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SUSTAINABLE EVALUATION OF DIFFERENT WATER SOURCES TO PRODUCE GREEN HYDROGEN

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Dissertação apresentada ao Programa de Pós-Graduação em Modelagem Computacional e Tecnologia Industrial do Centro Universitário SENAI CIMATEC como requisito parcial para a obtenção do título de Mestre em Modelagem Computacional e Tecnologia Industrial.
Orientador: Prof. Dr. Fernando Luiz Pellegrini Pessoa.

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Ao meu orientador, o professor Fernando, o famoso Brasinha, e aos meus amigos do centro de competência em hidrogênio verde.

RESUMO

A produção de hidrogénio a partir da eletrólise da água utilizando fontes de energia renováveis é essencial para descarbonizar a economia. Estudos mostram que a necessidade de hidrogênio seria de 2,3 Gt por ano num futuro renovável, aumentando a necessidade de água para eletrólise. Como resultado, os ecossistemas aquáticos podem ficar sob pressão significativa se não forem bem geridos. Assim, a escassez de água, tanto em qualidade como em quantidade, gera a necessidade de avaliar a adequação das fontes. Este trabalho tem como objetivo desenvolver um modelo para avaliar fontes de água sob as perspectivas econômica, ambiental e social para uso em eletrolisadores. A metodologia inclui a adaptação e aplicação do modelo de Valor Sustentável (SV) e o desenvolvimento de um modelo de Tomada de Decisão Multicritério (MCDM). O primeiro modelo utiliza 12 critérios com pesos diferentes para avaliar as fontes de água (águas subterrâneas, águas residuais industriais, água do mar, águas pluviais e rede hídrica) e é aplicado em 2 casos de estudo, um cluster de hidrogênio verde de 1MW e uma planta de hidrogênio de 60 MW em uma refinaria de petróleo. Os cálculos de custos consideraram todas as etapas do abastecimento de água (captação, transporte, tratamento e armazenamento). A avaliação demonstrou o baixo custo associado à água, comparado ao custo total da eletrólise (1,6%); assim, as dimensões social e ambiental devem ter um papel preponderante em comparação com a dimensão económica. Essa consideração foi aplicada no desenvolvimento do segundo modelo utiliza 14 critérios e considera o nível de escassez hídrica na região onde está implantada a planta de eletrólise, na forma do índice de explotação de água (WEI+). Este modelo foi aplicado em 3 casos de estudo, um parque industrial, uma refinaria de petróleo e clusters espalhados pelo estado da Bahia. Os resultados indicam variações na adequação das fontes de água, influenciadas por fatores como localização, custos de tratamento e considerações socioambientais. Conclui-se que uma abordagem multifacetada é essencial na seleção de fontes de água para a produção de hidrogénio verde, alinhada com os objetivos globais de sustentabilidade e transição energética. No geral, a água da chuva é a fonte mais adequada para pequena escala em locais com água disponível, e as águas residuais industriais são adequadas para escalas maiores e cenários de escassez.

Palavras-chave: Hidrogênio verde; Avaliação de fontes de água; Modelo de

Valor Sustentável; Tomada de Decisão Multicritério; Sustentabilidade.

ABSTRACT

Producing hydrogen from water electrolysis using renewable energy sources is essential to decarbonize the economy. Some studies show that the need for hydrogen would be 2.3 Gt per year in a renewable future. However, if the global economy achieves this hydrogen amount, the water requirement for electrolysis would be near $1x10^{14}$ *kg per year (1.8% of present global water consumption). As a result, water ecosystems can be under significant pressure if not well managed. Thus, water scarcity, both in quality and quantity, requires assessing the adequacy of the sources. Therefore, this work aims to develop a model to evaluate water sources from economic, environmental, and social perspectives for use in electrolyzers. The methodology includes adapting and applying the Sustainable Value (SV) model and developing a Multi-Criteria Decision Making (MCDM) model. Two models are discussed; the first model uses 12 criteria, with different weights, to evaluate the water sources; it is applied in 2 study cases, a 1MW green hydrogen cluster and a 60 MW hydrogen plant in a petroleum refinery. The available water sources were groundwater, industrial wastewater, seawater, rainwater, and water grid (applicable only for case 1). Cost calculations considered all steps of water supply (collection, transport, treatment (including disposal), and storage). The evaluation demonstrated the low cost associated with water compared to the total cost of electrolysis (1.6%); thus, the social and environmental dimensions must have a leading role compared to the economic dimension. This consideration, in addition to the concern with water scarcity, was applied in the development of the second model (MCDM model), which considers the level of water scarcity in the region where the electrolysis plant is implemented in the form of the water exploitation index (WEI+), in which the weights of the dimensions vary according to water availability. In addition, 2 new criteria were added to improve the model (14 criteria). This MCDM model was applied in 3 study cases in an industrial park (case 1), a petroleum refinery (case 2), and clusters across the state of Bahia (case 3). Groundwater, industrial wastewater, seawater, rainwater, water grid (applicable for cases 1 and 3), surface water, and urban wastewater (applicable only for case 3). The results indicate variations in the suitability of water sources, influenced by factors such as location, treatment costs, and socio-environmental considerations. It is concluded that a multifaceted approach is essential in selecting water sources for green hydrogen production, aligned with* *global sustainability and energy transition objectives. Overall, rainwater is the most suited WS for small scale in locals with water available, and industrial wastewater is suited for bigger scales and scarcity scenarios.*

Keywords: Green hydrogen; Water source evaluation; Sustainable Value model; Multi-Criteria Decision-Making; Sustainability; Energy transition.

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SUMMARY

1 INTRODUCTION

Hydrogen is recognized as an energy carrier for its operational absence of GHG emissions (greenhouse gases), thus rendering it environmentally benign, as highlighted by Beswick et al. (2021) in a future reliant on renewable energy, the demand for hydrogen is projected to reach 2.3 Gt per year; this transition could potentially reduce carbon emissions from the energy sector by up to 10.2 Gt annually. While the principal raw materials used to produce hydrogen derive from fossil fuels, notably natural gas, exploration into alternative renewable sources, such as biogas, water, ethanol, and glycerol, is actively underway. The methodologies employed for hydrogen generation encompass a diverse array of processes and energy inputs, with resultant types of hydrogen delineated by their production processes (Zawadzki, Kończak, & Smoliński, 2023), creating different colors.

Grey Hydrogen is predominantly yielded through steam reforming of natural gas or coal gasification. This process produces substantial CO_2 emissions, rendering these hydrogen technologies incompatible with a net-zero CO_2 emissions policy.

Blue Hydrogen involves coupling natural gas steam reforming with Carbon Capture Storage (CCS) or Carbon Capture and Utilization (CCU) technology. The CO_2 emissions are captured using CCS or CCU, reducing hydrogen production emissions. Nevertheless, the process is not entirely emission-free due to methane release during natural gas extraction and transportation.

Turquoise Hydrogen is derived from methane pyrolysis, with the primary feedstock being natural gas. The differentiating factor lies in the process being driven by electricity, preferably sourced from renewable energy, ensuring CO_2 neutrality (Zawadzki, Kończak, & Smoliński, 2023).

Green Hydrogen is harnessed from renewable energy sources and represents a linchpin in the sustainable energy transition paradigm. It is the most coveted due to its zero-emission nature. Green hydrogen is predominantly synthesized via electrolytic water splitting, employing a decarbonized electricity source. This process involves two electrodes, a cathode, and an anode, facilitating the electrochemical separation of water molecules. Approximately 4% of the total hydrogen production is attributed to electrolysis. However, as pointed out by Newborough & Cooley (2021), if green hydrogen were to replace all fossil fuels, it would necessitate approximately $1x10^{14}$ kg of water per year, equivalent to 1.8% of the current global water consumption. Consequently, there could be significant pressure on water ecosystems if not properly managed. Considering this, water scarcity, both in terms of quality and quantity, underscores the importance of evaluating the suitability of water sources, as discussed by Woods et al, (2022). Presently, hydrogen production through electrolytic cells is the most widespread method. With multiple electrolyzer technologies emerging (dos Santos, et al., 2017):

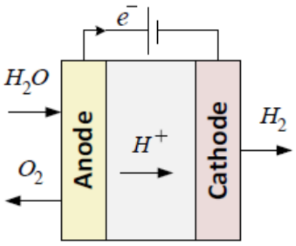
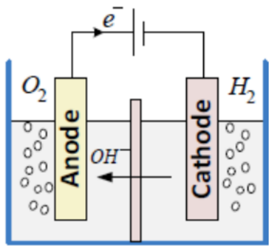
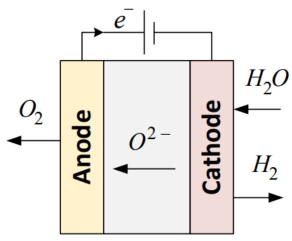
1. Alkaline Water Electrolysis: widely adopted, alkaline electrolyzers are favored for hydrogen production through electrolysis, being the most mature technology of water electrolysis with a 100-year history. This type of equipment operates by transporting hydroxide ions (OH^-) from the cathode to the anode.

2. Polymer Electrolyte Membrane (PEM) Electrolysis: also prevalent, PEM electrolyzers are characterized by lower power (ranging from 200 kW to 1150 kW) yet comparable efficiency (65% to 78%) relative to alkaline counterparts. Operate via the transport of protons through the solid polymeric electrolyte (normally Nafion®).

3. Solid Oxide Electrolysis (SOE): in the developmental phase, solid oxide electrolyzers leverage high-temperature steam (within 973 to 1173 K) to promise high-efficiency levels (approximately 85%). The electrolyte conducts oxygen ions (O_2^-) at elevated temperatures.

Table 1 presents an overview of these three most attractive and proven technologies for large-scale hydrogen production in the near term, shows a schematic of the electrolysis process of each technology, and lists its main characteristics, materials, maturity, advantages, and disadvantages (El-Emam and Özcan, 2019).

Table 1: Electrolysis technologies comparison.

	PEM	Alkaline	SOE(O)
	 Anode: $2H_2O \rightarrow O_2 + 2H^+ + 2e^-$ Cathode: $2H^+ + 2e^- \rightarrow H_2$	 Anode: $2OH^- \rightarrow H_2O + 0.5O_2 + 2e^-$ Cathode: $2H_2O + 2e^- \rightarrow H_2 + 2OH^-$	 Anode: $O^{2-} \rightarrow 0.5O_2 + 2e^-$ Cathode: $2H_2O + 2e^- \rightarrow H_2 + O^{2-}$
Materials	Pt, Ir, Ru	Ni, Ni alloys	LSM-YSZ, $CaTiO_3$, Ni-cermets
Maturity (TRL)	Early commercial (9)	Commercial (9)	R&D (6)
Advantages	• High current density • Design simplicity. • Compact system • Dynamic operation • Rapid response	• Well-established • Large stack size • Low capital cost • Non-noble materials	• High energy efficiency • Non-noble materials • Low capital cost • Reversible operation as fuel cell
Disadvantages	• High membrane cost • Noble materials • Acidic environment • Low durability	• Low current density • Corrosive electrolyte • Slow dynamics • Gas permeation	• Bulky design • Unstable electrodes • Brittle ceramics • Sealing issues

Source: El-Emam and Özcan (2019); Hobcraft (2024).

Among the technologies described in Table 1, PEM electrolyzers offer an attractive alternative compared to traditional solutions, with a higher efficiency, the potential for generation of ultrapure hydrogen (purity class >= 5.0, or that is, >= 99.999%), and a more compact design (Zawadzki, Kończak, & Smoliński, 2023). However, for optimal operation of the electrolyzer, the water supplied must comply with the specifications for deionized water with a conductivity of < 5 μS/cm.

Depending on the quality of the water used to feed the electrolyzer, several treatment processes may be necessary, including accelerated filtration, chemical treatment, ultrafiltration (UF), nanofiltration (NF), reverse osmosis (RO), ion exchange (IE) and electrodeionization (EDI), making the process more complex and expensive (Simões et al., 2021).

There are several sources of water available on the planet, such as seawater, surface water including creeks, streams, rivers, and lakes; groundwater, rainwater, water taken from the public network, recycled water from treated urban or industrial wastewater; or water obtained through processes such as condensation (e.g., cooling towers) (Simões et al., 2021). Water is a crucial resource to sustain life on Earth, being so important that the United Nations (UN) Sustainable Development Goals (SDGs) established two of the 17 SDGs directly related to water (6- Drinking water and sanitation, and 14 -Life below water) and at least 3 others indirectly associated with it (2- Zero hunger, 12- Responsible consumption and production and 13- Climate action). So, it is crucial to create strategies and adequately manage water resources, especially with a strategy considering economic, environmental, and social dimensions in final decisions (United Nations, 2024).

Sustainability must satisfy the triple bottom line of economic, environmental, and social pillars. However, numerous examples of sustainability solutions with good potential fail because one of the pillars is neglected. Thus, the relationship and connections between all three pillars are crucial because economic, social, environmental, and other semi-autonomous systems (including legal and political) connect and interact. A practical and pragmatic approach for translating sustainability science into action and application and for moving from theory to practice is the Three Pillars' framework (Santana et al, 2023).

According to Simões, et al. (2021), there is a lack of work assessing the suitability of different potential water sources and the extent this could influence decision-making regarding investing in hydrogen production via electrolysis. From their analysis, two publications specifically address water use for hydrogen production. Dincer & Acar (2015) qualitatively assess hydrogen production processes by considering global warming and acidification potential, the social cost of carbon, production cost, and energy and exergy efficiencies, looking into resource use such as water, biomass, and fossil fuels. (Turner, 2004) compares several production processes and states that water use for hydrogen production should be substantially lower than for other uses such as agriculture.

This dissertation, therefore, focuses on the guiding question: **What is the ideal type of water for the production of green hydrogen, considering the increase in water consumption and its potential environmental and social impacts?**

A gap in the literature is the lack of comprehensive studies on water sources (WS) for electrolysis. Most studies that associate *"water"* with *"electrolysis"* tend to focus on the electrochemical reaction in electrolyzers, often ignoring the broader water use perspective, particularly in selecting and evaluating suitable water sources for green hydrogen production. Winter et al. (2022) explore the non-traditional water sources for electrolysis, like seawater and wastewater, but could better specify other water sources, and the treatment costs and appropriate technologies for each source could be detailed. Baldinelli et al. (2022) also explore nontraditional water sources and present an excellent concept for water scarcity evaluation, the water exploitation index (WEI+), but do not show a methodology for water assessment. Finally, Simões et al. (2021) present an excellent method for water assessment but does not explore the local availability (just for each water source), which could be improved by incorporating new criteria and different weights for water evaluation. Thus, this dissertation aims to examine different water sources for electrolysis and propose a methodology to evaluate and choose the most appropriate sources.

In this perspective, the dissertation presents a comprehensive Multi-Criteria Decision Making (MCDM) model for evaluating water use in green hydrogen production. The model, evolving from the Sustainable Value methodology of Simões et al. (2022), addresses technical, social, economic, and environmental aspects necessary for decision-making in sustainable development (Santana, Almeida, & Pessoa, 2023). It integrates different concepts of value analysis, eco-efficiency, energy efficiency, and cleaner production, becoming a potential tool for evaluating water sources in the production of green hydrogen.

1.1 Objectives

1.1.1 Main objective

To create a model to evaluate the existing water sources around a green hydrogen plant from an economic, environmental, and social point of view to choose the most suitable source for electrolysis.

1.1.2 Specific objectives

- Identify possible water sources for hydrogen production.
- Establish socio-environmental criteria for evaluating water sources.
- Evaluate water source impact on green hydrogen efficiency.
- Compare water source viability across different geographies.

1.2 Document organization

This dissertation embraces an unconventional structure, adopting the multi-paper format. The multi-paper format, a relatively recent but increasingly popular structure in academic research, allows for a compilation of individual papers to be presented as chapters, each addressing distinct yet interconnected aspects of the overarching research theme. This structure is particularly suited to fields where research is dynamic and rapidly evolving, as is the case with green hydrogen production and the evaluation of water sources.

The advantages of the multi-paper format are manifold. Primarily, it allows for a more granular and focused exploration of the subject matter. By segmenting the research into discrete yet interconnected papers, the format facilitates a deeper dive into specific aspects of the topic, enabling the researcher to cover a broader range of perspectives and methodologies than might be feasible in a traditional dissertation format. This approach also lends itself well to the publication of findings in real-time, as each paper can be disseminated independently, contributing to the ongoing academic discourse even before the entire dissertation is completed. Moreover, the multi-paper format aligns well with the contemporary educational and research landscapes, where incremental but rapid dissemination of findings is increasingly valued.

However, the format is not without its challenges. One of the primary difficulties lies in maintaining a cohesive narrative throughout the dissertation. Each paper must be meticulously designed to contribute to the overarching thesis, ensuring that the dissertation, as a whole, presents a unified and coherent argument. This format requires a careful balance between the autonomy of each paper and their collective contribution to the central theme of the research.

The choice of the multi-paper format for this dissertation was driven by the evolving nature of the research in green hydrogen production, particularly the evaluation of water sources for electrolysis. As the study progressed, new findings and insights necessitated an agile and flexible approach to publishing. Utilizing modifications of the Sustainable Value (SV) model from Simões et al. (2021) as a foundational methodology, the research evolved through successive refinements, culminating in developing a comprehensive and robust model.

The dissertation is structured into three sections subdivided into six chapters (see Figure 1), starting with a general introduction (present chapter), followed by a discussion section (chapters two to five), where each chapter corresponds to one or two distinct (published or submitted) papers. Finally, it ends with a general conclusion of the dissertation (chapter six).

As it is a multi-paper format, the chapters of the discussion section are structured as follows: I) Introduction, containing Motivation, Purpose, Background, and information about objectives and goals; II) Methods used in the study; III) Major Results and Findings which includes quantitative references (key performance indicators, etc.), and IV) Conclusion of the chapter, which includes implications of findings, limitations of the study, and recommendations.

The second chapter, *"Water Sources Considerations for Green Hydrogen Production: Current Challenges, Innovative Insights, and Future Perspectives," is based on a published paper with the same name* and lays the groundwork for the research. It delves into the challenges and opportunities inherent in managing water resources for green hydrogen production, emphasizing the necessity of sustainable water management practices. This paper sets the stage by highlighting the current state of the art and the criticality of studying water sources for electrolysis.

Building on the foundation laid by the second chapter, the third one, *"Sustainable Value Approach to Evaluate Water Sources for Electrolysis,"* is based on two published works by the author (Santana et al. (2023a, 2023b)) and introduces the SV methodology as a strategic tool for evaluating water sources. This chapter discusses and applies the method to a hypothetical green hydrogen plant, demonstrating its practical applicability. It also extends the application of the methodology to real-world scenarios, evaluating different water sources in Brazil and providing a comprehensive sustainability analysis that includes technical, economic, environmental, and social criteria.

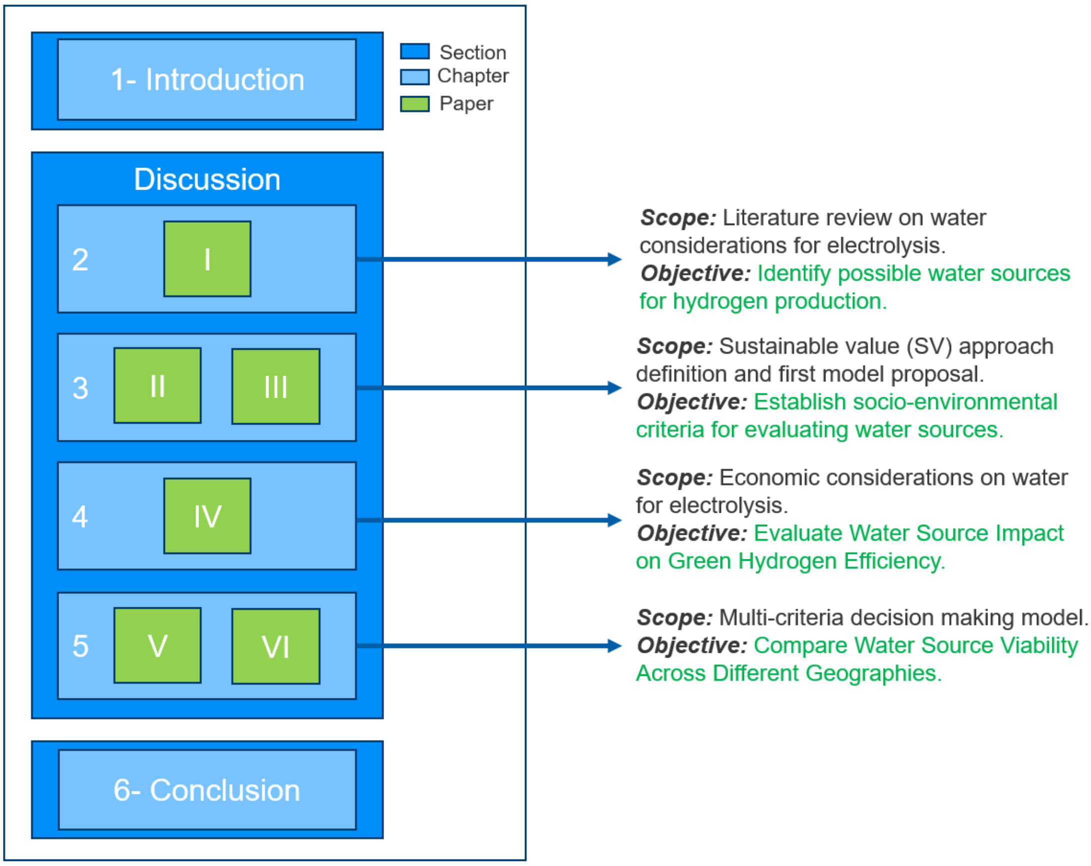
With a focus on economic aspects, the fourth chapter, *“Evaluating the Economic Influence of Water Sources on Green Hydrogen Production: A Cost Analysis Approach,” is based on a homonym paper and examines the impact of various water sources'* costs on the Levelized Cost of Hydrogen. This paper is crucial in establishing the economic viability of different water sources in green hydrogen production.

The fifth chapter, “*A Multi-Criteria Decision-Making (MCDM) Model for Water Assessment in Green Hydrogen Production*,” presents the culmination of the research and is based on two papers, the first, with the same name, and the second by Santana et al. (2024). This chapter introduces a new MCDM model, developed based on the sustainable value measurement MCDM AHP (Analytical hierarchical process) method. This model represents the synthesis of the research journey, incorporating advancements and refinements from previous papers, and applies the developed MCDM model to various sites in the State of Bahia, Brazil. The study cases of this chapter demonstrate the practical application and effectiveness of the model in diverse real-world contexts.

In summary, each paper in the dissertation progressively builds upon its predecessor. The dissertation presents a cohesive and detailed narrative from the initial exploration of the challenges in water management for green hydrogen production to developing and applying a sophisticated MCDM model. This narrative addresses the topic's complexities and showcases the efficacy and necessity of the multi-paper format in contemporary academic research, particularly in fields as dynamic and impactful as green hydrogen production.

Finally, the last chapter (sixth) is an overall conclusion of the dissertation, with some comments about the research journey and main findings of the master dissertation.

