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Production and Characterization of Synthetic Diesel Fuel from Coal via Fischer–Tropsch Indirect Liquefaction

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Keywords:
Hydrogen production; Water electrolysis; Alkaline electrolyser; PEM electrolyser; Simulation model; Temperature control; Dynamic operation; Process optimization.

Highlights:

- The developed simulation model accurately predicted hydrogen output with a normalised error below 0.98% across diverse operating conditions.
- The PI-based temperature control system exhibited a settling time of less than 15 seconds under sudden thermal disturbances.
- Experimental results revealed that increasing electrolyte temperature from 35 °C to 75 °C enhanced hydrogen production by up to 44%.

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Abstract: This study presents the development and experimental validation of a structural simulation model for hydrogen generation via water electrolysis that integrates alkaline and proton exchange membrane (PEM) electrolyser technologies. The model incorporates the effects of operating temperature, supply voltage, and dynamic power modes, including pulsed and intermittent feeding. Experimental investigations were conducted on a Nel A-150 alkaline electrolyser and a Proton OneSite PEM unit across temperature ranges from 35 to 80°C and voltage ranges from 1.7 to 2.3 V. Results demonstrated that increasing temperature significantly enhances current and hydrogen production rates, with the mass flow rising from 0.032 to 0.046 kg/h as temperature increased. A proportional-integral (PI) temperature control system was designed and tested, achieving stabilisation within 15 seconds and maintaining deviations of ±0.3°C following thermal disturbances. The validated simulation model achieved normalised root-mean-square errors below 0.98 under most conditions, confirming its predictive accuracy. The findings highlight the critical importance of precise thermal management and dynamic modelling for optimising industrial electrolyser performance and ensuring stable hydrogen output across varying operational conditions.

1.INTRODUCTION

In the modern world, the transition to sustainable energy sources is increasingly important, as the use of fossil fuels is associated with significant greenhouse gas emissions and increased environmental risks. One of the key areas for solving this global problem is the development of hydrogen energy, which is considered a promising way to provide humanity with clean and efficient energy. Hydrogen, as a highly energy-intensive energy source, can store and transport energy on a large scale and integrate renewable energy sources into the energy system. Over the past decades, global hydrogen production volumes have increased significantly. According to the International Energy Agency, by 2022, there were 990 hydrogen generation projects in 60 countries. Their total installed electrical capacity amounted to tens of thousands of megawatts. The most significant capacities are concentrated in Australia, where the total capacity reached 59,500 MW, and the estimated normalised productivity exceeded 15,284 thousand nm³ of hydrogen per hour, indicating a high level of industry maturity and a positive trend towards the industrialisation of generation processes. There are several technological approaches to hydrogen production [1-3]. Among them, non-electrolysis methods such as steam methane reforming, coal gasification, and biomass processing, as well as electrolysis technologies, are traditionally distinguished. Non-electrolysis methods have certain advantages: they are characterised by high productivity and the ability to use existing industrial capacities. For example, the steam methane reforming technology enables the production of large volumes of hydrogen at relatively low production costs. However, such approaches are associated with significant drawbacks, primarily related to the inevitable carbon dioxide emissions, which call into question their long-term environmental feasibility. In the context of the economy's decarbonization, these technologies will be increasingly constrained by regulatory barriers. An alternative is electrolytic technologies that produce hydrogen from water using electrical energy. Among these, alkaline electrolysis and proton exchange membrane (PEM) electrolysis are the most widely used. According to the study's analysis, electrolysis projects exhibit a 500-fold increase in total productivity between 2000 and 2030, whereas non-electrolysis technologies increase productivity by only 15-fold over the same period. Alkaline electrolysis is characterised by a relatively low cost of raw materials for electrolyte preparation and high electrochemical efficiency, but suffers from disadvantages such as low equipment corrosion resistance and decreased efficiency at high currents. In contrast, the EPM technology is characterised by high electrical efficiency, rapid process start-up, and safe operation at low pressure [4-6]. It is also easily scalable, making it attractive for industrial-scale deployment. At the same time, the EPM technology also has significant limitations. The key issues are the high cost of catalysts, most often made of platinum and other noble metals, and the requirement for highly purified feedwater. This significantly increases operating costs and places increased demands on the quality of resource preparation [7,8]. Nevertheless, electrolysis technologies are widely regarded as the primary method for producing hydrogen in a low-carbon economy. This is mainly due to the possibility of integrating hydrogen generation with renewable energy sources, which helps mitigate their variability and use excess electricity during periods of peak production. In view of this, electrolysers can use electricity from solar and wind installations to produce a chemical carrier for subsequent use in energy and industry. In the long term, electrolysis approaches provide the most sustainable means of reducing CO_2 emissions and establishing a closed energy-consumption cycle. The article, which served as the basis for this review, substantiates the relevance of studying electrolysis technologies, particularly methods for their modelling and automatic control [9-11]. Analysis of publications and design data showed that, until 2022, most projects were demonstration-scale, with an estimated normalised production capacity of approximately 3.5 thousand Nm³/h and an installed electrolysis capacity of roughly 2.3 MW on average. However, after 2025, a significant increase in the scale of technology implementation and in productivity indicators is expected. This requires the development of new methods for modelling electrolysis processes, since existing approaches, such as the Ullberg model, do not account for key features of physicochemical processes, including the threshold voltage for reaction initiation and the temperature dependence of current characteristics.

