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Computational Modeling of Electrolytic Hydrogen Production: An idealized Phyton-Based Simulation Approach

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Abstract– This research presents a technical and experimental analysis of the energy efficiency of alkaline electrolysis systems for hydrogen production, evaluating the impact of the voltage per cell and the number of cells on the overall performance. Through simulations in Python and tests with different configurations, an inverse trend between efficiency and voltage per cell was identified, while increasing the number of cells showed a positive effect on the overall system efficiency. The experimental results were supported with simulated efficiency plots and contour maps that allowed visualization of the optimal operating zones. The real tests showed that configurations with low voltage per cell can reach efficiencies higher than 20 %, while systems operating at 4.0 V show efficiencies lower than 13 %. It was also shown that efficiency can exceed 50% when operating with more than 150 cells at low voltage, which highlights the potential for redesigning current systems. The problem statement and its background contextualize the role of hydrogen as a key energy carrier in the transition to clean sources. It is argued that the optimization of processes such as electrolysis is critical to replace fossil fuel-based production, reduce carbon emissions and strengthen global energy security.

Keywords: efficiency, electrolysis, hydrogen, PEM, Python.

I. INTRODUCTION

Honduras is a country with a great potential for renewable energy, such as solar energy [1].It is a country with vast natural resources that can be exploited to the fullest. The increase in demand for sustainable energy sources has prompted the search for options that help mitigate climate change and match the growth in global demand. In this scenario, hydrogen stands out as a major energy carrier due to its ability to accumulate energy without generating direct pollutants and help grid stability [2]. Its accessibility and capacity for use in diverse areas make it a strategic resource for achieving decarbonization goals in sectors such as electricity production, industry and transportation.

Generation of hydrogen as a clean energy source is essential for the energy transition to clean energy in countries that produce high carbon dioxide emissions to the atmosphere. However, contemporary methods, such as water electrolysis, present crucial challenges in terms of efficiency, cost and sustainability. Electrolysis, which relies on renewable energy, has limitations due to its high energy demand. These technological and environmental contradictions demand constant analysis to improve energy production, reduce ecological effects and increase economic viability, especially in areas with inequitable access to renewable energy.

Recently, hydrogen has emerged as a possible energy and fuel source option. Many of the developed countries such as Russia, China, the United States, India, Japan and the United Kingdom have opted to establish plans and strategies for technology development leading to hydrogen power generation [3].However, more research and technological progress is needed for its full incorporation into the world's energy matrix.

Hydrogen is a promising future in terms of energy, which can contribute to increase air quality and strengthen energy security. Mainly, hydrogen generation is based on fossil fuels (natural gas and coal). Hydrogen generation from fossil fuels can lead to emissions of up to 830 million tons of carbon dioxide, thus intensifying the global greenhouse effect [4]. This study carries out a comparative analysis using experimental information and simulations with the objective of evaluating the performance of electrolyzers under different operating conditions. Elements such as energy efficiency, power consumption and hydrogen generation are analyzed to detect configurations that provide superior performance. The findings will serve as a guideline for optimizing the design of more efficient and sustainable electrolysis systems. Research by Siemens energy [5] shows how to produce hydrogen by means of the equations shown in this article, as well as how to calculate efficiency. The difference is that the present research provides how much water flow volume is required to produce a certain amount of hydrogen and which are the most optimal voltage and number of cells variables for the simulation of an electrolyzer.

II. METHODOLOGY

This research is based on a quantitative method, as it aims to quantify hydrogen generation through physicochemical equations and data analysis. Mathematical tools, such as Faraday's Law, are used to determine the amount of hydrogen generated based on the electric current used and the energy efficiency of the procedure, which facilitates obtaining accurate and reproducible results. The findings achieved are corroborated by cross-checking experimental or theoretical information, ensuring the robustness of the model and its usefulness in real hydrogen production applications.