Figure 1: Graphical abstract of the structure of the dissertation



Source: Author, 2024

2 WATER SOURCES CONSIDERATIONS FOR GREEN HYDROGEN PRODUCTION: CURRENTS CHALLENGES, INNOVATIVE INSIGHTS, AND FUTURE PERSPECTIVES

Abstract: The following chapter focuses on water source considerations for green hydrogen production, exploring the challenges and opportunities related to managing water resources in the electrolysis process. It assumes the role of a bibliographic review, being, in summary, a compendium of all the primary considerations regarding water for electrolysis. It plays an important position in this document, being the starting point of the research journey, Identifying possible water sources for hydrogen production. The aim is to ensure sustainable development and address the water usage implications. The importance of sustainable water management practices is emphasized. Alternative solutions, such as mass and energy-integrated water systems and alternative water sources, are explored to reduce the environmental impact of electrolysis. The future perspectives highlight technological advancements, collaboration, and increased adoption of green hydrogen. The research underscores the significance of sustainable water management for the success of green hydrogen in the transition to a low-carbon economy. The principal results highlight the need for careful consideration of water resources and the potential benefits of green hydrogen. The major conclusion is that sustainable water management practices are essential for the viability and scalability of green hydrogen production. In this sense, a decision support system could improve sustainable decision-making regarding water sources.

2.1 Introduction

The transition to a low-carbon economy is one of the most urgent challenges of our time, and the production of green hydrogen has emerged as a key solution in this effort. As a clean and sustainable alternative to fossil fuels, green hydrogen has the potential to transform the energy landscape and reduce greenhouse gas emissions. However, the production of green hydrogen requires significant amounts of water (Beswick et al. 2021).

The impact on water resources must be carefully considered to ensure that this promising technology can be developed sustainably and at scale (Winter et al. 2022). Green hydrogen is produced by using renewable energy sources to split water molecules into hydrogen and oxygen through a process called electrolysis (Woods et al. 2022). However, the water source and quality used in the electrolysis process can impact green hydrogen production's overall sustainability and environmental benefits (Baldinelli et al., 2022).

The hydrogen economy depends on clean water sources' availability (Simões et al. 2021). However, it is essential to ensure that the production of green hydrogen does not compete with other important water uses, such as drinking water or agricultural irrigation. Careful planning and management of water resources will be essential to ensure that the hydrogen economy's growth does not negatively impact water availability and quality (Beswick et al. 2021).

Water is an abundant renewable resource on Earth, which means that green hydrogen production has the potential to be a sustainable and environmentally friendly alternative to traditional fossil fuels. In addition, using green hydrogen can help reduce greenhouse gas emissions and improve air quality, positively impacting human health and the environment (Woods et al., 2022).

This chapter focuses on water source considerations for green hydrogen production, exploring the challenges and opportunities of managing water resources in the electrolysis process. We begin by discussing the importance of sustainable water management practices in producing green hydrogen and the current challenges of water usage and availability. We then examine alternative solutions such as mass and energy-integrated water systems, using alternative water sources, and integrating renewable energy sources to reduce the environmental impact of the electrolysis process.

Finally, we consider the future perspectives on water source considerations for green hydrogen production, highlighting the potential for technological advancements, more sustainable water management practices, collaboration between industry and government, and increased adoption of green hydrogen as a clean energy solution. As we delve into the current challenges, innovative insights, and future perspectives, we uncover a nuanced perspective that goes beyond conventional analyses, offering a holistic approach to ensure the viability of green hydrogen.

2.2 Methodology

A comprehensive study was conducted using an exploratory review and snowballing technique to achieve the objective. The primary focus was investigating various facets associated with water utilization in electrolysis. This encompassed diverse water sources such as seawater, groundwater, and others and the process of selecting the appropriate source. Additionally, the methodology aimed to determine cost calculations related to water, including water abstraction/capitation, transportation, and treatment, for its use in electrolysis. The selection process specifically targeted articles addressing potential water sources and their qualities.

The resultant compilation thoroughly explores key considerations surrounding water for electrolysis, encompassing challenges, usage limitations, and water quality aspects. Furthermore, innovative insights and prospects regarding water utilization in electrolysis are addressed in these studies.

The main findings for each topic about water considerations in electrolysis, including key factors, challenges, perceptions, and prospective insights, are summarized in tables. These findings are subsequently elaborated upon in the following sections of the manuscript.

2.3 The main considerations for water for electrolysis

Water studies are crucial issues on the topic of green hydrogen. Beswick et al. (2021) considered that the hydrogen demand would be 2.3 Gt/y and, assuming that all hydrogen will be produced by electrolysis, means that 20.5 billion m^3/y of water, which is a tiny amount of 1.5 ppm of the available water. However, freshwater is around 3% of the planet's total water, and less than this is accessible to humans (Baldinelli et al., 2022).

Table 2 shows some considerations for water sources regarding green hydrogen production. Some of these considerations are correlated, so they must be studied independently.

Table 2: Main considerations for water sources

Considerations	Description	References
Source of water	The source of water used in the electrolysis process should be carefully considered. Using freshwater sources such as rivers or lakes can strain local ecosystems, especially in areas where water scarcity is already an issue. Instead, using non-potable sources such as wastewater or brackish water can be a more sustainable option.	Simões et al. 2021
Water quality	The water quality used in the electrolysis process can impact the process's efficiency and the equipment's lifespan. High levels of impurities such as minerals, salts, or organic compounds can cause corrosion and fowling and reduce the efficiency of the electrolysis process. Therefore, water quality should be closely monitored and treated as necessary.	(Simões et al. 2021)
Water availability	Water availability in the region where green hydrogen is being produced is also an essential factor to consider. In areas with limited water resources, alternative water sources such as seawater or brackish water may need to be used.	(Simões et al. 2021)
Local regulations	Water usage and disposal regulations can vary depending on the region and country. Before starting a green hydrogen production project, it is essential to understand local water usage and disposal regulations to ensure compliance.	Moir et al. 2020.

Water treatment	Depending on the water source, treatment may be necessary to remove impurities and ensure the water is suitable for electrolysis. Treatment processes can include filtration, reverse osmosis, and distillation.	(Simões et al. 2021)
Water transportation	Depending on the location of the green hydrogen production facilities, transporting water to the site may be necessary. It can add additional costs and environmental impacts to the production process.	(Simões et al. 2021) Joksimovic, 2007
Water usage efficiency	The amount of water used in the electrolysis process can impact the overall efficiency of the process. Implementing water reuse systems and optimizing the electrolysis process can reduce the amount of water needed and increase efficiency.	Webber, 2007 (Simões et al. 2021)
Environmental impacts	Water extraction from natural sources and wastewater disposal can have environmental impacts such as habitat destruction and pollution. Implementing sustainable water management practices can minimize these impacts.	(Baldinelli, et al. 2022).
Climate considerations	Climate change can impact water availability and quality, making it essential to consider the long-term sustainability of water sources. Alternative water sources may need to be explored in areas with high water stress or vulnerability to climate change.	(Simões et al. 2021)

Source: Author.

In green hydrogen production, the water source should be carefully considered to avoid straining local ecosystems, and using non-potable sources like wastewater or brackish water can be more sustainable. Water quality must be monitored and treated to prevent corrosion and maintain process efficiency. Water availability, local regulations on usage and disposal, and the need for water treatment and transportation are essential considerations. Optimizing water usage efficiency and implementing sustainable water management practices can mitigate environmental impacts. Climate change necessitates considering alternative water sources in areas with water stress or vulnerability.

2.3.1 Water sources for electrolysis

Water sources for electrolysis can come from various sources, and the choice will depend on multiple factors, including the availability of water in the region, the cost of water treatment and transportation, and the environmental impacts of water use. It is essential to carefully consider these factors when planning and implementing green hydrogen projects.

The availability of water resources around the electrolysis plant is essential to guarantee the adequate production of green hydrogen. Thus, water sources must be appropriately identified and evaluated.

The identification goes through a hydrological study of the water sources in the surroundings of the electrolysis plant, and the term "surroundings" can be a little subjective. In addition, Simões et al. (2021) and Santana et al. (2023) concluded that the costs related to water transport are the most significant among all the costs associated with water use in the production of green hydrogen. Thus, a distance limit must be defined in advance.

The steps that guarantee the supply of water in the electrolyzers are defined by Simões et al. (2021) as being the following: water capture/collection, transport to the H_2 production plant, water storage, water treatment to the level required by the electrolyzer techniques, and disposal of wastewater treatment.

The water resources can be mainly classified as freshwater, anthropogenic wastewater, and low-quality natural water. In general, the most common sources of water in the area around an electrolysis plant, summarized in Table 3, are seawater, estuaries (with a saline concentration different from seawater), aquatic water (adding streams, rivers, and lakes), groundwater, rainwater, public water, urban wastewater, industrial wastewater, and cooling tower water.

There are typical examples of freshwater: surface water from rivers and lakes, groundwater, grid water, rainwater, and industrial feedwaters (cooling towers, deionized water, and distilled water). Freshwater is the most common water source for electrolysis. However, freshwater use for green hydrogen production must be managed carefully to avoid depleting local water resources and competing with other important uses such as agriculture, industry, and human consumption. Alternative water sources such as treated wastewater or brackish water may be more suitable in regions where freshwater is scarce.

Anthropogenic wastewater is water used in households, industries, and businesses and has undergone some treatment. It is generally classified as industrial effluents or wastewater and urban wastewater or sewage. The wastewater quality can vary depending on the source and the treatment processes used. Wastewater can be used for electrolysis but may require additional treatment to remove impurities and contaminants.

Finally, we have low-quality (salt-rich) natural waters, such as seawater and brackish water (from water wells or estuaries). Seawater is the most abundant source of water on Earth, presenting an average salinity of 36% due to the presence of Na (sodium), Cl (chlorine), Mg (magnesium), and K (potassium). Brackish water comes from underground reserves or basins (lakes, sea close to estuaries) and features low salinity, compared to seawater, which is about 10%.

Table 3: Overview of water sources

Water resource	**Water source**	**Main water pollutants and treatment parameters**	**Considerations on water quality**
Freshwater	surfaces, rivers, streams, lakes	Suspended solids (TSS), biochemical oxygen demand (BOD)	Good quality water, abundant flow rate in the closest river, can provide water all year round. The water stream can be dry in the summertime
	groundwater	Dissolved solids	Generally, it is of excellent quality due to soil filtration. It may contain specific ions (carbonates or metals such as iron/

			manganese).
	Water supply network (tap/grid water)	Dissolved solids	Good quality water. Tap water is a common water source for electrolysis, and it is usually readily available and may contain impurities such as minerals, dissolved gases, and contaminants such as chlorine. The quality of tap water can vary depending on the location and the treatment processes used by the local water authority.
	industrial feedwaters (cooling towers, deionized water, and distillate water)	Dissolved and suspended solids	It may be difficult or costly to collect and condense the water vapors. If these waters are of good quality, they will probably be condensed and reused in the respective industry.
	rainwater	Some dissolved solids, BOD, TSS	Usually, rainwater exhibits favorable characteristics and carries certain compounds because it absorbs gases while descending through the

			atmosphere or interacts with the soil during drainage. Utilizing such water mandates substantial storage capacity to ensure a year-round water supply.
Anthropogenic wastewaters	Treated industrial wastewater	Depending on the industry, suspended solids, BOD5, Chemical oxygen demand (COD), toxicity	Depending on the industry, it can produce organic pollution. It may be problematic to ensure the flow rate Throughout the year, due to possible variations in process production,
	urban wastewater	Suspended solids, BOD, COD, toxicity	Usually, the degree of treatment is secondary or secondary with nutrient removal. Thus, additional pretreatment (coagulation/ filtration) before reverse osmosis can be necessary.
low-quality natural water (Salt-rich)	Seawater	Salinity 36-37%	Seawater is used when no other sources are accessible. Encompasses elevated levels of dissolved solids (chloride and sulfate). While the abundance is notable, the distance

			might pose challenges.
	Estuary (low-quality groundwater)	Salinity 33-34%, algae, suspended solids	Estuarine water has high salinity, algae, and variable composition. The uptake can be complicated (more costly) due to the tide level fluctuations.

Source: Simões et al. 2021; Baldinelli, et al. 2022; winter et al. 2022.

2.3.2 Water quality for electrolysis

Water quality is an essential topic since impurities can affect electrolysis performance. Among the steps mentioned, synthesizing the treatment process is crucial to guarantee adequate water for electrolysis. Electrolyzer feed water specifications are defined by ISO 22734:2019 as being the responsibility of the manufacturer; deionized water is commonly used, usually type I or II ultrapure water (ASTM designation D1193, 1999. ASTM designation 5127 2007).

Some manufacturers sell electrolyzers with water purification units included. In these cases, it is common for the specification of water quality to be potable (intended for human consumption), according to Directive 2020/2184 of the European Union.

The main water quality parameters to be observed according to suppliers and ASTM designations are described in Table 4. There are nine main parameters to evaluate. However, these parameters can be summarized in two: conductivity and total organic carbon, given the high correlation between these two parameters and the previous ones, especially dissolved ions (Dubber & Gray, 2010) (Dabgerwal & Tripathi, 2016

Table 4: Requirements of water specifications according to ASTM D5127 and directive 2020/2184 of the European Union.

Parameter	**Inlet purification system (drinking**	**Purification system outlet (electrolyzer**

	water)	inlet)
Electric conductivity	220 microS/cm	0,056-1,0 microS/cm
Total organic carbon	2,3 mg/L	50 microg/L
Sodium	200 mg/L	1-5 microg/L
Chloride	1,3 mg/L	1-5 microg/L
Total silica	19 mg/L	3 microg/L
Iron	0,2 mg/L	0,05 microg/L
Manganese	0,04 mg/L	0,05 microg/L
Total dissolved solids	364 mg/L	0,05 ppm
Hardness (as CaCO3)	130 mg/L	0,05 ppm

Source: Adapted from ASTM (2007).

As mentioned by Woods et al. (2022), water impurities could lead to irreversible damage, which includes:

- Cations such as Fe^{+3}, Ca^{+2}, $Al^{+3,}$ and Na^{+}. Have the potential to reduce the proton conductivity of the membranes within polymer electrolyte membrane electrolyzers. Alternatively, they can accumulate on diaphragms due to concentration gradients in alkaline electrolyzers.
- Sulfates that poison the electrodes.
- Chloride concentrations higher than 0.1 ppm lead to extensive production of oxychloride (OCl) in alkaline electrolyzers and chlorine gas (Cl_2) in polymer electrolyte membrane electrolyzers, and these substances also poison the electrodes;
- Biofilms, which can generate organic compounds, can produce foam and contribute to Faradaic efficiency (the overall selectivity of an electrochemical process). It can lead to a notable decline in the effectiveness of water electrolysis.

The treatment technologies must be chosen according to the primary contaminants and have sufficient removal efficiency so the water meets the demand of the electrolysis plant. The required removal efficiency will depend on the water quality from each source.

Generally, each source mentioned will have a characteristic quality for each contaminant, but there are variations according to location. So, the water from each source must be analyzed to quantify these contaminants and screen the treatment processes.

2.3.3 Local regulations

And finally, local regulations are crucial to ensure that water is allocated fairly among stakeholders, including industry, agriculture, and local communities. They can also promote the use of sustainable water management practices.

Regulations on the use of water help understand how water bodies are classified and the environmental guidelines for their classification, as well as establishing the conditions and standards for effluent release and other measures. These regulations make it possible to know what is or is not possible in managing water resources. Since these regulations can change country by country, it is important to be mindful of them to manage water resources adequately and safely.

Ensuring sustainable water management practices in green hydrogen production requires careful consideration of various factors such as water treatment, transportation, usage efficiency, environmental impacts, and climate considerations. By prioritizing sustainable water management practices, using preferably non-potable sources, monitoring water quality, and adhering to local regulations, green hydrogen producers can minimize their environmental impact and contribute to a more sustainable future (Baldinelli et al. 2022).

2.4 Current challenges

Winter et al. (2022) cited that the challenges for achieving low-carbon energy storage and chemicals manufacturing will require an abundant supply of green hydrogen. Thus, the list of the main water for electrolysis considerations leads us to the key challenges of deploying a green hydrogen-based economy at scale.

Some current challenges related to water source considerations for green hydrogen production are described in Table 5.

Table 5: Current challenges on water source considerations.

Challenges	Description	References
Water scarcity	One of the main challenges for green hydrogen production is access to sufficient water resources, especially in arid regions. Water	(Simões et al. 2021)

	scarcity can lead to increased competition for water resources, impacting the availability and cost of water for green hydrogen production.	
Water quality	The quality of available water sources can also challenge green hydrogen production. Depending on the quality of the water, additional treatment processes may be required, which can increase the cost and environmental impact of the production process.	(Simões et al. 2021)
Infrastructure limitations	In some regions, the lack of water transportation and treatment infrastructure can limit the ability to access and use alternative water sources for green hydrogen production.	(Simões et al. 2021)
Regulatory hurdles	Water usage and disposal regulations can vary by region, creating challenges for green hydrogen producers seeking alternative water sources or implementing sustainable water management practices.	(Valleros-Romero et al. 2022) (Simões et al. 2021)
Climate change	Climate change is expected to increase water stress and impact water availability and quality, which could make green hydrogen production more challenging in some regions.	(Simões et al. 2021)
Energy consumption	The electrolysis process used to produce green hydrogen requires significant amounts of energy. Depending on the energy source used, this process can significantly impact water resources by increasing the demand for electricity or other energy sources, such as natural gas.	(Simões et al. 2021)
Water usage in fuel production	While green hydrogen is a clean and sustainable fuel, its production requires significant water. Depending on the production scale, it could lead to substantial water usage and environmental impacts.	Webber, 2007

Cost	Producing green hydrogen from renewable sources such as wind and solar power is currently more expensive than producing hydrogen from natural gas. The cost of producing green hydrogen will need to decrease to become a more competitive alternative to fossil fuels.	Winter et al. 2022
Scaling up production	As demand for green hydrogen grows, scaling up production to meet that demand will require significant infrastructure, technology, and human resources investments. Ensuring water sources are managed sustainably and efficiently will be a key consideration in scaling up production.	Blanco 2021
Public perception	Finally, the public perception of green hydrogen and its production process will be a significant challenge. Ensuring that green hydrogen is produced sustainably and environmentally friendly will be essential to its acceptance as a viable alternative to fossil fuels.	(Simões et al. 2021) (Valleros-Romero et al. 2022)

Source: Author.

2.4.1 Water scarcity

According to Blanco (2021), the water consumption for hydrogen production in 2050 will be much less than that of other water uses like agriculture, human use, and industrial use. Baldinelli et al. (2022) claim that the total water footprint will decrease, but on the other hand, the effects of climate change will soon be felt through the water (severe drought, melting glaciers). It will have dire implications for energy security. The balance of resources is at risk: as access to freshwater decreases, there are more use of energy-intensive processes such as desalination is expected.

In addition, in some situations, low-quality water (waste or saline) is not always available or can assume prohibitive costs (Simões et al., 2021), so potable water resources will be intensively exploited, contributing to droughts. It causes distress to the renewability and availability of hydric resources in each location and period– i.e., water is lacking when the resource is insufficiently sufficient to meet the request.

Also, the short-term reliability of availability (effect of weather factors on water sources such as droughts) is an important criterion to evaluate the water sources; this makes the use of tools that adequately assess the exploitation of these water resources significant, as is the example of the water exploitation index (WEI+) (Baldinelli et al. 2022).

The WEI+ metric demonstrates the ability to monitor localized pressure on renewable freshwater resources arising from water requisites. This involves assessing the variance between total water withdrawals (ABS) and replenishments (RET) in specific watersheds concerning the "average available water long-term annual report" (LAAW) for a particular moment and location (Baldinelli et al., 2022). Conventional wisdom dictates that a WEI+ value of 20% signifies a state of water scarcity, whereas a WEI+ value of 40% indicates an alarming level of unsustainable pressure and pronounced water scarcity (Baldinelli et al., 2022).

2.4.2 Water quality at the source level

As described in Table 3, each water source has a specific quality regarding some key contaminants. Zeng and Zhang (2010) research emphasized the critical role of water quality in electrolysis systems, shedding light on the potential deposition of impurities on electrode surfaces and membranes. Moreover, investigations by Dubber & Gray (2010) and Dabgerwal & Tripathi (2016) demonstrated a high correlation between key water quality parameters such as conductivity and total organic carbon with dissolved ions. These insights underscore the need for targeted water treatment processes to ensure optimal electrolysis performance. For this, the synthesis of the treatment train is crucial.

Once the contaminants and the recommended treatment processes for removing each one are identified, it is necessary to assemble the process. This process synthesis stage is the most critical stage of a process project, in which the equipment and how they are connected to form a flowsheet are defined. However, there are different possible combinations for structuring the process flowsheet. Seader et al. (2016) explain that to develop a certain flowsheet in the various industrial processes, the arrangement of equipment can vary greatly and grow to a prohibitive scale with the number of necessary equipment (combinatorial explosion), generating several plausible flowsheets, where each of these flowsheets represents a viable solution to the process synthesis problem. The difficulty caused by the combinatorial explosion in the synthesis is characterized as a classic optimization problem. It can be solved through intuitive knowledge-based methods, such as heuristic methods or mathematical programming (Perlingeiro, 2005).

Given this optimization problem to work around the issue related to the combinatorial explosion in the synthesis step, decision support tools (DSSs) are increasingly common in the development of water treatment and reuse networks as they help with problems of synthesis and simulation of treatment processes. (Santana et al., 2019)

Mannina et al. (2019) explain that using decision support tools allows the integration of issues related to sustainable development to provide helpful support to solve multi-scenario problems. They also make a bibliographical review the decision support tools developed between 2010 and 2019. Citing the disadvantages of existing prior techniques for managing wastewater treatment plants (WWTPs) before the deployment and use of DSS:

- difficulties in managing the high complexity of effluent treatment plants (ETPs) due to the interaction of heterogeneous components and elements (biological, chemical, physical, mechanical, etc.).
- Lack of control, automation, and instrumentation in the ETPs to deal with the dynamicity of the ETPs.
- No exhaustive alternative decision analysis support.
- No prognostic features for possible alternative decision evaluation.
- No broad data-driven models are used.

2.4.3 Water Cost and Infrastructure

While water is an available resource, producing green hydrogen at scale requires large quantities of water, and the cost of sourcing and treating this water can be significant. Additionally, the infrastructure needed to transport and store large amounts of water can be a barrier to the growth of green hydrogen production.

Simões et al. (2021) have identified all the required steps to ensure water supply and how each of these water supply steps (abstraction/capitation, transport, treatment, storage) can be translated into a water supply cost. Joksimovic (2007) has studied the modeling of a decision support system for planning integrated water reuse projects, and through his work it is possible to calculate the costs for each water supply step, since the abstraction/captation to the storage.

For Simões et al. (2021), ensuring water supply into the electrolyzers involves the following steps: water abstraction/capitation, transport to the H_2 production plant, water storage, water treatment up to the level required by electrolyzer technical specifications, and disposal of residues from water treatment. These water supply steps are not listed sequentially and depending on the specific water source site being considered can be ordered differently (for example, water storage being made before or after water treatment). Each step has associated costs and water losses, which will be estimated and presented in the following sections. In specific instances (particularly when using water from the public grid), established infrastructure exists to facilitate water transportation to the electrolyzer. For almost all the other water sources, it is necessary to build a whole infrastructure, or parts of it, to abstract, transport, store, and treat water.