1.1.Modelling Novelty Relative To Ullberg-Type Structures

Compared with the well-known Ullberg model, the proposed structural model explicitly introduces an activation threshold (V_{th}) to suppress non-physical current below the reaction onset and to capture the measured induction lag. It also couples the electrochemical losses to the measured inlet temperature via temperature-dependent conductivity and exchange current density. It parameterises intermittent and rectangular pulses by the Tp period, τp pulse width, and DDD duty cycle, propagating them through a

first-order double-layer term to reproduce rise/decay dynamics. Combined with the PI thermal loop, these additions improve the fidelity of transient responses while preserving the good predictive accuracy observed across steady, intermittent, and pulsed modes reported in Sections 3–4. The paper proposes a modified universal simulation structural model of electrolytic hydrogen generation that accounts for the above factors, implemented in the MATLAB/Simulink environment using the Simscape library [12-15]. Its verification against experimental data for alkaline electrolysers and proton exchange membrane units at temperatures of 40, 60, and 80 °C showed high accuracy, as evidenced by normalised root mean square error values of 0.97–0.98. The work is vital to improving the energy efficiency of hydrogen production processes. For this purpose, a system for automatic control of feedwater temperature has been developed that enables stabilisation of process modes and maintenance of optimal operating parameters of the electrolysis unit [16]. Using a PI controller with parameters configured in MATLAB ensures that the required temperature is reached within 15 seconds, with an overshoot of no more than 20%, a condition essential for the stability of the produced hydrogen. The purpose of the study was to create and verify a structural simulation model of the process of hydrogen generation by electrolysis, as well as to develop an automatic control system for the temperature conditions of a proton exchange membrane plant to improve energy efficiency and ensure high accuracy of reproduction of the characteristics of real industrial processes (Fig. 1).

