Student Industrial Project Report

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and
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Commisioning an Electrolyzer

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Abstract

This project focuses on optimizing a Proton Exchange Membrane (PEM) electrolyzer for efficient hydrogen production within the context of sustainable energy initiatives like Germany's Energiewende and the CO2InnO project. The study aims to address the challenges of varying power conditions and system integration to improve performance metrics such as Faraday efficiency, voltage efficiency, and overall cell efficiency. The experimental design includes monitoring hydrogen production under controlled variable conditions using advanced sensors and data acquisition systems. The Electrolyzer performs at highest efficiency when it was ran at around 25% Power level. Results highlight the potential of PEM electrolyzers in achieving climate-neutral energy systems, providing insights for broader applications in decarbonization strategies.

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1 INTRODUCTION

1.1 Background Study

The global shift towards sustainable energy has become increasingly urgent in the face of climate change. Hydrogen is emerging as a key energy carrier in the transition to a low-carbon future, particularly through water electrolysis powered by renewable energy sources. Proton Exchange Membrane (PEM) electrolyzers are a promising technology in this context, offering high efficiency, compact design, and flexibility in operation under varying power inputs.

Germany's "Energiewende" (Energy Transition) mission is a significant example of national commitment to achieving net-zero greenhouse gas emissions by 2045 [8]. Central to this mission is the decarbonization of energy production, where hydrogen plays a crucial role. By integrating hydrogen production with renewable energy and carbon capture technologies, Germany aims to reduce its reliance on fossil fuels and minimize its carbon footprint.

In line with these global and national goals, the Upper Rhine region is set to become a pilot for a greenhouse gas emission-free economic zone, focusing on sustainable energy and transport. The CO_2InnO project aims to contribute to the region's transformation into a climate-neutral hub, showcasing hydrogen-based solutions for power and heat generation, as well as e-mobility.[19] This initiative tests and promotes decentralized, climate-neutral energy and transport solutions, assessing their benefits for local and regional systems. Through this project, CO_2InnO investigates several key areas, including hydrogen-based combined heat and power (CHP) units, sustainable mobility and charging infrastructure, cybersecurity in energy systems, and societal acceptance. The collaboration involves close engagement with French and German citizens and stakeholders, ensuring that the project reflects the region's diverse needs and perspectives.

This project explores the optimization of a PEM electrolyzer, particularly within the context of CO_2InnO's initiatives and Germany's Energiewende goals, contributing to the broader aim of transforming the Upper Rhine region into a sustainable, climate-neutral economic zone.

1.2 Problem Statement

While PEM electrolyzers are advantageous for hydrogen production, optimizing their efficiency under different operating conditions remains a challenge. Moreover, understanding how to integrate these electrolyzers with hydrogen-based power and heat generation, as well as sustainable mobility infrastructure, is critical for maximizing their potential in sustainable energy systems.

This project aims to address these challenges by investigating the performance of a PEM electrolyzer under varying power conditions and assessing its integration with CO_2InnO's hydrogen-based solutions. The goal is to enhance hydrogen production efficiency while contributing to the broader objectives of CO_2InnO and Germany's Energiewende mission to reach net-zero emissions by 2045.

1.3   Relevancy of Project

As the world moves towards decarbonization, the role of hydrogen in energy systems becomes increasingly significant. This project holds high relevance as it aligns with Germany's Energiewende mission and the CO_2InnO project, both of which focus on transforming the Upper Rhine region into a climate-neutral economic zone. Furthermore, Malaysia has articulated its own aspirations towards achieving net-zero greenhouse gas emissions,[18] recognizing hydrogen as a important component in its sustainable energy strategy.

Being conducted by a Malaysian student from Universiti Teknologi Petronas (UTP), this research creates international efforts, drawing similarities between European initiatives and Malaysia's sustainability goals. The insights gained from this project can inform the design and operation of future energy systems not only in Germany but also in Malaysia and other countries pursuing similar objectives. Emphasizing hydrogen-based technologies, this study contributes to the global discourse on sustainable energy solutions, fostering knowledge transfer and collaborative opportunities across borders.

1.4   Objectives

1. Optimization of PEM Electrolyzer Efficiency:

   - Analyze performance under varying power inputs (20%-100%).
   - Evaluate operational parameters like Faraday efficiency, voltage efficiency, and overall cell efficiency.

2. System Integration:

   - Assess integration capabilities with hydrogen-based power and heat generation systems in CO2InnO projects.
   - Explore synergies with renewable energy sources to enhance operational feasibility.

3. Data-Driven Insights:

   - Develop operational curves and performance metrics for the electrolyzer to inform future designs.
   - Employ Tafel analysis to identify areas for efficiency improvements.

2 LITERATURE REVIEW

2.1 Hydrogen Production Techniques

Hydrogen, a promising clean energy carrier, must be separated from compounds such as water (H_2O) or methane (CH_4) to be utilized effectively. Several techniques for hydrogen production have been developed, each with varying efficiency, cost, and environmental impact.

Natural Gas Reforming / Gasification

Natural gas reforming is a well-established method for hydrogen production, utilizing existing natural gas infrastructure. According to U.S Department of Energy [7], currently, 95% of the hydrogen in the U.S. is produced using this technique, primarily through steam-methane reforming (SMR) .

Steam-Methane Reforming (SMR) involves reacting methane with high-temperature steam to produce hydrogen, carbon monoxide, and carbon dioxide. It is an endothermic process requiring heat input.
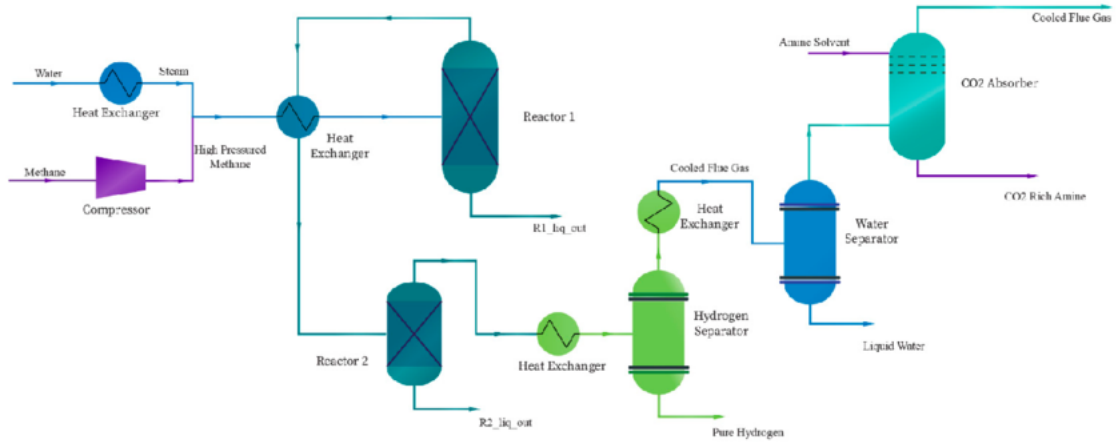
Figure 1: Steam-Methane Reforming (SMR) Process Flow [21]

Electrolysis

Electrolysis is a promising method for carbon-free hydrogen production using electricity from renewable or nuclear sources. The process involves splitting water into hydrogen and oxygen in a device called an electrolyzer, which can vary from small, distributed units to large-scale facilities powered by renewable energy. Electrolysis offers a versatile approach to generating hydrogen, and different electrolyzer types which is Polymer Electrolyte Membrane (PEM), Alkaline, and Solid Oxide Electrolyzers—function based on the specific electrolyte material used.

Polymer Electrolyte Membrane (PEM) Electrolyzers use a solid plastic membrane as the electrolyte. In this process, Water reacts at the anode, forming oxygen, hydrogen ions, and electrons. Hydrogen ions cross the membrane to the cathode, where they combine with electrons to form hydrogen gas.

$$4H^+ + 4e^- \rightarrow 2H_2 \qquad 2H_2O \rightarrow O_2 + 4H^+$$

2H₂ (displayed as 2H$_2$)

$2H_2$ O_2 $+ 4e^-$

Cathode H$^+$ Anode

H_2O
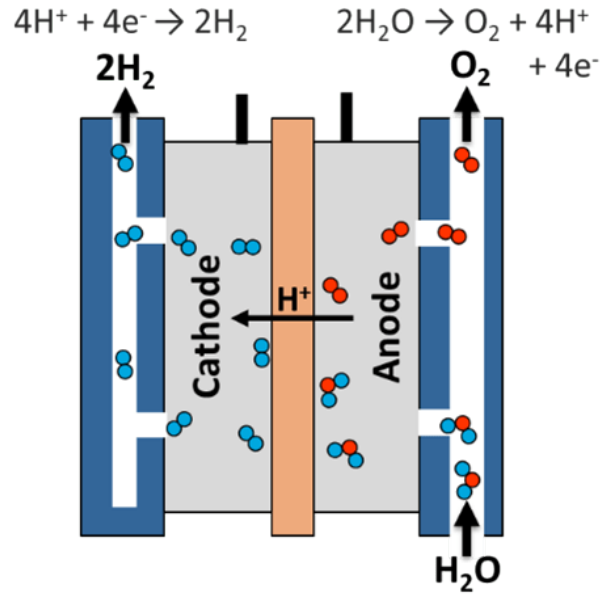
Figure 2: PEM Electrolyzer Illustration [6]

Alkaline Electrolyzers rely on transporting hydroxide ions through a liquid alkaline electrolyte, typically sodium or potassium hydroxide. Hydrogen is generated at the cathode side, and newer approaches using solid Alkaline Exchange Membranes (AEM) are being explored at the laboratory scale.

	Alkaline Electrolysis	Proton Exchange Membrane Electrolysis	Anion Exchange Membrane Electrolysis
Structure	Cathode — OH⁻ → Anode, Diaphragm	Cathode, PEM, Anode (H⁺)	Cathode, AEM, Anode (OH⁻)
Electrolytes	Aqueous KOH	Solid (Polymer)	Solid (Polymer)
Operating temperature	65-100 °C	50-90 °C	50-80 °C
Voltage	1.8-2.4 V	1.8-2.2 V	1.8-2.2 V

Figure 3: An illustration comparing traditional alkaline, PEM and AEM systems [14]

Solid Oxide Electrolyzers use a ceramic material as the electrolyte and operate at high temperatures (700–800°C). They leverage available heat to enhance efficiency, thereby reducing the need for electrical input. These electrolyzers form hydrogen at the cathode and oxygen gas at the anode.
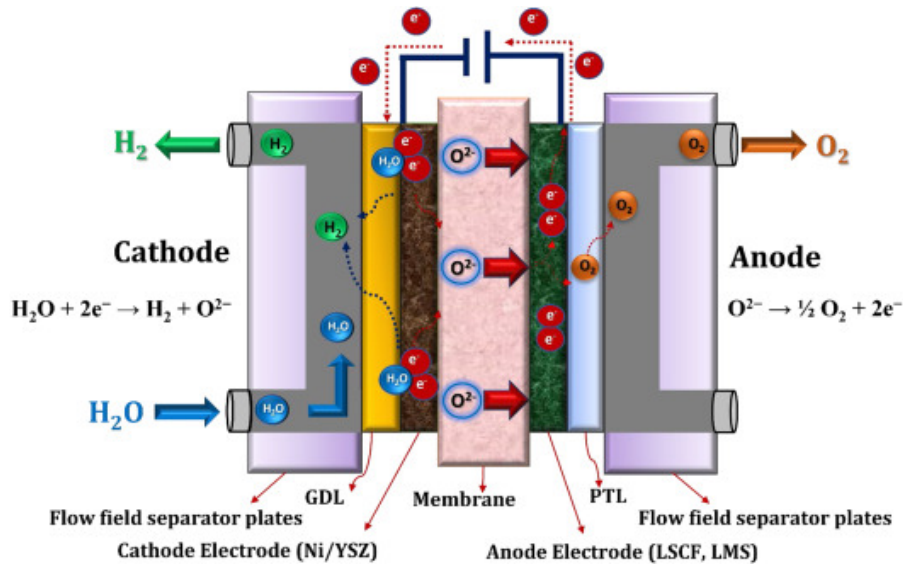
Figure 4: An illustration comparing traditional alkaline, PEM and AEM systems [24]

Synergy with Renewable Energy is particularly promising. Electrolysis could complement dynamic, intermittent power sources like wind, where surplus electricity can be used to produce hydrogen rather than being wasted.[6] This integration could enhance both the stability and utility of renewable power.
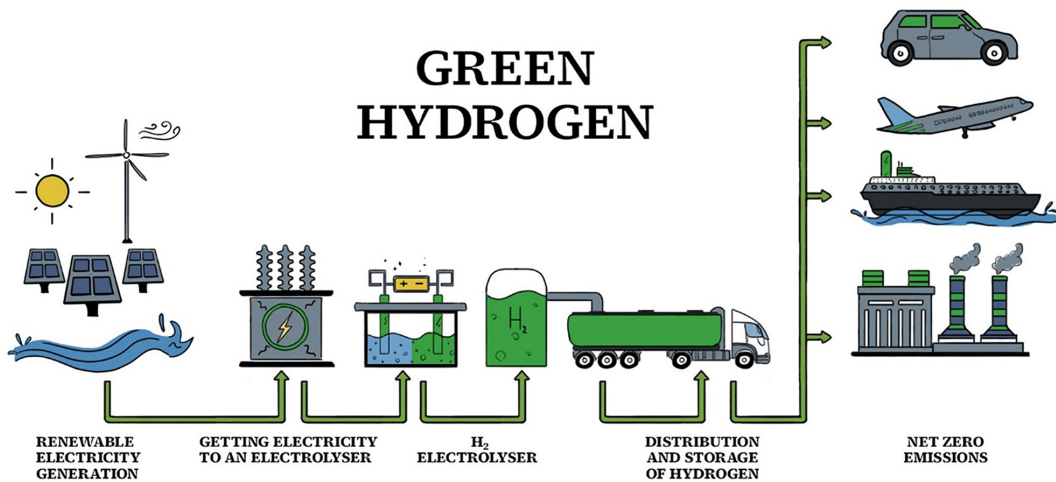
Figure 5: How hydrogen can be generated from excess renewable electricity [17]

The main challenge of electrolysis is its high cost, but ongoing research aims to reduce this by utilizing excess renewable electricity, particularly in "power-to-hydrogen" projects[4].

Electrolysis is a key pathway for clean hydrogen production, benefiting from renewable and nuclear energy integration. Its development could significantly reduce greenhouse gas emissions, particularly if linked to excess renewable energy. Continued research is vital to make electrolysis a viable large-scale hydrogen production solution.

Biomass-Derived Liquid Reforming and Microbial Biomass Conversion

Biomass-derived liquid reforming is a promising mid-term technology for hydrogen production. This process involves converting biomass resources, such as ethanol and bio-oils, into hydrogen using methods similar to natural gas reforming. Biomass-derived liquids have the advantage of being more easily transported compared to solid biomass feedstocks, enabling semi-centralized or distributed hydrogen production at refueling stations.[5].