In terms of infrastructure, transporting and storing large quantities of water can be challenging, especially in areas where water resources are scarce or infrastructure is limited. Developing a robust water supply and distribution infrastructure will be essential to support the growth of green hydrogen production. This infrastructure construction is not so trivial; factors such as the topography of the study site must be considered in the path between the source where the water will be collected and the destination, which helps to understand the geography of the place, to define the best locations for the implantation of the treatment plant, the areas where pumping stations will be placed, etc., and the barriers/constructions since the collection and distribution network cannot always go straight to the station; barriers, such as constructions, highways, rivers, and other kinds of zones where that may make it impossible for the pipeline to pass through, making it necessary to study these regions to define the best path for the collection and distribution networks (Santana et al., 2021).

In summary, addressing these challenges will require collaboration and innovation between industry, policymakers, civil society, and other stakeholders to ensure that water sources are managed sustainably and efficiently to support the growth of green hydrogen production in an environmentally sustainable and economically viable way.

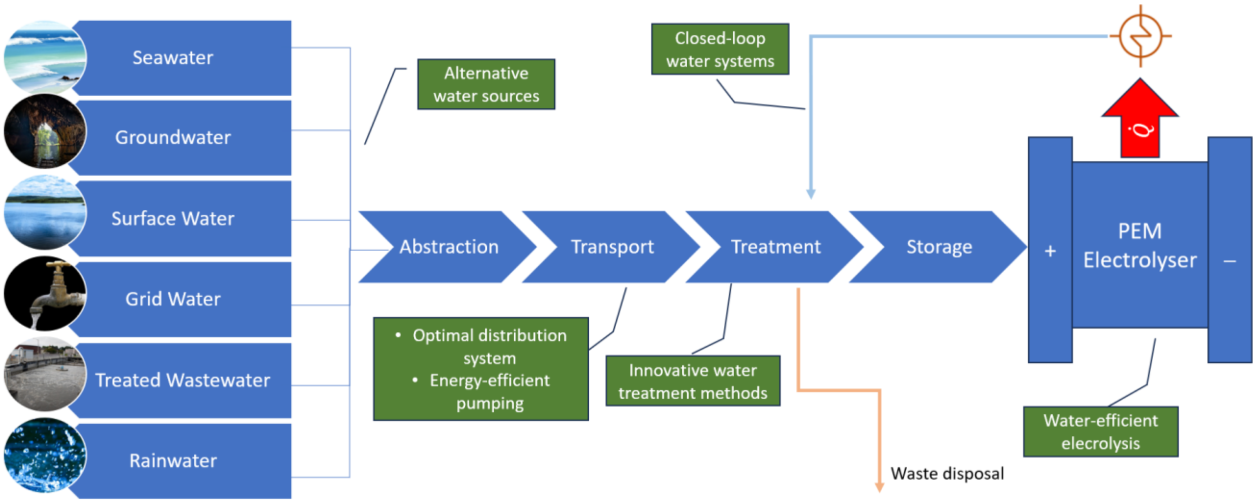
2.5 Innovative insights on the water for electrolysis

Given the challenges and the importance of water in a hydrogen-based economy, some innovative insights related to water sources for electrolysis are:

1. the use of alternative water sources is as follows: as water scarcity becomes a more significant concern in many regions, innovative solutions such as using alternative water sources, such as salty water or seawater, can be explored. Researchers are also investigating using non-conventional water sources, such as industrial wastewater, to reduce the impact on freshwater resources (Winter et al. 2022).
2. Mass and energy-integrated water systems: Closed-loop water systems that recycle and reuse water used in the electrolysis process can significantly reduce water consumption and minimize the environmental impact of the production process (Calixto et al., 2020). These systems can be implemented via fuel cells in hybrid hydrogen production and energy generation plants. Furthermore, thermal energy-based water purification technologies (such as membrane distillation) can reuse waste energy from the electrolysis process for water purification. Other process stages can be studied to minimize water and energy use.
3. Developing water-efficient electrolysis technologies: researchers are developing more efficient and water-saving electrolysis technologies that require less water to produce green hydrogen (Kumar & Lim, 2022; Webber, 2007).
4. Innovative water treatment methods: Developing innovative approaches such as membrane distillation and reverse osmosis can reduce the energy required to treat water for electrolysis, making the process more efficient and cost-effective (Saavedra et al., 2021).

Finally, these innovative solutions have the potential to significantly reduce the environmental impact of green hydrogen production while also addressing some of the challenges related to water sources. Continued research and investment in these and other innovative solutions will be essential to ensure that green hydrogen can be produced sustainably and at scale to help address the urgent challenges of climate change and energy transition. The primary considerations discussed in this work about water for electrolysis are illustrated in Figure 2.

Figure 2: Water considerations and insights on electrolysis



Source: Author.

2.6 Prospects and Future Challenges

The triple bottom line (sustainability) concept is the basis of all these challenges. With this new ecological awareness, engineers will be increasingly encouraged to consider economic aspects and social and environmental issues in developing their projects, always defining the most sustainable solution (Metcalf, 2013).

Although it is a commendable concept, it has proven difficult to apply and implement uniformly since it is still difficult in some cases to combine environmental and social issues with the economic aspect.

Evaluating a project's income and expenses in an economic evaluation is much easier than assessing that project's social and environmental costs and benefits. Therefore, for the social and environmental baselines to be satisfactorily met, it is necessary to assign monetary values to the respective costs and associated benefits. Even though it is impossible to assign economic values, social and environmental issues must still be considered. However, they have little impact on project implementation beyond those issues usually incorporated in the analysis of any project. The challenge is appropriately incorporating the concepts in the triple baseline tool into project planning, development, and deployment (Metcalf, 2013).

Some future perspectives on water source considerations for green hydrogen production are as follows:

1. Advancements in technology: future advancements in electrolysis technology and water treatment methods will continue to drive down the cost of

producing green hydrogen and increase the efficiency of the production process. It will make green hydrogen a more viable and cost-effective alternative to fossil fuels (Khan et al. 2021).

2. Increasing use of renewable energy: As renewable energy sources such as wind and solar power continue to grow, the production of green hydrogen will become more sustainable and less dependent on non-renewable energy sources. (Khan et al. 2021).

3. More sustainable water management practices: as the importance of sustainable water management becomes increasingly recognized, there will be greater emphasis on using alternative water sources and implementing mass and energy-integrated water systems to reduce water consumption and minimize the impact on freshwater resources. (Woods et al., 2022).

4. Collaboration between industry and government: cooperation between industry and government will be essential to drive the development of sustainable water management practices and support the growth of green hydrogen production at scale (Moir et al., 2020; Woods et al., 2022).

5. Increased adoption of green hydrogen: as the demand for clean energy continues to grow, green hydrogen as a sustainable alternative to fossil fuels is expected to increase, driving further investment and innovation in water source considerations for green hydrogen production (Blanco, 2021).

6. Hydrogen from wastewater: There are several methods to produce hydrogen through wastewater; a preliminary examination underlines that biological methods (dark fermentation and photofermentation) are economically suitable for active wastewater treatment and produce hydrogen. Still, environmental indicators suggest the advantages of two immature technologies, namely photocatalysis and microbial processes (Baldinelli et al., 2022; Metcalf, 2013).

7. Hydrogen from seawater: studies of direct electrolysis of seawater, chlor alkali process for which produces hydrogen or hybrid process are being developed to achieve high efficiency in the use of this non-traditional water source (Khan et al. 2021; Sharkh et al. 2022).

From the above-listed challenges, it appears that collaboration between industry and government and increased adoption of green hydrogen are the most critical factors in achieving a low-emission future. Furthermore, the possibility of hydrogen production from anthropogenic wastewater must be important since the increase in green hydrogen production can pressure freshwater scarcity. Metcalf et al. (2013) underline that this opportunity concerns the possibility of exploiting the energy and chemicals present in effluents, transforming waste into new raw materials. There is an unexplored potential in this waste, which makes room for a new type of income for companies that treat effluents and for innovative technologies, which, because of recovery, will reduce the exploitation of raw materials from nature, preserving natural resources. In addition to providing a new destination, resource recovery enables a source of wastewater that is increasingly free of impurities.

In addition, effluents rich in organic matter, such as food residues, oils, fats, and grease, which, once separated from the effluent, can undergo an anaerobic process, where microorganisms will consume these impurities and produce biogas (CH_4, CO_2, and H_2S), which can be burned in boilers to produce electricity. The challenge will be efficiently extracting the energy in such effluents (Metcalf, 2013).

The expectation is that in the future, the recovery of resources present in the effluents will occur simultaneously with energy recovery. Currently, the removal of nitrogen and phosphorus has received the most attention as the emission standards for these constituents have become increasingly rigorous. The option of recovery, instead of removing these constituents from the effluent, is becoming economically viable, attending to a crucial sustainable development issue (Metcalf, 2013).

Overall, the future of green hydrogen production depends on developing and implementing sustainable water management practices, adopting innovative technologies, and collaborating with industry, government, and other stakeholders. With suitable investments and policies, green hydrogen has the potential to play a significant role in the transition to a low-carbon economy and help address the urgent challenges of climate change.

2.7 Conclusion

In conclusion, the production of green hydrogen has the potential to transform the energy landscape and contribute to the urgent need for a low-carbon economy. However, as the production of green hydrogen requires significant amounts of water, the impact on water resources must be carefully managed to ensure sustainability.

Innovative solutions such as mass and energy-integrated water systems, using alternative water sources, and integrating renewable energy sources can reduce the environmental impact of the electrolysis process and contribute to sustainable water management practices.

The challenges related to water source considerations for green hydrogen production are significant, but the potential benefits are equally important. Continued research and investment in this area will be essential to ensure that green hydrogen can be produced sustainably and at scale to help address the urgent challenges of climate change and energy transition.

3 SUSTAINABLE VALUE APPROACH TO EVALUATE WATER SOURCES FOR ELECTROLYSIS[1]

Abstract: Based on the previous chapter, it was found that sustainable water management practices are essential for the viability and scalability of green hydrogen production. With a focus on the water sources for electrolysis previously discussed, this chapter presents the Sustainable Value (SV) methodology as a strategy to evaluate the most suitable water source (WS) for green hydrogen production from a sustainable point of view. Discussing the methodology and literature works that apply SV on companies and study cases of green hydrogen (GH2) HUBs; this chapter establishes the socio-environmental criteria for evaluating water sources. A new SV model is proposed here based on the model of Simões et al. (2021). Modifications on the “resources” term of the equation turned on 3 new criteria (Proportional cost for CAPEX and OPEX, and electricity consumption), and the weight of the requirements are proposed. Two study cases are presented here; the first applied to design a 1 MW green hydrogen cluster to be constructed in the future in SENAI-CIMATEC Park in Brazil. Five different WS were evaluated (seawater, treated industrial wastewater, tap water, rainwater, and groundwater),12 criteria were considered (Simoes et al., 2021), and economic calculations were performed to evaluate each source. The sum of each measure defined the best and worst water source for the case study. The results have shown that the best WS was tap and rainwater, and the worst was seawater, mainly due to the elevation of the hydrogen plant. The second is a case study on a hypothetical green hydrogen plant beside a petroleum refinery near the sea. For this one, the most suitable water source is the industrial effluent of the petroleum refinery.

[1] Based on Santana et al. (2023a). **Water sources evaluation for green hydrogen production: a case study in Brazil** and Santana et al. (2023b). **Sustainable value approach to evaluate water sources for electrolysis.**

3.1 Introduction

With the advent of the industrial revolution in the second half of the XVIII century, with the establishment of an economy centered on urban space and based on technologies that consume energy and raw materials, no civilization has ever had the destructive power that contemporary global society has. In terms of planetary devastation, humanity finds itself in a decisive moment of historical definition regarding the maintenance of the ecological and climatic balance of the planet (Camargo, 2012).

Ecological awareness can be found, although not yet of grand proportions, since the most remote times, but only in the 1960s did people begin to become aware of ecological problems, mainly related to actors in the social system; such issues were seen as concerns distinct and disconnected, each with perfectly identifiable causes (usually industry-related). Our Common Future, the report by the World Commission on Environment and Development, presented in 1987 and better known as the Brundtland Report (BR), is a milestone, not only because it represents the first institutional endorsement of the concept of sustainable development (SD), but because of its endorsement by the United Nations. (Hoyos et al., 2010; Camargo, 2012)

Since then, the United Nations has set sustainable development goals, and a new vision for production is taking place. Based on the three pillars or dimensions of sustainability:

1. Social Dimension – related to human needs, health, education, improvement of quality of life, and justice.
2. Economic Dimension – addresses the use and depletion of natural resources, waste production, and energy consumption.
3. Environmental Dimension - deals with the preservation and conservation of the environment, with actions ranging from reversing deforestation, protecting forests and biodiversity, combating desertification, and sustainable use of the oceans and marine resources to adopting effective measures against climate change.

Numerous examples of sustainability solutions with good potential fail because one of the pillars is neglected. The framework also broadly applies to institutional and market transformation by elaborating on how the SDGs operate and engage in ordinary and institutional practices (Santana et al., 2023).

Thus, this chapter aims to present SV methodology as a strategy to evaluate the most suitable water source for hydrogen production via electrolysis from a sustainable point of view. Discuss the methodology and some literary works that apply SV to companies and study cases of GH2 HUBs. Furthermore, two study cases were performed on a designed 1 MW green hydrogen cluster to be in the future in a pilot plant in a Brazilian industrial park (SENAI-CIMATEC Park) and on a hypothetical GH2 plant near the sea Petroleum refinery.

3.2 Sustainable value methodology (SV)

The SV methodology was developed to respond to the need for an approach to support companies in implementing Cleaner Production, Increasing Value, and improving their competitiveness by combining eco-efficiency and value analysis. Ecoefficiency means “doing more with less,” and it has become a management strategy towards sustainable development by improving the economic and ecological efficiency of companies, attaining a higher Value with fewer inputs, i.e., materials and energy, and more outputs but fewer waste, i.e., pollution in the form of emissions and waste. Value Analysis (VA) means satisfying needs using fewer resources. Its definition is an organized and creative approach using a functional and economical design process that aims at increasing the Value of a VA subject; also defined, in a Value Management (VM) context, as the relationship between the satisfaction of needs and the resources used in achieving that satisfaction (Henriques et al., 2008).

Thus, the complementarity between those two subjects is evident. Using tools from VM, such as Value Analysis and Cleaner Production from ecoefficiency, and profiting from the synergies between them enabled the development of the SV concept, which integrates the three aspects of sustainability (economic, environmental, and social) in the SV concept (Henriques and Catarino, 2015). The “Value” in SV is the relationship between the satisfaction of needs and the resources used to achieve it and explicitly considers the three dimensions of sustainability (Equation (1)). The performance is defined by criteria that are suitable for evaluating the WS. These criteria are evaluated for each WS by the performance level of each water source, which is determined by established criteria scaled from 1 to 4. Here, a score of 1 represents the lowest performance, while a score of 4 indicates the highest performance. The resources are defined by the costs related to each WS. The symbol α in Equation 1 means that the relationship between needs and resources is only a representation and that trade-offs from one against the other can result in the most beneficial balance. The optimization is achieved by balancing the amount to satisfy needs against the resources utilized.

$$SV\ \alpha\ \frac{Performance}{Resources\ (costs)} \tag{1}$$

3.3 SV applied to water sources evaluation.

Simões et al. (2021) have used Equation 1, applying the SV to assess the suitability of potential water sources for H_2 production via water electrolysis, combining technological, economic, environmental, and social criteria. From Equation 1, Equation 2 is proposed to measure the SV; the difference between the SV calculation is that Equation 2 considers that the SV is directly proportional to performance. In Equation 2, W represents the weight of the criteria *i*, and C the performance of the requirements *i*. The resources were evaluated as new performance criteria, as seen in Table 6. More details about the requirements can be found in Tables 23, 24, and 28 (Chapter 5).

$$SV\ \alpha\ Performance\ \alpha\ \sum_{1}^{n}(W_i\ \cdot C_i) \tag{2}$$

The decision to modify the original method of Simões et al. (2021) was driven by the need to directly address the limitations observed in the original model, particularly the difficulty in comparing water sources due to the disparity in the numerator and denominator values. Furthermore, the introduction of new criteria and the reweighting of existing ones were inspired by an improvement proposal suggested by Simões et al. (2021), acknowledging the importance of differentiating the weights of the water source evaluation criteria to reflect their contributions more accurately to the sustainability and economic viability of green hydrogen production.

When the outcomes obtained with the proposed model were compared to those of the original model, a preference for water sources that compete less with human consumption and have greater social acceptance was noted, indicating a potential reduction in environmental impact and better alignment with sustainable development goals. These findings validate the effectiveness of the revised model in providing a more comprehensive and contextualized assessment of water sources for green hydrogen production, highlighting the significance of considering a wide range of socio-environmental and economic criteria in the selection of water sources.

Table 6. Model's criteria and weight.

Criteria	Weight	
	SIMOES et al. (2021)	(SANTANA et al., 2023)
Reliability of availability (short time: weather)	1	2
Reliability of availability (climatic effect)	1	1
Reliability of availability (continuity of supply)	1	2
Competition with other uses [water collection]	1	2
Complexity of abstraction/ collection	1	1
Transport distance	1	2
Treatment needed	1	1
Social acceptance	1	4
Complexity of the permitting process	1	1
Proportional cost (Capex)	N/A	1
Proportional cost (Opex)	N/A	3
Electricity consumption	N/A	4

Source: Author, 2024.

The weights were defined based on the critical analysis of each criterion, the considerations relating to water for electrolysis in Chapter 2, and the degree of importance of these criteria in assessing water sources.

3.4 Pilot plant in an industrial park

The SV approach is applied to a 1 MW green hydrogen cluster at the SENAI-CIMATEC Park in Brazil. The park is located in the Camaçari industrial park in Bahia, about 45 km from Salvador. WS are evaluated for water availability, quality, transport options, abstraction costs, treatment, regulatory needs (including environmental restrictions), and social acceptance. The WS selected were grid water, seawater, rainwater (919 mm/year), industrial wastewater (from a near centralized effluent treatment plant), and good quality groundwater (from the São Sebastião aquifer). The necessary treatments were optimally generated using a decision support tool based on heuristic rules for water and effluent treatment, and the water Quality Specification (pre-purification) was established according to the electrolyzer data (according to Directive (EU) 2020/2184- the quality of water for human consumption).

The potential WS that can input the electrolyzer available around the green hydrogen cluster was identified, and then, information about distance and elevation (between the water source and the hydrogen plant) and treatment needs were summarized.

Five potential WS were identified (grid “Tap” water (TW), treated industrial wastewater (IWW), seawater (SW), rainwater (RW), and groundwater (GW)). Table 7 presents CAPEX and OPEX costs for water capitation, treatment, and water loss related to the treatment train required for each WS based on the literature. Besides this loss, an overall water loss of 10% was considered (due to evaporation, leaks, etc.) and water treatment (including installation costs, terrain preparation, etc.). The individual treatment technologies were Reverse Osmosis (RO), Reverse Osmosis (seawater) (RO*), Ultrafiltration (MF), Fine screening (FS), and Filtration/Coagulation (Chempre); data from Simões et al. were used to create the treatment train.

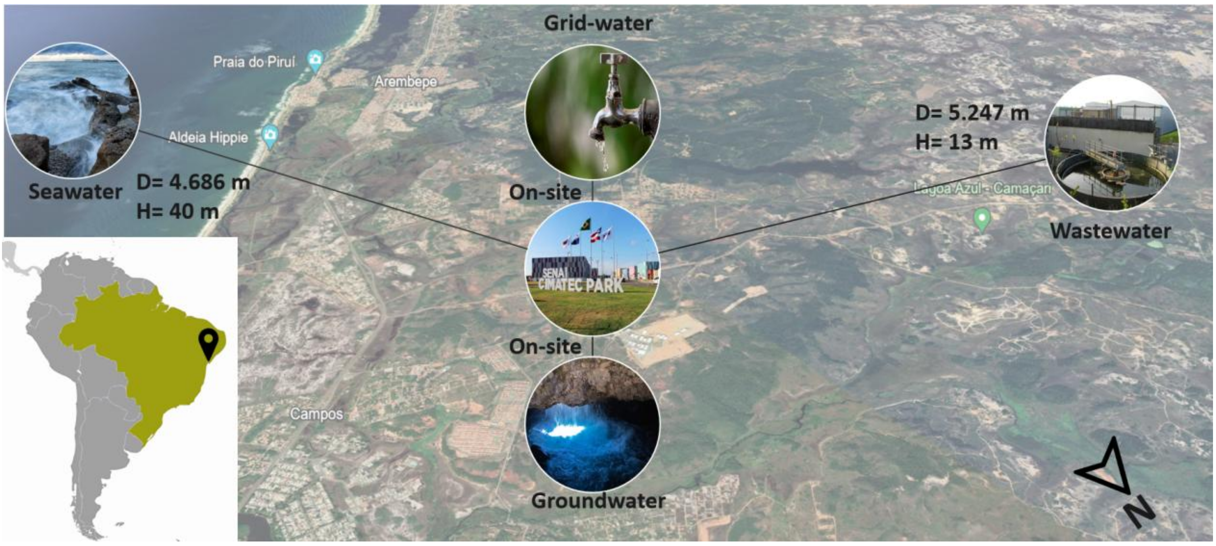
Table 7 – Treatment and capitation costs.

WS	Treatment train	W. loses	Process CAPEX (€)	Energy consumption kWh/m3	Capitation (€)	Capitation OPEX kW/m3
TW	RO	10%	500,000.00	4.5000	0.00	0
IWW	FS→MF→RO	25%	776,000.00	4.5635	25,000.00	180.0000
GW	Chempre→RO	20%	580,000.00	4.5500	150,000.00	600.0000
RW	FS→MF	10%	201,000.00	0.0635	-	-
SW	FS→RO*	37%	576,000.00	4.5010	80,000.00	-

Source: Author.

For investment cost calculations for water transport, the construction of the pipeline (considering the different transport distances in Figure 3) includes stainless steel piping with an internal diameter of 50 cm. For water transport via pipelines, purchase costs of welded and screwed pipe per unit length were assumed based on the equation in Table 8. The localization, specific distances, and elevation from each potential WS to the SENAI CIMATEC Park cluster (as in Figure 3) were considered.

Figure 3 – Distances and elevations considered for water transport.



Source: Author.

Water costs were calculated based on the work of Joksimovic (2007) and McGivney & Kawamura (2008), as shown by the equations in Table 3.

Table 8 – Water costs equations for transport storage and treatment

	CAPEX	OPEX
Water transport	$CC = 21{,}715 \cdot H \cdot Q^{0,52}$ $CP = C_1 \cdot e^{c_2 \cdot D}$ CC is the pumping station capital cost (BRL), H is the required pumping head (m) and Q the design flow rate. CP is the pipe unit cost (BRL/m), D is the diameter (m) and C_i is the pipe cost coefficients from Joksimovic, 2007,	$CE = \theta_{hp} \cdot C_e \cdot (V_{ann} \cdot H/2{,}7 \cdot \eta)$ CE is the annual cost of energy required for pumping (BRL); θ_{hp} is a conversion factor to kWh $\theta_{hp} = 0.746$; C_e is the electricity price [BRL/kWh]; V_{ann} the volume of water pumped annually (m^3) and η the pump efficiency (65 %).
Storage	$UCS = C_1 \cdot V^{C_2}$ UCS is the CAPEX unit cost of storage facility (BRL/m^3); C_i is the cost coefficients from literature and V is the storage volume (m^3).	
Treatment	$CT = Cost_{(1)} \cdot f$ CT is the capex cost for the treatment plant; $Cost_{(1)}$ is the sum of CAPEX cost of individual treatment process and f is the factor that includes other capex cost of treatment plat (f =1,8226)	$OT_{El} = E \cdot C_e$ $OT_{Total} = OPEX_{El} / 0{,}275$ OT is the OPEX of treatment plant in function of electricity and the total OPEX; E is the energy consumption [kWh/m^3] and C_e the electricity price [BRL/kWh]

Source: Author.

