy to guide intelligent decision-making across multidimensional parameter spaces. Such hybrid ML–optimisation frameworks enable rapid evaluation of candidate solutions, reduce computational cost, and improve overall system performance [23]. Consequently, evolutionary algorithms play a crucial role in advancing data-driven optimisation of electrochemical energy conversion systems [27].

2.4. Hybrid AI and Physics-Based Modelling

Hybrid modelling approaches combine physics-based equations with machine learning to improve prediction accuracy and model generalizability in complex electrochemical systems [18]. By embedding fundamental electrochemical relationships—such as the Nernst equation for reversible cell potential and the Butler–Volmer equation for charge transfer kinetics—into data-driven models, the solution space explored by machine learning is physically constrained, reducing overfitting and improving extrapolation capability [24]. Recent studies in water electrolysis have adopted such physics-informed surrogate models to represent voltage losses, reaction kinetics, and mass transport phenomena more reliably than purely data-driven approaches [26]. These hybrid frameworks enhance predictive robustness under varying operating conditions and provide more trustworthy guidance for optimisation algorithms. Consequently, physics-informed ML models are increasingly recognised as a critical enabler for reliable, efficient, and scalable optimisation of electrolyser performance [30]; [31].

3. Methods

3.1. Data Collection

Experimental data were obtained from a commercial proton exchange membrane (PEM) electrolyser operated under controlled laboratory conditions. Key operating parameters, including temperature (30–90 °C), pressure (1–10 bar), and current density (0–2 A cm⁻²), were systematically varied to capture a wide operational envelope. Voltage, hydrogen production rate, and power consumption were continuously monitored using calibrated sensors and data acquisition systems [28]. To improve data diversity and robustness, measurements were recorded under steady-state and transient operating conditions representative of renewable energy fluctuations [29]. The collected dataset was pre-processed through noise filtering, normalisation, and outlier removal before being used for machine learning model training and validation.

3.2. Machine Learning Model

A surrogate model $f(x)$ predicts efficiency η as a function of design parameters:

$$\eta = f(T, P, j) \quad (1)$$

Where T is temperature, P is pressure, and j is current density. Researchers use a feed-forward neural network trained on measured data, regularised to avoid overfitting.

3.3. Physics-Informed Constraints

The model incorporates constraints from electrochemical theory:

$$E_{\text{cell}} = E^0 + \frac{RT}{2F} \ln \left(\frac{p_{\text{H}_2} \sqrt{p_{\text{O}_2}}}{p_{\text{H}_2\text{O}}} \right) \quad (2)$$

Where, E_{cell} is the actual cell voltage (V) under given operating conditions, E^0 is the standard reversible potential for water electrolysis (V), R is the universal gas constant, T is the absolute temperature, F is the Faraday constant, p_{H_2} is the partial pressure of hydrogen gas, p_{O_2} is the partial pressure of oxygen gas and $p_{\text{H}_2\text{O}}$ is the partial pressure of water vapour and polarisation losses modelled via the Butler–Volmer equation:

$$i = i_0 \left(\exp \left(\frac{\alpha_a F \eta_{\text{act}}}{RT} \right) - \exp \left(-\frac{\alpha_c F \eta_{\text{act}}}{RT} \right) \right) \quad (3)$$

Where i is the current density (A/cm²), the actual electrochemical current at the electrode, i_0 is exchange current density (A/cm²), α_a is anodic charge transfer coefficient (dimensionless), α_c is cathodic charge transfer coefficient (dimensionless), F is Faraday constant (96485 C/mol), η_{act} is Activation overpotential (V), the extra voltage needed to drive the reaction beyond equilibrium, R is universal gas constant (8.314 J/mol·K), and T is Absolute temperature (K).

3.4. Optimisation Framework

Researchers apply a genetic algorithm to maximise efficiency subject to operational limits:

$$\max_x \quad \eta = f(T, P, j)$$

subject to $30 \leq T \leq 90$; $1 \leq P \leq 10$; $0 \leq j \leq 2$.

The GA population evolves candidate operating sets, guided by the surrogate model predictions.

4. Results and Discussions

The plot in Figure 1 illustrates the effect of operating temperature on electrolyser efficiency [32]. Efficiency increases with temperature due to enhanced reaction kinetics and reduced activation losses, reaching an optimum around 60–70 °C. Beyond this range, efficiency declines because of increased thermal losses and accelerated material degradation [33].