1. Steam Reforming: The biomass-derived liquid fuel reacts with steam at high temperatures in the presence of a catalyst to produce a reformate gas containing hydrogen, carbon monoxide, and carbon dioxide.

$$C_2H_5OH + H_2O \rightarrow 2CO + 4H_2 \tag{1}$$

2. Water-Gas Shift Reaction: The carbon monoxide from the first step reacts with steam to produce additional hydrogen and carbon dioxide.

$$CO + H_2O \rightarrow CO_2 + H_2 \tag{2}$$

Other Methods

Emerging techniques like Thermochemical Water Splitting, Photobiological Water Splitting, and Photoelectrochemical Water Splitting are under development, leveraging high temperatures and solar energy to produce hydrogen. These methods offer potential for low-emission hydrogen production, but they are still in experimental stages and require further research to become commercially viable[4].
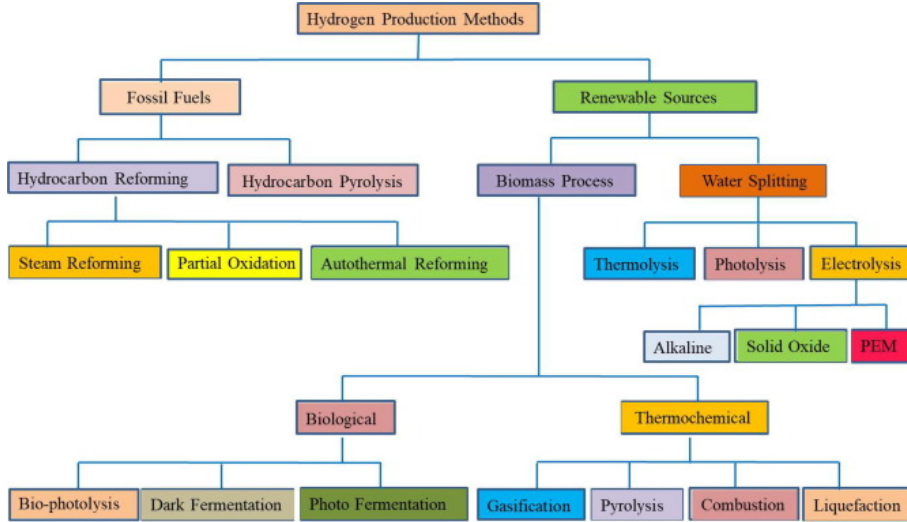

Figure 6: All Hydrogen Production Methods [23]

In summary, while natural gas reforming remains the dominant hydrogen production method, advances in electrolysis and biomass conversion, coupled with emerging technologies, are critical to reducing costs and environmental impacts. The future of hydrogen production lies in optimizing these processes to align with global decarbonization goals.

2.2 PEM Electrolyzer Technology

2.2.1 Challenges with Alkaline Electrolyzers

Alkaline electrolyzers have been widely used for hydrogen production, but they face several significant challenges that limit their efficiency and scalability. These drawbacks explain why newer technologies, like PEM electrolyzers, are gaining more traction in the industry. Below are some of the key challenges:

High Ohmic Resistance

Alkaline electrolyzers uses thick diaphragms, which result in increased ohmic resistance across the system. Thelower intrinsic conductivity of hydroxide ions (OH^-) compared to protons (H^+) in PEM electrolyzers further exacerbates this resistance, leading to lower performance efficiency. [11]

Gas Crossover Issues

The diaphragms used in alkaline electrolyzers are generally highly porous, allowing for ion transport but also leading to significant gas crossover. This occurs when hydrogen and oxygen gases mix across the diaphragm, reducing system efficiency and increasing the risk of creating hazardous conditions due to unwanted reactions.[11]

Catalyst Limitations

Nickel-based catalysts are predominantly used in alkaline electrolyzers due to their low cost and abundance. However, the catalytic activity of nickel is much lower compared to noble metals like platinum, making it less efficient for hydrogen production. Improving catalytic performance often involves alloying nickel with other metals, such as molybdenum or iron, but this increases fabrication complexity and costs.[11]

Performance Variability and Reproducibility

C. Karacan et al.[11] highlights the negative effects on reproducibility due to insufficient conditioning time of cells, affecting benchmarking and performance evaluation. Additionally, variations in material morphology, such as the formation of a passivation layer of nickel oxide (NiO) on the anode, contribute to inconsistent performance across different cells, making it difficult to ensure reliable operation.

Mechanical and Chemical Degradation

Mechanical and chemical degradation is a persistent issue in alkaline electrolyzers. Electrode materials, particularly nickel foams, are prone to mechanical erosion and chemical stresses, which degrade their performance over time[11]. These degradation processes are especially concerning for long-term operation, affecting the system's stability and efficiency.

Low Operating Pressure and Gas Management

Alkaline electrolyzers generally operate at low pressures, which necessitates additional compression for hydrogen storage and transport, increasing the overall system's energy consumption. The formation of gas bubbles during electrolysis often leads to bubble entrapment in the pores of nickel substrates, increasing resistance and reducing the effective surface area available for the electrochem-

ical reaction.[11]

2.2.2 PEM Water Electrolysis:

These issues with alkaline electrolyzers highlight why there was a push to develop alternative technologies for water electrolysis. In the 1960s, General Electric [27] addressed these drawbacks by developing the first PEM water electrolyzer based on a solid polymer electrolyte. The PEM design overcame many of the limitations of alkaline systems by using a solid membrane to separate the gases while allowing efficient proton conduction. It uses solid polysulfonated membranes (e.g., Nafion) as the electrolyte and operates under low temperatures (20–80°C). PEM electrolysis offers several advantages, including compact design, high current density, high efficiency, and the production of ultra-pure hydrogen. However, the use of noble metal electrocatalysts such as Pt/Pd (for HER) and IrO_2/RuO_2 (for OER) increases costs, making PEM electrolysis more expensive than alkaline water electrolysis. Research efforts continue to focus on reducing costs while maintaining high efficiency, moving the technology closer to commercial viability.

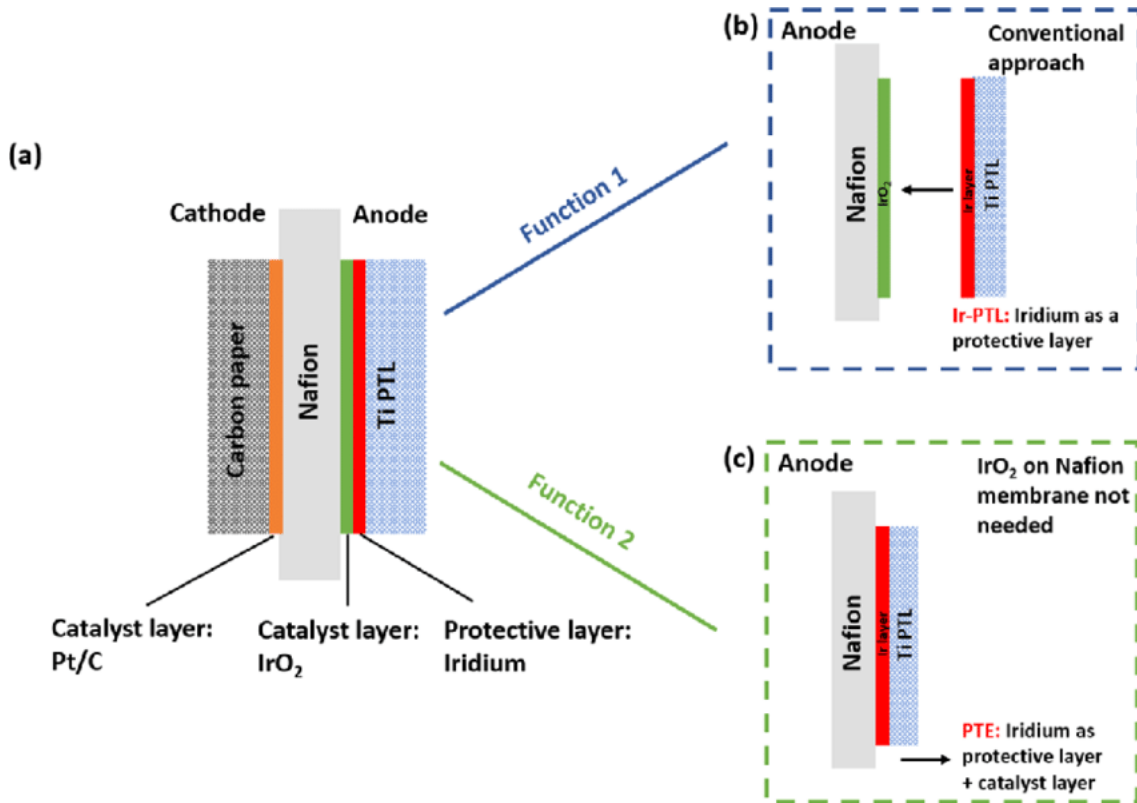Figure 7: (a) A schematic representation of the essential components within a PEM electrolyzer; (b) An Ir-coated porous transport layer (PTL) integrated with a standard catalyst-coated membrane (CCM), where the Ir layer on the PTL functions as a protective layer (Ir-PTL); (c) An Ir-coated PTL integrated with a CCM that lacks IrO_2 on the membrane, with the Ir layer acting as the catalyst layer (PTE). [15]

2.3   Principle of PEM Water Electrolysis:

Proton Exchange Membrane Electrolysis Cells (PEMECs) are advanced electrochemical devices used for splitting water into hydrogen and oxygen, relying on a solid polymer electrolyte. The fundamental operation of PEMECs is based on the principle of electrolysis, where an external electrical source drives the decomposition of water into its elemental components. The cell is divided into two compartments—an anode and a cathode—separated by a proton-conducting membrane.[13]

At the anode, deionized water is introduced and undergoes oxidation. Water molecules (H_2O) are catalytically split into oxygen gas (O_2), protons (H^+), and electrons (e^-). This reaction is facilitated by a catalyst, typically composed of unsupported iridium-based oxides, and can be represented by the half-cell reaction: [13]

$$H_2O \rightarrow \frac{1}{2} O_2 + 2\,H^+ + 2\,e^-$$
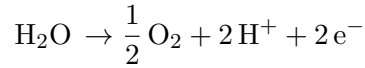
$$E_a = 1.23\,V \text{ vs. Standard Hydrogen Electrode (SHE)}$$

Oxygen is released as a gas, and the protons generated are transported across the proton-conducting membrane to the cathode.[13]

The membrane, usually made from perfluorosulfonic acid (PFSA) polymers such as Nafion®, serves two primary functions: facilitating the selective transfer of protons while preventing the mixing of hydrogen and oxygen gases. This ensures that the electrolysis process operates efficiently and safely.[13]

At the cathode, the protons that have migrated through the membrane are reduced by electrons supplied from the external power source. The reduction of protons leads to the production of hydrogen gas (H_2), following the half-cell reaction: [13]

$$2\,H^+ + 2\,e^- \rightarrow H_2$$
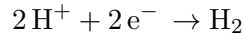
$$E_c = 0.00\,V \text{ vs. SHE}$$

Overall, the combined reactions at the anode and cathode result in the electrochemical splitting of water into hydrogen and oxygen: [13]

$$H_2O \rightarrow H_2 + \frac{1}{2} O_2$$
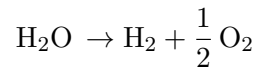
The energy required for this process can be calculated based on thermodynamic principles, where the Gibbs free energy change (ΔG^0) under standard conditions (25°C and 1 bar) is approximately +237.2 kJ/mol H_2O. This corresponds to a reversible cell voltage of 1.23 V. The external voltage applied must overcome this threshold to drive the reaction, with any excess voltage compensating for system inefficiencies, such as overpotentials associated with reaction kinetics and ohmic losses.

2.3.1 Thermodynamics of Water Electrolysis:

Water electrolysis is fundamentally governed by thermodynamic principles that dictate the energy requirements for splitting water molecules into hydrogen and oxygen. In Proton Exchange Membrane Electrolysis Cells (PEMECs), a clear understanding of the relationship between voltage, temperature, and pressure is crucial to optimizing the efficiency of the electrolysis process. This section focuses on the key thermodynamic parameters that affect cell performance, particularly from the perspective of electrical energy input and system efficiency.

Cell Voltage and Energy Requirements

In water electrolysis, the total energy required to decompose one mole of water (ΔH_{cell}) is derived from two components: the Gibbs free energy (ΔG_{cell}) and the reversible thermal energy (ΔQ_{rev}):

$$\Delta H_{\text{cell}} = \Delta G_{\text{cell}} + \Delta Q_{\text{rev}}$$

The Gibbs free energy corresponds to the minimum electrical energy required to drive the reaction, while the reversible thermal energy represents the heat needed to maintain thermodynamic equilibrium. The reversible voltage (U_{rev}) is the minimum voltage needed to initiate electrolysis under standard temperature and pressure (STP), which is calculated from ΔG_0 (237.2 kJ/mol at 25°C):

$$U_{\text{rev}} = \frac{\Delta G_0}{nF} = 1.23\,\text{V}$$

This voltage sets the theoretical lower bound for the process, and hydrogen production cannot occur if the applied cell voltage U_{cell} is less than this value. In practical systems, however, additional voltage is required to overcome inefficiencies like overpotentials and ohmic losses, which increase the energy demand above U_{rev}.

Thermo-neutral Voltage and Heat Management

Another key thermodynamic parameter is the thermo-neutral voltage (U_{tn}), which represents the voltage at which the system neither absorbs nor releases heat. For water electrolysis, the thermo-neutral voltage is typically 1.48 V. When $U_{\text{cell}} = U_{\text{tn}}$, the process is isothermal, meaning the heat produced by electrical inefficiencies is exactly offset by the reversible heat absorbed by the system.

The relationship between U_{cell} and U_{tn} can be summarized as follows:

- If $U_{\text{cell}} < U_{\text{tn}}$:
    - The system absorbs heat from the surroundings.
    - External heating may be required to sustain the electrolysis process at constant temperature.

- If $U_{\text{cell}} > U_{\text{tn}}$:

    - The system generates excess heat.

    - Cooling mechanisms are needed to dissipate this heat and prevent thermal degradation.

- If $U_{\text{cell}} = U_{\text{tn}}$:

    - The system operates isothermally (no net heat exchange).

    - No external heating or cooling is required as the heat produced by inefficiencies is exactly offset by the heat absorbed.

Temperature and Pressure Effects

Both temperature and pressure play critical roles in the efficiency and voltage requirements of water electrolysis systems. Increasing the temperature reduces the Gibbs free energy (ΔG) required for the reaction, thereby lowering the reversible voltage:

$$U_{\text{rev}}(T) = 1.481 - 0.000846T \text{ V}$$

This effect allows for more efficient operation at elevated temperatures, as less electrical energy is needed to maintain the electrolysis reaction. However, higher temperatures also increase the entropy (ΔS) of the system, which must be accounted for in the overall energy balance.

Pressure also influences the Gibbs free energy of the reaction. By increasing the pressure of the reactants (water) and decreasing the pressure of the products (hydrogen and oxygen), the system can operate at lower cell voltages. This relationship is governed by the Nernst equation, which describes how the cell voltage changes with variations in pressure.

Energy Efficiency and Losses

In practical electrolysis systems, energy losses occur due to overpotentials and ohmic resistances. These inefficiencies are responsible for the gap between the theoretical voltage (U_{rev}) and the actual operating voltage (U_{cell}). Overpotentials arise from the slow kinetics of the oxygen evolution reaction (OER) at the anode and hydrogen evolution reaction (HER) at the cathode. Ohmic losses result from resistance to ion transport through the electrolyte and electron transport through the electrodes.

The total energy efficiency of the electrolysis cell is therefore inversely related to the magnitude of these losses. Reducing overpotentials by optimizing catalyst materials and minimizing ohmic losses through improved cell design are key strategies to improving system performance.

Thermal Balance and Heat Flow

The thermal balance (ΔQ_{cell}) of the electrolysis process is determined by the interplay between reversible heat absorption ($\Delta Q_{\text{rev}} = T\Delta S$) and the heat generated by irreversible processes (ΔQ_{irrev}). The overall heat flow is given by:

$$\Delta Q_{\text{cell}} = nF(U_{\text{tn}} - U_{\text{cell}})$$

- If $U_{\text{cell}} < U_{\text{tn}}$: The system absorbs heat from the surroundings, and external heating may be required to sustain the process.

- If $U_{\text{cell}} > U_{\text{tn}}$: The system generates excess heat, necessitating cooling mechanisms to prevent overheating.

- If $U_{\text{cell}} = U_{\text{tn}}$: The system operates isothermally, with no net heat exchange required.

2.3.2   Efficiency Metrics in Electrolysis

Efficiency metrics are critical in determining the overall performance of water electrolysis systems, including Alkaline Electrolysis Cells (AEC), Proton Exchange Membrane Electrolysis Cells (PEMEC), and Anion Exchange Membrane Electrolysis Cells (AEMEC). Various definitions of energy efficiency exist in both research and industrial contexts, and these metrics help in evaluating how effectively these systems convert electrical energy into hydrogen. The four primary efficiency metrics used to assess electrolyzers are Faradic efficiency, voltage efficiency, cell efficiency, and energy efficiency.

1. Faradic Efficiency

Faradic efficiency, sometimes called current efficiency [13], measures how much of the electrical current supplied to the electrolyzer is effectively used to produce hydrogen. It is a measure of mass conservation efficiency, quantifying how closely the actual hydrogen production aligns with the theoretical hydrogen output predicted by Faraday's law.

