MATIAS CAMPOS HELMEISTER

ANALYSIS UNDER UNCERTAINTY OF THE LEVELIZED COST OF HYDROGEN PRODUCED BY AMMONIA DECOMPOSITION

São Paulo
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ANALYSIS UNDER UNCERTAINTY OF THE LEVELIZED COST OF HYDROGEN PRODUCED BY AMMONIA DECOMPOSITION

Thesis presented to the Polytechnic School of the University of São Paulo for the Industrial Engineering degree.

Supervisor:

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2024

A ship is always safe at shore, but that is not what it is built for
- Albert Einstein

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To my parents, to whom I owe the privilege of being able to study in one of the most prestigious universities in South America, my most sincerest thank you. From you, I learned to always give my best and strive to be an overachiever, with kindness and empathy along this stressful yet fulfilling journey. This achievement is as much yours as it is mine.

To my friends, it has been an honor to share this opportunity with you for the last five years. Thank you for being there, together, in the many challenging moments we've overcome, sharing the triumphs and managing to laugh at the painful and outraging moments. I am glad I managed to meet so many wonderful people that played a crucial role in such an important part of my life. Even though I am sure some of our paths will diverge, know that I am thankful for being a part of this chapter of your stories, and will always be here when you need me.

ABSTRACT

The growing demand for renewable energy and the transition to a green hydrogen economy have driven interest in hydrogen production technologies and carriers. This study evaluates the techno-economic feasibility of hydrogen production via thermocatalytic decomposition of ammonia in a fixed-bed reactor, using NREL's H2A Lite Model for deterministic and uncertain LCOH calculations. The obtained base case LCOH was \$5.46/kg, with ammonia cost contributing to 84% of the total. Sensitivity analysis identified ammonia price and quantity, capacity, and utilization as the most influential variables, aligning with the literature, while random simulations using Monte Carlo methods revealed an LCOH range of \$4.54/kg to \$6.34/kg and a 95th percentile Value-at-Risk (VaR) of \$6.08/kg. These results place ammonia decomposition in the lower-cost tier of renewable hydrogen production technologies but highlight its higher costs relative to fossil-fuel-based methods like steam methane reforming, even with carbon capture and storage technologies. This study underscores the importance of ammonia cost reductions and optimization of hydrogen production technologies for economic feasibility. It also demonstrates the utility of Monte Carlo Simulations for assessing cost uncertainties and establishes the H2A Lite Model as a reliable tool for hydrogen cost assessments. Future research should focus on renewable ammonia cost-reduction strategies and improved risk modeling to support investments and policy development in the hydrogen economy.

Keywords: LCOH, Monte Carlo Simulations, Hydrogen Economy, Ammonia Decomposition, Techno-Economic Analysis, Risk, NREL, H2A Lite Model

LIST OF FIGURES

LIST OF TABLES

LIST OF ABBREVIATIONS AND ACRONYMS

APR	Aqueous Phase Reforming
BoP	Balance of Plant
CAPEX	Capital Expenditures
CCS	Carbon Capture and Storage
DBT	Dibenzyltoluene
EPC	Engineering, Procurement, Construction
GAAP	Generally Accepted Accounting Principles
GHG	Greenhouse Gas
HydESS	Hydrogen-based Energy Storage Systems
IFRS	International Financial Reporting Standards
IRR	Internal Rate of Return
ISO	International Organization for Standardization
LCOA	Levelized Cost of Ammonia
LCOH	Levelized Cost of Hydrogen
LCOE	Levelized Cost of Energy
LOHCs	Liquid Organic Hydrogen Carriers
LSNG	Liquid Synthetic Natural Gas
MCS	Monte Carlo Simulations
NPV	Net Present Value
O&M	Operations and Maintenance
OPEX	Operational Expenditures
PEM	Proton Exchange Membrane
POX	Partial Oxidation
PSA	Pressure Swing Adsorption
RES	Renewable Energy Sources

SMR	Steam Methane Reforming
SOEC	Solid Oxide Electrolysis Cells
TRL	Technology Readiness Level
VaR	Value-at-Risk
WGS	Water-Gas Shift