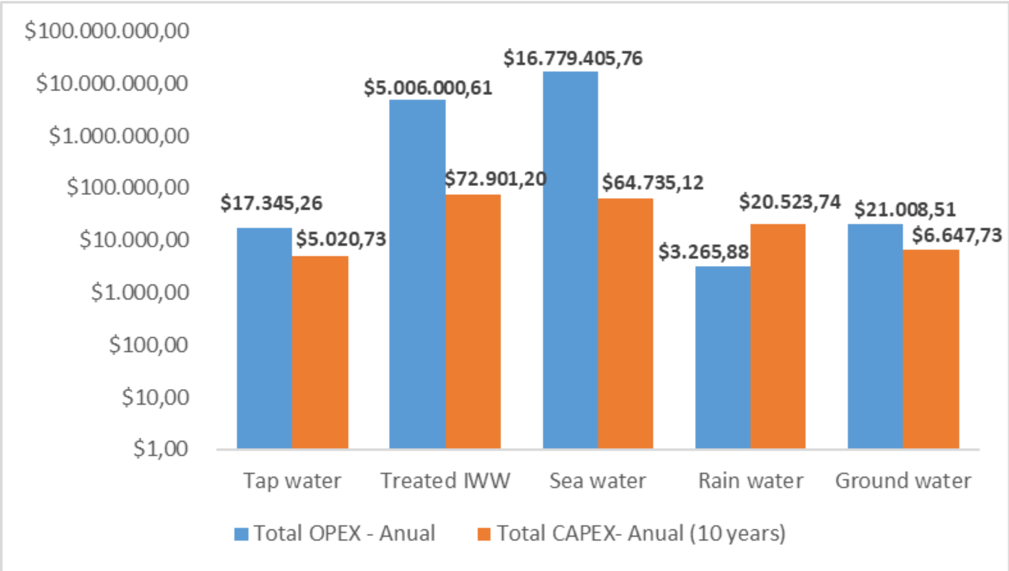
For this study, values of 10.00 L per kg produced H_2 are required to input for 1MW PEM electrolyzer and 25401.6 kWh per day of electricity consumption. The values are based on information publicly available from electrolyzer suppliers (Simões et al., 2022).

After cost calculations, each potential WS (Table 5) was qualitatively assessed for each site, adopting a functional value approach where the function is to supply water for hydrogen production.

3.4.1 Main results

The performed cost of the different water sources (Figure 4) shows that the more expensive source is seawater, especially in terms of OPEX; this is regarding the greater distance between the source and the treatment plant. Again, transporting the treated industrial wastewater is also an expensive source.

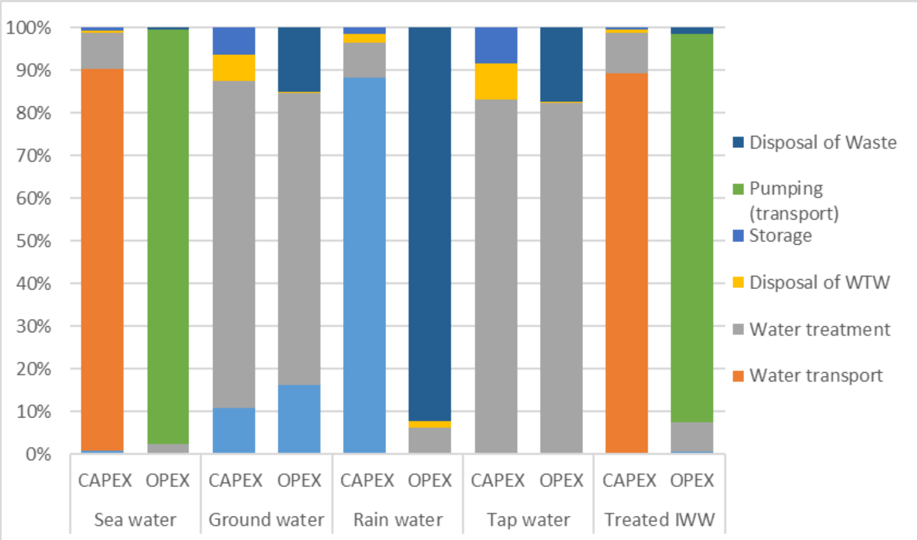
Figure 4 – Water sources CAPEX and OPEX



Source: Author.

The analysis of the distributed costs of water is presented in Figure 5. shows that costs related to transport (where necessary, for example, seawater and treated IWW) are the most relevant in a general context. Another high cost is the cost of water treatment itself.

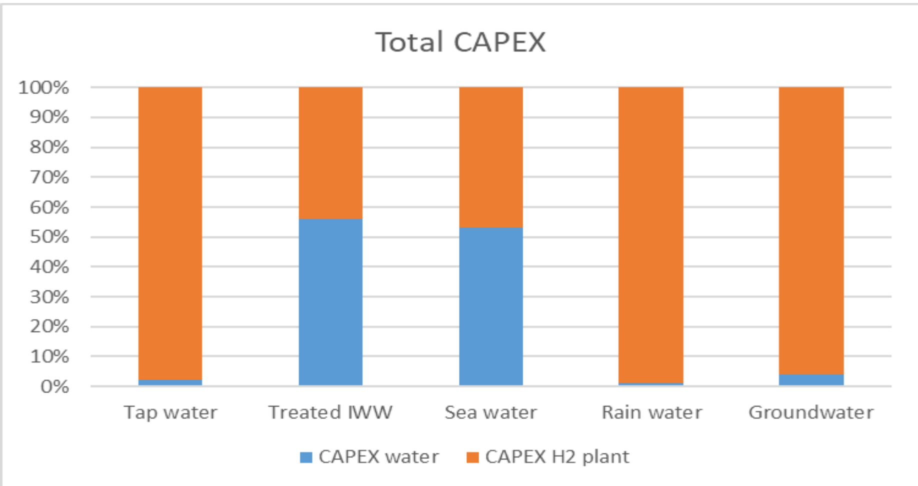
Figure 5 – Water sources distributed costs.



Source: Author.

Another significant result is the cost comparison. Figure 6 compares the investment cost related to water and the electrolysis process. The electrolysis process was calculated, but the results demonstrate that water-related expenses are low, except for water sources that require pumping. This preliminary result indicates the need for more rigorous calculations to validate that water-related costs are low (appearing insignificant) compared to the global price of hydrogen production.

Figure 6 – Water and electrolysis cost percentage.



Source: Author.

The results of the qualitative criteria are shown in Table 9 (based on Table 23, Chapter 5), in which the grading (1–4 points) follows the requirements presented in Table 6. The best qualitative water source performance was obtained for rainwater, treated industrial wastewater, and grid water. The water option with lower performance values for the site is seawater.

Table 9 – Sustainable Value analysis of water sources.

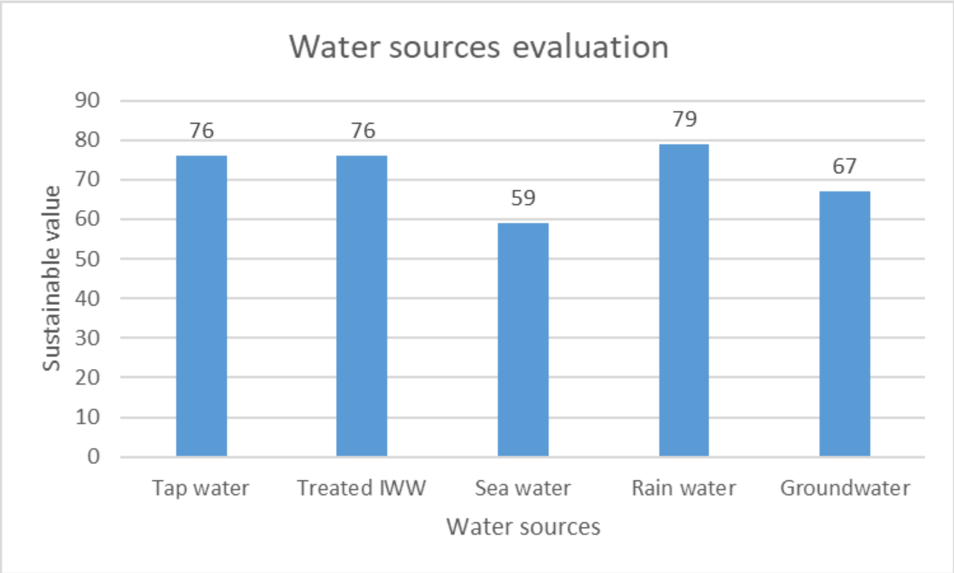
Weight		Criteria	TW	IW	SW	RW	GW
2	Reliability of availability (short time: weather)	A	3	4	4	1	2
1	Reliability of availability (climatic effect)	B	4	4	4	1	2
2	Reliability of availability (continuity of supply)	C	4	4	4	2	2
2	Competition with other uses [water collection]	D	1	4	4	4	1
1	Complexity of abstraction/ collection	E	4	2	1	2	2
2	Transport distance	F	4	2	2	4	4
1	Treatment needed	G	4	1	1	3	3
4	Social acceptance	H	1	4	4	4	2
1	Complexity of the permitting process	I	4	3	1	3	2
1	Proportional cost (Capex)	J	4	1	1	4	4
3	Proportional cost (Opex)	K	4	3	1	4	4
4	Electricity consumption	L	4	3	1	4	4
		Total points	76	76	59	79	67

Source: Author.

Rainwater was demonstrated to be a low-cost, easy-to-handle, and abundant resource at the study site, with water storage being managed in artificial ponds or cisterns. The capture infrastructure will utilize the rooftops of buildings at the CIMATEC Park to collect rainwater. Indeed, climate changes could affect rainwater availability; however, the region in which it is located is known for its high rainfall index, making this risk minimal in the medium term. Given the plant's low capacity (1 MW), which requires only a tiny amount of water, and the abundance of rainwater, the collected volume is deemed sufficient to meet the water demand of the hydrogen HUB.

It is important to take into account that these results (Figure 7) represent the best water source for this specific study case once the performance levels are location and capacity-dependent; for example, the high proportional capital and operational cost, the high energy consumption, and the complexity of collection make the seawater be a wrong choice for the study case plant. However, the proportional cost decreases as the hydrogen capacity increases and the hydrogen cluster is constructed near the sea, making seawater a better option.

Figure 7 – Results of water sources evaluation

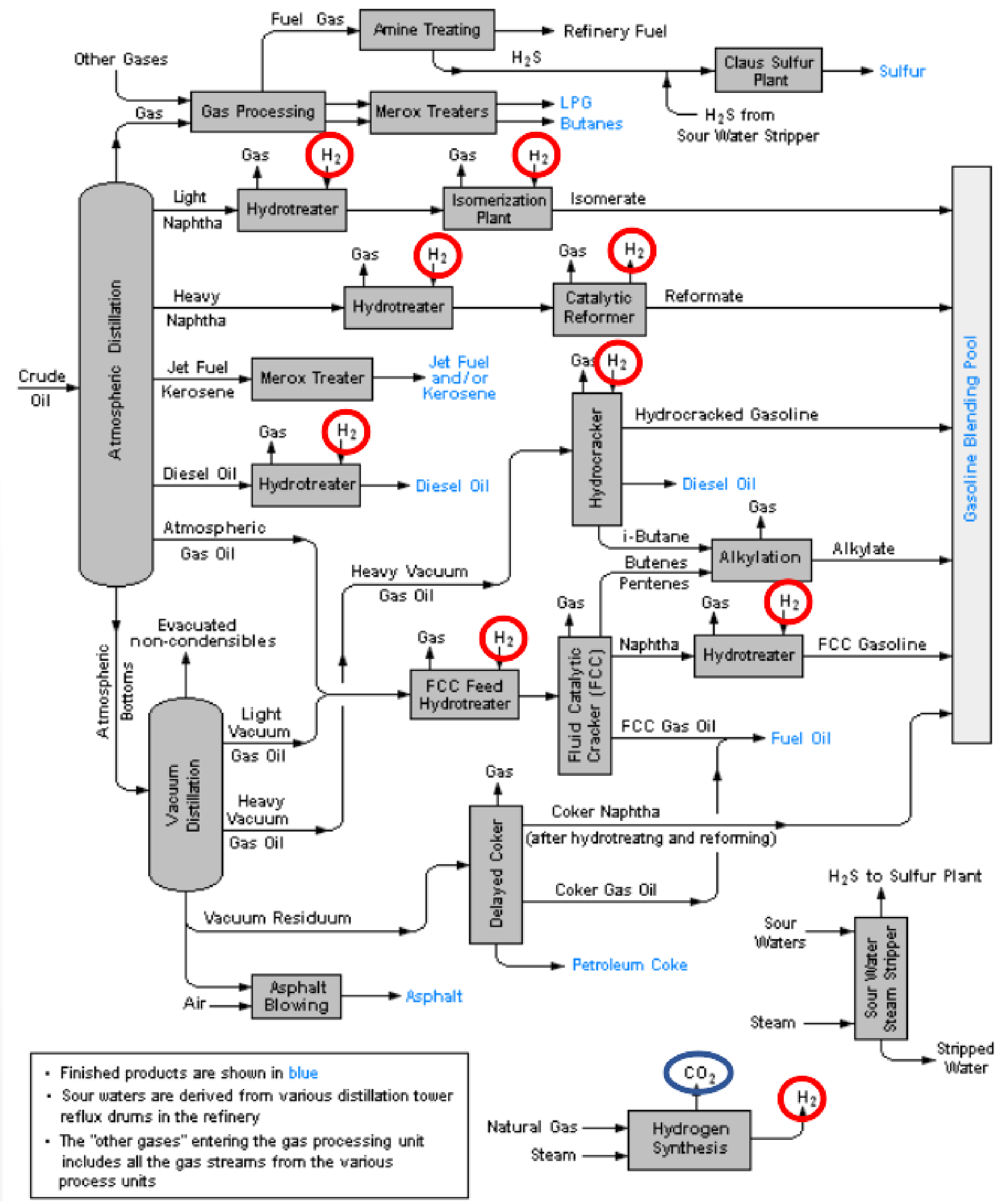


Source: Author.

3.5 Petroleum Refinery Study Case

To demonstrate the applicability of the SV model, a short study case is proposed to be analyzed, focusing on a hypothetical GH_2 HUB of 60MW installed near the sea at a petroleum refinery. Hydrogen customers, including oil refineries, rely heavily on hydrogen for several critical roles within the refinery. As illustrated in Figure 8, which is based on the work of Al-Moubaraki & Obot (2021) for refineries, the typical processes within a petroleum refinery are highlighted, along with the many applications of hydrogen. Figure 8 shows the extensive use of hydrogen in various refinery processes. It is common for these installations to possess an H_2 production unit due to the high consumption of hydrogen gas in oil refining. While production is usually carried out through natural gas steam reforming, the alternative of producing via electrolysis is being explored. The performance of each criterion of the SV model applied in this study case is presented in Table 10 (based on Table 23, Chapter 5).

Figure 8: Process flow diagram and hydrogen uses of a typical refinery.



Source: Adapted from Al-Moubaraki & Obot (2021).

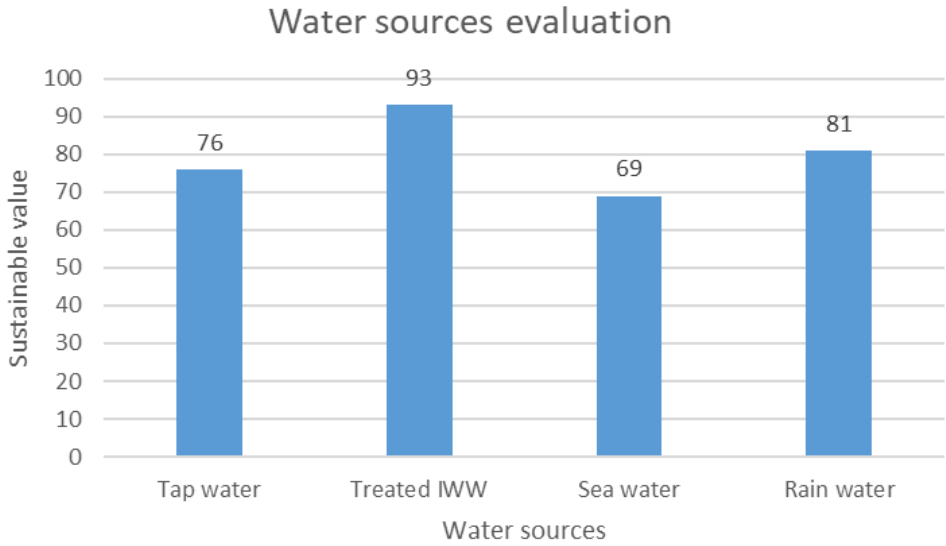
Table 10: SV analysis of water sources.

Weight	Criteria	IWW	RW	SW	GW
2	*Reliability of availability (short time: weather)*	*4*	*1*	*4*	*3*
1	*Reliability of availability (climatic effect)*	*4*	*1*	*4*	*4*
2	*Reliability of availability (continuity of supply)*	*4*	*2*	*4*	*4*
2	*Competition with other uses [water collection]*	*4*	*4*	*4*	*1*
1	*Complexity of abstraction/ collection*	*4*	*4*	*4*	*4*
2	*Transport distance*	*4*	*4*	*4*	*4*
1	*Treatment needed*	*2*	*3*	*1*	*4*
4	*Social acceptance*	*4*	*4*	*4*	*4*
1	*Complexity of the permitting process*	*3*	*3*	*1*	*4*
1	*Proportional cost (Capex)*	*4*	*4*	*4*	*4*
3	*Proportional cost (Opex)*	*4*	*4*	*1*	*4*
4	*Electricity consumption*	*4*	*4*	*1*	*1*
	Total	*93*	*81*	*69*	*76*

Source: Author.

Four different on/ near site water sources were evaluated: seawater, grid water, rainwater, and treated industrial wastewater. The distance between WS and the plant was not considered. As all four water sources are already being used on the refinery site, social acceptance, transport distance, and abstraction complexity are considered negligible. As industrial wastewater depends only on the productivity of petroleum refineries, its availability is considered good. Thus, as shown in Figure 9, treated wastewater is the most suitable water source for GH2 production in this study case.

Figure 9: Results of water sources evaluation



Source: Author.

It is important to note that each case study's results are only valid for the respective circumstances analyzed, showing the hierarchy of values for the present moment and considering that any SV Indicator may result differently, depending on how technical achievements or political decisions occur in time.

This classification refers to a time horizon of the next 1-2 years and differs for small H2-producing units (<10 MW) and larger units, which consume more significant volumes of water. Likewise, these results will vary in areas of the country with greater water scarcity.

3.6 Conclusion

A sustainable value indicator allows a relative quantitative comparison of the performance of different water sources for electrolysis and the costs involved. For the SENAI-CIMATEC Park case study, rainwater is the most suitable water source for electrolysis due to the lower risk of supply, lower costs, and the avoidance of complex licensing processes. Likewise, grid water and effluent from the effluent treatment plant proved to be possible sources of water, where the factors that most affect suitability are the costs of transporting water and disposing of waste from effluent treatment. For the petroleum refinery case, treated industrial wastewater is the most suitable water source for electrolysis due to lower supply risk. It was possible to note that water costs are minimal compared with hydrogen costs; thus, the next chapter will discuss the impact of water costs on the levelized cost of hydrogen.

4 EVALUATING THE ECONOMIC INFLUENCE OF WATER SOURCES ON GREEN HYDROGEN PRODUCTION: A COST ANALYSIS APPROACH

Abstract: In Chapter 3, it was found that the economic impact of water treatment and use is shallow when compared with overall hydrogen costs. To evaluate water source impact on green hydrogen efficiency, this chapter aims to assess the water source costs impact on the Levelized Cost of Hydrogen (LCOH) in green hydrogen production by investigating the economic implications of utilizing various water sources, including seawater, groundwater, grid water, industrial wastewater, and rainwater, in the green hydrogen production by PEM (Proton Exchange Membrane) technology. The study evaluates the costs associated with water abstraction, transport, treatment, and storage and assesses their impact on the LCOH for different hydrogen plant sizes (1MW, 10MW, 20MW, 50MW, and 100MW). By analyzing these factors, the chapter provides valuable insights into the cost-effectiveness and sustainability of utilizing different water sources for green hydrogen production. The results show that the costs related to water are minimal (less than 2%), corroborating with the works of Bruce et al. (2018) and Khan et al. (2021), when compared with other economic influences on the LCOH, such as electricity price and electrolyzer costs; however, the water source distance must be considered, once in some cases can bring a strong influence on hydrogen final cost (more significant than 10%), corroborating the results founded on Chapter 3 and by Simões et al. (2021) regarding the influence of pumping costs. The findings confirm the idea that regarding the water issue for electrolysis, the economic dimension of sustainability could play a secondary role compared to social and environmental dimensions in the sustainability triple bottom line.

4.1 Introduction

The production of green hydrogen requires substantial quantities of water for several purposes, including electrolysis, cooling, and hydrogen purification. The costs associated with water sourcing, such as abstraction or collection, water transport, water treatment, disposal of wastewater (WTW), and water storage, significantly impact the overall production process cost (Santana, et al., 2023). To accurately assess the GH_2 economic feasibility and sustainability, evaluating the impact of different water sources on the Levelized Cost of Hydrogen (LCOH) is essential. The LCOH is a metric used to estimate the total cost of producing hydrogen over the lifetime of a plant, considering various cost components. (Santos, et al., 2023).

According to Santana, et al. (2023) and Woods, et al. (2022) the accessibility to water should also be considered in the hydrogen context. However, (Beswick, et al., 2021) and (Newborough & Cooley, 2021) talk about the increasing necessity for water in a hydrogen-based future, with this concern (SIMÕES, et al., 2021) listed all the potential water sources for electrolysis, and as a general rule, higher the treatment requirements, the more expensive the price of water. Regarding the scarcity scenario (Baldinelli, et al., 2022) and (Winter, et al., 2022) discuss the challenges of using non-traditional water sources for electrolysis. For instance, fresh water is cheaper than purifying groundwater and desalination, and (Bruce, et al., 2018) claim that, but even with this variability, the cost of water typically makes up less than 2% of the cost of hydrogen production. Even though this research is about water and hydrogen, a gap in the literature was noticed when trying to reconcile the costs of different water sources and their impact on the global price of hydrogen.

To address the gap in existing literature, this research paper aims to evaluate the cost implications of utilizing different water sources on the LCOH of green hydrogen production (by PEM technology). To assess their economic feasibility and environmental impact, the study considers multiple water sources, including seawater, groundwater, grid water, industrial wastewater, and rainwater. Furthermore, the analysis accounts for different plant sizes to provide scalability and cost optimization insights. Additionally, the impact of these water sources on the LCOH components, including stack, BOP, replacement, compression, storage of hydrogen, water, and electricity for BOP, will be thoroughly analyzed.