Faradic efficiency can be calculated as the ratio of the amount of hydrogen actually produced during electrolysis (ΔN_{H_2}) to the theoretical amount of hydrogen that should be produced based on the electrical current applied (ΔN_{th}):

$$\eta_{\text{Faradic}} = \frac{\Delta N_{H_2}}{\Delta N_{\text{th}}} = \frac{I - 2F\frac{\Delta N_{H_2,\text{loss}}}{\Delta t}}{I} = \frac{I - I_{\text{loss}}}{I} = 1 - \frac{I_{\text{loss}}}{I}$$

where:

- I is the current intensity,

- Δt is the duration of operation,

- F is Faraday's constant, and

- $\Delta N_{H_2,\text{loss}}$ accounts for hydrogen losses due to cross-permeation or side reactions.

- $I_{\text{loss}} = 2F\dot{n}_{H_2,\text{loss}}$, where $\dot{n}_{H_2,\text{loss}}$ is the molar flow rate of hydrogen loss.

The Faradic efficiency can also be expressed as this [20, 3]:

$$\eta_{\text{Faradic}} = \frac{\dot{m}nF}{IM_{H_2}}$$

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Where:

- $\dot{m}$: Represents the mass flow rate of hydrogen.

- n: the number of moles or a mole ratio.

- F: Faraday's constant.

- I: Current intensity.

- M_{H_2}: Represents the molar mass of hydrogen.

If there are no losses, the Faradic efficiency reaches a maximum of 100%, meaning all the supplied current contributes to hydrogen production. However, parasitic processes such as hydrogen leakage or side reactions can reduce the Faradic efficiency. For example, cross-permeation of hydrogen through the membrane from the anodic to cathodic compartment can lead to a lower hydrogen yield. Studies by Grigoriev et al [10]. report that Faradic efficiency decreases from nearly 100% at low pressures to about 90% at higher pressures, such as 130 bar, due to increased gas permeation through the membrane.

In industrial systems, the Faradic efficiency is a practical measure because it directly correlates with the amount of hydrogen produced, which is critical for optimizing electrolyzer performance. The Faradic efficiency can drop significantly at lower current densities, as parasitic reactions become more prominent. Below 50–100 mA/cm², the efficiency can significantly decrease, making it a key factor in the design and operation of both AEC and PEMEC systems [10].

In industrial electrolyzers, the Faradic efficiency typically reaches 98–99.9% at nominal operating conditions, but it can decrease at higher pressures or lower current densities due to the increase in parasitic reactions and resistive losses [10]. Understanding and optimizing cell efficiency is crucial for minimizing operational costs and ensuring the maximum hydrogen yield.

2. Voltage Efficiency

Voltage efficiency is another key metric used to evaluate electrolyzer performance. It measures how efficiently the supplied voltage is converted into the electrochemical work required for water splitting. In essence, it quantifies the ratio of the reversible cell voltage (U_{rev})—the minimum voltage needed to split water—over the actual cell voltage (U_{cell}) applied to the system.

The voltage efficiency is given by:

$$\eta_{\text{voltage}} = \frac{U_{\text{rev}}}{U_{\text{cell}}} \times 100$$

Where:

- U_{rev} is typically around 1.23 V at standard temperature and pressure (STP),

- U_{cell} is the total voltage applied during electrolysis.

Voltage efficiency indicates how much of the electrical potential is effectively used in driving the water-splitting reaction versus how much is lost due to overpotentials and ohmic resistances. Overpotentials arise from the sluggish kinetics of the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER) [13], while ohmic losses occur due to resistance in the electrolyte, membrane, and electrodes.

If the system is perfectly efficient with no losses, the voltage efficiency would be 100%. However, practical systems experience losses, and the voltage efficiency can drop significantly, especially at higher current densities where overpotentials increase. For instance, voltage efficiency is reduced as the current intensity increases because the cell voltage rises due to overpotentials and resistive losses [26].

3. Cell Efficiency

Cell efficiency integrates both the Faradic efficiency and voltage efficiency, providing a comprehensive measure of the electrolyzer's overall performance at the cell level. It accounts for both the electrical and thermal losses and is defined as the ratio of the theoretical power input (based on reversible conditions) to the actual power input supplied to the electrolyzer.

The overall cell efficiency can be expressed as[3, 13, 20]:

$$\eta_{\text{cell}} = \eta_{\text{voltage}} \times \eta_{\text{Faradic}}$$

By multiplying the voltage efficiency and Faradic efficiency, cell efficiency provides a more complete picture of the electrolysis process's performance. If either the voltage efficiency or the Faradic efficiency is low, the overall cell efficiency will be reduced. This metric is particularly useful for evaluating how both electrical and mass-based inefficiencies (such as hydrogen losses) impact the overall system performance.

4. Energy Efficiency

The energy efficiency of an electrolyzer is the most general metric used to evaluate the system's performance. It compares the ideal thermodynamic energy required for hydrogen production (based on the lower heating value or higher heating value of hydrogen) to the actual energy input supplied to the system. This metric is critical because it includes both the electrical energy and any heat exchanged with the environment.

According to M.Schalenbach et al. [22] and Lamy [13],Energy efficiency of electrolyser is expressed as:

$$\eta_{\text{energy}} = \frac{P_{\text{ideal}}}{P_{\text{real}}}$$

Where:

- P_{ideal} is the theoretical power required to produce hydrogen,

- P_{real} is the real power input, including both electrical and thermal energy.

Two commonly used reference points for energy efficiency are the higher heating value (HHV) and the lower heating value (LHV) of hydrogen. The HHV includes the energy required to vaporize the water formed in the reaction, while the LHV excludes this energy. This distinction is important because industrial processes typically operate based on LHV, while HHV is often used in thermodynamic analyses.

When calculating energy efficiency based on the HHV:

$$\eta_{\text{HHV}} = \frac{\dot{V}\,\text{HHV}}{P_{\text{el}}}$$

where $\dot{V}$ is the hydrogen production rate and P_{el} is the total electrical power input [13]. Similarly, for LHV-based efficiency, the equation is:

$$\eta_{\text{LHV}} = \frac{\dot{V}\,\text{LHV}}{P_{\text{el}}}$$

Energy efficiency can sometimes exceed 100% if the cell is absorbing heat from the environment, particularly when the cell voltage is between the reversible voltage and the thermo-neutral voltage ($U_{\text{rev}} < U_{\text{cell}} < U_{\text{tn}}$). This endothermic behavior means the system is drawing energy from the environment to complete the reaction, which can lead to unusually high efficiency values [13].

However, Lamy and Millet [13] argued that the definitions of η_{HHV} (or η_{LHV}) lack consistency because the denominator accounts solely for the electric power $P_{el} = U_{cell}I$, while the numerator, $HHV_{H_2} = \Delta H_{\text{liquid}}$ (or $LHV_{H_2} = \Delta H_{\text{gas}}$), incorporates the reversible heat exchanged $\Delta Q_{\text{rev}} = T\Delta S$. In practical terms, the real energy efficiency should take into account all losses, including resistive losses, overpotentials, and any heat exchange from the electrolyser. Schalenbach et al. [22] propose that a comprehensive definition of energy efficiency includes all sources of energy, both electrical and thermal, to provide an accurate assessment of system performance under real-world operating conditions.

The energy efficiency can be expressed as:

$$\eta_{\text{energy}} = \frac{\dot{V}\,\text{LHV}_{H_2}}{W_{\text{irrev}} + \Delta Q_{\text{heat},H_2O}}$$

Where:

- LHV_{H_2}: Represents the lower heating value of hydrogen.

- W_{irrev}: Represents the irreversible work done during the electrolysis process.

- $\Delta Q_{\text{heat},H_2O}$: Represents the heat exchanged with water during the electrolysis.

5. Critical Analysis of Efficiency Metrics

While each of these efficiency metrics—Faradic, voltage, cell, and energy efficiency—provides valuable insights into the performance of electrolyzers, it is important to recognize their limitations:

- Faradic efficiency is focused on mass conservation and does not consider the energy required to produce hydrogen, making it less relevant for energy-based comparisons.

- Voltage efficiency is an excellent indicator of how effectively the electrical potential is used, but it does not account for mass-based losses or other inefficiencies such as hydrogen leakage.

- Cell efficiency is a more comprehensive metric but can still overlook the thermal energy input, especially in systems that operate at high temperatures.

- Energy efficiency offers the most complete measure but can be difficult to standardize due to differences in how the heating value of hydrogen is defined (LHV vs. HHV), and it may sometimes yield misleading results if external heat is absorbed by the system especially for the electrolyzer that operates at high temperature. It should not be a problem for Near Ambient Temperature (NAT) Electrolyzer.

To make meaningful comparisons between different electrolyzer systems and technologies, it is crucial to adopt standardized definitions for these metrics and understand the contexts in which they are applied.

2.4 Tafel Equation

Definition

The Tafel Equation is a fundamental mathematical expression in electrochemical kinetics that relates the overpotential (η) of an electrode to the current density (i) during an electrochemical reaction. It describes the kinetic behavior of electrode processes under high overpotentials, where either the anodic or cathodic reaction dominates.

Mathematical Expression

The Tafel Equation is expressed as:

$$\eta = a + b \log(i)$$

where:

- η: Overpotential in volts (V),

- a: Tafel constant (related to the exchange current density, i_0),

- b: Tafel slope in volts per decade (mV/decade),

- i: Current density in amperes per square meter (A/m^2).

The Tafel slope (b) is given by:

$$b = \frac{2.303RT}{\alpha nF}$$

where:

- R: Universal gas constant ($8.314\,\text{J/mol}\cdot\text{K}$),

- T: Temperature in kelvins (K),

- α: Charge transfer coefficient (typically ~ 0.5),

- n: Number of electrons transferred,

- F: Faraday constant ($96485\,\text{C/mol}$).

Physical Meaning

The Tafel Equation provides insights into the relationship between the reaction rate and the energy required to drive it:

- Overpotential (η): Represents the additional energy needed to overcome the activation barriers of the reaction.

- Tafel Slope (b): Indicates how much the overpotential must increase to achieve a tenfold increase in current density.

- Exchange Current Density (i_0): The reaction rate at equilibrium ($\eta = 0$), reflecting the intrinsic catalytic activity.

Relationship with Butler-Volmer Equation

The Tafel Equation is derived from the Butler-Volmer Equation under conditions of high overpotentials ($|\eta| > 0.1\,\text{V}$), where either the anodic or cathodic reaction dominates. For an anodic reaction:

$$i = i_0 \exp\left(\frac{\alpha_a F\eta}{RT}\right)$$

Taking the logarithm leads to the Tafel form:

$$\eta = a + b\log(i)$$

2.4.1 Derivation of the Tafel Equation from the Butler-Volmer Equation

At high overpotentials ($|\eta| > 0.1\,\text{V}$), the Tafel Equation can be derived as an approximation of the Butler-Volmer Equation [12]. Under these conditions, one reaction (either anodic or cathodic) dominates, simplifying the kinetic expression. [2, 9, 16]

For Anodic Reactions ($\eta > 0$)

When the overpotential is positive, the second exponential term in the Butler-Volmer Equation ($\exp(-\alpha_c F\eta/RT)$) becomes negligible. This leaves:

$$i \approx i_0 \exp\left(\frac{\alpha_a F\eta}{RT}\right)$$

For Cathodic Reactions ($\eta < 0$)

When the overpotential is negative, the first exponential term ($\exp(\alpha_a F\eta/RT)$) becomes negligible. This reduces the equation to:

$$i \approx i_0 \exp\left(-\frac{\alpha_c F\eta}{RT}\right)$$

Taking the natural logarithm of the current density, we obtain:

$$\ln i = \ln i_0 + \frac{\alpha F\eta}{RT}$$

where α is the charge transfer coefficient, and $\alpha = \alpha_a$ for anodic processes or $\alpha = \alpha_c$ for cathodic processes. Solve the equation as n as overpotential as the subject will lead to the standard Tafel form:

$$\therefore \eta_s = \frac{RT}{\alpha_a F}\ln i - \frac{RT}{\alpha_a F}\ln i_o$$

To convert from natural logarithms to base-10 logarithms, a factor of $\ln 10 = 2.3$ must be included. With this adjustment, the Tafel Equation is expressed as [2, 9, 16]:

$$\eta_s = -\frac{2.3RT}{\alpha_a F}\log i_o + \frac{2.3RT}{\alpha_a F}\log i$$

Simplify :

$$\eta = A \cdot \log\left(\frac{j}{j_0}\right)$$

- j = Current Density

- j_0 = Exchange Current Density

- $A = \frac{2.3RT}{\alpha_a F}$ (Tafel slope)

The Tafel Plot

The Tafel Plot is a key tool in electrochemical analysis that provides insights into reaction kinetics and catalyst performance. It is a graph plotting overpotential (η) against the logarithm of current density ($\log i$), with the linear region corresponding to the "Tafel region," where the reaction kinetics follow the Tafel Equation.

How to Construct a Tafel Plot

- Plot the log j value along the x-axis and overpotential η along the y-axis

- Extract the region of the polarization curve where η and $\log i$ exhibit a linear relationship.

- Fit a straight line to this region using the Tafel Equation to determine:

    - The slope (b): Related to reaction kinetics and activation energy.
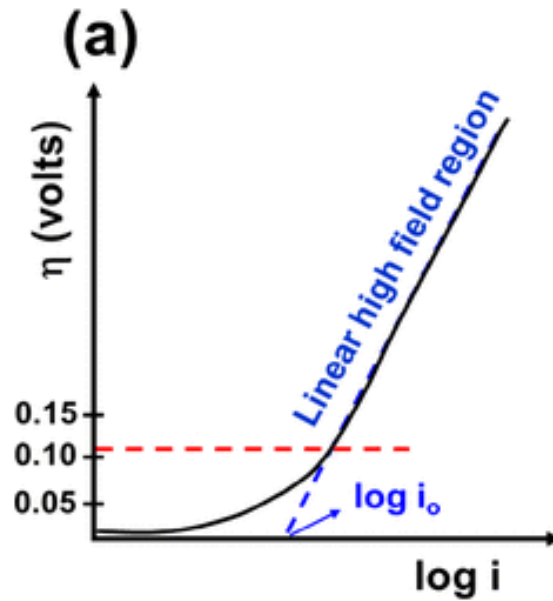   - The intercept (a): Related to the exchange current density (i_0).

Figure 8: log j against Overpotential [25]

How to Interpret a Tafel Plot

- Tafel Slope (b):

    - Represents the overpotential required to increase the current density by a factor of 10.
    - Indicates the energy barrier and rate-determining step of the reaction:
        * Low b: Fast kinetics, low activation energy.
        * High b: Slow kinetics, high activation energy, or poor catalytic performance.

- Intercept ($\log i_0$):

    - Reflects the exchange current density (i_0), which represents the reaction's intrinsic activity at equilibrium.
    - Higher i_0: Indicates better catalytic activity and efficient reaction kinetics.

Significance of the Tafel Equation

The Tafel Equation is a simplified form of the Butler-Volmer Equation, valid for conditions of high overpotential where either the anodic or cathodic reaction dominates. It can be used to analyze how much overpotential needed to increase a decade of current density of the Electrolyzer by extracting key parameters such as the Tafel slope (b) and exchange current density (i_0).

Practical Insights from Tafel Plots

- Comparing Catalysts:

    - Lower Tafel slopes (b) and higher i_0 values indicate superior catalyst performance.

- Assessing Reaction Mechanisms:

    - The Tafel slope can help identify the rate-determining step, such as electron transfer or adsorption/desorption processes.

Limitations

- Valid only at high overpotentials ($|\eta| > 0.1\,\mathrm{V}$).

- Assumes constant i_0, which may vary due to surface changes.

- Sensitive to mass transport limitations, especially at very high overpotentials.

2.5   Previous Research and Case Studies

Project Overview

Alexander and Kitzbichler from Hochschule Karlsruhe [1] initiated a research project aimed at investigating the performance of a PEM (Proton Exchange Membrane) electrolyzer for hydrogen production. The main focus of the project was to analyze how different hydrogen/natural gas mixtures affect the operation of a Combined Heat and Power (CHP) unit. Hydrogen was to be produced through electrolysis, stored, and later blended with natural gas for combustion in a CHP engine.