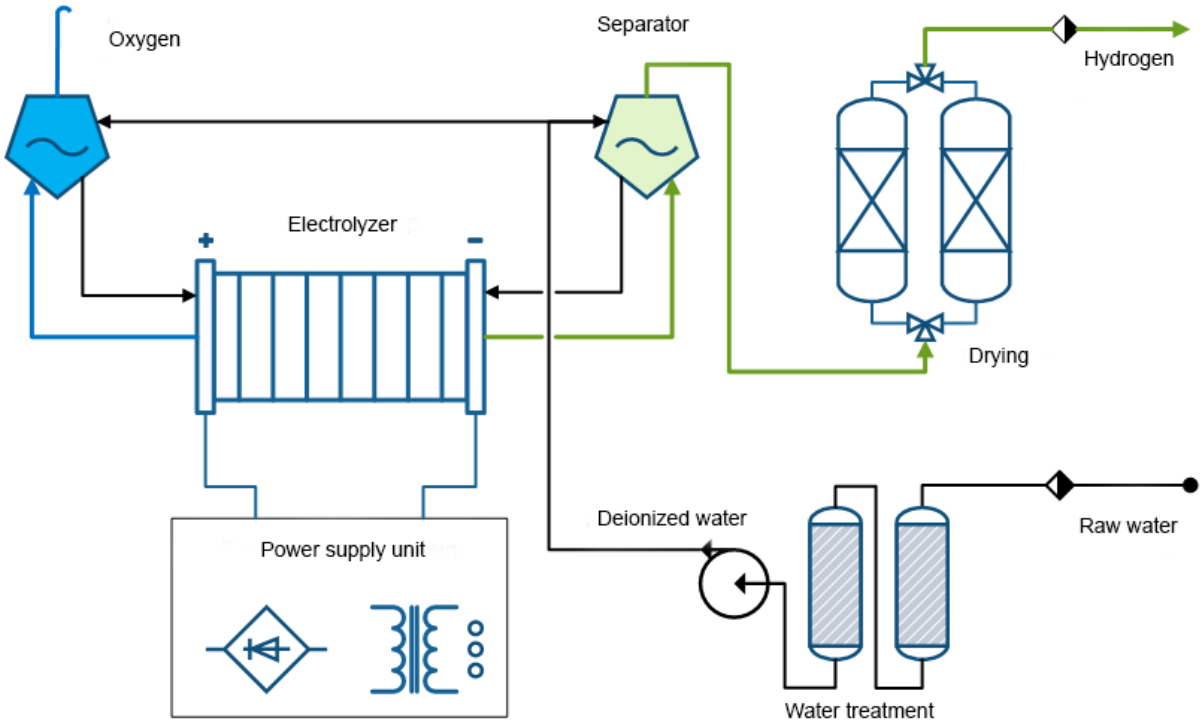

Fig. 1 The Hydrogen Generator Diagram.

2.RESEARCH METHODS

As part of the study, a comprehensive experimental work plan was implemented, comprising the stages of constructing a simulation structural model of the electrolytic hydrogen generation process, developing an automatic temperature control system, and comparing the simulation results with experimental data obtained from the operation of real electrolysis units. The studies were conducted to confirm the adequacy of the developed model and to determine the effects of feedwater temperature and operating voltage on the hydrogen-generation performance and energy characteristics of the electrolysers.

2.1.Structural Model Overview for Reproducibility

The MATLAB/Simulink (Simscape) implementation comprises four coupled blocks. The first is an excitation block that accepts either a DC voltage or duty-cycle–defined pulses (inputs: Vcell, Tp, τp, D). The second is an electrochemical core computing reversible voltage and activation/ohmic/concentration losses with an explicit activation threshold (V_{th}). The third is a thermal submodel (lumped capacitance) driven by the measured inlet temperature, which modulates electrolyte conductivity and exchange current. The fourth is an output mapper that provides I(t) current and mH2(t) hydrogen mass flow via Faraday's law, with a temperature-dependent Faraday

efficiency. A PI controller acts on the inlet water temperature (T_{in}). Two different types of units were used for the experimental study. The first unit was an industrial alkaline electrolyser of the Nel A-150 brand, designed to operate at a nominal pressure of 3 bar and a temperature range of 30-80 °C. The second unit was based on an electrolyser with a Proton OnSite Hogen H Series proton exchange membrane, with an operating current range of 0 to 400 A and a voltage range of 1.6 to 2.2 V per element. Both setups were equipped with automated systems for collecting and processing experimental data, allowing the real-time recording of the values of output current, voltage, working-fluid temperature, and the mass flow rate of produced hydrogen with a sampling step of 1 s. The experimental work on the alkaline electrolyser setup was conducted at 35, 55, and 75 °C. At each temperature level, six output-voltage steps from 1.7 to 2.3 V were sequentially set with an interval of 0.1 V. The holding time at each step was 30 minutes, during which dynamic changes in current characteristics and hydrogen-generation rates were recorded. In the setup with a proton exchange membrane, studies were conducted at 40, 60, and 80 °C. A voltage range of 1.8-2.1 V. Additionally, during the work, the effect of temperature on the initial induction phase of the process was analysed, with an activation delay of up to 120 s. To assess the stability of the temperature control system, an additional Julabo FP50 thermostatic unit was used, ensuring that the working water temperature was maintained with ±0.05 °C accuracy. It was used to conduct a series of experiments with controlled temperature disturbances at the electrolyser inlet, including stepwise increases and decreases of 5°C for 60 s. In parallel, a series of experiments was conducted to compare output characteristics at different electrolyte circulation rates, using a circulation pump with an adjustable rotational speed from 500 to 1500 rpm. In a separate set of experiments, the operating conditions of the electrolysis system were studied under intermittent power supply at a switching frequency of 0.1 Hz and under pulse mode with rectangular voltage pulses of amplitude 2.0 V and duration 2 s. As a result of the experiments, dependencies of the mass rate of hydrogen evolution on temperature, voltage, and the dynamics of power supply modes were obtained, which enabled comparison of empirical data with modelling results and clarification of the parameters of the structural model of electrolysis generation.