CONTENTS

1 INTRODUCTION

1.1 Motivation

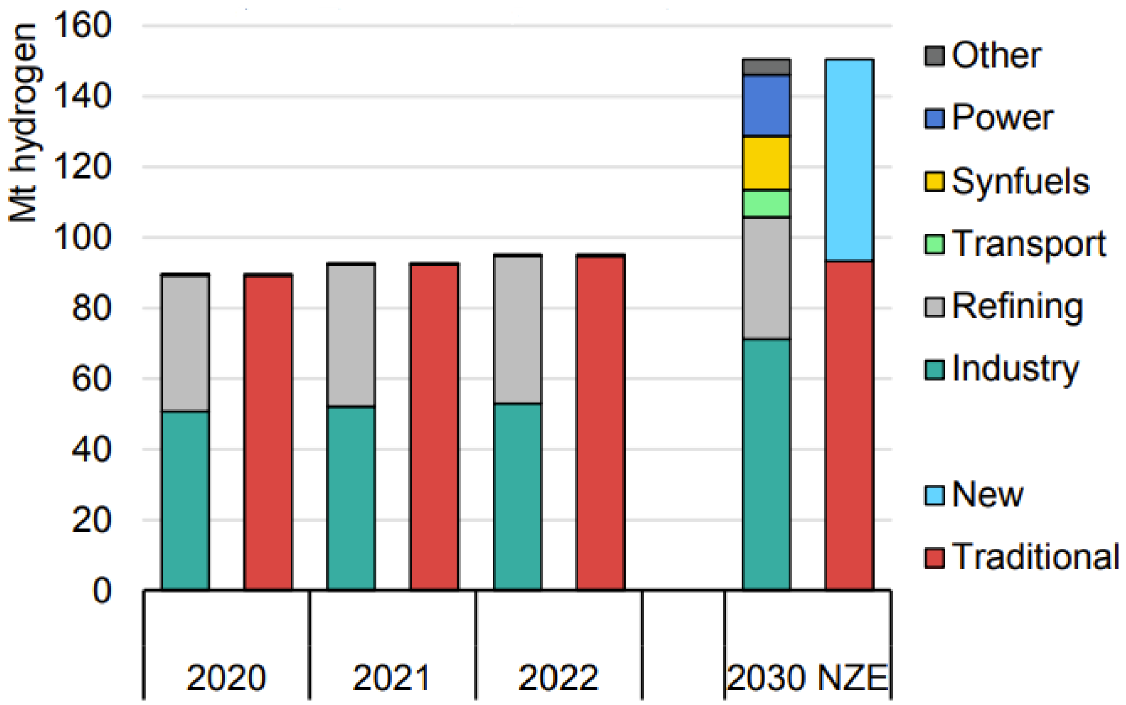
The world faces a critical challenge regarding the sources of energy used to power up all of mankind's technologies and industries at the core of the countries' economies. Energy consumption is increasing at tremendous speed ever since the First Industrial Revolution, and recent technological developments, population increase projections and urbanisation show us that energy consumption will only get bigger: forecast provided by the International Energy Agency (2023b) predicts a yearly increase in total energy demand of 0,7% until 2030. To supply this increasing demand, non-renewable energy sources have been used, primarily fossil fuels such as natural gas, oil and coal (International Energy Agency, 2023a). Their efficiency is high, but also their environmental impacts, which includes mainly air pollution and greenhouse gas (GHG) emissions. These two consequences are concerns because of the impact on health due to bad air quality and climate change.

Therefore, alternative sources of energy are being considered to mitigate the effects of GHG emissions and air pollution. There is consensus from the literature that renewable energy is one of the main feasible drivers to mitigate climate change effects (Gielen et al., 2019). While these sorts of energy have had important technological and financial breakthroughs, making them more popular and competitive in markets worldwide, there is still a gap to be closed when comparing to fossil fuels. Also, when considering electricity, there is a problem regarding energy availability. Due to its dependency on climate, such as water, sun and wind, it is necessary some form of energy storage, so that it is available when those natural elements are unavailable (Dawood; Anda; Shafiullah, 2020).