The project had a strong focus on developing operational curves for the electrolyzer, optimizing the control system, and understanding the effects of hydrogen enrichment in traditional fuel systems. Despite facing some challenges in implementation, the project provided key insights into system design, data collection methods, and control mechanisms for future hydrogen projects.

System Components

Electrolyzer Details:

- Type: PEM Electrolyzer (Sylatech GmbH).

- Power Consumption: 1.9 kW.

- Hydrogen Production Rate: 0.3 Nm³/h of hydrogen gas.

- Hydrogen Purity: Greater than 99.99%, suitable for direct use in applications like fuel cells and combustion systems.

- Operating Pressure: The system operates at a pressure range between 3 and 10 bar, making it suitable for direct storage or further compression for higher-pressure storage systems.

Control System:

Initially, the system used a two-point control mechanism for regulating hydrogen production and pressure. However, this method proved insufficient as it caused frequent power cycling that could reduce the electrolyzer's operational life. To address this issue, the system was upgraded to use a Proportional-Integral (PI) controller, which allowed smoother adjustments in voltage and current to maintain constant pressure without the rapid cycling of power.

Data Collection and Communication:

The system incorporated Modbus communication to enable real-time monitoring and control. This allowed the team to log critical parameters such as:

- Hydrogen pressure,

- Stack voltage and current,

- Total system power consumption,

- Hydrogen flow rate.

The control system was designed to collect this data for performance analysis and feed into a graphical user interface (GUI) developed in Python (PyQt) to ensure user-friendly system control and data visualization.

Project Objectives

Hydrogen/Natural Gas Combustion Testing:l System:

The primary objective was to test different hydrogen/natural gas mixtures in a single-cylinder CHP engine and analyze the impact on combustion efficiency, emissions, and overall performance. The blending of hydrogen with traditional fossil fuels is seen as a way to reduce CO emissions and enhance the sustainability of conventional energy systems.

Optimization of Electrolyzer Efficiency:

The research aimed to measure and optimize the efficiency of the PEM electrolyzer by developing characteristic curves (performance maps) based on various operating conditions. The goal was to understand the relationship between power input, hydrogen production rate, and hydrogen purity to

enhance the overall efficiency of the system.

Control and Safety:

The project also focused on ensuring that the electrolyzer operated within safe pressure ranges and that the hydrogen flow was precisely controlled to match the CHP unit's requirements. An important part of the project was to develop a robust control system that could balance hydrogen production with energy consumption while maintaining safety protocols.

Challenges and Issues

Software Malfunction:

During the testing phase, a software error in the electrolyzer's control system halted operations. The issue stemmed from the memory capacity of the control system becoming full, which prevented the electrolyzer from saving crucial operational parameters, such as power usage and pressure values. This error caused the electrolyzer to stop functioning and prevented the team from collecting the necessary data to complete the testing phase.

Component Delays:

In addition to software issues, there were delays in the delivery of key components, such as a backpressure valve that was essential for maintaining stable operation during hydrogen production and storage. This delay further stalled the project and limited the ability to run full tests with the CHP unit.

Operational Setbacks:

Although a temporary workaround allowed the electrolyzer to reach its desired pressure, the incomplete installation of necessary components meant that full testing, particularly with respect to long-term hydrogen production and blending with natural gas, could not be completed.

Key Insights and Learnings

Although the project did not reach full operational capacity, several important lessons were learned from the setup and partial operation of the electrolyzer:

- Control System Optimization: The transition from a two-point control to a PI controller demonstrated how smooth voltage regulation is crucial in maintaining electrolyzer stability and efficiency. This insight is valuable for future projects where power cycling needs to be minimized to preserve the electrolyzer's lifespan and maximize hydrogen production efficiency.

- Importance of Software and Data Logging: The software malfunction highlighted the importance of robust data logging and software capacity in hydrogen production systems. As hydrogen systems scale, data management and error handling become critical to ensuring long-term reliability and avoiding unexpected shutdowns.

- Hydrogen/Natural Gas Mixture Potential: Even though full tests with hydrogen/natural gas mixtures were not completed, the project's foundation showed that hydrogen blending has the potential to improve combustion efficiency and reduce CO emissions. This aligns with the broader trend of decarbonizing energy systems by combining hydrogen with traditional fossil fuels.

2.5.1 Next Steps and Future Work

Resolving Software Issues:

The project team plans to resolve the software issues with the manufacturer's assistance. Once the control system is functioning correctly, the next steps will involve re-testing the electrolyzer and collecting performance data on hydrogen production rates and energy efficiency.

Component Installation and Full Testing:

With the final installation of the delayed components (like the backpressure valve), the project will be able to proceed with the long-awaited tests of the hydrogen/natural gas mixtures in the CHP unit. This data will be crucial in understanding how different ratios of hydrogen affect combustion dynamics, emissions, and efficiency.

Further Development of Operational Curves:

Once the system is fully operational, the team will develop specific performance curves (e.g., voltage-current characteristics, hydrogen production vs. power consumption) to provide deeper insights into how varying operating conditions impact the efficiency of the PEM electrolyzer.

Conclusion

The Karlsruhe University of Applied Sciences Electrolyzer Project demonstrates the potential for using hydrogen in CHP applications as a means to reduce emissions and improve efficiency. While the project faced significant technical challenges, especially with respect to software and component delays, it offers valuable lessons on system control, data management, and the importance of detailed operational planning in hydrogen production systems. The project underscores the complexities of integrating hydrogen production with traditional energy systems, but also highlights the potential benefits of hydrogen blending in future energy applications.

3 DESIGN SPECIFICATION

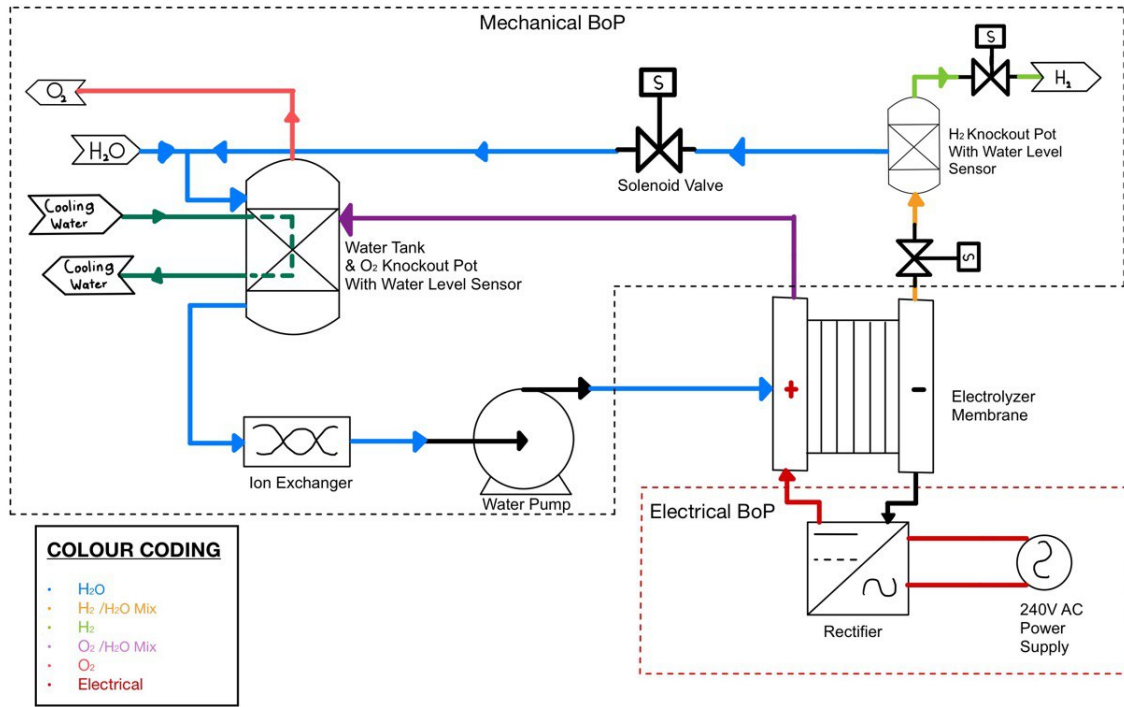## 3.1 Piping and Instrumentation Diagram (P&ID)

Figure 9: Overall mechanism of the electrolyzer

3.1.1 Water Input and Initial Handling

The process begins with water being introduced into the system through a narrow metal tube. This tube directs the water to a water container (combined with Oxygen Knockout Pot) .The excess water from Hydrogen Knockout (KO) Pot will directs the water back to the water container. The water container serves a dual purpose: it stores the incoming water and facilitates the separation of oxygen gas. As the water enters this container, it prepares for the next steps in the electrolyzer system.
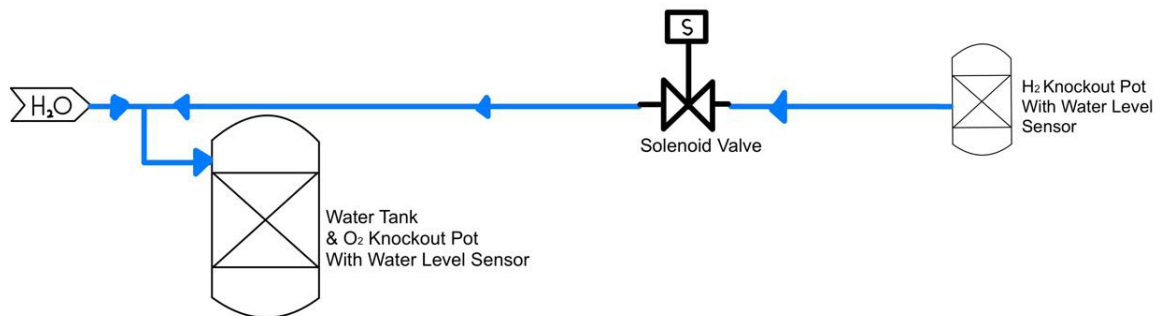
Figure 10: Water Input and Initial Handling

3.1.2 Hydrogen Knockout (KO) Pot

Within the hydrogen knockout (KO) pot, a water level sensor continuously monitors the water level. This sensor is crucial for maintaining the correct amount of water within the pot. If the water level reaches a predetermined threshold, the sensor triggers a solenoid valve positioned before the Hydrogen KO pot. This valve then closes to prevent additional water from entering, thereby controlling the water flow into the pot. This mechanism ensures that the KO pot does not overflow and maintains optimal operating conditions.

3.1.3 Water Purification

After the solenoid valve closes, water flows into the water container. From here, it is directed to the ion exchanger tank, also known as the Ionenaustauscher. This tank is essential for purifying the water by removing various ions such as calcium and magnesium. The ion exchanger works to produce deionized water, which is crucial for the efficient operation of the electrolyzer membrane. The purity of the water enhances both the efficiency and longevity of the electrolyzer system.
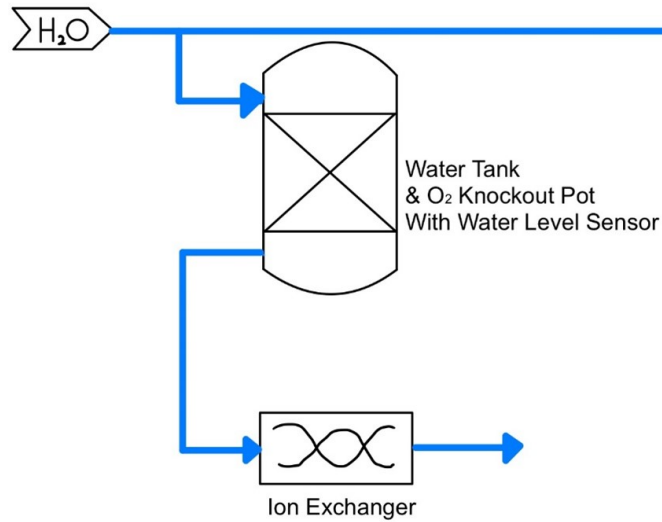

Figure 11: Water Purification

3.1.4 Water Pump

To maintain a steady flow of water through the system, a water pump is installed. This pump plays a vital role in creating a continuous flow from the water container through the ion exchanger tank and finally to the electrolyzer membrane. The consistent flow ensures that the water is properly purified and delivered to the electrolyzer for the electrolysis process.
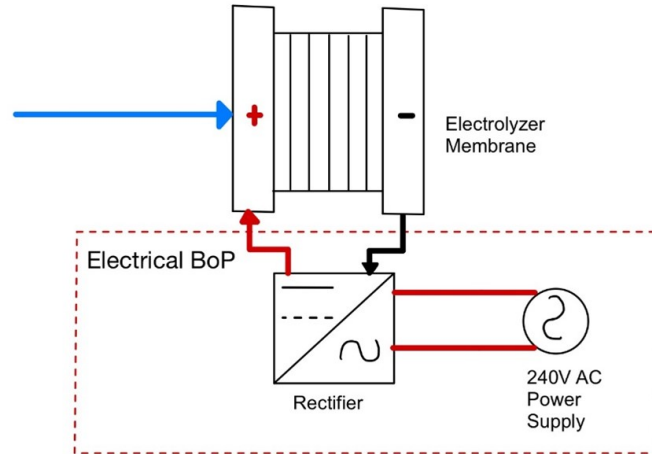
3.2 Electrolysis Process

Figure 12: Electrolysis Process

The core of the system is the electrolyzer membrane, where the actual electrolysis process takes place. Here, the purified water is split into hydrogen and oxygen gases. The system includes a rectifier that converts the incoming 240V AC power supply to DC, as electrolysis requires direct current. The positive wire from the rectifier is connected to the anode, and the negative wire is connected to the cathode of the electrolyzer membrane. During electrolysis, water molecules are split into hydrogen ions (protons) and oxygen. The protons move through the membrane to the cathode, where they combine with electrons to form hydrogen gas, while oxygen gas is produced at the anode.