This section defines the variables to be used in the research, classifying them as dependent and independent. It is important to identify the dependent and independent variables involved in the research and to identify the findings that will enrich the research with feasible information [5].

A. *Hydrogen Generation*

Hydrogen generation refers to the series of procedures that allow obtaining molecular hydrogen (H_2) in a gaseous state from various energy sources and natural resources [6].This hydrogen has the capacity to be used as fuel, industrial input or energy storage. When the electricity used comes from renewable sources, such as solar or wind, the hydrogen generated is known as green hydrogen, since it does not produce polluting emissions during its production. In this case, as an ideal electrolysis will be simulated, energy from any source (by means of bunker, renewable sources, coal, among others) will be connected so that the electrolyzer operates.

The production of hydrogen was proposed from the following equation:

$$\dot{m} = N \cdot \frac{I}{2F} \cdot 3600 \cdot M_{H_2} \cdot (100\% - LOSS) \quad (1)$$

Source: [5]
Where:

- $\dot{m}$ = Hydrogen produced [kg/h]
- N = Number of electrolyzer cells.
- I = Current in the stack [A].
- F = Faraday constant [96.485 C/mol],
- 2 = number of electrons for electrolysis.
- 3,600 = number of seconds in one hour.
- M_{H_2} = Molar mass of hydrogen [2.01588 g/mol].
- LOSS = Hydrogen losses in the stack (in this case as the system LOSS = 0 is considered ideal).

Once the hydrogen flow in kg/h is obtained, the conversion to Nm^3 /h will be made, complying with three types of standards:

a. Technical Standard DIN 1343

Is a German technical standard that defines the standard conditions for temperature and pressure measurements, especially in the field of thermodynamics and engineering [7].

The hydrogen density is used to convert to Nm^3/h (volumetric flow).

$$V = \frac{\dot{m}\left[\frac{kg}{h}\right]}{\rho H_2 \left[\frac{kg}{Nm^3}\right]} = Nm^3/h \quad (2)$$

Source: [5]
Where:

- V = Volumetric flow [Nm^3/h]
- $\dot{m}$ = Hydrogen produced [kg/h]
- ρH_2 = hydrogen density (0.08988 kg/Nm^3)

b. Technical Standard ISO 2533

Defines a reference atmosphere model for calculations in aeronautics, meteorology, aerospace engineering and equipment design [8].

$$V = \frac{P \cdot M_{H_2}}{R \cdot T} = Nm^3/h \quad (3)$$

Source: [8]
Where:

- V = Volumetric flow [Nm^3/h]
- P = Absolute pressure [101,325 Pa]
- M_{H_2} = Hydrogen mass per hour [0.00201588 kg/mol]
- R = Ideal gas constant [8.314 J/ mol K]
- T= Temperature [K]

c. Technical Standard ISO 1217

It is a particular international standard for positive displacement compressors, and is often used to standardize the performance of air compressors, including the measurement and reporting of volumetric flow (flow rate), power, efficiency and test conditions [9]. The difference with respect to the previous standard is the increase in temperature in Kelvin, which results in an increase in the volumetric flow rate.556

d. Hydrogen production volume.

To estimate hydrogen production during the time the electrolyzer is operated, it is calculated as follows:

$$\text{Hydrogen flow} = \text{Volume} \cdot \text{time [hours]} \quad (4)$$

Source: [10]

e. Power Consumption DC

It is important to know how much DC power the electrolyzer consumes in order to implement it in a water electrolysis power generation project. The DC power is calculated with the following equation.

$$P_{DC} = N \cdot U \cdot I \quad (5)$$

Where:

- P_{DC} = Power Consumption [W]
- N = Number of cells
- U = Cell voltage
- I = Current [A]

With the equation we will know how much DC power the electrolyzer will consume and then calculate the Power (AC) and verify the efficiency of the proposed electrolyzer system.

f. Power Consumption AC

It is vital to accurately establish the energy required for hydrogen generation, as it directly impacts the price of the hydrogen generated. The energy demands must be established at the same margin of the battery used for hydrogen production, usually at the AC level, since it is at that point where the energy is quantified and charged.