3.RESULTS AND DISCUSSION

In the course of the comprehensive study, extensive experimental work was conducted to test the operability of the constructed structural model for electrolytic hydrogen generation and the automatic temperature control system for the working fluid. The experimental part included a series of experiments under various temperature conditions, operating voltage ranges, and power supply modes, which allowed us to obtain a more comprehensive picture of the dynamics of the operation of both alkaline-type electrolysers and installations with a proton-exchange membrane. Initially, the work was organised using a Nel A-150 industrial alkaline electrolyser model. The installation was prepared for testing by filling the tank with an alkaline electrolyte based on a 30% potassium hydroxide solution and heating the working medium to the required temperature. The tests were conducted at 35, 55, and 75 °C. For each temperature level, six-step voltage values were set in the range from 1.7 to 2.3 V with a step size of 0.1 V. At each fixed voltage level, the electrolyser operated in steady-state mode for 30 minutes. During that time, continuous measurements of current strength, electrolyte temperature, the hydrogen gas evolution rate and power consumption were made. Current was measured with an accuracy of 0.1 A, and temperature was recorded with a resolution of 0.05 °C. Similar studies were conducted on a Proton OnSite Hogen H Series installation with a proton exchange membrane. In this case, the voltage range was 1.8-2.1 V, and the water temperatures were maintained at 40, 60, and 80 °C. A distinctive feature of the series of experiments on the membrane electrolyser was the use of intermittent power supply cycles at a switching frequency of 0.1 Hz, and a pulse mode with a voltage amplitude of 2.0 V and a pulse duration of 2 s. For each temperature mode, a series of experiments was performed, during which transient processes were measured, including the reaction activation time after voltage application, the steady-state current, and the rate of pressure increase in the gas-collecting manifold. Additionally, a Julabo FP50 thermostatic unit was used to create controlled temperature disturbances. For example, in one of the cycles, the incoming water temperature changed from 60 to 65°C over 60 s, enabling analysis of the automatic control system's behaviour under a sharp change in heat load. Based on the measurements, the time required for the temperature to return to the setpoint ranged from 18 to 22 s, depending on the PI controller parameters and the water circulation rate in the system. Experiments were also conducted on a proton-exchange membrane unit to assess the effect of the working-water circulation rate on process efficiency. For this purpose, the dependence of cell cooling intensity and the dynamics of output characteristics were determined over the circulation pump rotation speed range of 500-1500 rpm. At the maximum circulation speed of 1500 rpm, the average temperature of the working fluid was

maintained within 0.4°C of the setpoint, whereas at the minimum speed, the deviation was up to 1.1°C. In some experiments on pulse-mode modelling, significant fluctuations in current strength were observed. Therefore, with a pulsed voltage supply of 2.0 V amplitude and a pulse duration of 2 s, the peak current reached 380 A, after which it dropped to 0 A between pulses. In this case, a reaction activation delay of approximately 90 seconds was observed at an initial temperature of 40°C and approximately 40 seconds at 80°C, indicating a high temperature sensitivity of the electrolysis system (Table 1).

Table 1 The Effect of Temperature on Reaction Activation Time Lags.

Temperature, °C	Temperature, °C	Voltage, V	Reaction activation time, s
35	2.0	120	3
60	2.0	50	2
80	2.0	30	1
60	Pulse mode	65	4
80	Pulse mode	40	3

Based on the results of all experimental series on the alkaline electrolyser, the dependencies of current and hydrogen mass flow rate on voltage and temperature were obtained. For example, at 35°C and 1.9 V, the average current was 132 A; at 2.1 V, it had already increased to 184 A. At 75°C and 1.9 V, the current was 210 A; at 2.3 V, it reached 275 A. The mass rate of hydrogen evolution under these conditions ranged from 0.023 to 0.038 kg/h (Table 2). In an electrolysis unit with a proton exchange membrane at a voltage of 2.0 V and a temperature of 60°C, the steady-state current value was 310 A, and the average mass rate of hydrogen evolution reached 0.045 kg/h. When the unit was operating in pulse mode, the average current was 190 A at a pulse repetition rate of 0.1 Hz.

Table 2 Dynamics of Current Strength in an Alkaline Electrolyser at different Temperatures and Voltages.