3.3 Oxygen Handling

The byproducts of the electrolysis process include oxygen gas and some water, which are directed back to the water container. The oxygen gas is vented out through a vapor outlet to prevent pressure build-up within the system. This recycling of water helps maintain the water level within the container and ensures efficient use of resources. The vapor outlet is designed to allow the safe release of oxygen, maintaining a stable and controlled environment within the container.
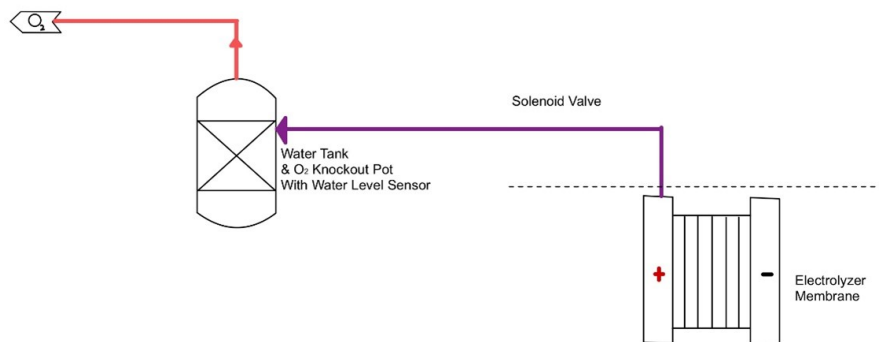

Figure 13: Oxygen Handling

3.4 Temperature Control

The electrolysis process generates heat, leading to an increase in the temperature of the water within the container. To manage this, a cooling system is integrated into the design. A cooling water inlet introduces cool water into a separate tube within the water container. This tube, designed with a large surface area, acts as a heat sink, facilitating efficient heat transfer from the warm water to the cooling water. This mechanism ensures that the water temperature remains within optimal limits, preventing overheating and maintaining system efficiency.
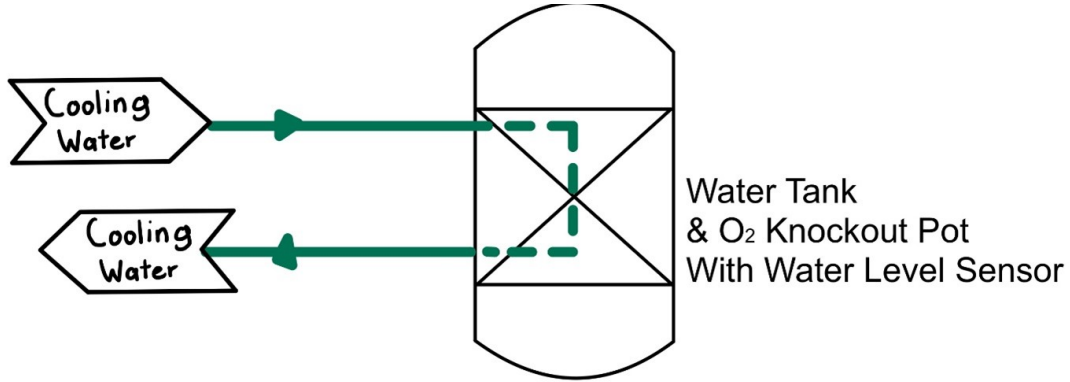

Figure 14: Temperature Control

3.5 Hydrogen Handling

Hydrogen gas, produced at the cathode, is directed to the Hydrogen KO Pot. Before entering the KO Pot, the hydrogen passes through another solenoid valve. This valve prevents hydrogen leakage when the electrolyzer is turned off, ensuring safety and efficiency. The Hydrogen KO Pot is designed as a vertical cylinder, allowing hydrogen, being lighter, to rise to the top. At the top of the KO Pot, there is an outlet for collecting hydrogen gas. Another solenoid valve controls the release of hydrogen, ensuring it can be safely managed and stored.
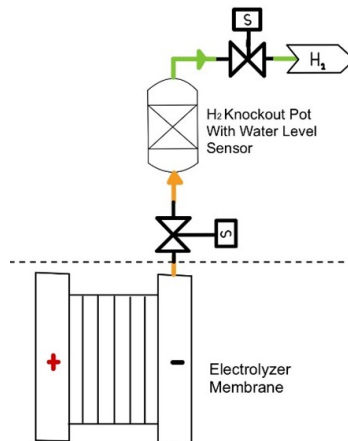

Figure 15: Hydrogen Handling
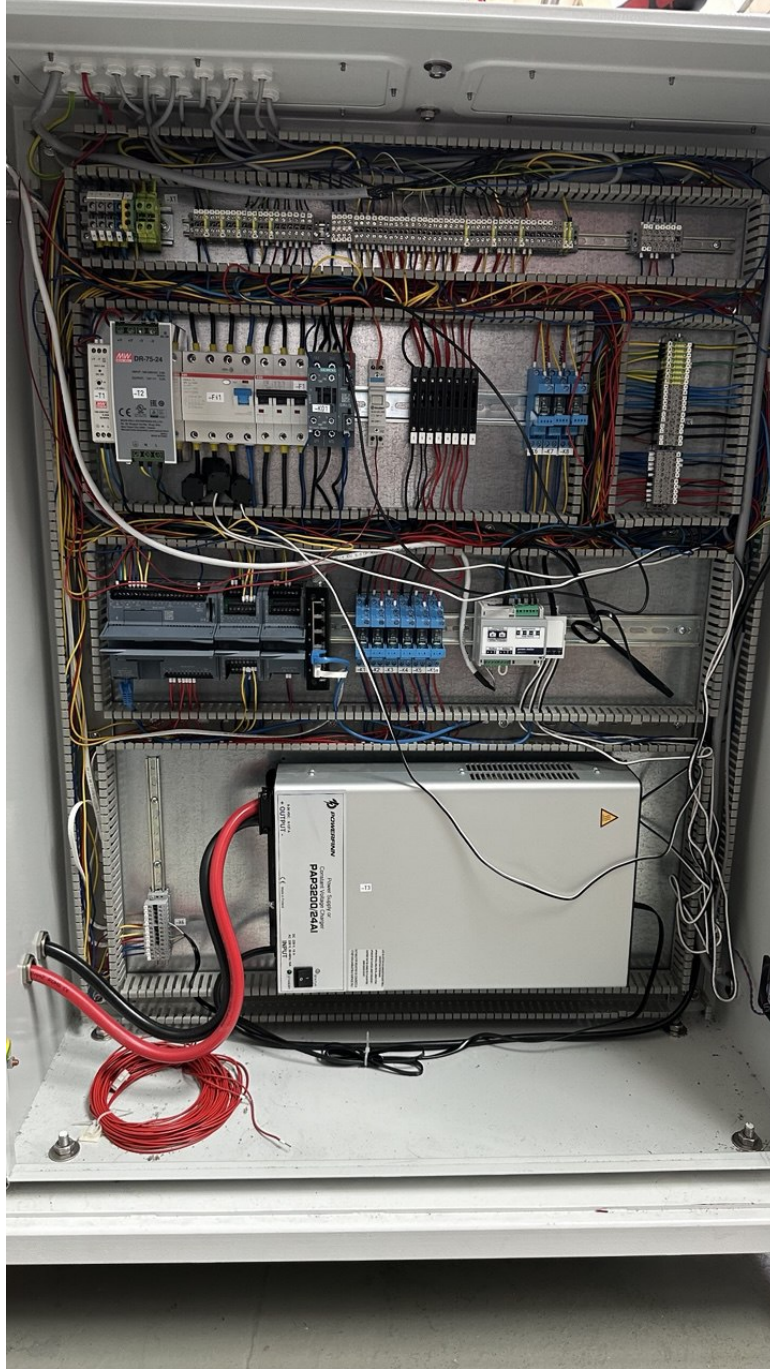
3.6 Electrical Design

Figure 16: Electrical Connection of the Electrolyzer

The electrolyzer system is powered by a three-phase 400/230 V supply, with each phase allocated to specific components to ensure balanced distribution and efficiency. One phase powers the DC charger, which supplies regulated DC power to the electrolyzer cells for the electrolysis process. Another phase supports the pump and auxiliary systems, such as heating or cooling devices, while the third phase is dedicated to sensors and the programmable logic controller (PLC) for system monitoring and automation. All connections are centralized through a terminal block, providing an organized and secure hub for power distribution, simplifying maintenance, and ensuring operational reliability.

4   METHODOLOGY

This chapter explains the research methods and procedures used to conduct the study. It includes the following subsections:

4.1   Research Methodology

An overview of the research approach, including experimental design, data collection, and analysis methods.

4.1.1   Experimental Design

The experiment is designed to measure the impact of controlled variables on hydrogen production. The experimental setup includes the following key components:

- The PEM electrolyzer is connected to a deionized water input, a rectifier for direct current (DC) supply, and a Siemens PLC (S7-1200) to control solenoid valves, pumps, and monitor water flow rates.

- The Siemens PLC manages several sensors, including a water level sensor in the hydrogen knock-out (KO) pot. If the water level reaches a certain threshold, the PLC triggers a valve to open, transferring excess water from the KO pot back into the water container to prevent leakage from the hydrogen outlet.

- The independent variable is the power input, varied from 20% to 100% with 5% increments. The dependent variable is the hydrogen production rate, and the efficiency is measured at each power level.

The experiment will proceed in two phases: baseline testing and variable condition testing. The baseline phase will measure performance under standard conditions, while the second phase will vary power input to observe the effect on hydrogen production.

4.1.2   Data Collection

Data is gathered using various sensors connected to the Siemens PLC. The key instruments include flow rate sensors, temperature sensors, and pressure sensors, which monitor real-time conditions of the electrolyzer. The Bronkhorst El-Flow Prestige FG-201Cv mass flow meter measures hydrogen gas production, and the data is logged through the FlowSuite 2 software on a separate PC. This data is manually entered into an Excel spreadsheet for analysis.

The collected data includes:

- Pressure of hydrogen

- Cell temperature

- Current cell

- Water temperature

- Voltage across the cell (voltage of 9 cells)

4.1.3   Data Analysis

The collected data is analyzed to calculate the following parameters:

- Current density

- Voltage for a single cell

- Power

- Faradaic (current) efficiency

- Voltage efficiency

- Cell efficiency

- Overall efficiency

Additional analyses include determining the Tafel equation and slope for the electrolyzer to study its performance. Data from Excel is processed using Python scripts to generate graphs and perform calculations.
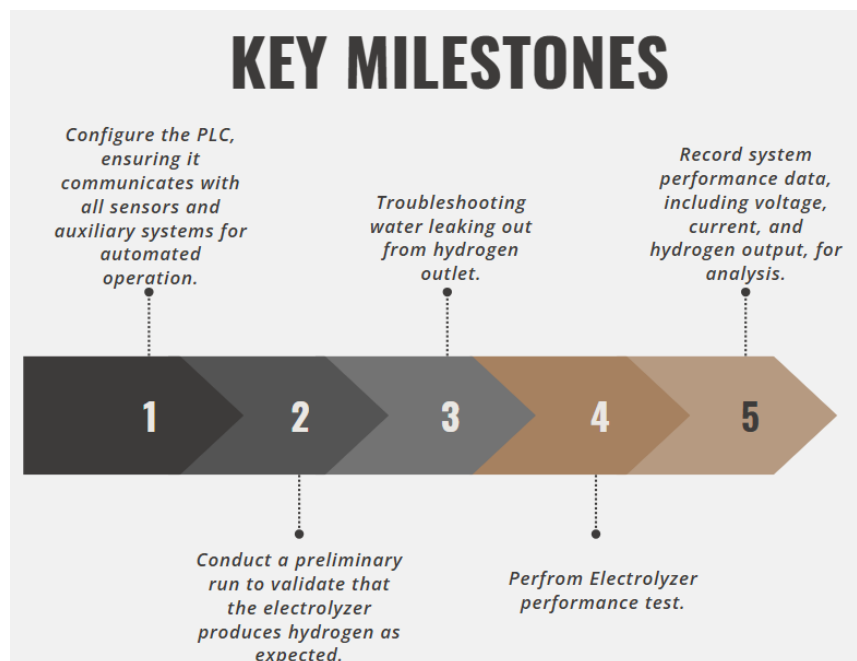
4.2   Key Milestones

Figure 17: Key Milestones

4.3 Gantt Chart

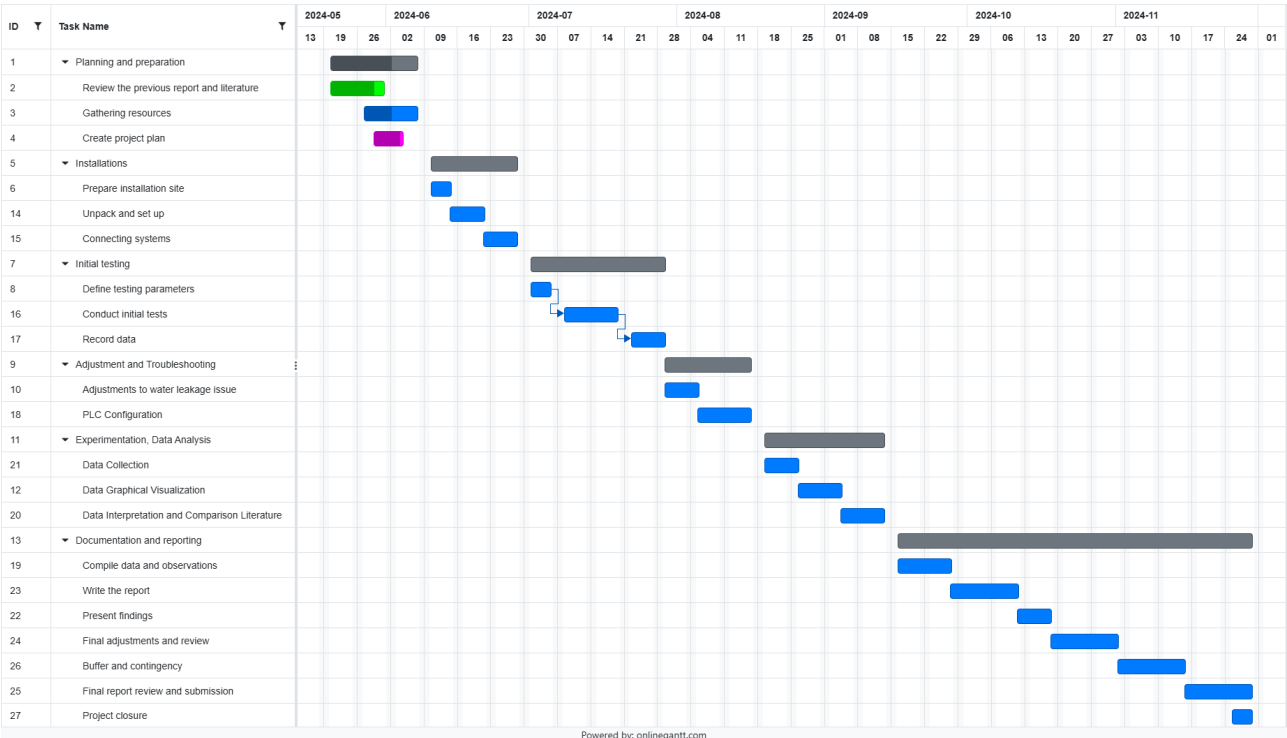A visual timeline of the project, showing the schedule for each major task.

Figure 18: Gantt Chart of the Project

4.4 Tools Required

4.4.1 Instrumentation

Key instruments for the experiment include sensors and devices that monitor and control various parameters necessary for the hydrogen production process:

- Mass Flow Meter (Bronkhorst El-Flow Prestige FG-201CV): This mass flow meter is used to measure the precise flow of hydrogen gas produced in the electrolysis system. It allows real-time data collection, enabling accurate analysis of hydrogen production rates.

- Siemens PLC (S7-1200): The Siemens PLC is used to integrate and manage the data from various sensors, as well as to control the electrolysis process. It communicates with the sensors and other instruments, ensuring that the system operates smoothly and according to preset conditions.

- Power Meter (Modbus Interface): The power meter is connected to the electrolyzer system to measure the electrical power consumption. The power meter transmits real-time power data via Modbus protocol, which is then read and logged by the system for analysis of efficiency at different operating conditions.
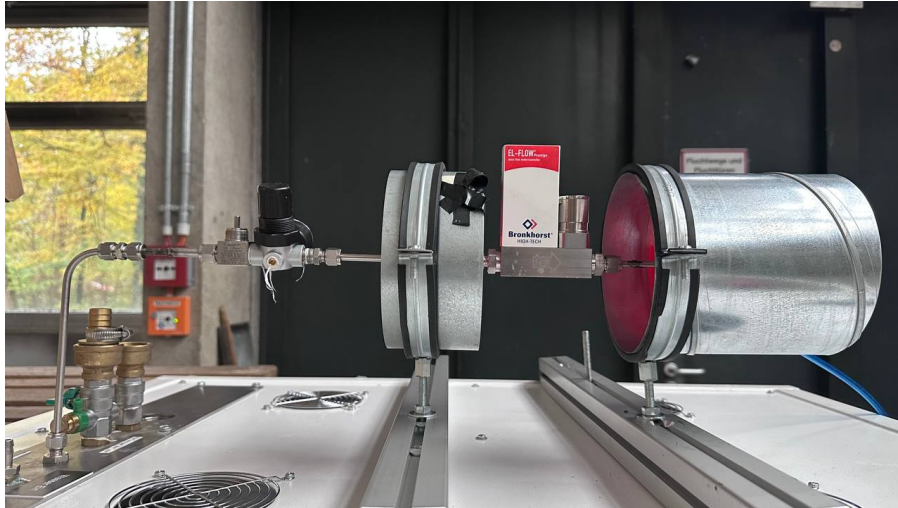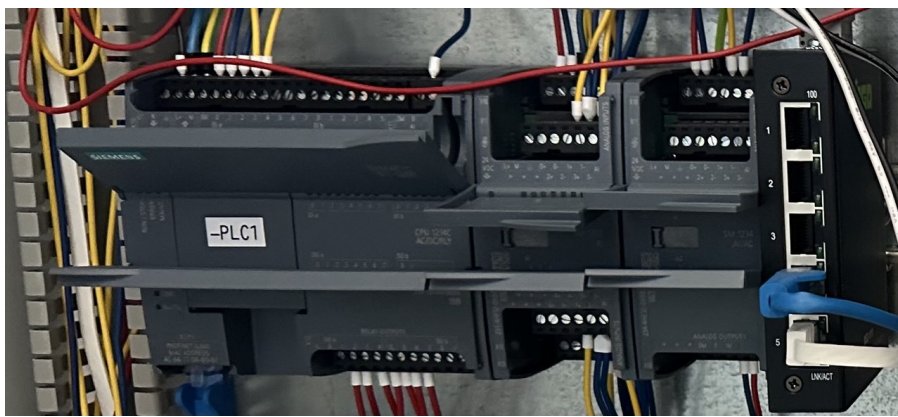
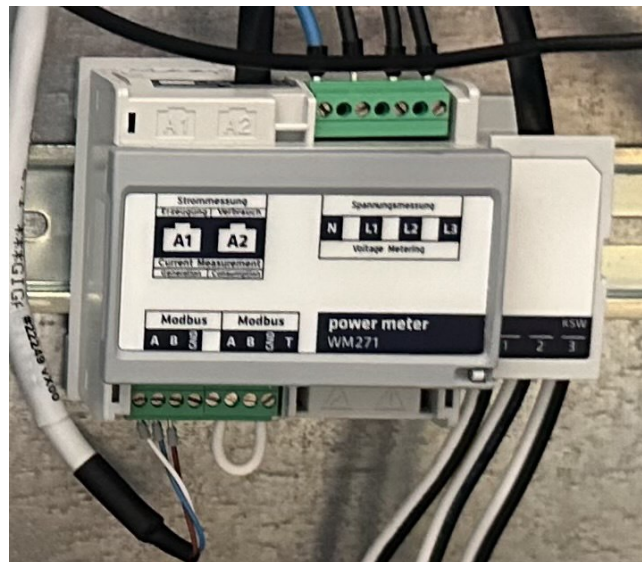Figure 19: Bronkhorst Mass Flow Controller