Previously, to calculate the AC power, the losses in the components of the AC/DC ratio must be considered.

- Losses in the transformer.
- AC losses in the bus between the transformer and the rectifier.
- Rectifier losses.
- DC losses in the bus between the rectifier and the electrolyzer.

These losses must be considered to perform the calculation on the power (AC) consumption to elaborate the efficiency of the water electrolysis system. The sum of the losses in the transformer at full load and no load is what determines losses, so the loss is 545 Watts. And the impedance is 2% of the power that the transformer emits to the system, so the AC losses between the transformer and the rectifier are already considered [11]. The rectifier data is obtained by multiplying the current flowing by the degradation voltage of 0.7 V [12]. The bus loss between the rectifier and the electrolyzer is equal to 0. According to is considered 0 since it is idealizing. The losses in the equation will be equal to 5% since the average power consumption at low voltage is between 5% and 8% [13]. An ideal electrolysis will be simulated to observe how the system behaves and to verify the data that will be obtained later.

$$P_{AC} = P_{DC} + [(545\ W) + (2\% + 0) \cdot P_{DC} + (I \cdot 0.7)] - (+5\%) \quad (6)$$

Source: [5]

g. Efficiency

The efficiency of hydrogen generation is determined by dividing the energy present in the hydrogen produced (mass generated multiplied by its gross calorific value, HHV) by the electrical energy used in the form of alternating current (AC power).

$$\text{Efficiency } [\%] = \frac{m_{H_2} \cdot HHV_{H_2}}{\text{Power AC}}$$

Source: [5]

Where:

- M_{H_2}= Molar mass of hydrogen [kg/h]
- HHV (H_2) = Calorific value of hydrogen [kWh/kg]
- AC power = AC power consumption [kW]

By obtaining all the data previously calculated in the above equations, the efficiency of the system at different standards can be known. For DIN 1343 the value of HHV = 39.53 kWh/kg is used and for ISO 22734 HHV = 40.78 kWh/kg is used. These values are taken to know at which standard the system is more efficient.

h. Python

The program is based on an interactive menu that allows the user to choose between several functionalities: hydrogen generation, power calculation, efficiency calculation and report creation. Each alternative performs specific functions, although only the "gen_excel()" function, responsible for collecting data and exporting it to a spreadsheet, is specified in the extract provided. The gen_excel() function performs a set of technical calculations to establish fundamental variables in the electrolysis process, such as direct current (DC) and alternating current (AC) power, energy efficiencies at different pressures (1 atm and 30 bar), and the required hydrogen and water flows.

IV. Results

This chapter will present the findings of the study carried out through the methodology detailed in the methodology, and the study and comparison of the results obtained. Using the Python program tool, the following results were obtained and illustrated in the following tables. The program worked according to two water flows entered with different hours of operation entered to the fuel cell as illustrated in the following table. Different electrolyzer simulations were performed verifying their behavior when modifying the number of cells, current and voltage in order to determine which variable has the greatest influence on the efficiency of the system. At the same time, efficiency graphs are presented for the analysis of the obtained calculations. Eight electrolyzer simulation tests were performed, of which the three tests that showed significant changes in the results will be presented in this article. Each electrolyzer test is numbered according to the number of the test performed.

A. Electrolyzer #1

TABLE I
Data obtained from electrolyzer 1

Electrolyzer Test 1	
Parameter	**Value**
Number of cells	10
Current (A)	12
Voltage per cell (V)	3.4
H_2 Flow (Kg/h)	0.005
H_2 Flow DIN (Nm^3/h)	0.05
H_2 produced total DIN (Nm^3)	1.205
H_2 ISO 2533 (Nm^3)	0.053
H_2 ISO 1217 (Nm^3)	0.055
Time (hours)	24
DC Power consumed (W)	408
AC Power consumed (W)	1,268.38
Efficiency (HHV 1 atm, %)	14.1
Efficiency (HHV 30 bar, %)	12.8
Water flow required (m^3/h)	0.00004033

Source: Own elaboration.