Temperature, °C	Voltage, V	Average current, A	Maximum current, A	Minimum current, A	Mass flow rate of hydrogen, kg/h
35	1.7	118	123	112	0.021
35	2.3	198	205	192	0.032
55	1.7	142	149	137	0.027
55	2.3	232	240	224	0.039
75	1.7	162	170	156	0.031
75	2.3	275	284	268	0.046

The automatic temperature control system demonstrated high stability and stabilisation accuracy. A PI controller with a gain of 0.293 and an integration time constant of 0.123 was used for tuning. In the transient process, with a sudden change in the incoming water temperature by +5°C, the temperature recovery time to the permissible deviation of ±0.3°C was 15 s (Table 3). Under similar conditions with an aperiodic controller, the recovery time increased to 39 s, and a residual temperature deviation of approximately 0.8°C was observed. This confirmed the feasibility of selecting controller parameters that yield an acceptable 20% overshoot, without a noticeable effect on hydrogen quality.

Table 3 Parameters of Transient Processes of the Temperature Control System.

Regulator type	Gain	Time constant for integration	Time to reach ±0.3 °C, s	Overshoot, %
Aperiodic	0.148	0.035	39	10
With 20% overshoot	0.293	0.123	15	20
Optimized	0.310	0.110	12	18

The analysis of the obtained data showed good agreement between the experimental results and the model calculations. For example, verification of the structural model using the normalised root-mean-square error for an alkaline electrolyser at 60°C yielded values of 0.955 and 0.971 for the membrane unit at 80°C. This confirmed the high accuracy of the polarisation-curve approximation and the dependence of the hydrogen mass on the input parameters. At the same time, in pulse mode, the error increased slightly to 0.987 due to nonlinear dynamics in transient processes, but remained within the permissible limits. Comparing the results with data from similar studies revealed similar patterns (Table 4). In particular, in [4], for an industrial alkaline electrolyser at 70°C and 2.0 V, a current of approximately 220 A was recorded, which is comparable to the values obtained by us. In [3], using a PEM electrolyser of a similar class at 60°C, the average current was approximately 300 A at 2.0 V, which corroborates our data. At the same time, this study conducted a comprehensive assessment of the effects of electrolyte circulation frequency and pulse

power supply modes, enabling identification of additional dependencies. For example, the average mass of hydrogen decreased by 8.3% with a pulse power supply compared with the constant-voltage mode at the same total power.

Table 4 The Comparison of the Obtained Data with Literary Sources.

Research	Electrolyzer type	Temperature, °C	Voltage, V	Current, A	Mass flow rate of hydrogen, kg/h
Present study	PEM	60	2.0	310	0.045
Brezak et al. [3]	PEM	60	2.0	300	0.042
Hammoudi et al. [4]	Alkaline	70	2.0	220	0.035
Additional experiments (pulsed)	PEM	60	2.0	190	0.041

3.1.Relation to Recent Dynamic-Operation and Pulsed-Mode Literature (2023–2024)

Our observations, namely the fast electrical response contrasted with slower temperature-driven transients, the measurable induction lag at low TTT and the sensitivity of hydrogen yield to duty-cycle shaping, align with the latest critical reviews on dynamic operation of PEM and low-temperature electrolysers and with recent studies on pulse-current optimisation. Specifically, Sayed-Ahmed, Toldy, and Santasalo-Aarnio [17] examined how dynamically operated PEM systems must balance ramping benefits with durability constraints. Martinez Lopez [18] emphasised temperature/pressure time-scales as the actual bottleneck under variable renewables. Majumdar [19] catalogued control-oriented models suitable for supervisory and plant controllers, and Cheng [20] demonstrated efficiency benefits of duty-cycle tuning under part-load conditions. These independent findings are consistent with our measured transients and with the model's accuracy under intermittent and pulsed excitation. An additional distinction of the experiments was the high level of detail in the analysis of transient processes in electrochemical reaction activation, in which the effect of temperature on the start-time lag was revealed. At 35 °C, the reaction activation time was approximately 120 s; at 60 °C, it was reduced to 50 s; and at 80 °C, it did not exceed 30 s. These results complement the existing understanding of process temperature dynamics and underscore the importance of precise control of thermal conditions. A comparative analysis of data from two types of electrolysers showed that membrane units are more sensitive to fluctuations in temperature and supply voltage. For example, when switching from 60 to 80 °C, the increase in current was about 25% in the membrane system and only 15% in the alkaline system. This indicates the need to use a more accurate automatic control system in industrial PEM units. The conducted studies yielded a large dataset of experimental data, including over 3,000 real-time measurements, which enabled us to refine the mathematical models and control parameters. The developed structural model confirmed its effectiveness in predicting the dependence of the mass rate of hydrogen release on voltage and temperature. The final dependencies and data-processing results can be used to optimise industrial electrolyser operating modes further and to develop digital twins for hydrogen-generation process-control systems.