Figure 20: Siemens PLC S7-1200

Figure 21: Power Meter WM271

4.4.2   Software

The software tools used for this project include a combination of specialized software for programming, data collection, and analysis:

- TIA Portal V16: This software is used for programming the Siemens PLC (S7-1200). It enables the creation of control logic to manage the operation of the sensors and electrolysis process. The software provides an intuitive graphical interface for configuring hardware, programming control sequences, and troubleshooting the system.
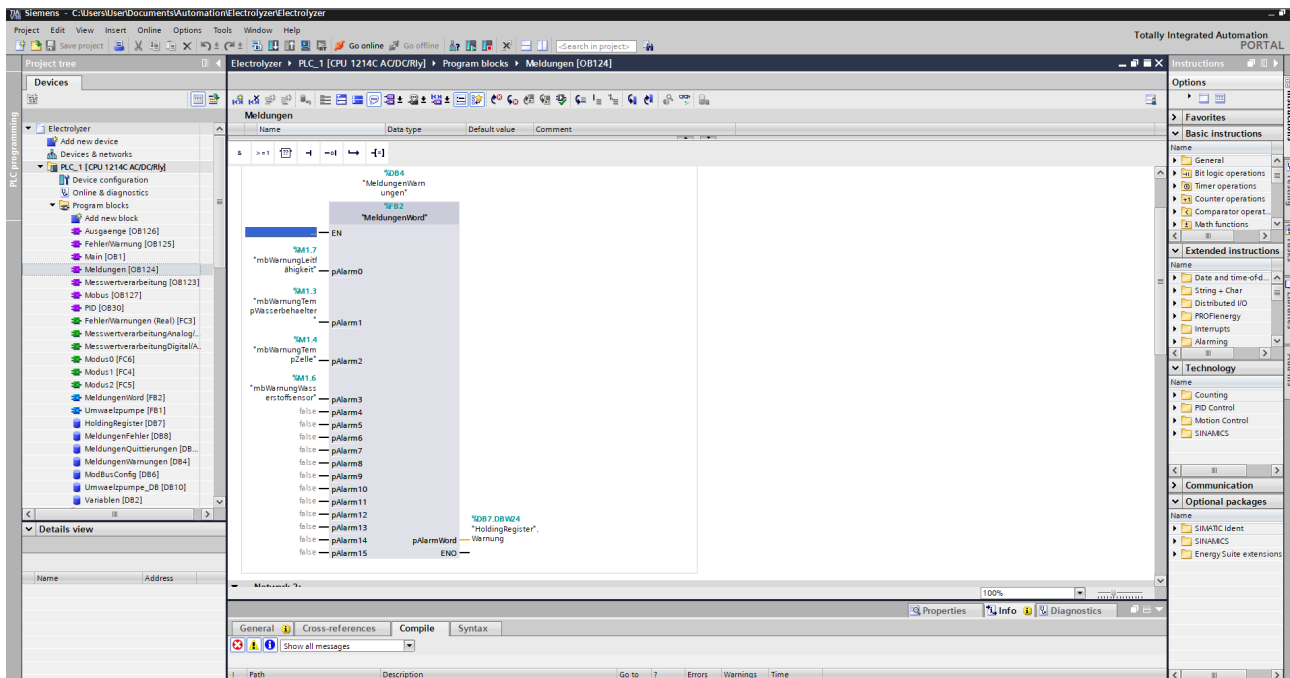

Figure 22: Screenshot of TIA Portal V16

- Bronkhorst FlowSuite 2: This software is specifically designed for monitoring and controlling Bronkhorst flow meters, such as the El-Flow Prestige FG-201CV used in the experiment. It allows real-time monitoring of hydrogen production, logging data for analysis, and configuring flow meters for precise control.
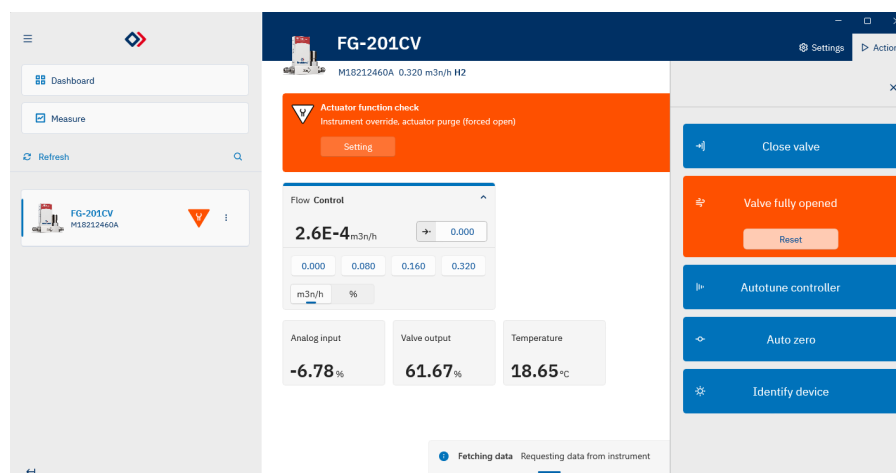

Figure 23: Screenshot of Bronkhorst FlowSuite 2

- Modbus Software: This software allows communication with the power meter, enabling the retrieval of real-time power consumption data through the Modbus protocol. The power values are logged alongside other experimental parameters for subsequent analysis.
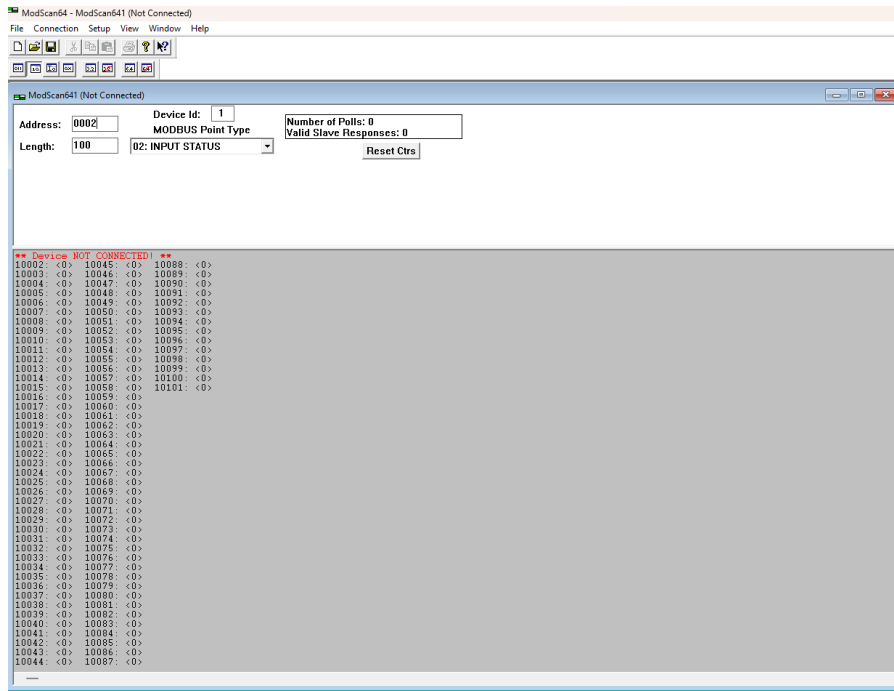
Figure 24: Screenshot of ModScan64

- Python: Python is utilized for reading data from Excel, performing necessary calculations, and generating graphs to visualize results. Python libraries such as Pandas are used to manage data, and Matplotlib or Seaborn is used for data visualization, providing insights into the performance of the system.


```python
# Generate smooth x-axis values for interpolation
power_smooth = np.linspace(power_level.min(), power_level.max(), 200)

# Function to plot and save each graph as an individual image
def save_individual_graphs():
    # Power Level vs Current Density
    plt.figure()
    plt.plot(power_level, current_density, 'o', markersize=5, color='orange')
    plt.plot(power_smooth, poly_current_density(power_smooth), '-', label='Current Density (smoothed)', color='orange')
    plt.title('Power Level vs Current Density')
    plt.xlabel('Power Level (%)')
    plt.ylabel('Current Density (mA/cm^2)')
    plt.grid(True)
    plt.savefig('Power_Level_vs_Current_Density.png')

    # Power Level vs Voltage Cell
    plt.figure()
    plt.plot(power_level, voltage_cell, 'o', markersize=5, color='purple')
    plt.plot(power_smooth, poly_voltage_cell(power_smooth), '-', label='Voltage Cell (smoothed)', color='purple')
    plt.title('Power Level vs Voltage Cell')
    plt.xlabel('Power Level (%)')
    plt.ylabel('Voltage Cell (V) ')
    plt.grid(True)
    plt.savefig('Power_Level_vs_Voltage_Cell.png')

    # Current Density vs Real Hydrogen Volume Flow (m³)
    plt.figure()
    plt.plot(current_density, real_hydrogen_volume_flow_m3, 'o', markersize=5, color='red')
    plt.plot(np.linspace(current_density.min(), current_density.max(), 200),
            Polynomial.fit(current_density, real_hydrogen_volume_flow_m3, 10)(np.linspace(current_density.min(), current_density.max(), 200)),
            '-', label=' Hydrogen Volume Flow (smoothed)', color='red')
    plt.title('Current Density vs  Hydrogen Volume Flow')
    plt.xlabel('Current Density (mA/cm^2)')
    plt.ylabel('Hydrogen Volume Flow (m³n/h)')
    plt.grid(True)
    plt.savefig('Current_Density_vs_Hydrogen_Volume_Flow.png')

    # Voltage Cell vs Real Hydrogen Volume Flow (m³)
    plt.figure()
    plt.plot(voltage_cell, real_hydrogen_volume_flow_m3, 'o', markersize=5, color='green')
    plt.plot(np.linspace(voltage_cell.min(), voltage_cell.max(), 200),
            Polynomial.fit(voltage_cell, real_hydrogen_volume_flow_m3, 10)(np.linspace(voltage_cell.min(), voltage_cell.max(), 200)),
            '-', label=' Hydrogen Volume Flow (smoothed)', color='green')
    plt.title('Voltage Cell vs  Hydrogen Volume Flow')
    plt.xlabel('Voltage Cell (V)')
    plt.ylabel(' Hydrogen Volume Flow (m³n/h)')
    plt.grid(True)
```

Figure 25: Python Script for Data Analysis

5 DATA COLLECTION

5.1 Raw Data

All the data presented here has been collected from both the electrolyzer system and the Bronkhorst FlowSuite software, providing insights into the operation parameters at different power levels. The data captures key variables necessary for evaluating the performance and efficiency of the electrolyzer, including voltage, current, surface area, hydrogen volume flow rate, valve output, temperature, and pressure. Each of these metrics contributes to a complete understanding of the electrolysis process at incremental power levels, as represented in the table below.

Table 1: Raw Data

Power Level (%)	Voltage (V)	Current (A)	Surface Area (cm^2)	H_2 Volume Flow (m^{3}n/h)	Valve Output (%)	Temperature (°C)	Pressure (bar)
20	13.1	15.2	702	0.028644	61.67	16.9	4.7
25	13.3	31.5	702	0.070595	61.67	17	4.9
30	13.5	37.8	702	0.085591	61.67	16.9	4.9
35	13.7	44.2	702	0.100306	61.67	17	4.8
40	13.9	51.6	702	0.11521	61.67	17.2	4.9
45	14.1	58.9	702	0.129879	61.67	17.1	5.0
50	14.3	66.3	702	0.144287	61.67	17.2	5.1
55	14.4	73.6	702	0.15888	61.67	17.3	5.1
60	14.6	81.0	702	0.171569	61.67	17.3	5.2
65	14.8	88.3	702	0.185378	61.67	17.4	5.3
70	14.9	95.6	702	0.19887	61.67	17.4	5.3
75	15.1	102.9	702	0.21205	61.67	17.5	5.4
80	15.2	110.3	702	0.226123	61.67	17.5	5.4
85	15.4	117.6	702	0.23957	61.67	17.6	5.5
90	15.5	125.0	702	0.25345	61.67	17.6	5.5
95	15.7	132.3	702	0.26715	61.67	17.7	5.6
100	15.8	139.7	702	0.28079	61.67	17.7	5.6

5.2 Processed Data

From the raw data obtained in the previous section, additional critical parameters were calculated to provide insights into the electrolyzer's operational characteristics and hydrogen production efficiency. These parameters include the voltage across each electrolyzer cell, current density, and real hydrogen flow rates in various units. Below are the formulas used to derive each parameter:

- Voltage (V) per Cell:

$$\text{Voltage}_{\text{cell}} = \frac{\text{Total Voltage (V)}}{\text{Number of Cells}}$$

  This formula divides the total applied voltage by the number of cells in the electrolyzer stack (if applicable), yielding the voltage across each cell. This is useful for assessing cell efficiency and uniformity.

- Current Density (mA/cm^2):

$$\text{Current Density} = \frac{\text{Current (A)}}{\text{Surface Area (cm}^2)} \times 1000$$

  Here, current density is calculated by dividing the measured current by the total electrode surface area and converting it to mA/cm^2 (by multiplying by 1000). This value is key for evaluating the electrochemical reaction rate.

- Real Hydrogen Volume Flow (m^3n/h): This value is measured directly from the hydrogen gas output flow in normalized cubic meters per hour, standardized to normal temperature and pressure (STP).