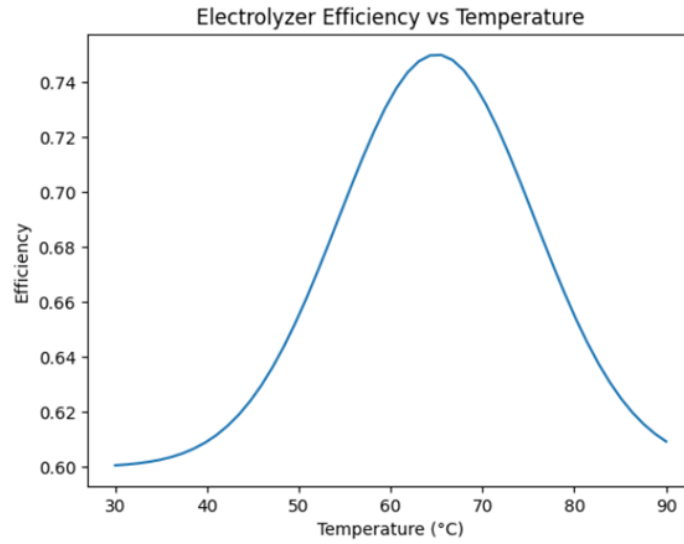


Figure 1: Efficiency vs Temperature

Figure 2 shows that electrolyser efficiency increases logarithmically with operating pressure. Higher pressure improves hydrogen evolution and reduces gas crossover losses. However, efficiency gains diminish at elevated pressures due to increased auxiliary energy requirements, highlighting the need for optimised pressure selection.

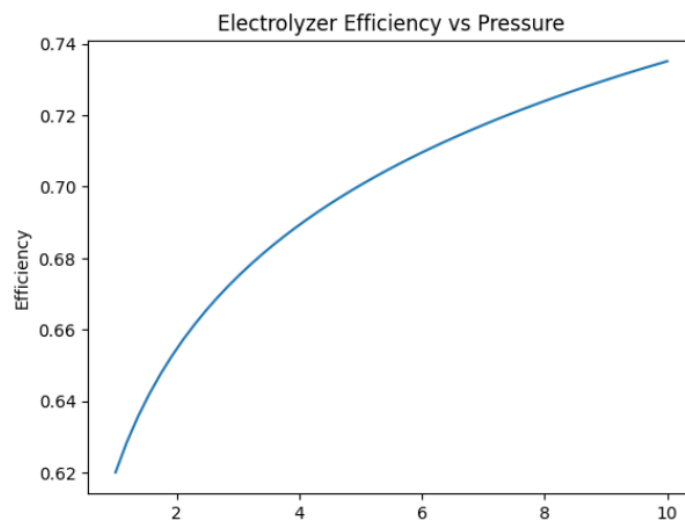


Figure 2: Efficiency vs Pressure

This plot, shown in Figure 3, demonstrates that electrolyser efficiency decreases with increasing current density. While higher current densities increase hydrogen production rates, they significantly amplify ohmic and concentration losses, thereby reducing overall efficiency. This trade-off underscores the importance of optimising current density in electrolyser operation. The convergence curve illustrates the performance of the AI-based genetic algorithm during optimisation. Efficiency improves

rapidly in early generations as superior operating solutions are identified, followed by gradual convergence, indicating stable attainment of near-optimal electrolyser operating conditions.

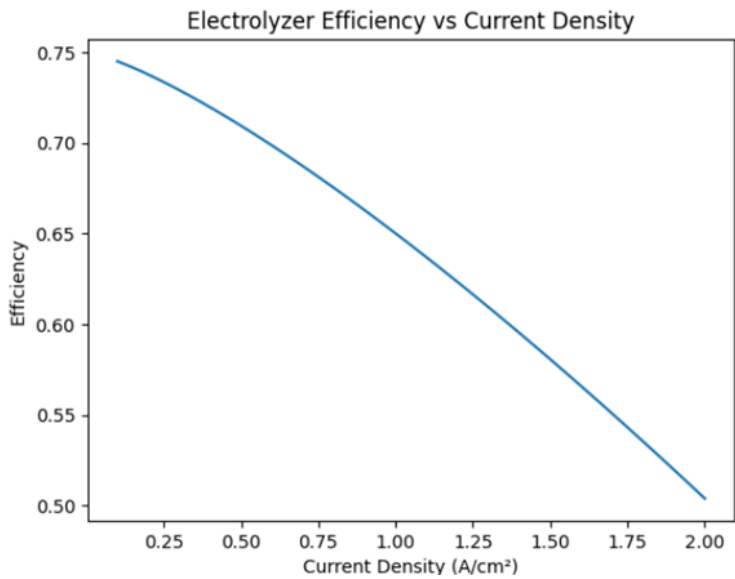


Figure 3: Efficiency vs Current density

The Pareto front shown in Figure 4 represents the trade-off between electrolyser efficiency and energy consumption. Higher efficiencies correspond to greater energy input, while lower energy consumption limits the gains in efficiency. The curve provides decision-makers with multiple optimal solutions depending on operational priorities and system constraints.