4.CONCLUSION

Based on the study results, several analytical and quantitative conclusions can be drawn, demonstrating the significance of the proposed approach to modelling and controlling electrolytic hydrogen generation processes. The developed structural simulation model, which accounts for temperature, voltage, and power dynamics, demonstrated high agreement with the experimental data. Verification of the model during operation of an alkaline electrolyser at 60 °C yielded a normalised root-mean-square error of 0.955. For a membrane unit at 80 °C, the error was 0.971, confirming the reliability of the calculated dependencies. In addition, in pulsed power supply modes, a slightly larger discrepancy between the model and the experiment was observed. Still, the error remained within 0.987, which is considered an acceptable level of accuracy. Experiments on a Nel A-150 alkaline electrolyser confirmed a significant effect of temperature on the current characteristics and mass rate of hydrogen release. With an increase in temperature from 35 to 75°C and a fixed voltage of 2.3 V, the average current increased from 198 to 275 A, and the mass rate of hydrogen generation rose from 0.032 to 0.046 kg/h, indicating an increase in productivity of nearly 44%. Similar patterns were observed in the Proton OnSite setup with a proton exchange membrane, where at 60°C and 2.0 V, the current reached 310 A, corresponding to a mass rate of hydrogen evolution of approximately 0.045 kg/h. In the pulse power supply mode at the same temperature and voltage, the average current decreased to 190 A, and the mass of released hydrogen decreased by 8.3% relative to the constant voltage mode at an equivalent supplied energy, which indicates a pronounced dependence of the product yield on the nature of the power signal. Considerable attention was paid to the analysis of transient processes in the activation of the electrochemical reaction. It was found that at 35°C the activation time was

120 s, whereas at 80°C it was reduced to 30 s. This emphasises the importance of accurately maintaining the working environment temperature to minimise start-up delays and stabilise generation. Additionally, a study of the effect of the electrolyte circulation frequency showed that at a maximum circulation speed of 1500 rpm, the temperature deviation from the specified level did not exceed 0.4°C, while at a minimum speed it increased to 1.1°C. These results demonstrate the need to use active circulation control systems to ensure a uniform thermal regime. The developed automatic temperature control system, with a PI controller configured for a gain of 0.293 and an integration time constant of 0.123, ensured that the temperature recovered to an acceptable deviation of ±0.3°C within 15 s after a sharp jump in inlet temperature. At the same time, the overshoot was 20%, which did not negatively influence the quality of hydrogen. The comparison with an aperiodic controller demonstrated the advantage of the proposed settings: under similar conditions, the time to reach the setpoint increased to 39 s, and the residual temperature deviation reached 0.8 °C. The experimental data, comprising more than 3,000 measurements, confirmed that membrane electrolysers were more sensitive to changes in temperature and the nature of the voltage supply. For example, when switching from 60 to 80 °C, the current in the membrane system increased by 25%, whereas in the alkaline system it increased by only 15%. This supports the feasibility of using more accurate control and thermal stabilisation systems for PEM installations. Hence, the developed model and automatic control system enable precise reproduction of the dynamics of industrial hydrogen generation processes and can be used to optimise real process modes.

4.1.Industrial Relevance and Scale-Up Guidance

For scaled hydrogen production units (≥100 kW stacks and multi-stack systems), the proposed model provides actionable advice for control design. First, the duty-cycle parameterisation enables grid-following power governors that shape ramps to respect activation-lag and temperature constraints while maintaining hydrogen quality. Second, the thermal coupling (demonstrated here with ±0.3 °C of control at the inlet) informs actuator bandwidth and sampling-rate selection for the robust operation under fluctuating power. Third, the explicit mappings ($I(t) \rightarrow m_{H_2(t)}$) and pressure/temperature states support plant-level set-point optimisation (energy-specific consumption, purity) under renewables-driven variability. These control-oriented features are consistent with current roadmaps and reviews that call for dynamic-ready electrolyser architectures for industrial deployment.

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