There are multiple energy storage systems. There are short-term storage systems, such as capacitors, flywheels or batteries, which are helpful for temporary energy storage. However, for the problem at hand, they can't be fully relied on, as they are solutions that last from seconds to hours. To solve the problem of global clean energy availability, energy must be stored for much longer periods of time. Other useful systems can be compressed air energy storage systems and hydroelectric pumping stations, but these depend on quite specific infrastructure that might not be feasible worldwide.(Dutta; Hussain, 2020)

In this scenario, hydrogen appears as a possible solution. Since it can be produced using renewable energy sources and its use for generating energy releases only water in the environment, it can be an efficient alternative for energy storage with low to zero emissions. This idea has gained notoriety on the literature due to the potential of hydrogen as a cost-effective solution for storing renewable energy in large scale, as it is the most abundant substance in the universe and is considered the fuel with the most energy content, at 120 MJ/kg (El-Shafie; Kambara; Hayakawa, 2019). The term Hydrogen-based Energy Storage Systems (HydESS) is key in understanding the so called hydrogen economy, which perceives a world that is fully supplied by renewable energy using HydESS (Dawood; Anda; Shafiullah, 2020). According to the International Energy Agency (2023a), global hydrogen demand reached 95Mt in 2022, with main use cases being refining and industry. As it can be seen on Figure 1, it is expected that hydrogen begins to be used for new applications, such as transport, synfuels, power and others.

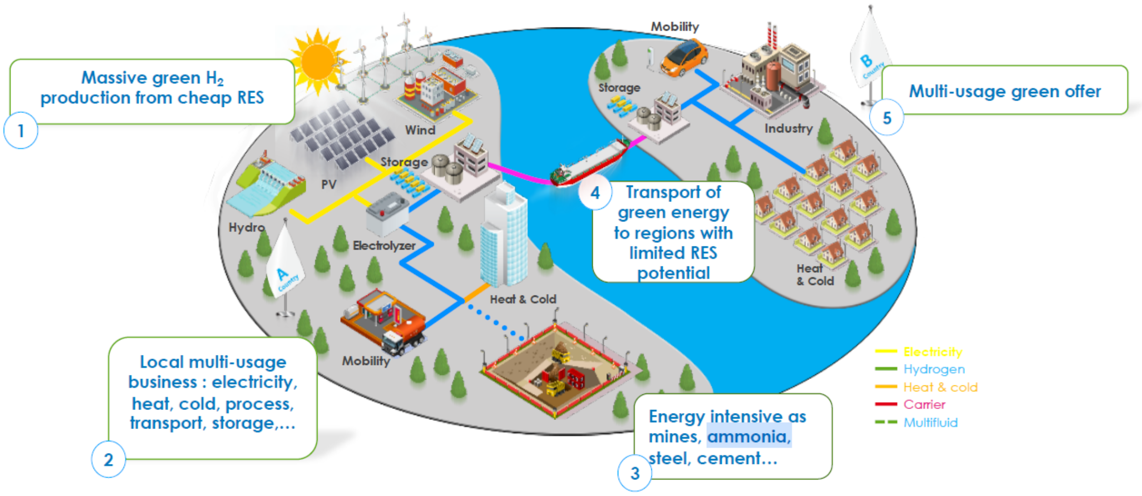
Figure 1: Hydrogen Use Cases 2020-2030



Source: International Energy Agency (2023a)

A sustainable energy transition model based on a hydrogen-powered economy can be depicted in Figure 2, provided by Makhloufi and Li (2019). The first component of this model is the capacity to produce green hydrogen in a massive scale, from cheap renewable energy sources (RES), such as solar and wind. As second and third components, the model emphasizes local usage of this energy for multiple purposes, such as heating, cooling and transport, and also including energy-intensive industries such as mining and steel, which are major current carbon-emitters. Finally, the fourth and fifth components highlight the ability to transport green energy to regions with limited RES potential, enabling worldwide sustainable energy utilization. Hence the importance of an integrated value chain for transitioning to a hydrogen-driven economy.

Figure 2: Sustainable Hydrogen Economy



Source: Makhloufi and Li (2019)

There is certain consensus among the literature that hydrogen will compose around 20% of total global energy demand by 2050 (Hydrogen Council, 2020), driven by already announced hydrogen national strategies such as Germany, which bets on green hydrogen to achieve decarbonization by 2045 (Federal Ministry for Economic Affairs and Energy (BMWK), 2020).