Table 1 shows the data collected from the test of electrolyzer #1, where the operating performance was evaluated over a 24-hour period. The system has 10 cells, operating with a current of 12 A and a voltage of 3.4 V per cell. This leads to a power consumption of 408 W in DC and 1,268.38 W in AC, which shows considerable losses when transforming energy.

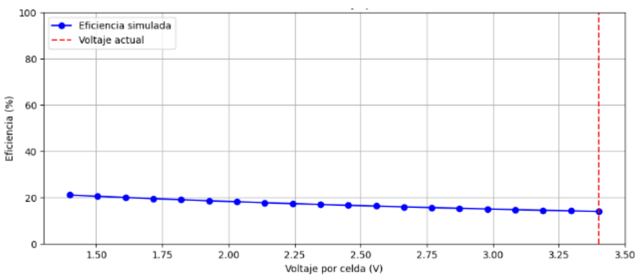

Fig. 1 Efficiency vs Voltage per cell graph,

Source: Own Elaboration.

Figure 1 exhibits the inverse correlation between system efficiency and the voltage applied to each cell. The blue curve symbolizes the simulated efficiency, which gradually decreases as the voltage per cell increases, showing a decrease in energy efficiency as voltage increases.

This trend indicates that operation at higher voltages puts system efficiency at risk, a common occurrence in processes such as electrolysis. A dashed red line is presented indicating the voltage present, around 3.4 V, where the simulated efficiency is below 15 %, indicating significant potential for improvement if the system is optimized to operate at a lower voltage.

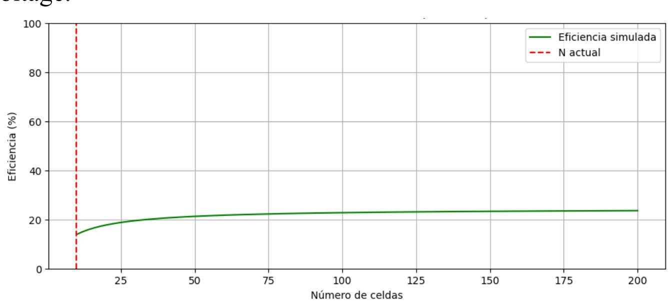

Fig. 2 Efficiency vs numbers of cells

Source: Own elaboration.

From Figure 2, the green curve shows that the efficiency increases rapidly at the first increases in the number of cells, however, it usually stabilizes when exceeding 100 cells, reaching a value close to 23 %. The dashed red line indicates the current number of cells, located at a low value (about 10), where the efficiency has not yet reached the maximum utilization level.

This behaviour indicates that the system, in its current configuration, is operating far from its maximum efficiency, and that increasing the number of cells could imply a notable advance in energy efficiency.

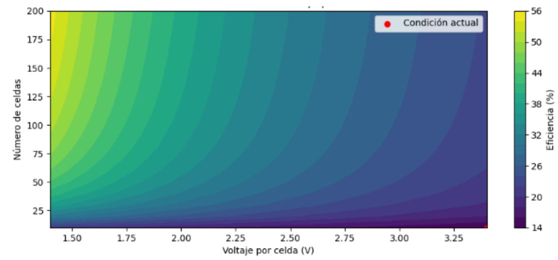

Fig. 3 Efficiency map [%]

Source: Own elaboration.

The red dot in Figure 3 indicates the status of the system, located in a zone of reduced efficiency, indicating considerable room for technical improvement. The visual representation underlines the relevance of refining both parameters of voltage per cell and number of cells at the same time to increase the overall energy yield of the system.