- Real Hydrogen Mass Flow (kg/h): To convert the hydrogen volume flow rate to mass flow, we use the density of hydrogen gas under normal conditions:

$$\text{Mass Flow (kg/h)} = \text{Volume Flow (m}^3\text{n/h)} \times \text{Hydrogen Density (kg/m}^3)$$

  where:

$$\text{Hydrogen Density} = 0.08988\,\text{kg/m}^3$$

- Real Hydrogen Mass Flow (g/s): The hydrogen mass flow rate in grams per second can be derived by converting kg/h to g/s:

$$\text{Mass Flow (g/s)} = \frac{\text{Mass Flow (kg/h)} \times 1000}{3600}$$

- Real Hydrogen Flow (mol/s): To determine the molar flow rate, the mass flow rate is divided by the molar mass of hydrogen (M_{H_2}):

$$\text{Molar Flow (mol/s)} = \frac{\text{Mass Flow (g/s)}}{M_{H_2}}$$

  where:

$$M_{H_2} = 2.016\,\text{g/mol}$$

Table 2: Processed Data

Power Level (%)	Voltage cell (V_{Cell})	Current Density (mA/cm^2)	Current cell (A)	Real H_2 Volume Flow (m^{3}n/h)	Real H_2 Mass Flow (kg/h)	Real H_2 Mass Flow (g/s)	Real H_2 Flow (mol/s)
20	1.31	21.65	15.2	0.04645	0.004175	0.00116	0.000575
25	1.33	44.87	31.5	0.114479	0.010289	0.002858	0.001418
30	1.35	53.85	37.8	0.138796	0.012475	0.003465	0.001719
35	1.37	62.96	44.2	0.162659	0.01462	0.004061	0.002014
40	1.39	72.02	51.6	0.186249	0.016748	0.004653	0.002307
45	1.41	81.09	58.9	0.209774	0.018864	0.00524	0.002599
50	1.43	90.15	66.3	0.233018	0.020962	0.005822	0.00289
55	1.44	99.22	73.6	0.25645	0.023074	0.006409	0.003182
60	1.46	108.28	81.0	0.278846	0.025071	0.006964	0.003454
65	1.47	117.35	88.3	0.302635	0.027196	0.007555	0.003744
70	1.49	126.42	95.6	0.324679	0.029187	0.008108	0.00402
75	1.50	135.48	102.9	0.347174	0.031161	0.008656	0.004297
80	1.52	144.57	110.3	0.370429	0.033305	0.009251	0.004586
85	1.53	153.64	117.6	0.392091	0.035244	0.009789	0.004856
90	1.55	162.71	125.0	0.416246	0.037423	0.010395	0.005153
95	1.56	171.77	132.3	0.43988	0.039543	0.010984	0.005448
100	1.58	180.85	139.7	0.461804	0.041533	0.01154	0.005719

5.3   Efficiency Metrics

To evaluate the performance of the electrolyzer system, several efficiency metrics were calculated. These metrics assess the efficiency of the voltage, Faraday, cell, and overall energy conversion processes. The formulas used for each efficiency metric are explained below.

- Voltage Efficiency (η_{voltage}): Voltage efficiency represents the ratio of the thermodynamic reversible cell voltage (V_{rev}) to the actual cell voltage (V_{cell}) applied. The formula is:

$$\eta_{\text{voltage}} = \frac{V_{\text{rev}}}{V_{\text{cell}}}$$

  where:

- V_{rev} is the reversible cell voltage, typically around 1.23 V at standard temperature and pressure (STP).

- V_{cell} is the measured voltage applied to the electrolyzer cell.

Faradaic Efficiency (η_{Faradic}): Faradic efficiency, also known as current efficiency, reflects the efficiency with which electric current produces hydrogen. The formula is given by:

$$\eta_{\text{Faradic}} = \frac{\dot{m}\,n\,F}{I}$$

  where:

- $\dot{m}$: Mass flow rate of hydrogen, expressed in moles per second (mol/s).

- n: Number of moles involved in the reaction per mole of H_2 produced (usually $n = 2$ for electrolysis of water).

- F: Faraday's constant, approximately 96485 C/mol.

- I: Electric current supplied to the electrolyzer, in amperes (A).

Cell Efficiency (η_{cell}): Cell efficiency is the product of the voltage and Faradic efficiencies, representing the overall efficiency of the electrolyzer cell in converting electrical energy into chemical energy (hydrogen production):

$$\eta_{\text{cell}} = \eta_{\text{voltage}} \times \eta_{\text{Faradic}}$$

Overall Efficiency (η_{LHV}): The overall efficiency, based on the lower heating value (LHV) of hydrogen, measures how effectively the input electrical power is converted into hydrogen's chemical energy. It is calculated as:

$$\eta_{\text{LHV}} = \frac{\dot{V} \cdot \text{LHV}}{P_{\text{el}}}$$

where:

- $\dot{V}$: Volume flow rate of hydrogen, in moles per second (mol/s).

- LHV: Lower heating value of hydrogen, 241881 J/mol.

- P_{el}: Electrical power input to the electrolyzer, in watts (W).

Table 3: Calculated Efficiency Metrics

Power Level (%)	Voltage Efficiency	Faraday (Current) Efficiency	Cell Efficiency	Power (W)	Overall Efficiency
20	0.9389	0.8114	0.7619	199.12	0.6988
25	0.9248	0.9650	0.8925	418.95	0.8185
30	0.9111	0.9750	0.8883	510.3	0.8147
35	0.8978	0.9772	0.8773	605.54	0.8046
40	0.8844	0.9792	0.8657	707.5	0.7925
45	0.8712	0.9805	0.8546	810.1	0.7818
50	0.8578	0.9820	0.8431	922.6	0.7692
55	0.8445	0.9835	0.8313	1047.8	0.7566
60	0.8311	0.9850	0.8191	1176.1	0.7442
65	0.8178	0.9865	0.8071	1306.7	0.7321
70	0.8042	0.9880	0.7943	1412.8	0.7190
75	0.7908	0.9895	0.7815	1551.3	0.7061
80	0.7773	0.9900	0.7694	1664.5	0.6940
85	0.7639	0.9910	0.7571	1782.4	0.6812
90	0.7506	0.9920	0.7446	1912.7	0.6691
95	0.7372	0.9930	0.7322	2032.4	0.6566
100	0.7238	0.9940	0.7199	2164.3	0.6443

5.4   Tafel Analysis

The Tafel plot is a crucial tool in electrochemistry used to analyze the kinetics of electrochemical reactions, such as hydrogen evolution, by examining the relationship between overpotential (η) and the logarithmic current density (j).

Overpotential : The overpotential (η) represents the additional potential required beyond the standard electrode potential to drive the reaction. For this analysis, overpotential is calculated by:

$$\eta = (V_{\text{cell}} - E_0) \times 1000\,\text{mV}$$

where:

- V_{cell} is the cell voltage recorded during electrolysis,

- E_0 is the standard potential for the hydrogen evolution reaction, typically 1.23 V, and

- 1000 is used to convert the overpotential from volts to millivolts.

Tafel Slope and Linear Fit:

The Tafel plot can be obtained by plotting the logarithm of current density ($\log j$) on the x-axis and overpotential (η) on the y-axis. The Tafel slope is determined by performing linear regression on the linear region of the plot, where η versus $\log(j)$ is approximately linear. The calculated Tafel slope provides insights into the reaction mechanism and can reveal information about the rate-determining step of the reaction. The equation of the linear can be expressed as:

$$\eta = a \cdot \log(j) + b$$

where:

- a is the Tafel slope, indicating the voltage increase per decade increase in current density, and

- b is the intercept.

Exchange Current Density (j_0):

The exchange current density is a critical kinetic parameter indicating the reaction rate at equilibrium (when $\eta = 0$). It is derived from the intercept b of the linear fit:

$$j_0 = 10^{-\frac{b}{a}}$$

where:

- a is the Tafel slope,

- b is the intercept.

<u>Tafel Equation of the Electrolyzer:</u>

The Tafel equation of the electrolyzer, the equation that can be used to estimate the current density at given overpotential is expressed as:

$$\eta = slope \cdot \log\left(\frac{j}{j_0}\right)$$

where j is the current density, and j_0 is the exchange current density. This equation and plot provide a clearer understanding of the reaction kinetics and efficiency of the electrolysis process under study.
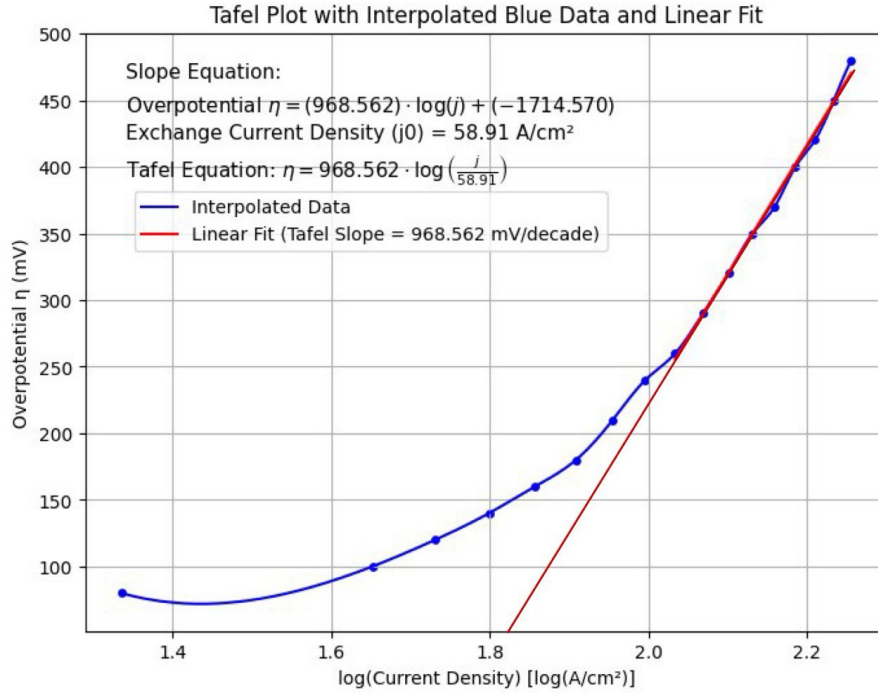
<u>Data Plot and Interpretation:</u>

Figure 26: Tafel Plot with Interpolated Blue Data and Linear Fit

The Tafel plot below shows the overpotential data points with an interpolated curve in blue. The linear fit is illustrated by a red line, from which the Tafel slope and exchange current density are calculated. In this example, the Tafel slope was calculated to be approximately (slope) mV/decade, and the exchange current density, j_0, was found to be approximately (value) A/cm², providing insight into the efficiency of the electrochemical system.

6 ANALYSIS AND DISCUSSION
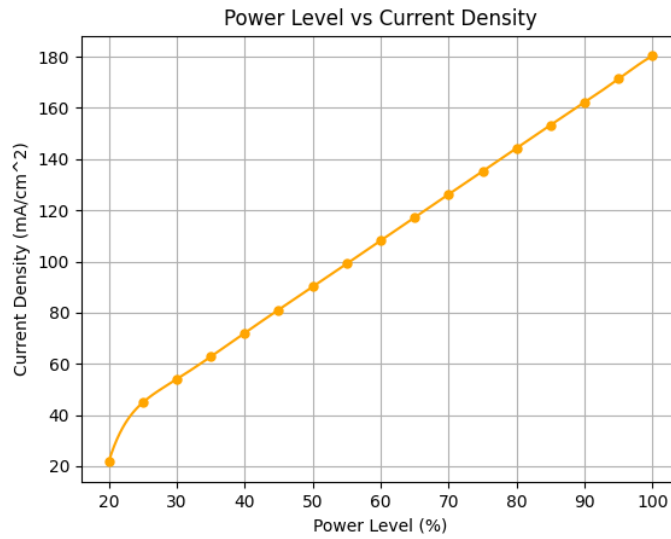
6.1 Power Level vs Current Density

Figure 27: Power Level vs Current Density

The graph of power level versus current density initially shows a logarithmic increase up to 25% power, after which it transitions to a linear relationship. This behavior occurs because, at low power levels, the electrolyzer must first overcome activation energy barriers for the electrochemical reactions, requiring more energy to initiate. Once the reactions reach a stable regime, further increases in power contribute directly to higher current density in a proportional manner. The linear phase after 25% power suggests that the electrolyzer reaches a state where additional power inputs are directly and efficiently converted into current density, indicating that activation and resistance effects are minimized.
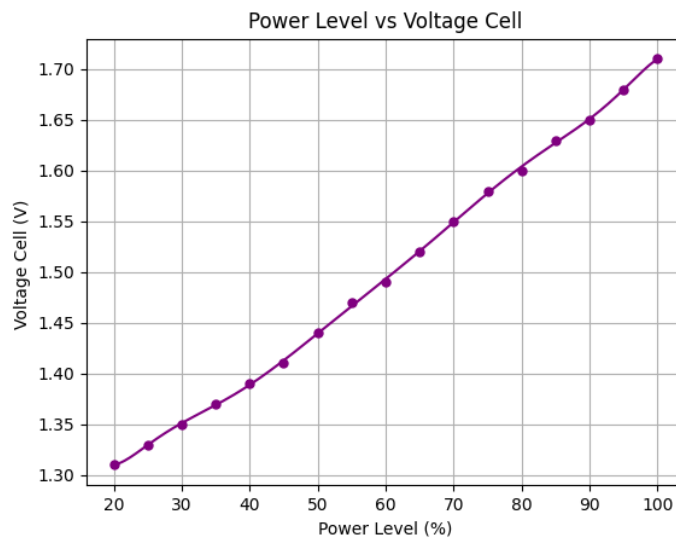
6.2 Power Level vs Voltage

Figure 28: Power Level vs Voltage

In the power level versus voltage graph, the linear increase in voltage as power level rises indicates stable system resistance and consistent electron transport across the electrolyte membrane and electrodes. This linearity implies that the system's internal resistance and ionic conductivity are relatively constant within the examined power range, allowing voltage to scale predictably with power. Additionally, this behavior reflects the effective design of the PEM, which efficiently maintains ion conductivity without significant changes in resistance as power increases.

6.3 Current Density vs Hydrogen Volume Flow
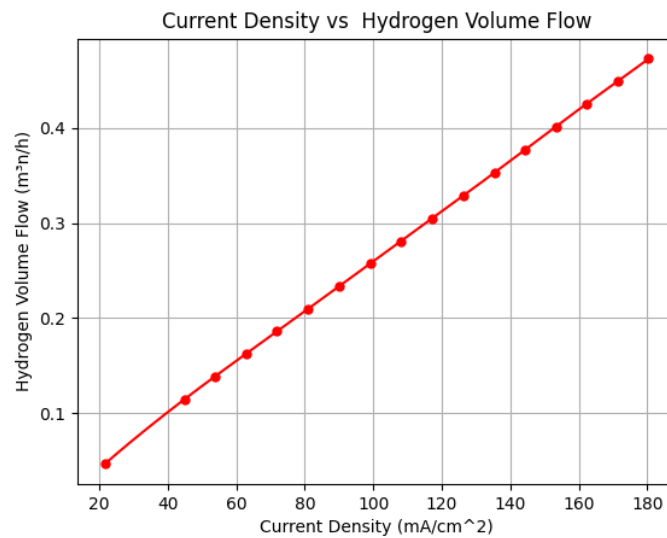
Figure 29: Current Density vs Hydrogen Volume Flow

The linear relationship between current density and hydrogen volume flow demonstrates that hydrogen production scales directly with current density, as expected in electrolysis. This behavior is

due to Faraday's Law of Electrolysis, which states that the amount of gas produced is proportional to the current passed through the electrolyte. In this system, each increment in current density corresponds to a proportional increase in hydrogen production, reflecting the efficiency of the electrolyzer's electrodes and membrane in supporting the hydrogen evolution reaction (HER).
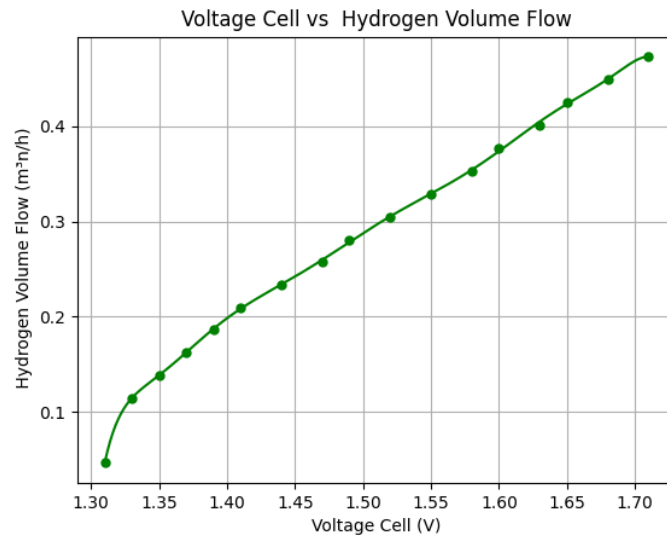
6.4 Voltage vs Hydrogen Volume Flow

Figure 30: Voltage vs Hydrogen Volume Flow

The graph of voltage versus hydrogen volume flow exhibits a piecewise linear trend, with an initial logarithmic rise up to around 1.33V, after which the relationship becomes linear. The initial steep increase suggests that at lower voltages, even small voltage increases significantly enhance hydrogen production by overcoming kinetic barriers in the electrochemical reactions. Once the voltage reaches the 1.33V threshold, the system stabilizes into a linear phase, where further voltage increments directly contribute to proportional hydrogen output. This stability suggests that above a certain voltage, activation overpotentials have been effectively overcome, enabling a more predictable scaling of production with voltage.