The problem with hydrogen is that it is highly reactive and flammable in its molecular form (H_2), so it requires cautious handling. Multiple accidents have happened since the 20th century (Simpson, 2024), creating a bad reputation for its use. Recent studies have assessed the safety of using hydrogen as a fuel, and while it is known that for every fuel there is a concern of not combining the three combustion factors (ignition, oxidant and fuel) unwantedly, hydrogen requires special attention as it demands only 10% of the gasoline's ignition energy and can ignite with a low concentration of 4% in air (Dawood; Anda; Shafiullah, 2020). Not only that, but hydrogen can cause embrittlement if leaked, which damages the materials and reduces the lifespan of the components due to changes in their mechanical properties. Other problems regarding H_2 pointed out by Kanaan et al. (2023) are a low gravimetric hydrogen density when compressed, which means less molecules of hydrogen per weight unit; and a high energy demanded for transporting hydrogen in its liquid form.

In this sense, hydrogen carriers play a crucial role in addressing the challenges associated with handling hydrogen directly. By storing hydrogen in other compounds such as ammonia, methanol, or liquid organic hydrogen carriers (LOHCs), these carriers offer safer and more efficient ways to transport and store hydrogen. They mitigate issues like low gravimetric density, the need for high compression or liquefaction energy, and the risks of embrittlement. Additionally, hydrogen carriers allow for easier integration into existing infrastructure, reducing costs and avoiding the construction of an entirely new infrastructure for this renewable energy option.

To make a proper techno-economic assessment (TEA) on hydrogen, it is essential to use a metric that accurately compares different hydrogen production methods. Among the literature, there is consensus in using the Levelized Cost of Hydrogen (LCOH), for this purpose. This metric derives from the Levelized Cost of Energy (LCOE), which is used to evaluate the lifetime costs of a power generation project in comparison to the amount of energy produced it produces, expressed in terms of cost per unit of energy produced ($/MWh). It allows for the comparison of different energy technologies, as it is calculated by gathering all costs at present value and dividing by the total energy output over the project's lifetime.

Applying the same principle, specific metrics were created for hydrogen (LCOH) amd ammonia (LCOA), for example. For these, however, the metric is discussed in terms of amount of hydrogen or ammonia produced, in kilograms, rather than an energy measure. Therefore, the LCOH compares the amount of hydrogen produced in a plant to its total costs of installation and operation, at present value.

Currently, many scientific studies explore the LCOH of various hydrogen production techniques, but some rely on deterministic results, which don't account for the uncertainties of key variables. This limits the practical application of these findings, as real-world factors like fluctuating energy prices, market conditions, technology and operational efficiency gains are not fully considered (Andrade et al., 2024). Incorporating risk and sensitivity analysis into LCOH studies would provide a more robust ground for decision-making in hydrogen economics.

1.2 Scope and Objectives

The purpose of this study is to understand the techno-economic viability of a green hydrogen economy enabled by ammonia as carrier. To address the issue of evaluating the feasibility of a hydrogen-based energy system, Dawood, Anda and Shafiullah (2020) has introduced a framework that analyzes four main stages (corners): production, storage, safety and utilization. This study will tackle the production aspect, focusing on LCOH using ammonia as carrier, but will also explore storage and safety themes. While most studies on this matter deploy a deterministic approach, in this study an uncertainty approach will be used to account for the randomness regarding key cost components that influence the LCOH, an essencial metric to determining the cost-efficiency of a hydrogen economy. This method enables investors to make proper decision-making, as the return of a project has to be analyzed considering its risk, represented by the variance of the results.

Andrade et al. (2024) used a similar method to compare the LCOH of two projects, one in Brazil and the other in Germany. This approach selects variables to be considered random, choosing probability distributions to each of them, and uses Monte Carlo Simulations (MCS) to calculate the Value at Risk (VaR) with a confidence level of 95% of randomly generated LCOH values. The range of results that consider uncertainty will be compared to the deterministic results to get a better understanding of economic risk. Furthermore, a sensitivity analysis will be executed to point out the most influential variables in the model, which will enable discussing risks, drivers and expected scenarios for the near future.