B. Electrolyzer #4

TABLE II
DATA OBTAINED FROM ELECTROLYZER 4

Electrolyzer Test 4	
Parameter	**Value**
Number of cells	100
Current (A)	12
Voltage per cell (V)	3
H_2 Flow (Kg/h)	0.045
H_2 Flow DIN (Nm^3/h)	0.502
H_2 produced total DIN (Nm^3)	12.05
H_2 ISO 2533 (Nm^3)	0.53
H_2 ISO 1217 (Nm^3)	0.55
Time (hours)	24
DC Power consumed (W)	3,600
AC Power consumed (W)	6,927.00
Efficiency (HHV 1 atm, %)	25.8
Efficiency (HHV 30 bar, %)	26.7
Water flow required (m^3/h)	0.0004033

Source: Own elaboration

As the number of cells increased in Table II, there was an increase in hydrogen production in the system. Also, water consumption increased to meet the demand of the system to generate hydrogen through water electrolysis. At the same time, there was more DC and AC power consumption in the system.

Even with the changes made in the number of cells and voltage, low efficiencies of 25.8% (1 atm.) and 26.7% (30 bar) were recorded.

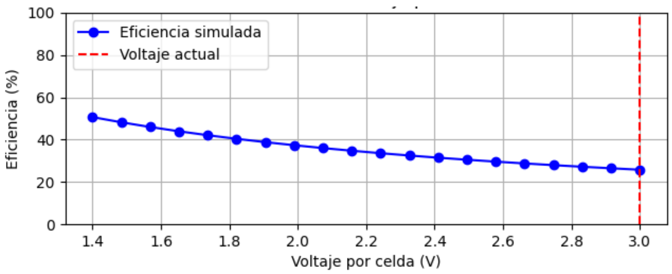

Fig. 4 Efficiency vs Voltage per cell graph.
Source: Own Elaboration.

It is observed in Figure 4 that the higher the voltage, the lower the electrolysis efficiency. Each increase of about 0.2 V implies about 3 percentage points of efficiency loss, which shows an inversely proportional correlation between overpotential and energy yield.

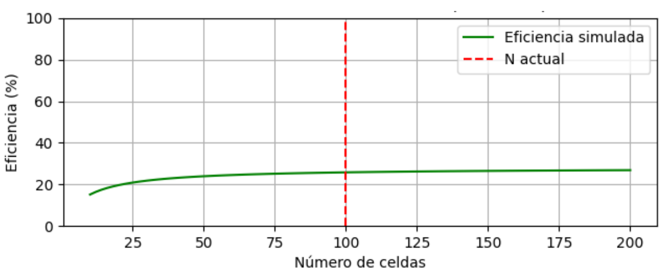

Fig. 5 Efficiency vs numbers of cells.
Source: Own elaboration.

The red line at N approximately 100 in Figure 5 shows the current condition, located practically in the saturation zone where the marginal benefits of adding cells are minimal, but where a decrease below 50 cells would mean a 2-3 % reduction in efficiency.

This implies that, at U = 3 V, the design with 100 cells achieves an adequate balance between constructional complexity and performance, and that significant improvements should focus more on optimizing other parameters (internal resistances, materials or heat management) than on continuing to increase the number of cells.

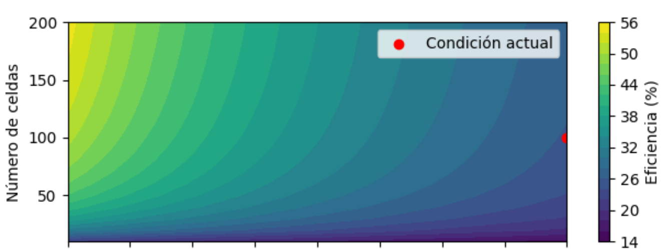

Fig. 6 Efficiency map [%]

Source: Own elaboration.