Understanding the economic implications of different water sources on the LCOH of green hydrogen production will contribute to strategic decision-making, allowing for developing more sustainable and cost-effective hydrogen production systems.

4.2 Methodology

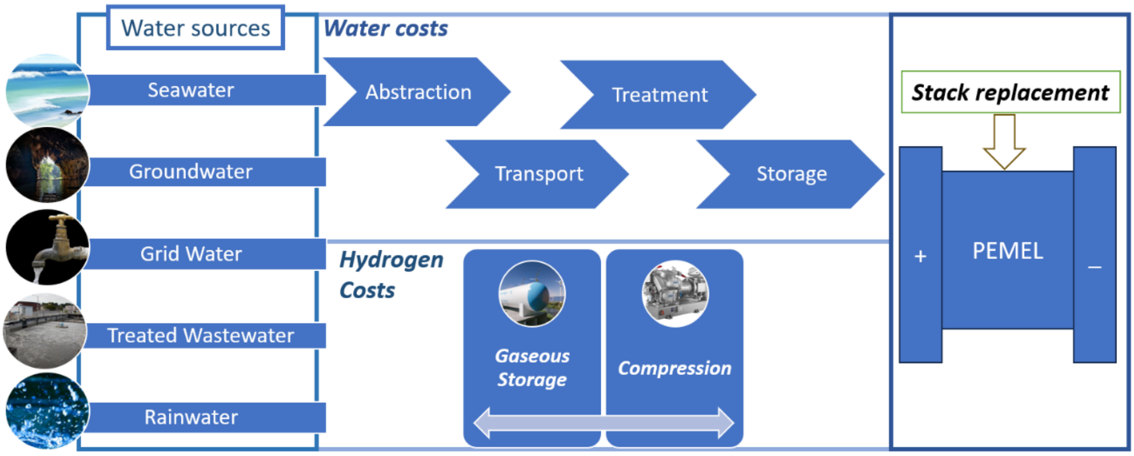
The study evaluates the costs associated with water abstraction, transport, treatment, and storage for different water sources and assesses their impact on the LCOH for different hydrogen plant sizes (1MW, 10MW, 20MW, 50MW, and 100MW).

Five potential WS were identified (grid “Tap” water (TW), treated industrial wastewater (IW), seawater (SW), rainwater (RW), and groundwater (GW)), based on the work of (Santana, et al., 2023), the case study is based on the location of the SENAI CIMATEC Park, a semi-urban location along the Atlantic coast, located in the industrial hub of Camaçari, in the Brazilian state of Bahia, in the vicinity of the petrochemical park. The SENAI CIMATEC Park is situated above the São Sebastião water table, an aquifer with good water quality. Furthermore, the proximity to the CETREL’s effluent treatment plant (ETP) (a centralized ETP of the petrochemical hub of Camaçari) allows for the easy use of treated industrial effluent. The park is supplied by the local water company (EMBASA), and the proximity to the ocean makes seawater an option for use.

The LCOH costs in this study consider the sum of costs related to the PEM electrolysis stack, the balance of plant (BOP), stack replacement, compression, hydrogen storage, water-related costs (subdivided as mentioned above), and electrical energy consumption by the electrolysis plant, as can be seen in Figure 10, five water sources are analyzed, and the considered water costs are abstraction, transport (pumping), treatment and storage. Electrolysis costs are considered stack replacement; other hydrogen costs are compression and storage. Furthermore, a sensitivity analysis was carried out by varying the price of electricity.

The costs are I) Capital Expenditures (CAPEX), which are mainly associated with the investment made to build infrastructure and equipment, and 2) operating expenses (OPEX), including maintenance costs (O&M).

Figure 10 Developed approach

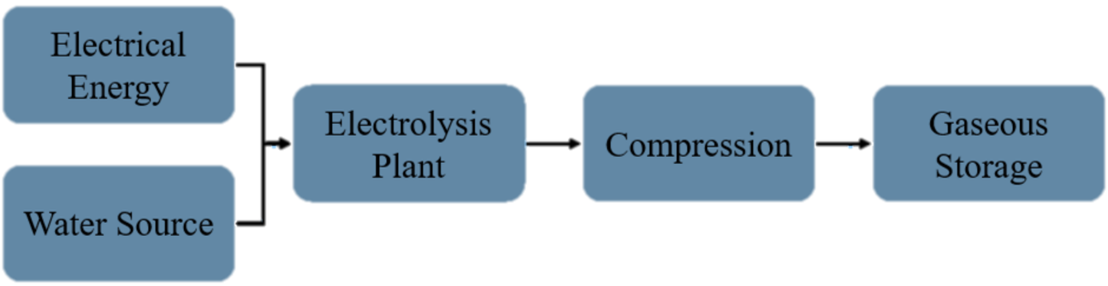


Source: Author.

4.2.1 Proposed scheme of modeling

To achieve the goal of this study, the scheme in Figure 11 was considered, where the required energy is first evaluated for the electrolysis system and the respective BOP. Water sources are assessed according to the proposed methodology, and costs for each source are generated. The electrolysis plant comprises a standard PEM system with a stack and the required accessories. Then, a reciprocating compressor system is evaluated for hydrogen storage at 350 bar in cylinders type I for local use[2].

Figure 11 Scope of economic analysis



Source: Author.

[2] Type 1 gas cylinders are usually manufactured from steel or aluminum. They are the lowest cost and heaviest cylinder type. This makes them most suitable for static applications and high-volume industrial use.

Electricity Cost Estimation

The electricity cost is crucial for the electrolysis process because it is necessary for hydrogen production and the primary power source for the equipment, such as compressors and pumps, in the hydrogen process and all water management steps.

In this study, the electricity cost is BRL 0.575/kWh, based on data from the Brazilian National Confederation of Industry (CNI, 2021).

Tow the costs related to water and LCOH behaved, a sensitivity analysis concerning the price of electricity was carried out, with the value of electricity being varied to values of BRL 0.144/kWh; BRL 0.287/kWh; BRL 0.575/kWh; BRL 0.862/kWh; BRL 1.15/kWh; based on the current price of BRL 0.575/kWh of electricity, multiplying this value by 0.25; 0.5; 1; 1.5 and 2.0 respectively.

Water Cost Estimation

The CAPEX and OPEX information were calculated considering capitation (abstraction or collection) and transport. Table 12 presents investment costs for water capitation, storage for each water source, and an overall water loss of 10% was taking in account (due to evaporation, leaks, etc.); water treatment (including installation costs, terrain preparation, etc.) was considered for supplying 700 m3/day. The individual treatment technologies were Reverse Osmosis (RO), Reverse Osmosis (seawater) (RO*), Ultrafiltration (MF), Fine screening (FS), and Filtration/Coagulation (Chempre). The primary contaminants for each water source are as follows: Table 11, and literature was used to create the best treatment train and costs presented in Table 12.

Table 11 Key contaminants for each water source

WATER SOURCE	MAIN WATER POLLUTANTS AND TREATMENT PARAMETERS
Groundwater	Dissolved solids
Water supply network	Dissolved solids
Rainwater	Some dissolved solids, BOD, TSS
Treated industrial wastewater	Depending on the industry, suspended solids, BOD5, Chemical oxygen demand (COD), toxicity
Seawater	Salinity 36-37%

Source: Simões et al. (2022).

Table 12 Treatment and capitation costs.

WS	Treatment train	W. loses	Process CAPEX (€)	Energy consumption kWh/m3	Capitation (€)	Capitation OPEX kW/m3
TW	RO	10%	500,000.00	4.5000	0.00	0
IW	FS→MF→ RO	25%	776,000.00	4.5635	25,000.00	180.0000
GW	Chempre→ RO	20%	580,000.00	4.5500	150,000.00	600.0000
RW	FS→MF	10%	201,000.00	0.0635	-	-
SW	FS→RO*	37%	576,000.00	4.5010	80,000.00	-

Source: Author.

Water costs were calculated based on the work of (Joksimovic, 2007) and (McGivney & Kawamura, 2008) as shown by the equations in Table 14. For investment cost calculations for water transport, water is the sum of pumping and infrastructure; for pumping costs, the specific distances and elevation from each potential WS to the SENAI CIMATEC Park cluster (Table 13) were considered. Transport infrastructure was considered transport via pipelines, and the purchase costs of welded and screwed pipe per unit length were assumed based on the equation in Table 14. The construction of the pipeline (considering the different transport distances in Table 13) includes stainless steel piping with an internal diameter of 50 cm.

Table 13 Considered distances and elevation for water transport.

Potential water source	SENAI CIMATEC Park cluster distance (m)/ Elevation (m)
Groundwater	On-site
Industrial wastewater	5.247/13
Seawater	4.686/40
Water grid	On-site
Rainwater	On-site

Source: Author.

Table 14 Water costs equations.

	CAPEX	OPEX
Water transport	$CC = 21{,}715 \cdot H \cdot Q^{0{,}52}$ $CP = C_1 \cdot e^{c_2 \cdot D}$ CC is the pumping station capital cost (BRL), H is the required pumping head (m) and Q the design flow rate. CP is the pipe unit cost (BRL/m), D is the diameter (m) and C_i is the cost coefficients from literature.	$CE = \theta_{hp} \cdot C_e \cdot (V_{ann} \cdot H/2{,}7 \cdot \eta)$ CE is the annual cost of energy required for pumping (BRL); θ_{hp} is a conversion factor to kWh $\theta_{hp} = 0.746$; C_e is the electricity price [BRL/kWh]; V_{ann} the volume of water pumped annually (m^3) and η the pump efficiency (65 %).
Storage	$UCS = C_1 \cdot V^{C_2}$ UCS is the CAPEX unit cost of storage facility (BRL/m^3); C_i is the cost coefficients from literature and V is the storage volume (m^3).	
Treatment	$CT = Cost_{(1)} \cdot f$ CT is the capex cost for the treatment plant; $Cost_{(1)}$ is the sum of CAPEX cost of individual treatment process and f is the factor that includes other capex cost of treatment plat (f =1,8226)	$OT_{El} = E \cdot C_e$ $OT_{Total} = OPEX_{El} / 0{,}275$ OT is the OPEX of treatment plant in function of electricity and the total OPEX; E is the energy consumption [kWh/m^3] and C_e the electricity price [BRL/kWh]

Source: Santana et al. (2023)

For this study, values of 10.00 L per kg produced H_2 are required to input for 1MW PEM electrolyzer and 25401.6 kWh per day of electricity consumption. The values are based on information publicly available from electrolyzer (stack) suppliers (Simões et al., 2022).

PEM Electrolysis

The costs of the PEM electrolysis system were informed by a series of supplier information and compiled for different sizes. A correlation between electrolyzer size and price was gathered based on previous work from (Santos, et al., 2023), a correlation between electrolyzer size and cost was gathered. In this case, a useful life of 90,000 h was considered for the stack replacement on the plant sizes of 1, 10, 20, 50, and 100 MW, and the hydrogen output pressure of 40 bar at 70 ºC.

Compression

The compression system evaluates the work necessary to compress hydrogen from 40 to 350 bar in a reciprocating compressor. (Santos, et al., 2023) describes a series of required equations for specific work, isentropic efficiency, and finally the power in kW for the compressor.

Storage

Hydrogen storage was analyzed for tanks with 90 kg of capacity and selected based on supplier information. The number of tanks was evaluated according to each proposed system's demand for local use.

4.2.2 LCOH evaluation and economic assessment

Economic assessment and LCOH parameters are the performance indicators for each system. It was considered for the cash flow of LCOH in the first year of implementation and construction of the plant, and 10 years were selected for equipment replacement. Annualized costs were adapted when necessary. Equation 8 describes the LCOH.

$$\mathrm{LCOH}\left(\frac{\$}{\mathrm{kg}}\right)=\frac{\mathrm{AEE + WT + BoP + CS + GS}}{\mathrm{H2Prod(kg)}} \quad (8)$$

Where, AEE is the Annual electrical energy cost ($), WT, is the water treatment cost ($), BoP is the electrolysis plant BoP costs ($), CS is the compression system cost($), GS the gaseous storage ($), and H2Prod is the total hydrogen production (kg)

The costs and data necessary to estimate total CAPEX and O&M are presented in Table 15; the conversion factor from euro to dollar is considered to be € 1.09 = US$ 1.00 (values from november 2023).

Table 15 Economic data for H2 Production.

	CAPEX	O&M (%CAPEX)	Notes	Reference
Total PEM	$C(€) = 1.7 \cdot Pw \cdot (6064 \cdot Pw^{-0.2})$	4%	Pw=Power (kW)	(Hyjack, 2022)
Replacement	N/A	20% Total PEM	N/A	(Singlitico, et al., 2021)
Compressor	$C(€) = (75700 \cdot Pw^{-0,62}) \cdot Pw$	8%	Pw=Power (kW)	(Hyjack, 2022)
Storage	$C(€) = Cap \cdot N \cdot (0.0015 \cdot P^2 + 0.2521 \cdot P + 448.54$	5%	Cap=Capacity N= number of tanks P=pressure (Bar)	(Hyjack, 2022)

Source: Author.

4.2.3 Graphical and Statistical Analysis

After calculation, the LCOH results were subjected to graphical evaluation, initially correlated with water supply (WS) costs. Initially, the study delved into the relationship between water-related costs and LCOH. The methodology employed leveraged statistical process control, specifically the NP chart, also recognized as the control chart for defects (D chart). This approach typically monitors the incidence of nonconforming or defective items in the measurement process, utilizing a binomial distribution to quantify defects or nonconformities within a sample. A boxplot chart, a graphical tool for visualizing metric distributions, enhanced the analysis. This visualization, grounded in quartiles, facilitated the identification of data outliers. The subsequent step involved carefully examining outliers and their potential impact on the analysis. Notably, the decision to retain or remove outliers was made judiciously, with a transparent documentation process. Utilizing these statistical tools and outlier analysis contributed to a more nuanced understanding, enabling the determination of the most probable values for water costs in the context of LCOH.

Another statistical analysis was performed using the Pearson correlation and sample covariance of the calculated cost data to see which had the most significant impact on LCOH. Covariance and Pearson correlation are measures that indicate the relationship between two variables. Covariance measures the extent to which two random variables change together, while Pearson correlation measures the strength of the relationship between two variables. The difference between the two is the correlation values are standardized, while the covariance values are not.

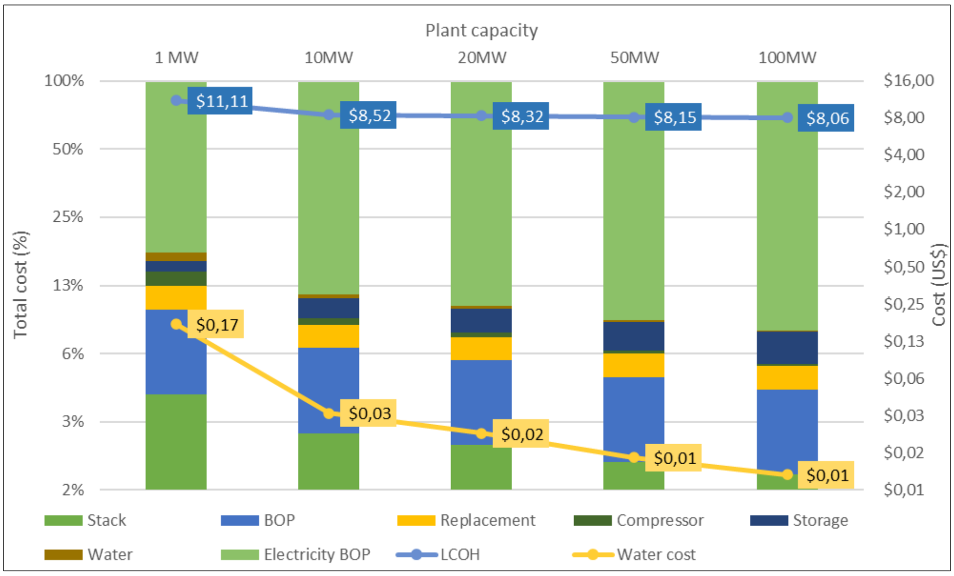
Microsoft Excel software was used for cost calculations, graphs, and statistical analyses for all steps described in this methodology. For all steps described in this methodology, Microsoft Excel software was used for cost calculations, graphs, and statistical analyses.

4.3 Main results

The results from the cost calculations are summarized in the following tables and figures, where it is possible to see the percentage of each sub-item impact on LCOH. The lines show each plant capacity's LCOH and water cost (in US$).

Figure 12 shows the analysis of the groundwater. It was assumed that the hydrogen plant is located above a water table, so the distance between the water source and the plant is disregarded. Figure 3 shows the decrease in hydrogen cost with plant capacity growth, and the water cost follows the same decreasing trend on the graph. However, with a look at Figure 12, it is possible to note that the percentage of the cost of water concerning LCOH decreases at the highest rate; on the other hand, it is possible to notice the percentage increase in the influence of the cost of electricity on the final price of hydrogen.

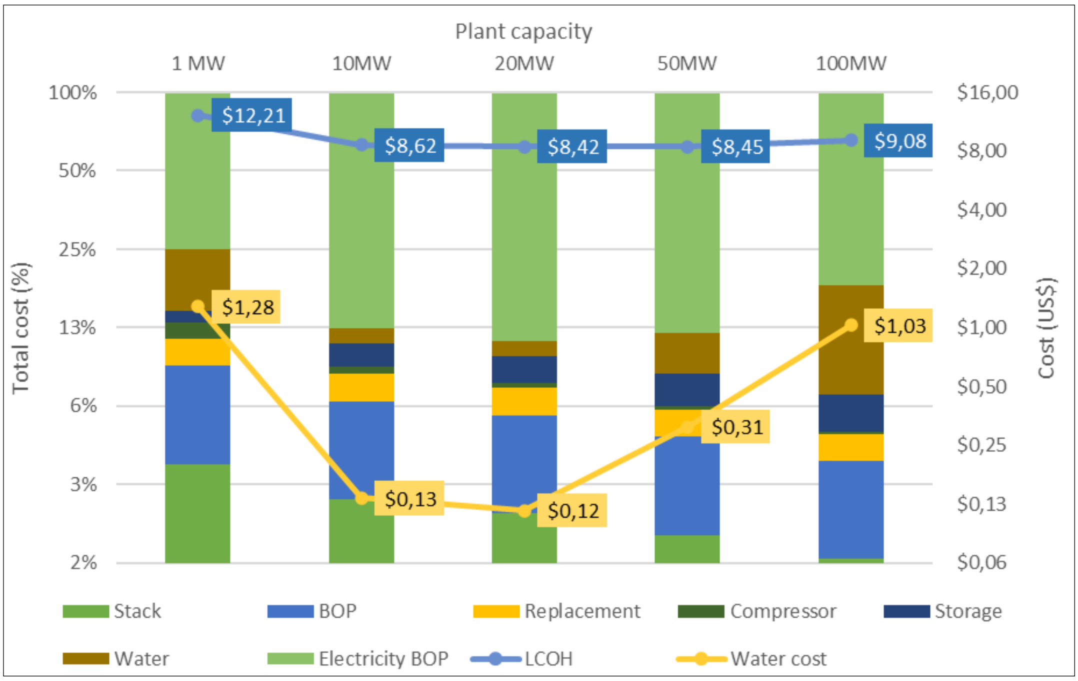
Figure 12 Groundwater analysis



Source: Author.

In the case of industrial wastewater (figure 13) as the water source, with a considerable distance of 5.247 m and an elevation of 13 m to the hydrogen plant, the impact on the LCOH exhibits an intriguing pattern. For smaller-scale hydrogen production (1MW and 10MW), the cost of water transportation contributes significantly to the LCOH, resulting in higher hydrogen prices. However, as the plant capacity increases to 20MW, the LCOH experiences a reduction in water costs. This unexpected decrease is attributed to economies of scale in production, which can partially offset the increased water transportation cost. Nevertheless, the water cost for larger plants (50MW and 100MW) rises again, potentially exceeding the LCOH for smaller-scale facilities. Thus, the choice of industrial wastewater as a water source warrants careful consideration, considering both the production scale and the distance to the water source.

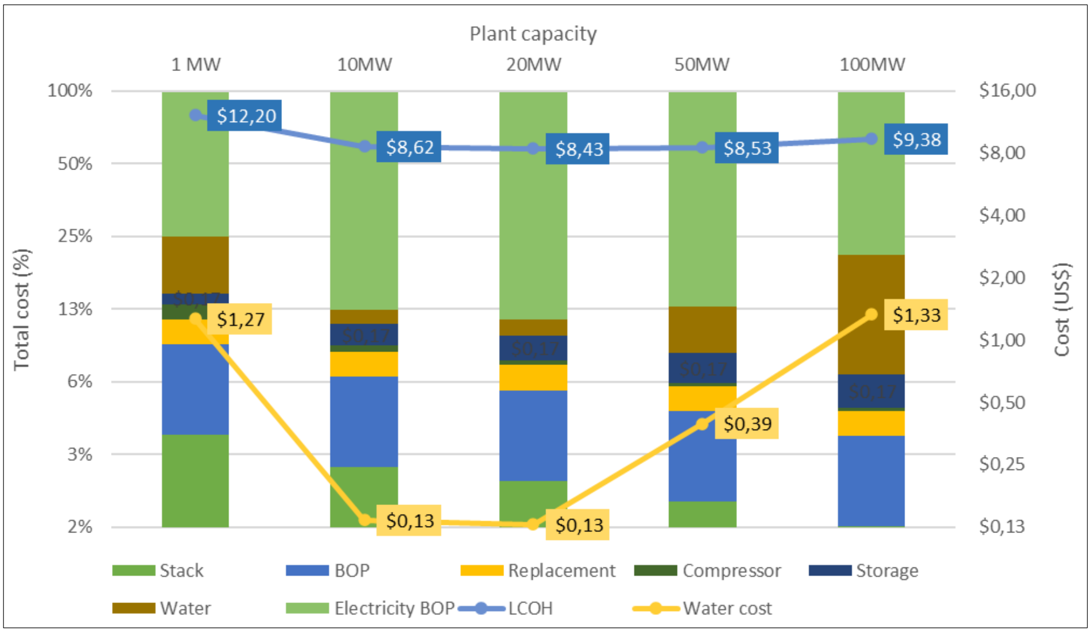
Figure 13 Industrial Wastewater Analysis



Source: Author.

Like industrial wastewater, seawater (illustrated in Figure 14) poses unique challenges as a water source, primarily due to its considerable distance from the hydrogen plant. In facilities with 1 MW and 10 MW capacities, the substantial cost of transporting seawater significantly impacts the Levelized Cost of Hydrogen (LCOH), leading to higher hydrogen prices. Surprisingly, as plant capacity increases to 20 MW, there is a noticeable reduction in water costs associated with the LCOH. This reduction likely stems from economies of scale that counteract the expenses related to transportation. However, for larger plants (50 MW and 100 MW), the costs linked to seawater transport once again escalate, potentially surpassing the LCOH for smaller-scale operations. Therefore, harnessing seawater demands a meticulous assessment of the production scale and the distance to the water source to ensure optimal cost-effectiveness.