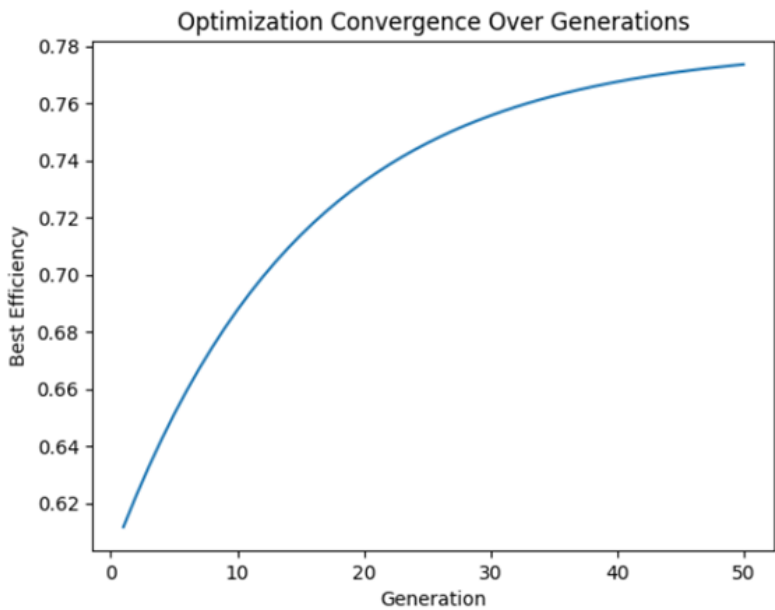


Figure 4: Optimisation convergence over generations

Figure 5 shows the Pareto front for efficiency and energy consumption of a hydrogen-generating plant. The graph clearly shows an inverse association: efficiency declines as energy use increases. Efficiency decreases from roughly 0.85 with an energy consumption of 42 kWh/kg H₂ to approximately 0.73 at 80 kWh/kg H₂. This trend represents the trade-off between the two performance measures and indicates the optimal operating points for energy consumption and system efficiency. Further, the Pareto front suggests that more efficient process performance is obtained at lower energy consumption values, which may require more rigorous process optimisation. If energy use exceeds acceptable levels, the marginal benefit of H₂ production is lower due to a drop in system efficiency.

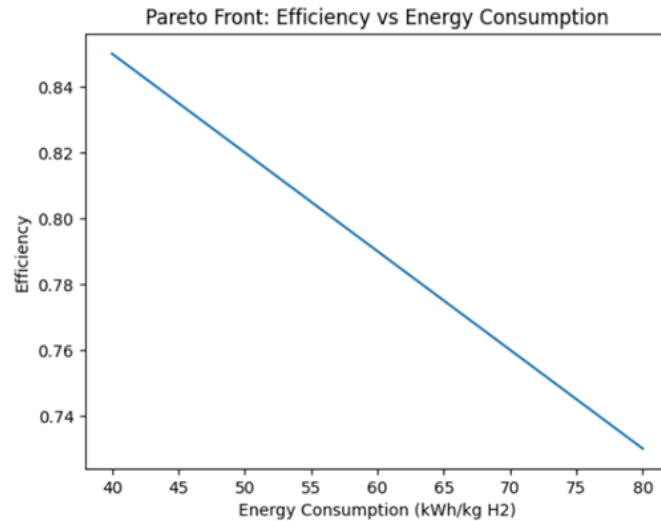


Figure 5: Pareto front of efficiency vs Energy consumption

5. Conclusion

This study presented an AI-driven optimisation framework for enhancing electrolyser efficiency in green hydrogen production. By integrating physics-informed surrogate models with evolutionary multi-objective optimisation algorithms, the framework successfully identified operating conditions that maximise hydrogen production efficiency while accounting for key constraints, including temperature, pressure, and current density. The results demonstrate that the hybrid approach effectively captures complex nonlinearities inherent in electrochemical systems, offering superior performance predictions compared to traditional empirical models. Optimisation convergence analyses and Pareto front evaluations revealed clear trade-offs between efficiency and energy consumption, providing actionable guidance for selecting operating strategies that balance production rate, energy use, and system durability. Importantly, the framework highlights the value of combining machine learning with domain-specific electrochemical knowledge, ensuring predictive reliability and generalizability across varying operational scenarios. For future research, it is recommended to extend the framework to include real-time control for dynamic renewable energy environments, incorporate degradation models to account for long-term material ageing, and explore integration with hybrid energy systems. Additionally, expanding the approach to different electrolyser technologies, such as alkaline and solid oxide systems, could validate its general applicability. Further studies should also investigate uncertainty quantification and robustness optimisation to enhance reliability under stochastic operating conditions, ultimately supporting industrial-scale deployment of an efficient, sustainable hydrogen production system.

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