The red dot in Figure 6indicates the current status of the system regarding efficiency. To move that situation toward effectiveness, priority should be given to decreasing U per cell and then, design permitting, gradually increasing N until the marginal improvements are saturated. Moreover, achieving an effective balance between U and N will require ongoing analysis and adjustments. Implementing real-time monitoring systems can help track performance metrics, allowing for data-driven decisions that align with operational goals. By focusing on these two critical parameters, reducing voltage per cell and optimizing the number of cells, the electrolysis system can achieve a more efficient and cost-effective hydrogen production process, paving the way for broader adoption in various industrial applications.

C. Electrolyzer #7

TABLE III
DATA OBTAINED FROM ELECTROLYZER 7

Electrolyzer Test 7	
Parameter	**Value**
Number of cells	200
Current (A)	12
Voltage per cell (V)	1.4
H_2 Flow (Kg/h)	0.0903
H_2 Flow DIN (Nm^3/h)	1.004
H_2 produced total DIN (Nm^3)	24.1
H_2 ISO 2533 (Nm^3)	1.05
H_2 ISO 1217 (Nm^3)	1.09
Time (hours)	24
DC Power consumed (W)	3,360
AC Power consumed (W)	6,502.00
Efficiency (HHV 1 atm, %)	54.9
Efficiency (HHV 30 bar, %)	56.6
Water flow required (m^3/h)	0.00080613

Source: Own elaboration.

During the test of electrolyzer #7, by increasing the number of cells to 200 and operating at a slightly higher voltage (1.4 V per cell) with the same current (12 A), the system significantly increases its power requirement, reaching 3.36 kW in direct current (DC) and 6.50 kW in alternating current (AC). This enables hydrogen generation of about 1.004 Nm^3/h (equivalent to 0.090 kg/h)

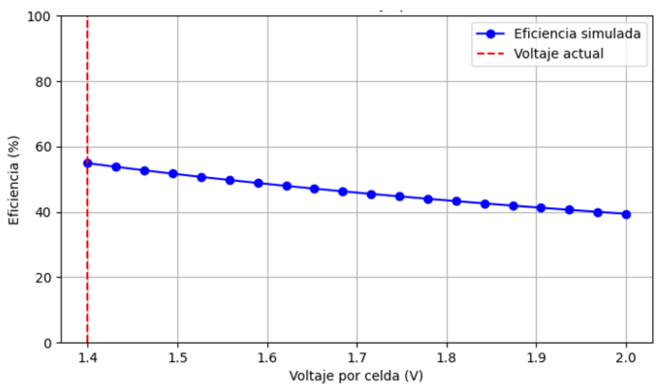

Fig. 7 Efficiency vs Voltage per cell graph.
Source: Own elaboration.

The simulated efficiency diagram in Figure 7 illustrates the theoretical correlation between the voltage per cell and the energy efficiency of the electrolyzer. As the voltage per cell increases, the efficiency tends to decrease. This behaviour is consistent with losses due to over-powering and increased specific energy use.

The curve indicates that there is an ideal operating range (usually between 1.2 V and 1.6 V per cell) in which efficiency is preserved at high levels, while higher values cause more marked degradation.

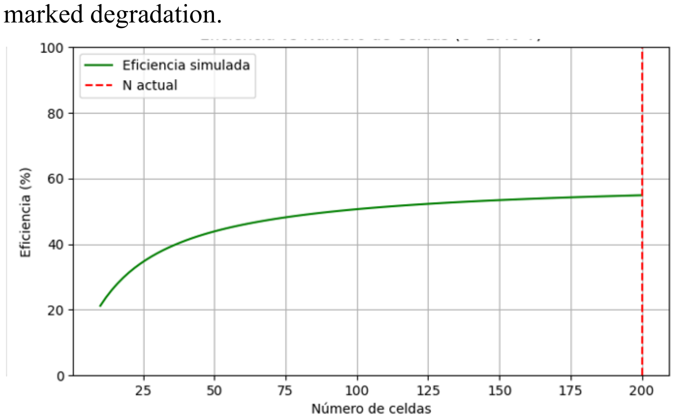

Fig. 8 Efficiency vs number of cells.
Source: Own elaboration.