6.5 Voltage vs Voltage Efficiency

The linear decrease in voltage efficiency as voltage increases reflects the increasing impact of resistive losses and overpotentials at higher voltages. In electrochemical systems, applying higher voltages typically exacerbates internal resistances within the membrane and electrodes, leading to increased energy losses. This decline in efficiency with rising voltage suggests that the system experiences growing electrical resistance as it operates at higher voltages, which reduces the portion of input power that is effectively converted to hydrogen production.
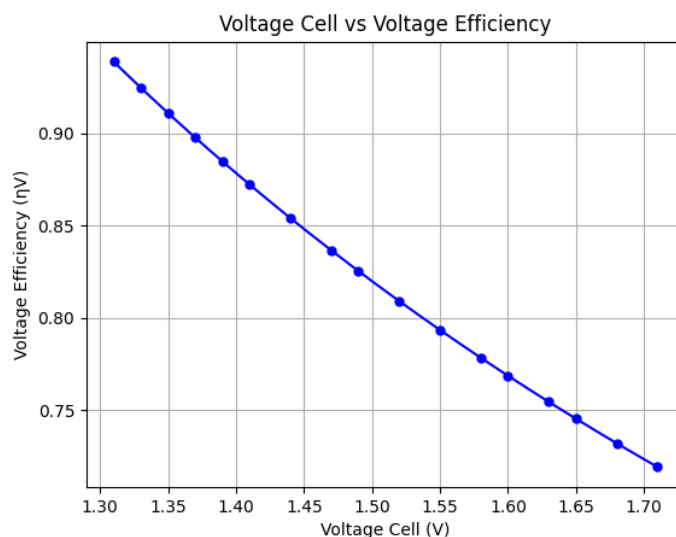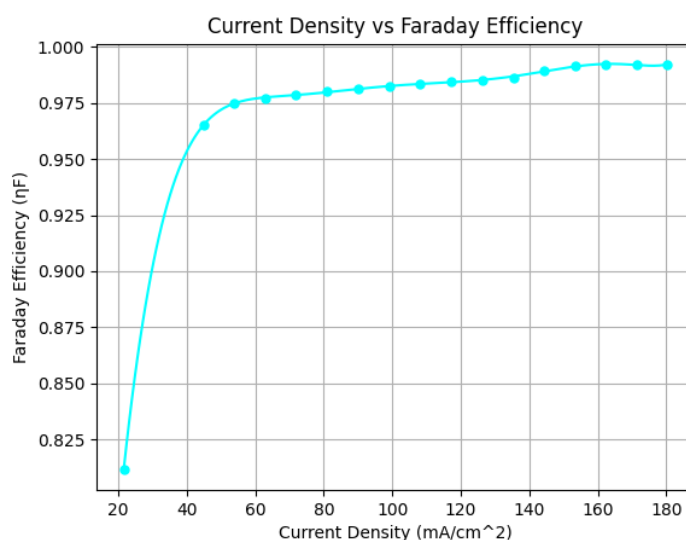
Figure 31: Voltage vs Voltage Efficiency

Figure 32: Current Density vs Faraday Efficiency

6.6 Current Density vs Faraday Efficiency

The logarithmic increase in Faraday efficiency with rising current density indicates that, initially, small increases in current density lead to significant gains in efficiency. At low current densities, inefficiencies such as gas crossover or side reactions are more prominent, causing lower Faraday efficiency. As current density increases, however, these inefficiencies are less impactful relative to the total hydrogen produced, resulting in higher Faraday efficiency. The plateau near maximum efficiency reflects the point at which nearly all electrons contribute to hydrogen production, though minor losses prevent it from reaching 100%.
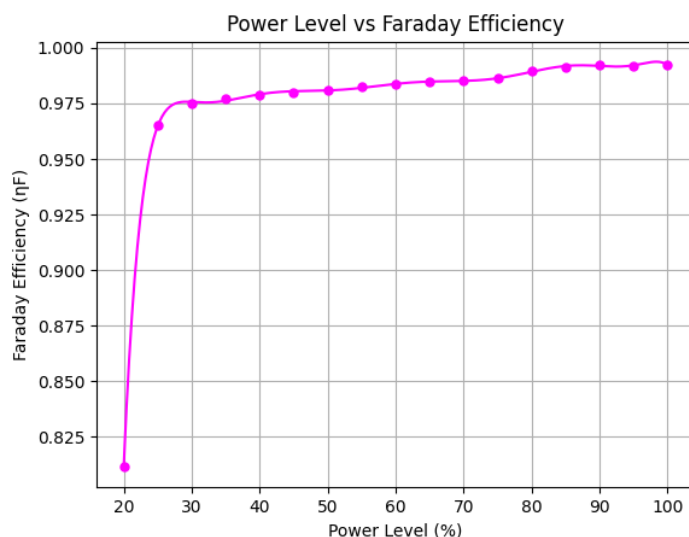
Figure 33: Power Level vs Faraday Efficiency

6.7 Power Level vs Faraday Efficiency

The trend in power level versus Faraday efficiency is similar to current density, showing a rapid logarithmic rise in efficiency up to 25% power, after which the rate of efficiency gain slows. This logarithmic increase suggests that at lower power levels, Faraday efficiency is initially limited by side reactions or incomplete utilization of the applied current. As power level increases, the electrolyzer overcomes these inefficiencies, achieving near-optimal efficiency as the power level reaches 25%. Beyond this point, Faraday efficiency approaches its maximum, as most input power effectively drives hydrogen production.
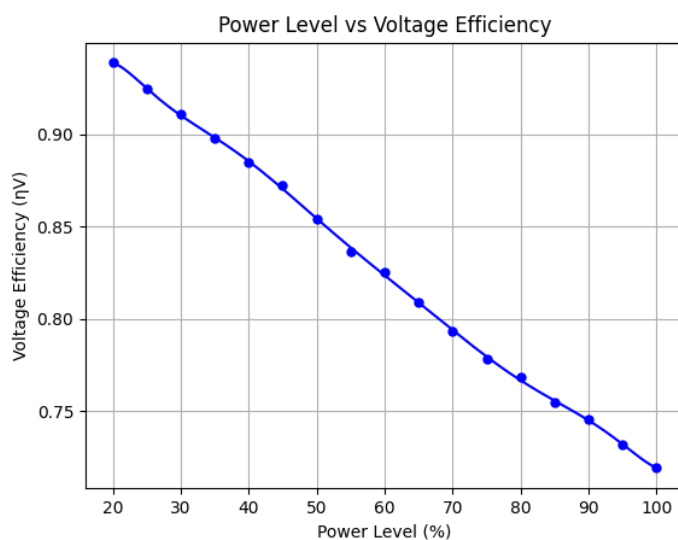
6.8 Power Level vs Voltage Efficiency

Figure 34: Power Level vs Voltage Efficiency

The power level versus voltage efficiency graph reveals a linear decrease in efficiency as power level increases. This decline suggests that as power input grows, so do resistive and overpotential losses, which contribute to the system's inefficiency in voltage usage. The linearity of this decrease highlights that power input beyond the optimal range exacerbates energy losses, underscoring the importance of maintaining a balanced power level to limit these inefficiencies.

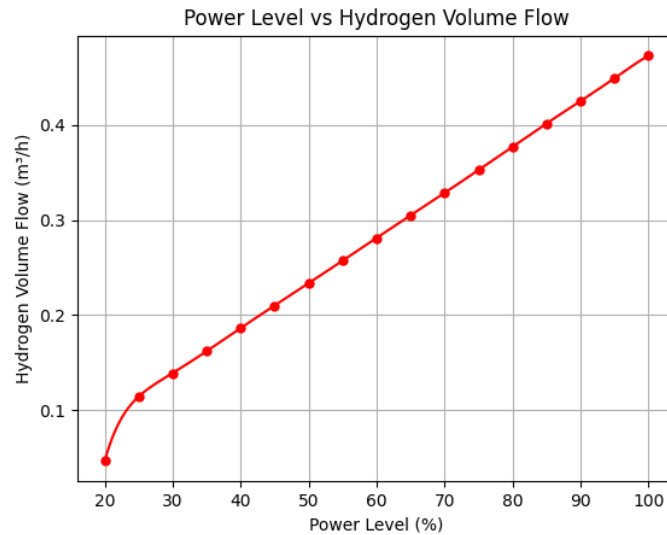## 6.9   Power Level vs Real Hydrogen Volume Flow

Figure 35: Power Level vs Real Hydrogen Volume Flow

The graph of power level versus real hydrogen volume flow exhibits a piecewise linear trend, similar to the power level versus current density graph, with an initial logarithmic increase up to 25% power, followed by a linear relationship. This trend suggests that hydrogen production is highly sensitive to power input changes at lower levels, achieving maximal response below 25%. After this point, hydrogen production scales more predictably and linearly with power, supporting a balanced output in relation to power input.

6.10   Power Level vs Cell Efficiency

In the power level versus cell efficiency graph, efficiency increases sharply up to 25% power and then declines linearly as power continues to increase. This trend occurs because at lower power levels, the system operates in a highly efficient regime with minimal energy losses. However, beyond 25% power, resistive and overpotential losses become more prominent, leading to a steady decline in cell efficiency. This pattern indicates that the electrolyzer operates most effectively within a moderate power range before additional input results in diminishing efficiency.
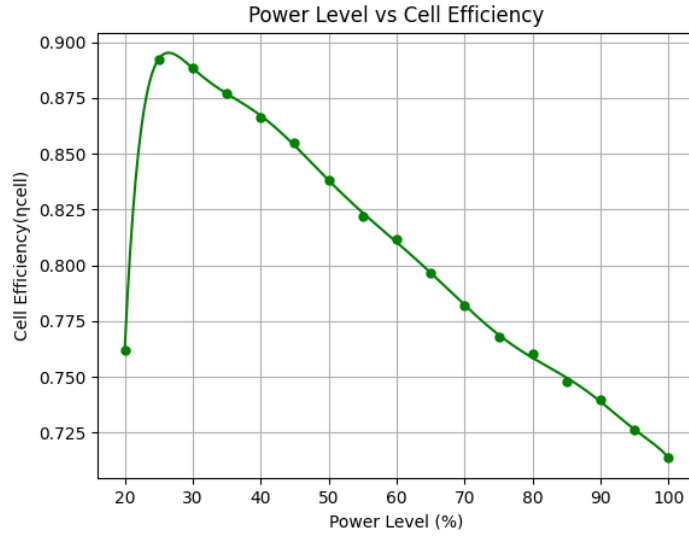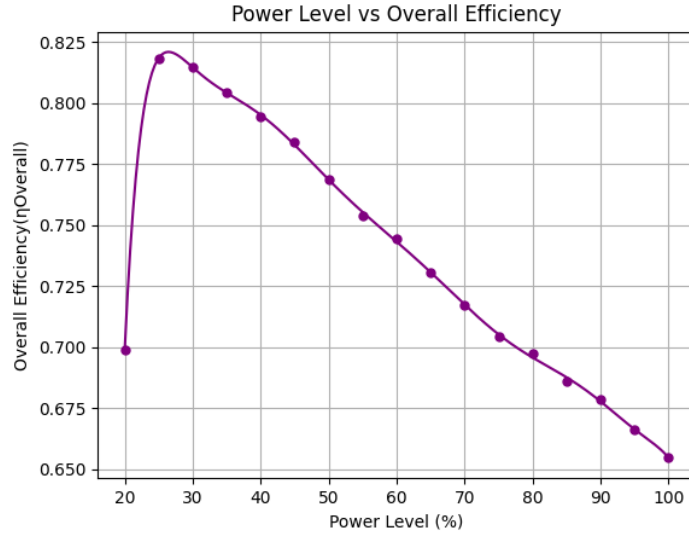
Figure 36: Power Level vs Cell Efficiency

Figure 37: Power Level vs Overall Efficiency

6.11 Power Level vs Overall Efficiency

The graph of power level versus overall efficiency closely follows cell efficiency, with an initial steep increase up to 25% power, after which efficiency decreases linearly. This similarity in behavior suggests that both cell and overall efficiencies peak at around 25% power, where resistive and overpotential losses are minimized. The steady decline in overall efficiency at higher power levels reflects not only electrical losses but also the need for thermal management as more energy is dissipated as heat. This highlights 25% power as the optimal level to maximize hydrogen output while limiting energy waste.
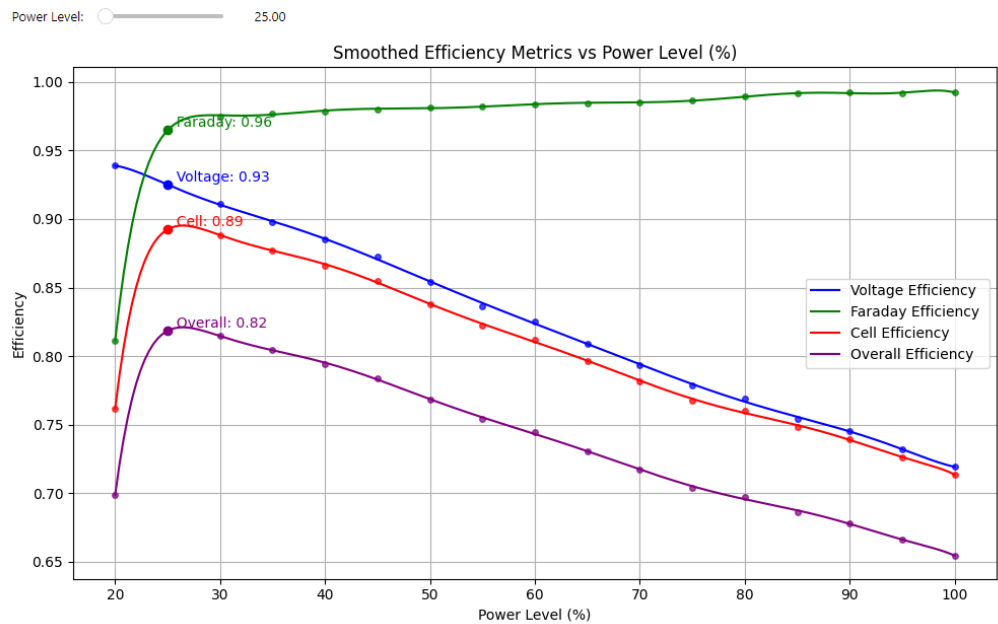
6.12 Power Level vs All Efficiency Metrics

Figure 38: Power Level vs Efficiency Metrics (Faraday, Voltage, Cell, and Overall Efficiency)

When comparing all efficiency metrics—Faraday, voltage, cell, and overall—on a single graph, it becomes evident that the 25% power level is the most efficient point across all metrics. This convergence confirms that 25% is an ideal operating power level, offering the best balance between hydrogen production and energy efficiency. It provides a practical guide for operational settings, where maintaining this moderate power level maximizes efficiency while avoiding the excessive losses seen at higher power levels.

7 CONCLUSION

7.1 Summary

The research successfully validated the potential of PEM electrolyzers as a key technology in sustainable hydrogen production. By systematically varying power inputs and analyzing corresponding operational data, the study revealed critical insights into the relationships between power level, current density, hydrogen volume flow, and efficiency metrics. The project underscored the significance of advanced control systems like Siemens PLC and data acquisition tools in achieving stable and efficient electrolyzer operations. These findings align with global decarbonization efforts, particularly in integrating renewable energy with hydrogen production technologies.

7.2 Recomendations

1. Integration with Renewable Energy:

   - Expand the system's compatibility with variable renewable energy inputs, to align with Energy transition Project.

2. Addition of Backpressure Regulator:

   - Incorporate a better backpressure regulator to maintain optimal pressure levels within the electrolyzer, preventing pressure fluctuations that could reduce efficiency and potentially damage the system.

7.3 Future Work

1. Study of Catalysts to Reduce Tafel Slope:

   - Investigate alternative catalysts and materials to reduce the Tafel slope, improving the efficiency of electrochemical reactions and reducing energy consumption during hydrogen production..

2. Advanced Data Analytics:

   - Implement AI and machine learning tools to predict and optimize system performance under diverse operational conditions.

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