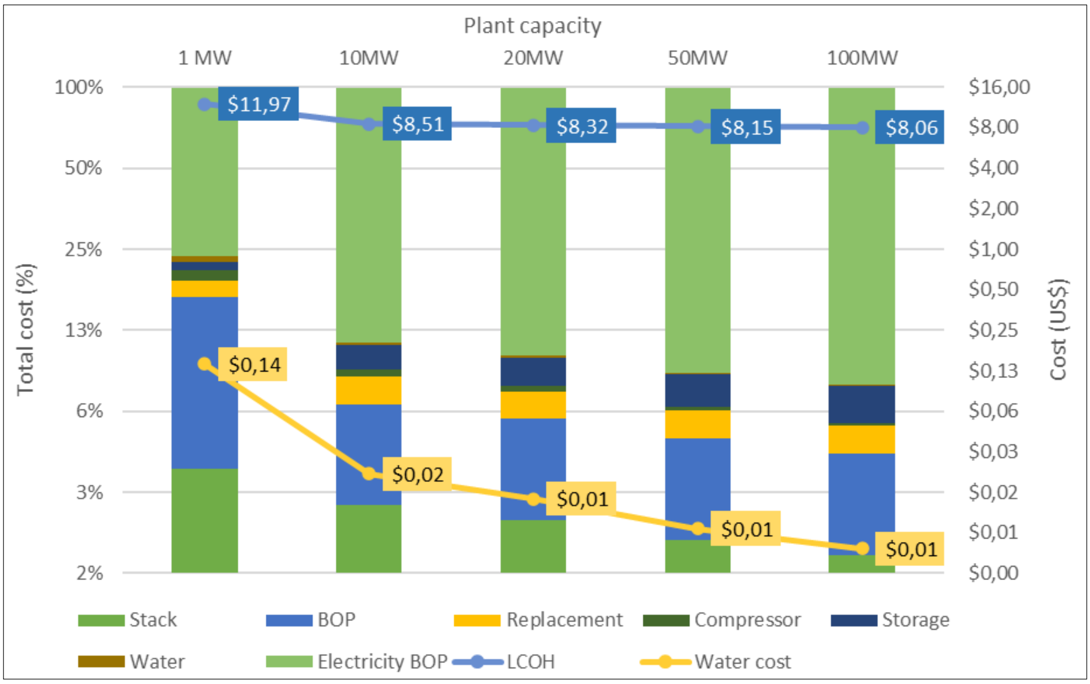
Figure 14 Seawater analysis.



Source: Author.

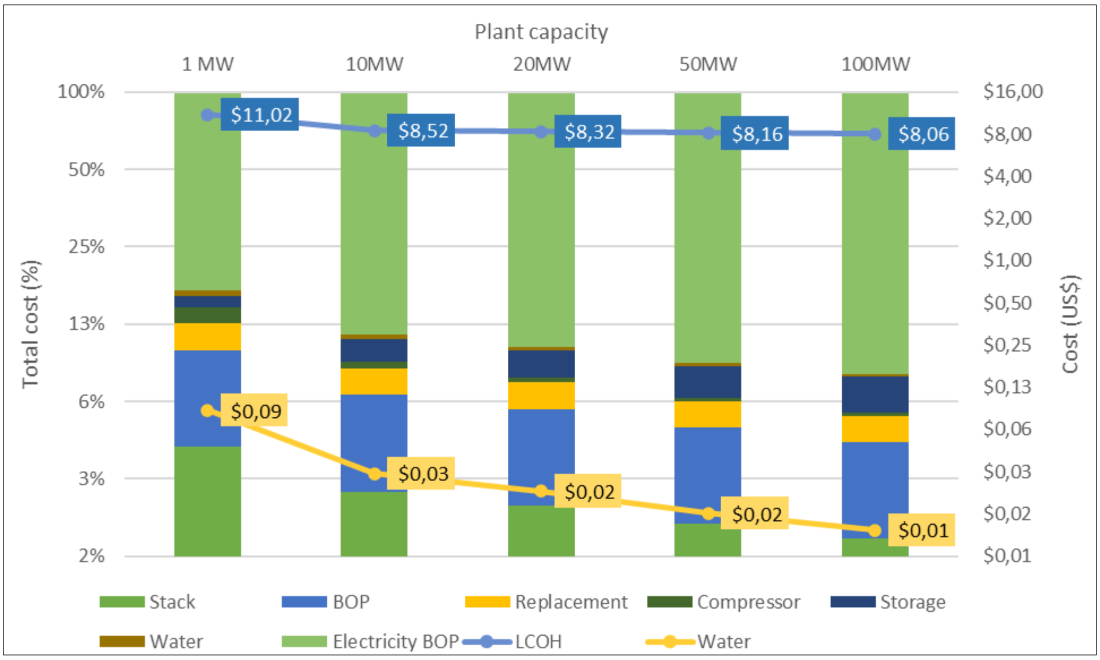
In contrast to industrial wastewater and seawater, the results for tap "grid" water and rainwater (figure 15 and Figure 16) closely resemble those for groundwater. Assuming these sources are located nearby and the distance is negligible, the LCOH exhibits a consistent decreasing trend with increasing plant capacity. Water costs for tap "grid" and rainwater follow the same pattern, decreasing with the facility’s growth. As with groundwater, these sources demonstrate minimal water-related cost impact on the LCOH (less than 2%). Thus, for locations where tap "grid" water or rainwater is readily available and the distance to the source is short, these options appear to be economically favorable for green hydrogen production.

Figure 15 Tap “grid” water analysis.



Source: Author.

Figure 16 Rainwater analysis



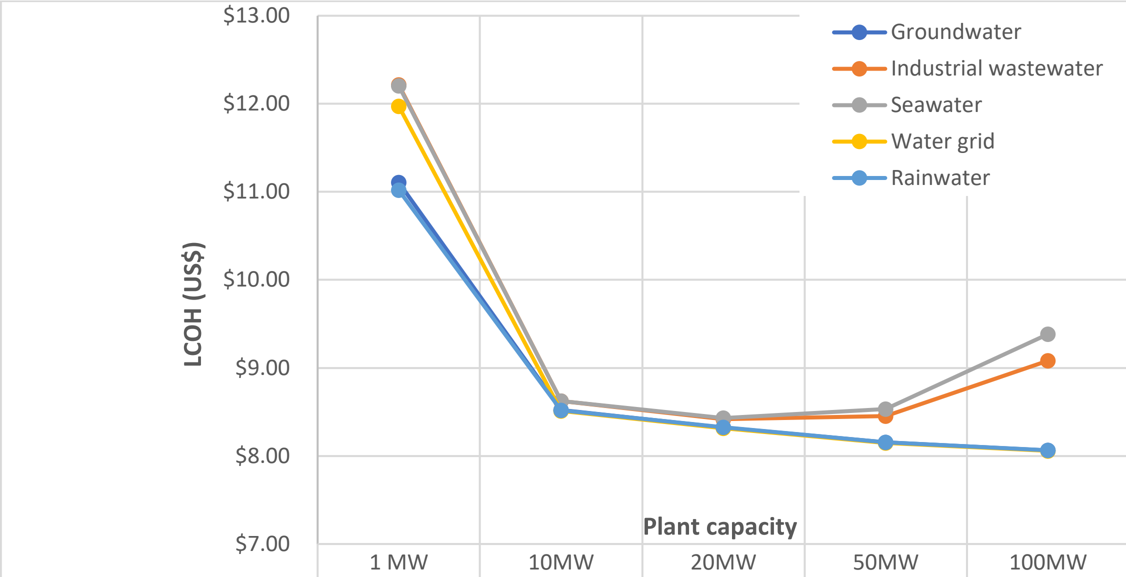
Source: Author.

As expected, LCOH generally decreases as the scale of production increases; in addition, the stack costs, plant balance, replacement, compression, and storage in the form of compressed gas, water, and electricity costs were analyzed. It is possible to notice that the percentages related to each of these costs change according to the scale of production; storage and electricity costs tend to become more significant within the total cost. Conversely, expenses related to water or the price of the electrolyzer tend to be less and less important in LCOH.

This behavior is only modified for cases where the water source needs transport. Simões et al. (2021) and Santana et al. (2023) show that the costs related to pumping water are the most significant among the expenses related to water. It demonstrates that the distance between the electrolysis plant and the respective water source must influence the choice of water source for electrolysis. This impact even modifies the behavior of the hydrogen cost curve, pointing to an increase in LCOH with scale (figure 17). Since larger plants require more water, the cost of transporting water increases significantly.

Figure 17 shows the values of LCOH for each WS. The results highlighted the necessity of a decision support system based on social and environmental parameters. Once, hydrogen prices present little difference between different WSs.

Figure 17 Hydrogen cost for each WS.

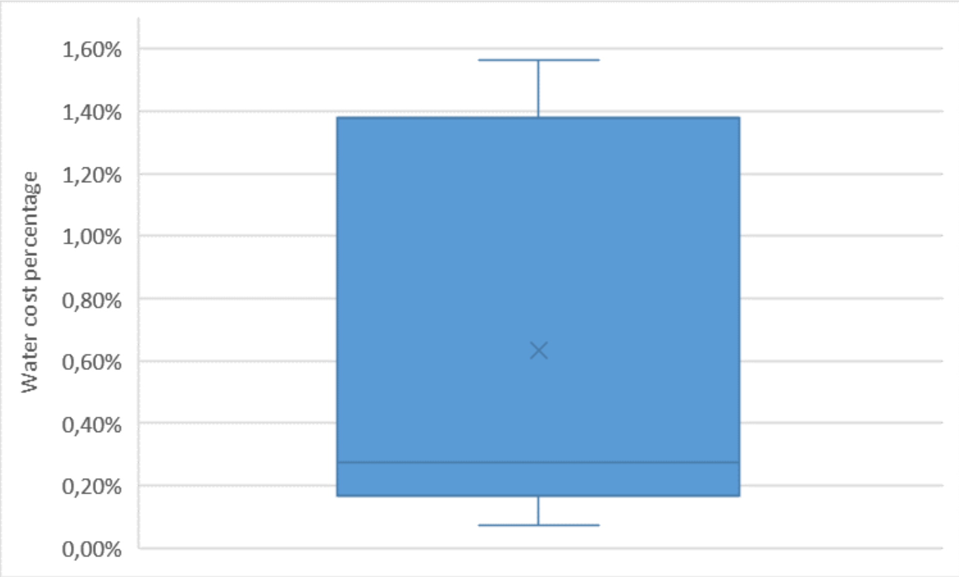


	1 MW	10MW	20MW	50MW	100MW
Groundwater	$11.11	$8.52	$8.32	$8.15	$8.06
Industrial wastewater	$12.21	$8.62	$8.42	$8.45	$9.08
Seawater	$12.20	$8.62	$8.43	$8.53	$9.38
Water grid	$11.97	$8.51	$8.32	$8.15	$8.06
Rainwater	$11.02	$8.52	$8.32	$8.16	$8.06

Source: Author.

All percentage results of water cost about LCOH were organized and statistically analyzed using the boxplot chart. The process was carried out successively until there were no discrepant data (outlines), resulting in the graph in Figure 18, where it is possible to see that the impact of the cost of water concerning the total cost of hydrogen is insignificant, generally not exceeding 1.6%.

Figure 18 Economic influence of water on hydrogen cost.



Source: Author.

The final analysis shows the correlation and covariance (Table 16 and Table 17) between each item and the LCOH. With a unique look at the variation in the cost of water, it is possible to observe that the influence of water is generally smaller than that of other items on the final price of hydrogen. Reiterating what was already stated above, the analysis of the type of water must focus on aspects beyond the economic dimension, appealing to a vision of sustainability, which consequently encompasses environmental and social factors. In addition, the reduction of LCOH must be considered carefully for other items, such as electricity and stack prices.

Table 16 Data covariance

	Stack	*BOP*	*Replacement*	*Compressor*	*Storage*	*Water*	*Electricity BOP*	*LCOH*
Stack	0,01250							
BOP	0,02487	0,07573						
Replacement	0,00800	0,01592	0,00512					
Compressor	0,00845	0,01699	0,00540	0,00580				
Storage	3,4E-18	7,8E-18	2,2E-18	2,8E-18	6,6E-33			
Water	0,01341	0,01376	0,00858	0,01071	1,3E-17	0,18593		
Electricity BOP	0,07400	0,15013	0,04736	0,05137	2,8E-17	0,10365	0,45901	
LCOH	0,14122	0,29741	0,09038	0,09872	5,8E-17	0,33604	0,88553	1,84931

Source: Author.

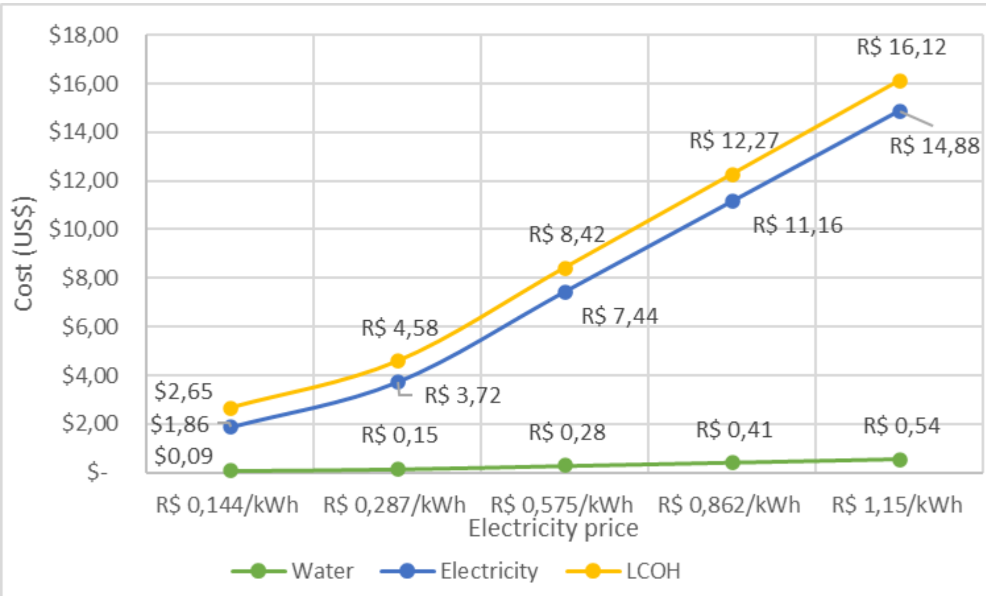
Table 17 Data correlation

	Stack	*BOP*	*Replacement*	*Compressor*	*Storage*	*Water*	*Electricity BOP*	*LCOH*
Stack	1							
BOP	0,80143	1						
Replacement	1	0,80143	1					
Compressor	0,99274	0,80393	0,99274	1				
Storage	0,42145	0,38488	0,42145	0,50368	1			
Water	0,24088	0,08084	0,24088	0,29332	0,40104	1		
Electricity BOP	0,97852	0,79859	0,97852	0,99614	0,55565	0,32583	1	
LCOH	0,92578	0,78729	0,92578	0,95136	0,57256	0,54942	0,96045	1

Source: Author.

The analysis was conducted considering a 50 MW plant, and the WS chosen was underground water. Finally, it can be seen (in Figure 19) that the correlation between the price of electricity and the LCOH is very high. Hence, an essential highlight of this work is that the efforts of companies, governments, and other institutions to reduce the cost of green hydrogen should focus on the reduction in the price of electricity, both due to the high degree of correlation and the percentage that electricity-related costs represent in the LCOH.

Figure 19 Graphical analysis of electricity and water costs on LCOH



Source: Author.

4.4 Conclusions and next steps

The study evaluated the associated costs of hydrogen production through PEM electrolysis with a unique look at water abstraction, transport, treatment, and storage costs. Assessing their impact on the Levelized Cost of Hydrogen (LCOH) for different hydrogen plant sizes (1MW, 10MW, 20MW, 50MW, and 100MW). Some valuable insights were obtained into the cost-effectiveness and sustainability of utilizing different water sources for production. This study demonstrates that for most cases, the cost of water has little impact on the final cost of hydrogen production (less than 2%); however, as described in the literature and demonstrated in this work, the transport distance plays an important factor in water cost, with the value of the cost growing exponentially depending on the distance and elevation between the source and the place of use. Thus, the pumping distance of the water must be a decisive factor, as it impacts the natural behavior of the hydrogen cost curve; the water source distance must be considered, once in some cases, it can have a strong influence on hydrogen final cost (more significant than 10%). The results also show that water costs are minimal compared to other economic impacts on the LCOH, such as electricity prices and electrolyzer costs. The findings of this research can provide critical insights for policymakers, industry stakeholders, and researchers involved in green hydrogen technology.

From the results obtained in this study, since there is no clear choice for the best source, based on economic factors, a proper water analysis as a reagent for the electrolysis process must consider other factors such as technical, social, and environmental feasibility. Thus, models that consider life cycle analysis or sustainable criteria whose metrics go beyond costs but follow social, ecological, and technical dimensions will be studied and developed as the following steps.

5 A MULTI-CRITERIA DECISION-MAKING (MCDM) MODEL FOR WATER ASSESSMENT IN GREEN HYDROGEN PRODUCTION

Abstract: Based on the minimal influence of water costs in the electrolysis process reported in the last chapters, this chapter presents a New Multi-Criteria Decision-Making (MCDM) model for water assessment, capable of comparing the water sources' viability across different geographies. A decision support tool was developed using a sustainable value measurement (SV) MCDM method. The model is an improvement of the first model proposed, with the addition of 2 more criteria (ecological impact and regulatory compliance); a hierarchical approach is implemented by adding the requirements divided into 4 sustainable dimensions (environmental, social, economic, and technical), and with the criteria ordered according to their level of importance within the dimensions. Also, the level of water scarcity in the region where the electrolysis plant is considered, in the form of the Water Exploitation Index (WEI+), changes the criteria and dimensions weights for each level of WEI+. To implement the model, the approach was applied to two sites in regions with different WEI+, which is the quantitative availability of local water resources. The most suitable water sources for the cases were rainwater and industrial wastewater. It is possible to conclude that the model well assesses the most sustainable water source for electrolysis in a chosen location. Finally, the approach was applied to three different sites (A, B, and C) in the Brazilian state of Bahia. As a result, the most suitable water sources differed for each site (seawater, rainwater, and treated urban wastewater), depending on the distinct characteristics of each territory.

5.1 Introduction

An adequate model to access a more suitable water source for electrolysis plants with a vision of sustainable development must consider the necessary political, social, economic, and environmental aspects (Santana et al, 2023).

To solve such complex problems concerning this type of issue, multi-criteria decision-making (MCDM) is one of the better approaches to developing a decision support system. MCDA originated from operations research involving various methodologies, with an amusing rational foundation in other disciplines (Kumar, et al., 2017).

MCDM can be classified as Multi-Attribute Decision Making (MADM) and Multi-Objective Decision Making (MODM); otherwise, both share similar characteristics. MODM is suitable for evaluating continuous alternatives for which we predefine constraints as decision variable vectors. In MADM, inherent characteristics are covered, leading to the consideration of fewer alternatives, and thus, evaluation becomes difficult as prioritizing becomes more difficult. (Kumar, et al., 2017)

Broadly, we have three types of MCDM models, namely value measurement models, goal, aspiration, and reference level models, as well as outranking models. The value measurement models are utility-based and are mostly preferred for ranking energy technologies like using energy storage devices in renewable energy. When multiple objective functions are considered, the goal, aspiration, and preference level models are used. Outranking models consider various parameters and provide a broad perception of the problem, making them suitable for evaluating scenarios (Kumar, et al., 2017).

In our Previous work (Santana, et al., 2023) we presented a methodology to evaluate water sources based on the multi-criteria approach of sustainable value measurement (SV) methodology proposed by (Simões, et al., 2021). It was developed by integrating concepts from distinct subjects such as value analysis, ecoefficiency, energy efficiency, and cleaner production.

Literature shows that value measurement models are suitable for achieving the objective of choosing water sources. The value measurement models include methods like Multi-Attribute Utility Theory (MAUT), Analytical

Hierarchy Process (AHP), Weighted Sum Method (WSM), and Weighted Product Method (WPM).

The WSM is a decision-making technique where each criterion is assigned a weight, and the alternative with the highest weighted sum is chosen. The weights represent the relative importance of each criterion, and the decision is based on the aggregated score for each alternative (Wimmler et al., 2015).

The WPM is another decision-making approach in which each criterion is assigned a weight, and the alternatives are scored based on the product of their performance values raised to the power of their respective weights. The alternative with the highest overall product is selected as the best choice (Wang et al., 2010).

The AHP is a structured decision-making method that decomposes a complex decision problem into a hierarchical structure of criteria and sub-criteria. Pairwise comparisons are then used to determine the relative importance of criteria and a mathematical process is applied to derive a weighted score for each alternative, which will lead to a final decision. (Shahroodi, et al., 2012).

MAUT is a decision-making framework that considers both quantitative and qualitative aspects of decision problems. It involves assessing alternatives based on multiple criteria, assigning utility functions to represent decision-makers preferences, and then combining these utilities to determine the overall desirability of each alternative (Jiménez-Martin et al., 2014). The steps, strengths, and weaknesses of these methods are described in Table 18.

Table 18 Value measurement MCDM methods, strengths, and weaknesses.

Methods	Steps	Strength	Weakness	References
WSM	Where wi (i=1, 2…m) is a weighing factor for ith objective function and J is a function of designed vector. The best alternative is chosen as max (Jweightedsum).	1. Simple computation. 2. Suitable for single dimension problem	1. Only a basic estimate of one's penchant function 2. Fails to integrate multiple preferences	(Wimmler, Hejazi, de Oliveira Fernandes, Moreira, & Connors, 2015)
WPM	where Pi is the alternative's overall score and mij is an attribute's normalized value.	1. Labelled to solve decision problems involving criteria of the same type. 2. Uses relative values and thus eliminates the problem of homogeneity	1. Leads to undesirable results as its priorities or deprioritizes the alternative, which is far from average	(Wang, Liu, Wang, & Lai, 2010)
AHP	1. Defining objectives into a hierarchical model. 2. Determining weights for each criterion. 3. Calculating the score of each alternative	1. Adaptable 2. Doesn’t involve complex mathematics 3. Based on hierarchical structure and thus each criterion can be better	1. Interdependency between objectives and alternatives leads to hazardous results. 2. The involvement of more decision-	(Shahroodi, et al., 2012)

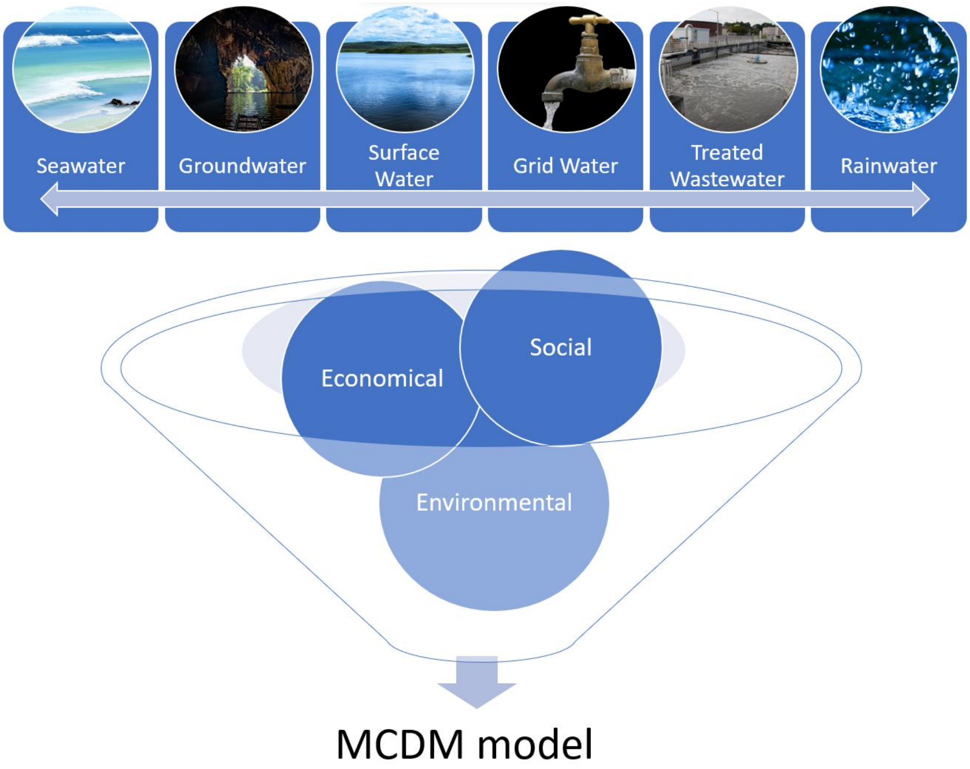
	considered criteria. 4. Calculating the overall score of each alternative.	focused and transparent	makers can complicate the problem when assigning weights. 3. Demands data collected based on experience	
MAUT	1. Identify the dimensions of each objective and assign weight to each. 2. Calculation of % weight and updating values based on the weight assigned to options of each dimension. 3. Multiplication of updated values of weight and previously obtained values 4. Add the product of each dimension to get the final sum for each option and thereby determine the decision	1. Accounts for any difference in any criteria 2. Simultaneously compute preference order for all alternatives 3. Dynamically updates value changes due to any impact.	1. Difficult to have precise input from decision-makers. 2. The outcome of the decision criteria is uncertain.	(Jiménez-Martín, Mateos, & Sabio, 2014)

Source: Author.