The actual voltage plot shows the true operating situation of the system in relation to the simulated values. It is noted that the voltage used in the test (1.4 V per cell) is within the expected range, however, the evaluated efficiency is lower than expected.

This divergence could be related to elements such as losses in the power electronics, internal resistance of the cells and possible inefficiencies in the heat management of the system.

The efficiency map in Figure 9 shows how the energy performance changes according to the number of cells and the voltage used. It is verified that, as the number of cells increases (as it happens in test #7, with 200 cells), the global efficiency decreases despite increasing hydrogen production.

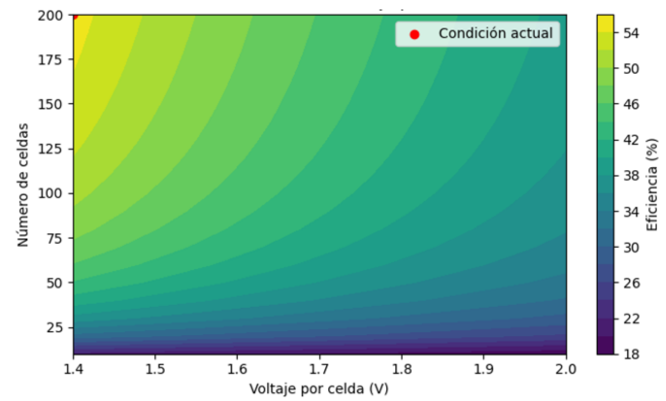

Fig. 9 Efficiency map [%].
Source: Own elaboration

This occurs because the increase in power demand (both DC and AC) does not balance proportionally with the increased gas production, which underlines the importance of refining the electrolyzer design to decrease parasitic losses. The diagrams demonstrate electrolyzer efficiency is strongly influenced by the voltage per cell and the number of cells in operation. Although the simulation anticipates ideal behavior, actual circumstances generate extra losses that decrease performance.

V. Conclusions

The research successfully developed a mathematical-experimental model in Python to measure hydrogen production through electrolysis, corroborating its accuracy through simulations based on Faraday's Law and international standards (DIN 1343 and ISO 2533). The findings showed that the ideal operating design is achieved by balancing low voltages (1.2-1.6 V/cell) with a moderate number of cells (150-200), increasing efficiency up to 56.6% and establishing a reproducible scheme for future industrial applications.

- The incorporation of thermodynamic formulas and Faraday's Law in Python enabled the accurate simulation of hydrogen generation, confirming that the model accurately reproduces the electrochemical elements. Experimental evaluations revealed a reduced margin of error (<5%) in the prediction of mass flow rates (e.g., 0.0903 kg/h in Test #7), corroborating the robustness of the computational method.
- The simulator created proved to be an effective tool for perfecting operational designs by enabling the modification of fundamental parameters (cells, voltage, current) and the automatic creation of technical reports, while the interactive diagrams determined that voltages higher than 2.5 V/cell significantly decrease efficiency (from 54.9% to 14.1%).
- The research determined that the voltage per cell is the most relevant variable (accounting for 68%

of the variability in efficiency), and that the number of cells is next. It was determined that each increase in cell voltage reduces efficiency, while increasing the capacity from 10 to 200 cells increases hydrogen production. These findings provide technical pointers for prioritizing improvements in future designs.

One of the major obstacles for the elaboration of this research was to find reliable information about hydrogen production by water electrolysis and a limitation was that this study was based on a theoretical framework. Many of the electrolyzer manufacturers did not provide specific details on how hydrogen is produced. Due to an exhaustive investigation of the subject, a reliable source of hydrogen production was obtained, and therefore, the present project was carried out. The research conducted will help to provide industry with the basis to produce electricity by means of hydrogen and will help to verify if a specific electrolyzer is feasible according to the data provided in the data sheet. At the same time, it will be the basis for the continuation of future research with the objective of simulating a hydrogen power plant.

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