(Santana, et al., 2023) have used the SV methodology as a WSM; however, as described in Table 18, even though it is a simple mathematical model, it is only suitable for one-dimensional problems, in addition to presenting weaknesses, being only a basic estimate of its pending function.

Thus, this work aims to evaluate the water sources eligible for electrolysis from a sustainable point of view using a value measurement MCDM AHP method, as summarized and illustrated in Figure 20. It will be compared with case studies similar to those in our previous works (Santana, et al., 2023) and (Santana, Almeida, & Pessoa, 2023).

Figure 20 – Description of Sustainable Water Sources Evaluation



Source: Author.

5.2 Methodology

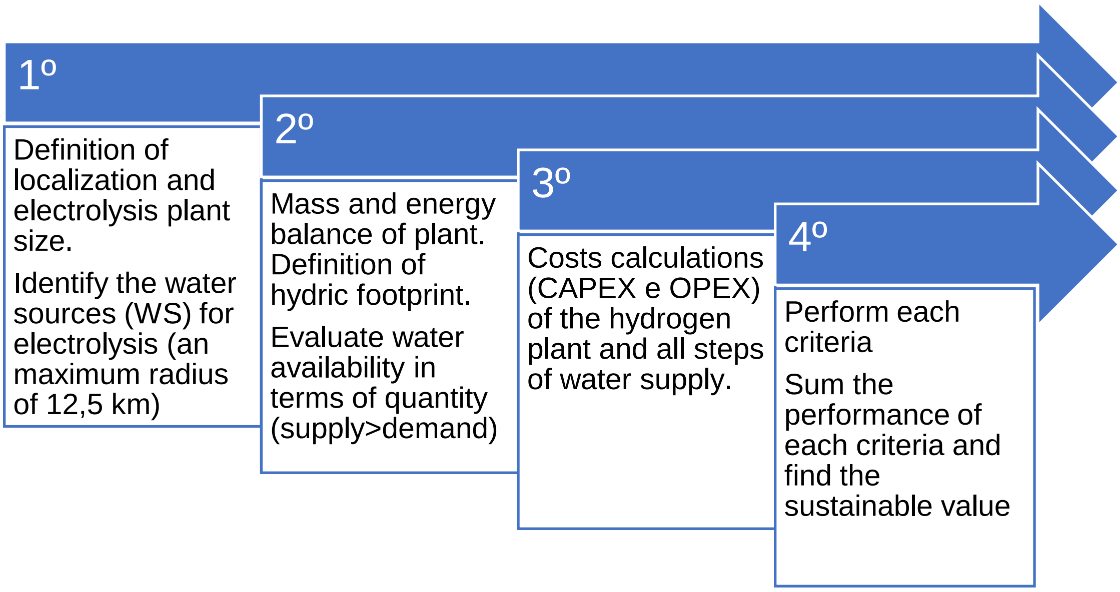
The methodology of this work will be discussed in this section. An overview of the considered approach is presented in Figure 21. The methodology is divided into 3 parts: a quantitative evaluation of the green hydrogen site and water costs. The second part discusses the multi-criteria method, a qualitative assessment of the water sources with a description of the chosen criteria. At last, the modeling and optimization presented how the weights for each dimension and criteria were obtained.

5.2.1 Water Cost Estimation

The first step of this work was to identify and map all potential WS that can input the electrolyzer available around the green hydrogen cluster. Then, information about distance, elevation (between the water source and the hydrogen plant), and treatment needs were summarized.

The potential WS around a green hydrogen plant must be identified and evaluated from this list. Seven potential WS were identified for this study, namely: Grid “Tap” water (TW), treated industrial wastewater (IW), urban wastewater (UW), seawater (SW), rainwater (RW), surface “lake/river” water (LW), and groundwater (GW). It’s important to define the capacity of the green hydrogen plant and run out of the mass and energy balance to determine the hydric footprint; an average of 10L of water per kg of hydrogen produced was considered, and a production of 18kg of H_2 per kW (plant power). The CAPEX and OPEX information were calculated by considering the collection and water transport.

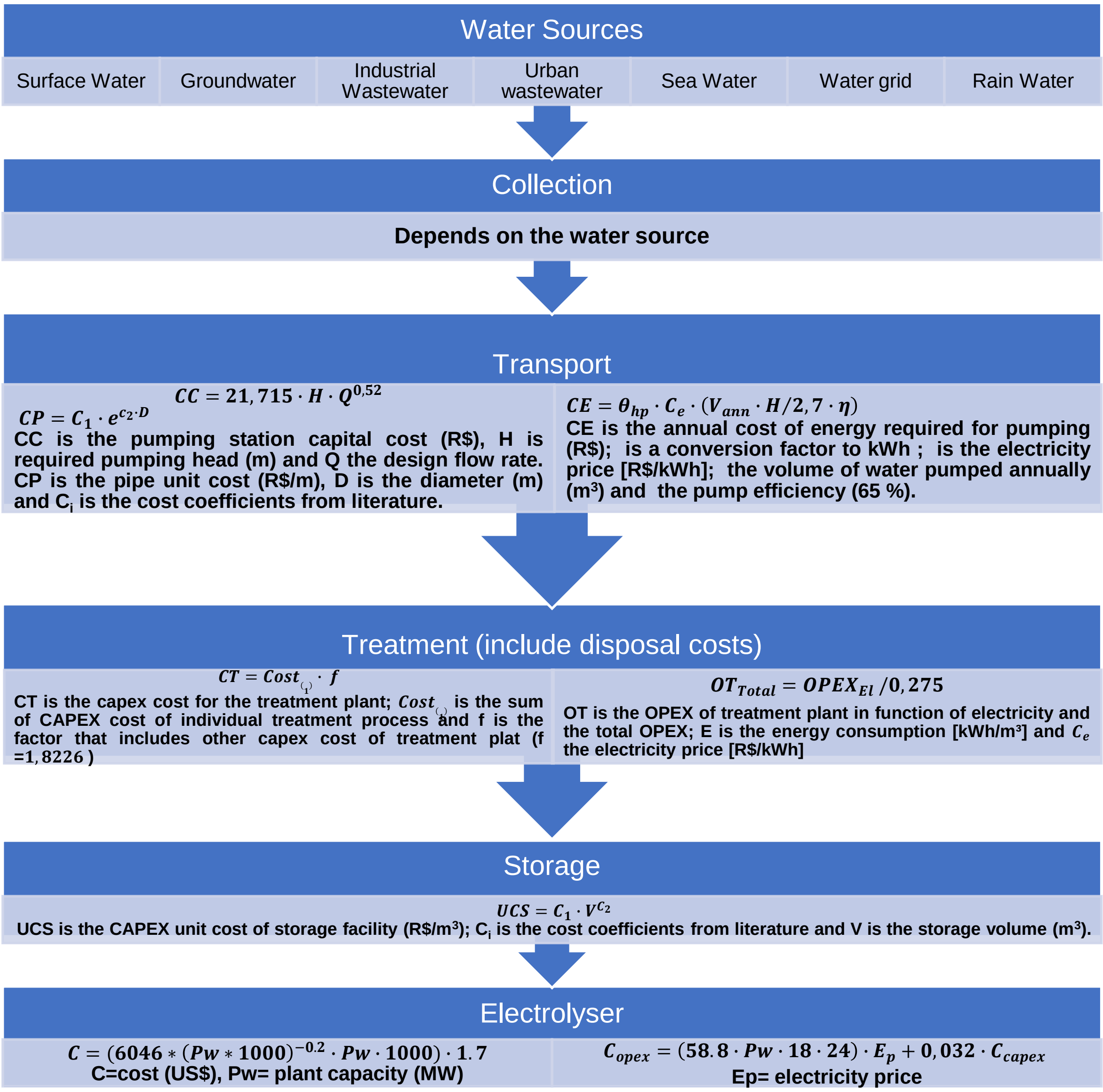
Figure 21 Overview of the approach considered for assessing potential water sources for electrolysis.



Source: Author.

Water costs were calculated based on the work of (Joksimovic, 2007) and (McGivney & Kawamura, 2008) as shown by the equations in Figure 22. A baseline scenario for calculation was established, considering a water flow of approximately 700 m^3/day (equivalent to 255,500 m^3/year), which includes water losses. The plant was assumed to operate for 365 days/year (8,760 hours), and this calculation was applied uniformly regardless of the plant's location. Figure 22 contrasts with the mentioned 389-386 m^3 of water per day, accounting for water losses during collection, transport, and treatment, resulting in an 85% increase. This baseline scenario is presented in Table 19 and Table 20.

Figure 22 Water supply steps and costs equations.



Source: Author.

Table 20 Treatment and collection costs.

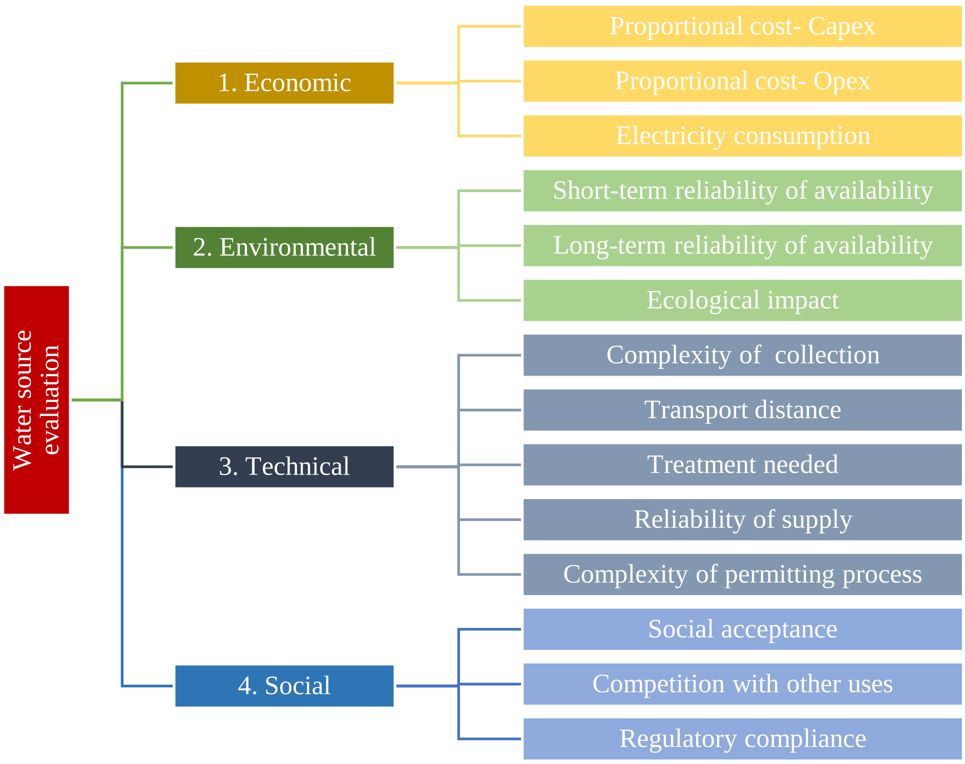
WS	Treatment train	Water loses	Process CAPEX (€)	Energy consumption kWh/m3	Collection (€)	Collection OPEX kW/m³
TW	RO	10%	500,000.00	4.5000	0.00	0
IW	FS→MF→ RO	25%	776,000.00	4.5635	25,000.00	180.0000
UW	FS→MF→ RO	25%	701,000.00	4.5635	25,000.00	-
GW	Chempre→ RO	20%	580,000.00	4.5500	150,000.00	600.0000
RW	FS→MF	10%	201,000.00	0.0635	-	-
LW	FS→ Chempre→MF	15%	281,000.00	0,1135	50,000.00	-
SW	FS→RO*	37%	576,000.00	4.5010	80,000.00	-

Source: Author.

5.2.2 SV based on AHP approach.

As the objective of the MCDM model is single and well-defined (choose the more suitable water source), it is classified as MADM. The proposed model will consider 14 criteria divided into 4 sustainability dimensions to evaluate the WS well. Figure 23 shows how a hierarchical tree's criteria and dimensions are related. In Table 21, each criterion’s description is given. It is possible to see that in terms of the number of criteria, the technical dimension is the most relevant.

Figure 23 Hierarchical tree of the water source evaluation.



Source: Author.

Table 21 Criteria Description.

Criteria	***Dimension***	***Description***
Short-term reliability of availability	Environmental	Short-term reliability of availability (effect of weather factors on water sources as droughts);
Long-term reliability of availability	Environmental	Long-term reliability of availability, which can affect authorization on water use by environmental authorities (perceived future impact of climate change on water source related to water scarcity);
Ecological impact	Environmental	ecological impact on the environment, effect on flora and fauna, related to ecosystem health
Social acceptance	Social	Social acceptance of the water source. Population's general opinion about the use of that source of water for non-human consumption
Competition with other uses	Social	Competition with other uses at the water collection level
Regulatory compliance	Social	Water usage and disposal regulations. Understanding of local regulations regarding water usage and disposal to ensure compliance.
Complexity of	Technical	The complexity of collection (number of involved entities

collection		and the existence of previous experience with this type of water for a similar use);
Transport distance	Technical	Transport distance from water source to H_2 production plant site; (from water source to H_2 production plant site)
Treatment needed	Technical	Degree of water treatment needed up to electrolyzer input requirements;
Reliability of availability	Technical	Reliability of supply (possibility for non-weather-related intermittencies, such as maintenance pauses, that could damage ensuring continuity of water supply);
Complexity of the permitting process	Technical	The permitting process's complexity required previous experience with this type of water for similar use, including transport).
Proportional Capex	Economical	Proportional cost related to CAPEX, comparison between the water sources
Proportional Opex	Economical	Proportional cost related to OPEX, comparison between the water sources
Electricity consumption	Economical	Electricity consumption, comparison between the water sources

Source: Author.

The Criteria can also be divided into local or source-dependent and related to one or more steps of water supply described in Figure 22. These dependencies are essential to understand the criteria and the scenarios better. It is important to mention the related steps, and Table 22 shows the dependence of these criteria.

Table 22 Criteria dependence

Criteria	***Dependence***	***Dimension***	***Related Step of water supply***
Short-term reliability of availability	Local dependent*	Environmental	Collection
Long-term reliability of availability	Local dependent*	Environmental	Water source
Ecological impact	Local dependent*	Environmental	Collection
Social acceptance	Source dependent⁑	Social	Water source
Competition with other uses	Source dependent⁑	Social	Water sources
Regulatory compliance	Local dependent*	Social	Collection

Complexity of collection	Source dependent	Technical	Collection
Transport distance	Local dependent	Technical	Transport
Treatment needed	Source dependent	Technical	Treatment
Reliability of availability	Local dependent	Technical	Transport
Complexity of the permitting process	Source dependent	Technical	Water source
Proportional cost-Capex	Source dependent	Economical	All Steps
Proportional cost- Opex	Source dependent	Economical	All Steps
Electricity consumption	Source dependent	Economical	All steps

(*) This means that the performance level of the criteria can vary with the hydrogen hub production scale. It is leading to water availability and ecological and regulatory issues.

(⁑) This means that the performance level of the criteria can vary with the WEI+, impacting the use and acceptance by society.

Source: Author.

5.3 Modeling and assessment of potential WS

The SV of the evaluated water sources can be defined by equation 4, where the subscripts C and D are the criteria and dimension, respectively; and P and W represent performance (which varies from 1 to 4), and the weight assigned to each criterion or dimension according to the model. The definition and optimization of Dimensions and Criteria Weights are discussed in detail below.

$$SV = \sum_{D=1}^{4} \left(\frac{\sum_{C=1}^{n} P_c \cdot W_c}{4} \right) \cdot W_D \qquad \text{Eq. 4}$$

As a sustainable decision-making support system, the model proposed includes population trends, socioeconomic development, climate, and its implication on the availability of renewable freshwater resources in the form of the Water exploitation index (WEI+) defined by equation 5.

$$\overline{WEI} += \frac{ABS - RET}{LAAW} \qquad \text{Eq. 5}$$

The water exploitation index (WEI+) is defined as the pressure on renewable freshwater resources due to water demand, relating the difference between total water abstractions (ABS) and returns (RET) to water basins with the “long-term annual average available water” (LAAW) at a given time and place.

5.3.1 Criteria’s Performance Level Description

The classification of the performance level for each water source is based on identified criteria, ranging from 1 to 4, where 1 indicates worse performance, and 4 signifies the best performance, as outlined in Table 23. Evaluating water source performance for each criterion is grounded in a literature review. Consequently, there is a degree of subjectivity; nevertheless, the assessment for each case study should maintain transparency and incorporate objective information for the sites and all potential water sources. Some performance level recommendations for each water source are shown in Table 24.

Table 23 Performance Level description for Criteria for Sustainable qualitative assessment of water sources.

Criteria	***Dependence***	***Dimension***	***Performance Level***			
			1	***2***	***3***	***4***
Short-term reliability of availability (effect of weather factors on WS as droughts).	Local dependent	Environmental	Highly dependent on weather factors (water source not available throughout the whole year)	Medium dependent on weather factors (annual water source flow can vary and can be lower than needed by electrolyzer)	Low dependence on weather factors (annual water source flow can vary but will not be lower than needed by electrolyzer)	Not dependent on the weather
Long-term reliability of availability (perceived future impact of climate change on water source- related to water scarcity)	Local dependent	Environmental	High climate change impact expected	Medium climate change impact expected	Low climate change impact expected	No climate change impact is expected.
Ecological impact (Related to ecosystem health)	Local dependent	Environmental	High ecological has implications at the collection level	Medium ecological has consequences at the collection level	Low ecological impacts at the collection level	No ecological impacts at the collection level
Social acceptance	Source dependent	Social	Difficult acceptance due to the possibility of exhaustion of the resource	Weak acceptance due to the possibility of rejection of brines in the ecosystem	Possibly difficult acceptance due to the impact on water availability	No anticipated problems with acceptancy

Competition with other uses [water collection]	Source dependent	Social	Competition with human water supply and/or agricultural uses	Competition with agricultural uses	Competition with other uses	Without expected competition
Regulatory compliance	Local dependent	Social	High difficulty of environmental licensing and water use granting; involvement of multiple entities with complex procedures and lengthy approval timelines	Moderate difficulty of environmental licensing and water use granting; involvement of a few entities with relatively streamlined procedures and reasonable approval timelines.	There is low difficulty in environmental licensing and water use granting; a single entity is involved with straightforward procedures and efficient approval timelines.	There is minimal difficulty in environmental licensing and water use granting; there is no involvement of additional entities or regulatory hurdles.
Complexity of collection (number of involved entities and the existence of previous experience with this type of water for a similar use)	Source dependent	Technical	Very difficult and with potentially unexpected complications	Requires permit and payment of charges	Requires negotiations and eventually payment of charge/tariff	Freely accessible
Transport distance (from water source to H_2 production plant	Local dependent	Technical	Long distance	Medium	Short distance	In situ

site)						
Treatment needed (up to electrolyzer input requirements)	Source dependent	Technical	Very high [fine screening (or microfiltration) + coagulation/ filtration (or ultrafiltration) and reverse osmosis]	High [microfiltration (or ultrafiltration)]	Medium [fine filtration (or fine screening) and ultrafiltration]	Light [fine filtration (or fine screening) and ultrafiltration]
Reliability of availability (continuity of supply)	Local dependent	Technical	Strong possibility of interruptions in the supply	Medium possibility of disruption in the supply	Light possibility of disruption in the supply	No disruption in the supply
Complexity of permitting process (Existence of previous experience with this type of water for a similar use, including transport)	Source dependent	Technical	High complexity	Medium complexity	Low complexity	Permit not necessary
Proportional cost-Capex (total cost of H2 production/water cost)	Source dependent	Economical	75-100% of H_2 plant Maximum CAPEX	50-74% of H_2 plant Maximum CAPEX	25-49% of H_2 plant Maximum CAPEX	0-24% of H_2 plant Maximum CAPEX
Proportional cost-Opex (total cost of H2 production/water cost)	Source dependent	Economical	75-100% of H_2 plant Maximum OPEX	50-74% of H_2 plant Maximum OPEX	25-49% of H_2 plant Maximum OPEX	0-24% of H_2 plant Maximum OPEX

Electricity consumption	Source dependent	Economical	75-100% of H_2 plant Maximum electricity consumption	50-74% of H_2 plant electricity Maximum consumption	25-49% of H_2 plant electricity Maximum consumption	0-24% of H_2 plant electricity Maximum consumption

Source: Author.

Table 24 Performance of water sources according to qualitative assessment of selected value analysis criteria.

WATER RESOURCE	**Freshwater**					**Anthropogenic wastewaters**		**low-quality natural water (Salt-rich)**	
WATER SOURCE	**Surfaces, rivers, streams, lakes**	**Groundwater**	**Water supply network (tap/grid water)**	**Industrial feedwaters (cooling towers, deionized water, and distillate water)**	**Rainwater**	**Treated industrial wastewater**	**Urban wastewater**	**Seawater**	**Estuary (low-quality groundwater)**
Short-term reliability of availability	Local dependent- To assess water availability for electrolysis, the mass balance must determine the need for water flow and then calculate whether the water availability in the water source is sufficient.								
Long-term reliability of availability	Local dependent- Studies of the water availability of that resource over the years must be done to predict if there are future water scarcity risks due to climate change.								

Ecological impact	Local dependent- Environmental impact studies to determine whether water collection or brine disposal will affect the ecosystem.								
Social acceptance	1	2	1	4	4	4	4	4	4
Competition with other uses	1	2	1	3	4	4	4	4	4
Regulatory compliance	Local dependent- The difficulty of environmental licensing and granting of water use. Number of entities involved. Check if the water catchment area is an environmental preservation area, if there is already a catchment infrastructure, etc.								
Complexity of collection	4	2	4	4	2	2	2	1	3
Transport distance	Local dependent- Map existing water sources for use in the electrolyzer and measure distances. A radius of 12,5 km (approx. $50x10^3$ ha) from the electrolysis plant is considered suitable for mapping. ((1) long-distance: 8,5-12,5 km; (2) medium distance: 4,6-8,5; (3) Short distance: 0,5-4,5; (4) less than 0,5 km- In situ)								
Treatment needed	3	3	4	4	3	1	1	1	1
Reliability of supply	Local dependent*- the distance, elevation, and existing barriers between the water source and the plant, among other factors, can add or decrease reliability.								
Complexity of the permitting process	4	2	4	4	3	3	3	1	1

Proportional cost- Capex	4	4	4	4	4	1	1	1	1
Proportional cost- Opex	4	4	4	4	4	3	3	1	1
Electricity consumption	4	4	4	4	4	3	3	1	1

Source: Author.

5.3.2 Dimensions and Criteria Weights definition and optimization

The different numbers of criteria in each dimension and their importance in evaluating the WS for electrolysis highlight the need to assign different weights to each criterion and dimension. Thus, it was defined that the environmental dimension is the most important, followed by the social, technical, and economic dimensions, as shown in Table 25, indicating the qualitative classification of each criterion within the dimension.

Table 25 Qualitative classification of criteria and dimensions

1. Environmental	1.1. Short-term reliability of availability
	1.2. Ecological impact
	1.3. Long-term reliability of availability
2. Social	2.1. Competition with other uses
	2.2. Regulatory compliance
	2.3. Social acceptance
3. Technical	3.1. Transport distance
	3.2. Treatment needed
	3.3. Complexity of collection
	3.4. Complexity of permitting process
	3.5. Reliability of supply
4. Economic	4.1. Electricity consumption
	4.2. Proportional cost- Opex
	4.3. Proportional cost- Capex

Source: Author.

The weights of the dimensions were defined based on qualitative modeling and optimized using the Excel Solver tool. Extensive literature studies were conducted for this purpose. The region's water scarcity level played a crucial role in this determination since the literature defines a WEI+ of 40% as a very high level of water scarcity, with a value of 20% considered the water security threshold Baldinelli et al. (2022). The scale was divided into 5 intervals. The first interval ranges from 0 to 8% (indicating very satisfactory water security levels), and the range from 8.1 to 16% is considered an adequate security level. The water security limit falls between 16.1 and 24%, representing an insecure level from 24.1 to 32%. In the interval between 32.1 and 40%, it is considered a critical level, and for values above these, the risk of water scarcity is very high, making the scale prohibitive. Consequently, locations with WEI+ values above 40% should not receive green hydrogen production plants.

Based on this, it was established that the maximum sustainable value (SV) for the sum of the 4 dimensions (technical, economic, social, and environmental) would be equal to 100 (as in equation 6).

Table 26 Dimension weights modeling

	SWEI+				
	0-8%	**8.1-16%**	**16.1-24%**	**24.1-32%**	**32.1-40%**
Environmental (D_1)	D_2*1	D_2*1,125	D_2*1,25	D_2*1,375	D_2*1,5
Social (D_2)	D_3*1	D_3*1,25	D_3*1,5	D_3*1,75	D_3*2
Technical (D_3)	D_4*1	D_4*1,25	D_4*1,5	D_4*1,75	D_4*2
Economic (D_4)	OF	OF	OF	OF	OF

Source: Author.

The data in Table 26 defines the dimension weights, and the Excel target function is used to calculate the objective function (OF) (economic dimension weight) for each local water availability scenario. The variation of the cell containing D4 gives the objective function to satisfy 3.

$$\sum_{D=1}^{4} W_D = 100 \qquad \text{Eq. 6}$$

Once the weights of each dimension were defined, it was possible to find the value of the weights for each criterion through optimization. The non-linear GRG solution method was used; the objective is for the cell containing Equation 7.

$$\sum_{D=1}^{4} \left(\sum_{C=1}^{n} W_C\right)_D = 4 \qquad \text{Eq. 7}$$

The weights for each criterion would add up to 1 for each dimension. In addition to these constraints, the order of importance of the dimensions and each criterion within the dimensions and among the dimensions was defined so that the less critical criterion within a dimension of more significant importance should have a smaller influence on the SV than the more critical criterion within a dimension of lesser importance. This influence is attributed to the impact of the criterion (*CI*), Equation 8, defined in the equation weight of the dimension within the global (SV model). Table 27 details Excel's model constraints for the solver and goal seek. The resulting modeling data are presented in Table 28 and are used to assess the most suitable WS in the study cases in the following section. It is possible to consult the values of the weights of the dimensions and criteria for each WEI+ range defined in the model presented.

$$CI_{D,C} = W_D \cdot W_C \qquad \text{Eq. 8}$$

Table 27 Modelling constraints

Solver Constraints	
$W_C > W_{C+1}$	$\left(\sum_{C=1}^{n} W_C\right)\Big\|_{D=1}^{4} = 1$
$CI_{3,5} \leq CI_{4,1}$	$CI_{1,3} \leq CI_{2,1}$
$CI_{2,3} \leq CI_{3,1}$	$CI_{4,1} \leq CI_{2,1}$
$CI_{1,3} \leq CI_{3,5}$	$CI_{1,3} \leq CI_{4,1}$

Source: Author.

Table 28 Dimensions and Criteria Weights for each WEI+

Dimension	***Criteria***	***WEI+***									
		8%		***16%***		***24%***		***32%***		***40%***	
		W_D	W_C	W_D	W_C	W_D	W_C	W_D	W_C	W_D	W_C
Environmental	*Short-term reliability of availability*	**25**	*0,51*	**32**	*0,57*	**37**	*0,61*	**42**	*0,61*	**46**	*0,64*
	Long-term reliability of availability		*0,16*		*0,10*		*0,06*		*0,06*		*0,03*
	Ecological impact		*0,33*		*0,33*		*0,33*		*0,33*		*0,33*
Social	*Social acceptance*	**25**	*0,21*	**28**	*0,11*	**30**	*0,11*	**31**	*0,11*	**31**	*0,11*
	Competition with other uses		*0,43*		*0,48*		*0,48*		*0,48*		*0,48*
	Regulatory compliance		*0,36*		*0,41*		*0,41*		*0,41*		*0,41*
Technical	*Complexity of collection*	**25**	*0,20*	**22**	*0,20*	**20**	*0,19*	**17**	*0,19*	**15**	*0,2*
	Transport distance		*0,22*		*0,25*		*0,24*		*0,24*		*0,24*
	Treatment needed		*0,21*		*0,21*		*0,22*		*0,22*		*0,22*
	Reliability of supply		*0,18*		*0,16*		*0,17*		*0,17*		*0,16*
	Complexity of the permitting process		*0,19*		*0,18*		*0,18*		*0,18*		*0,18*
Economical	*Proportional cost- Capex*	**25**	*0,32*	**18**	*0,31*	**13**	*0,31*	**10**	*0,31*	**8**	*0,31*
	Proportional cost- Opex		*0,34*		*0,34*		*0,34*		*0,34*		*0,34*
	Electricity consumption		*0,35*		*0,35*		*0,35*		*0,35*		*0,35*

Source: Author.

5.4 Case studies

5.4.1 Industrial Park and Petroleum Refinery Cases

The case studies discussed here are based on our previous works (Santana, et al., 2023) and (Santana, Almeida, & Pessoa, 2023) and aims to evaluate and compare the simplified models with the MCDM model proposed in this work.

From each case study (Table 29), the water sources available for electrolysis and the distances and elevations from each source to the electrolysis plant were reproduced. However, 4 scales of hydrogen production were evaluated, and 4 levels of scarcity (WEI+). Case 1 is based on (Santana, et al., 2023), the site is a pilot plant (1 MW) located in an industrial park with groundwater, industrial wastewater, seawater, rainwater, and water from the grid available for electrolysis. Case 2 is based on (Santana, Almeida, & Pessoa, 2023), the site is located inside a petroleum refinery, with groundwater, industrial wastewater, seawater, and rainwater available.

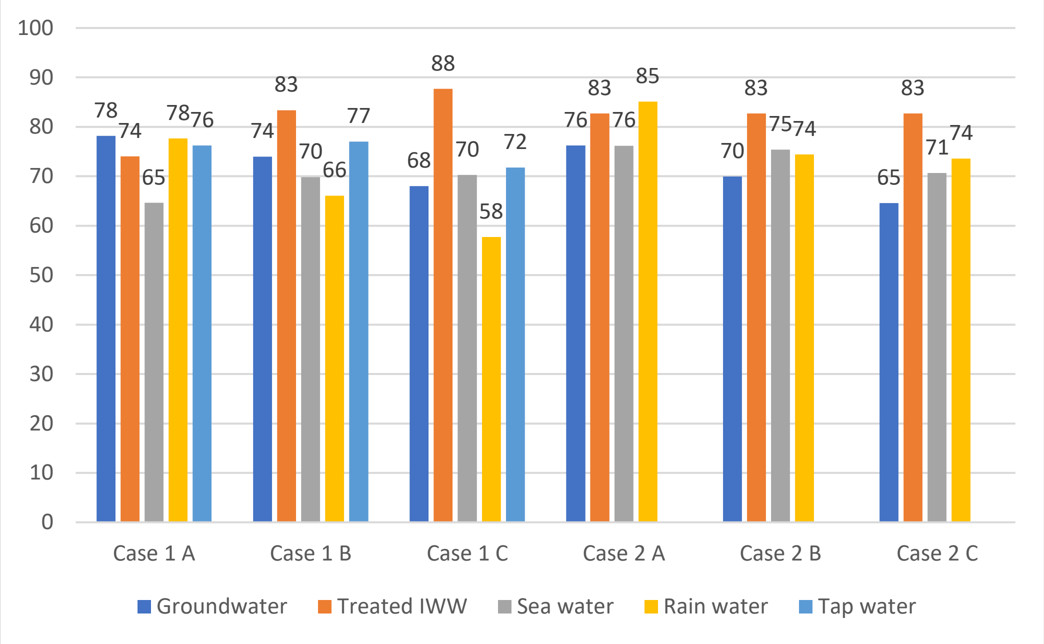
Table 29- Study case description

	Case 1- Pilot plant in an industrial park			***Case 2- Electrolysis in petroleum refinery***		
	1A	***1B***	***1C***	***2A***	***2B***	***2C***
Plant capacity	1MW			20 MW	60 MW	100 MW
WEI+	<8%	<24%	<40%	<16%		
	Water sources and distances/elevation (m)					
Groundwater	On-site			On-site		
Industrial wastewater	5.247/13			On-site		
Seawater	4.686/40			On-site		
Rainwater	On-site			On-site		
Water grid	On-site			Not applicable for case 2		

Source: Author.

Each case study can unfold into three additional sub-cases, with variations in the hydrogen plant capacity (and consequently water demand) and the water scarcity index (WEI+). The results from this study case are presented in Figure 24.

Figure 24: MCDM results



Source: Author.

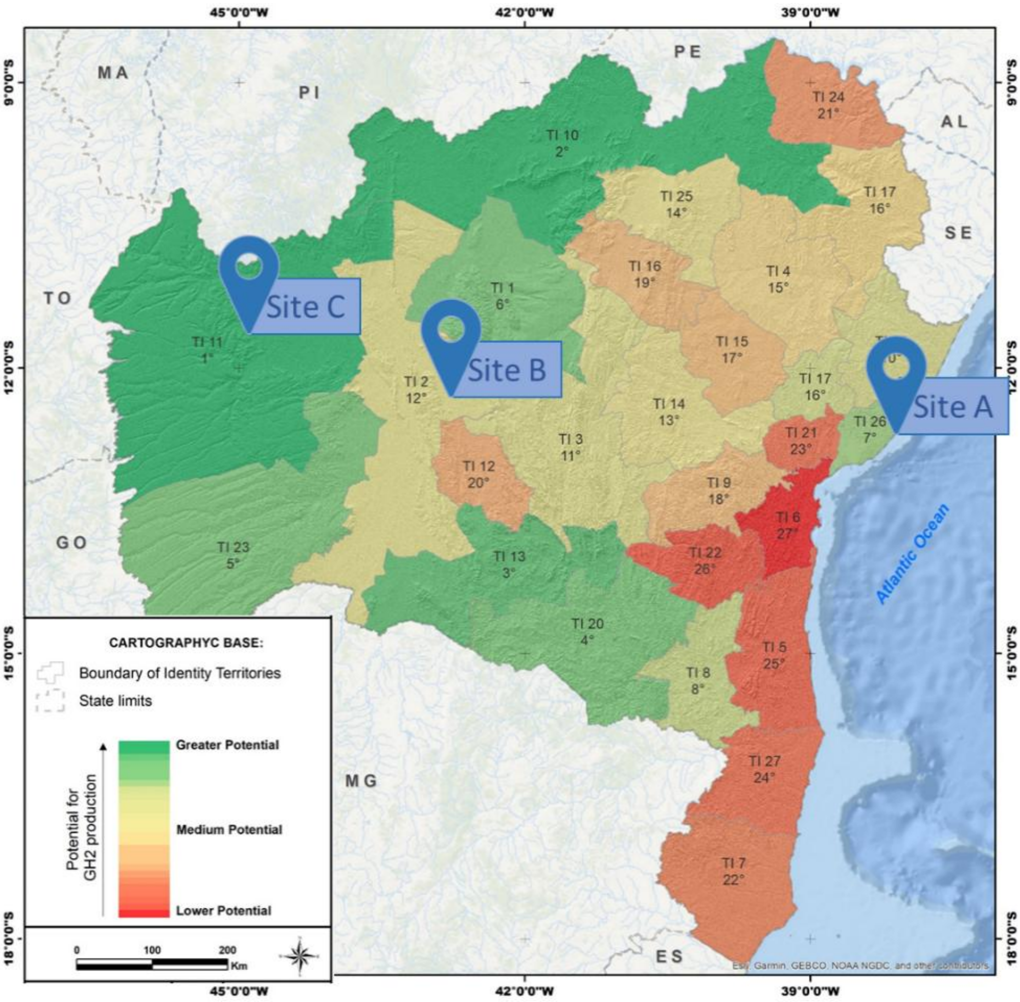
In Figure 24, it can be observed that, in the cases studied, the best water sources are treated industrial effluent and rainwater (for cases where the scale or scarcity index is lower). On the other hand, industrial effluent proves to be a viable alternative in all studied cases. Still, it is directly dependent on the existence of industrial plants near the electrolysis plant. It is possible to note that the viability of rainwater and groundwater decreases, as expected for WS for human consumption.

5.4.2 Study case of the priority regions for green hydrogen production in the state of Bahia

In this study case, the approach is implemented using three different sites in the Brazilian state of Bahia, the fifth largest state in terms of territory. The State of Bahia is energetically strategic, Brazil's second wind energy generator and eighth in solar Photo Voltaic (PV), according to Santos et al. (2023).

The choosing locations of the clusters were based on the green hydrogen map of the state of Bahia (Figure 25): a semi-urban location along the Atlantic coast with cooler summers (site A); a rural area far from the coast with slightly hotter summers (site B); and a semi-urban location far from the coast with intermediated summers (site C). The model uses the analytical hierarchy process to define the weight of each criterion. The weights of each sustainable dimension are determined according to the study area's water exploitation index (WEI+).

Figure 25 – Site locations in the Bahia's GH2 Map



Source: Author.

A total of seven potential WS were identified (grid “Tap” water (TW), treated industrial wastewater (IW), Treated Urban wastewater (UW), Surface “river/lakes” water (SFW), seawater (SW), rainwater (RW), and groundwater (GW)). The CAPEX and OPEX information were calculated considering water abstraction, transport, and treatment, as in our previous work, Santana et al. (2023a). The hydrogen site capacity was 60MW, and the electricity cost was BRL 0.575/kWh (CNI, 2021).

For site A, a semi-urban location along the Atlantic coast with cooler summers, all potential WS are available; for the rural area plant, far from the coast with slightly hotter summers (named site B), only three WS were available (SFW, GW, RW); for the site C, the semi-urban location far from the coast with intermediated summers, TW, UW, SFW, GW, and RW are available. It is important to highlight that the sources available for each case have already undergone quantitative mass balance assessment.

Table 30 – Water sources and distances/elevation (m) for each site

Site	A	B	C
Groundwater (GW)	On-site	On-site	On-site
Industrial wastewater (IW)	5,247/13	NA	NA
Seawater (SW)	4,686/40	NA	NA
Rainwater (RW)	On-site	On-site	On-site
Water grid (TW)	On-site	NA	On-site
Urban wastewater (UW)	10,000/10	NA	5,247/13
Surface water (SFW)	5,000/10	On-site	4,686/40

Source: Author.

The considered distance between the local water collection and the electrolysis plant is listed in Table 30. This study classified the regions into five types, depending on the WEI+, regions with water exploitation greater than 40% can not afford an electrolysis plant. For this study, the WEI+ considered were 20%, 30%, and 30% respectively.

After performing each criterion for the water sources of all the sites, the results are presented in Table 31 and Figure 26. It is possible to visualize the performance of each WS divided into the four sustainable dimensions of the study. The better WS for each criterion is underlined in Table 31.

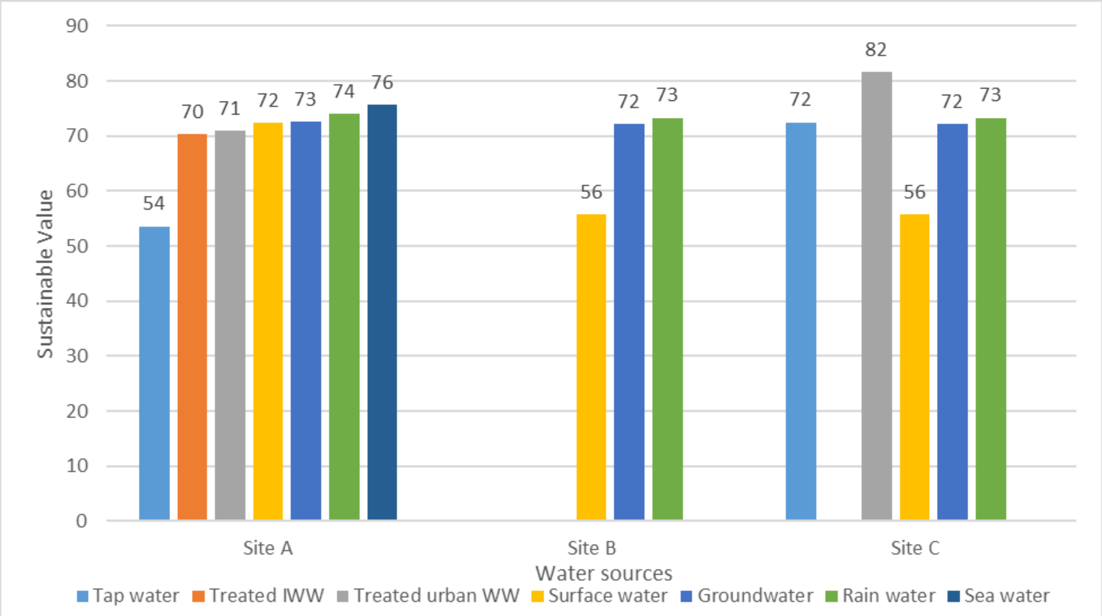
Table 31 – Sustainable Value analysis of water sources.

		TW	IW	UW	SFW	GW	RW	SW
Site A	***Envir***	19	28	25	24	28	20	36
	Social	15	17	20	24	17	30	24
	Tech	12	20	20	16	20	13	8
	Econ	8	5	5	9	8	11	8
Site B	***Envir***				22	32	23	
	Social				16	17	31	
	Tech				10	17	11	
	Econ				8	6	8	
Site C	***Envir***	29		42	22	32	23	
	Social	21		28	16	17	31	
	Tech	17		6	10	17	11	
	Econ	6		6	8	6	8	

Source: Author.

Figure 26 shows the overall performance of the water sources. Comparing them, it is possible to note that the higher sustainable value is for the urban wastewater at site C. However, the most suitable WS for each site is seawater for site A, Rainwater (site B), and Urban wastewater for site C. The results show that the most suitable WS depends on the plant capacity and local issues. This type of evaluation is essential when a hydrogen hub is being built.

Figure 26 – Results of water source evaluation for each Site



Source: Author.

As a result, the most suitable water sources were different for each site (seawater, rainwater, and treated urban wastewater), depending on the distinct characteristics of each location. At Site A, for example, a region with diverse water sources and greater water availability (about other places), the model points to seawater as the most sustainable. Still, there is little variability between the results, except tap water, which has a much lower sustainable value than other water sources. A technical tie can then be considered between rainwater, seawater, and groundwater, with the choice of any of these considered sustainable according to the proposed model.

At Site B, few water sources are available; in this scenario, rainwater and groundwater are the best options. On the other hand, at site C, there is great emphasis on the sustainable value score of urban effluent; on the other hand, surface water is not recommended.

5.5 Conclusions

In this study, a new MCDM model for water source evaluation in green hydrogen production was proposed, employing a sustainable value methodology enhanced by AHP in four distinct steps to identify the optimal water source for electrolysis. Application of the model across case studies, including a pilot plant situated within an industrial park and a refinery, underscored rainwater and industrial wastewater as the most fitting choices, emphasizing the criticality of mindful water source selection in sustainable hydrogen production. Nevertheless, it is acknowledged that the methodology could benefit from further expansion to include a detailed examination of climate change effects on water availability and the incorporation of advanced simulation techniques for forecasting future water supply scenarios. Future research directions should encompass a comprehensive assessment of climate change impacts on water source reliability and the development of a dynamic framework adaptable to changes in water legislation, electrolysis technological advancements, and shifts in socio-economic factors influencing water resource management. Addressing these gaps, future iterations of the model could provide a more holistic tool for stakeholders in the green hydrogen sector, ensuring water resource management aligns with sustainability objectives and the evolving global energy production landscape.

6 CONCLUSIONS

This dissertation presents the main aspects of the required quality and quantity of water used in hydrogen production via electrolysis. It proposes creating a model for evaluating and choosing water sources around a green hydrogen production plant using economic, environmental, and social criteria for this purpose.

The SV methodology emerged as a fundamental tool for diagnosing the main problems related to water sources and quantifying the resources used, considering environmental and social aspects. Case studies in Brazil and elsewhere have provided concrete examples of how different water sources – from industrial wastewater to rainwater – can be assessed for suitability, costs, and overall impact on sustainability.

The economic analysis emphasized that although water costs have a minimal direct impact on the LCOH, factors such as water transportation distance can significantly influence the overall cost efficiency of hydrogen production. This finding is critical for decision-making in locating hydrogen plants and selecting water sources.

The proposed MCDM model offered a robust framework for evaluating the most sustainable water source for electrolysis. The model has demonstrated versatility and effectiveness when applied at various scales and conditions, from pilot plants to larger plants in industrial environments. The results of these applications highlighted rainwater and industrial wastewater as the most suitable sources under certain conditions, emphasizing the need for a contextual approach to water source selection.

6.1 Suggestions for future works

The MCDM model used here to evaluate water sources could be used to explore green hydrogen production.

The weights defined in the modeling could be obtained from specialist knowledge, using a survey, for example.

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