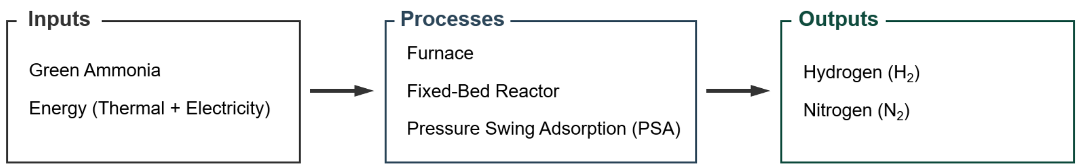
The National Renewable Energy Laboratory (NREL) of the Department of Energy of the United States government provides a range of tools and resources to calculate the LCOH, one of which is their H2A Lite Model. This model is available as a spreadsheet and it is a comprehensive tool that calculates LCOH of any production technology, given that the user inputs key data such as capital expenditures (CAPEX), operational costs (OPEX), capacity, energy efficiency and others. The model also includes built-in risk and sensitivity analysis. Though a reliable tool, few studies in the literature have used it to calculate LCOH. In this study, it will be used to ensure accuracy and consistency in cost modeling.

Since the objective is analyzing the feasibility of an economy powered by green hydrogen using ammonia as a carrier, the most common method for hydrogen production via ammonia will be considered. Among the literature, it is a consensus that the most popular method is the thermocatalytic decomposition of ammonia in a fixed-bed reactor using ruthenium as a catalyzer (Rizi; Shin, 2022). Green ammonia production will not be explored in this analysis, as the hydrogenation process is the one of interest, so it will be assumed that green ammonia is available at a determined cost.

In the modeling of this work, the data for the process will be used based on a project conducted by Alves, Avilez and Mereguete (2024), which seeks to evaluate the technical feasibility of the thermocatalytic decomposition of ammonia in a fixed-bed reactor. The chemical modeling has been completed and validated by the team, however, while the authors have agreed to share relevant data for this study, details will remain partially undisclosed to respect their ongoing publication efforts. Despite this non-disclosure, the general process was shared.

The modeled plant performs centralized ammonia decomposition, at an import terminal in Rotterdam, in the Netherlands. Ammonia is stored in liquid form and pumped into a furnace reactor, which burns part of the ammonia to generate thermal energy, heating the system up to the decomposition temperature, defined by the catalyst, which is ruthenium, thus producing hydrogen and nitrogen. The mixture is then separated in a PSA (Pressure Swing Adsorption) unit. The process outline is defined in Figure 3.

Figure 3: Process Outline



Source: Own elaboration based on Alves, Avilez and Mereguete (2024)

In this sense, this study aims to make a number of contributions to the literature. Firstly, it deepens the discussion on the techno-economic viability of using ammonia as a hydrogen carrier in a green economy by exploring multiple hydrogen productions technologies and providing a detailed LCOH analysis specific to a novel ammonia decomposition plant, idealized by Alves, Avilez and Mereguete (2024). Additionally, this study brings the risk analysis using MCS for the ammonia case, incentivizing this type of methodology as a standard for LCOH studies of any nature, due to the inherent uncertainties of long-term projects. Finally, this work is the first to showcase the NREL's H2A Lite model as a practical tool for hydrogen TEAs, emphasizing its flexibility and reliability.

In the context of an industrial engineering course, this topic is highly relevant, as it permeates multiple different subjects. As a first, when analyzing the mathematical basis of the study, there are multiple concepts from statistics that are used in the risk analysis. Secondly, another relevant matter in this study is economic background and modeling, which is present in the course through quite a few subjects, such as accounting, economical engineering and others. Thirdly, the background behind chemical processes, present in the course, is a pre-requisite for grasping the structure and peculiarities of different examined articles, with different technologies, inputs and outputs. Finally, as a study that is inserted in the energy transition discussion, sustainability concepts are embedded in every discussion. Therefore, there is a lot of intersection between the objectives of this study and the general learning objectives of the industrial engineering course.

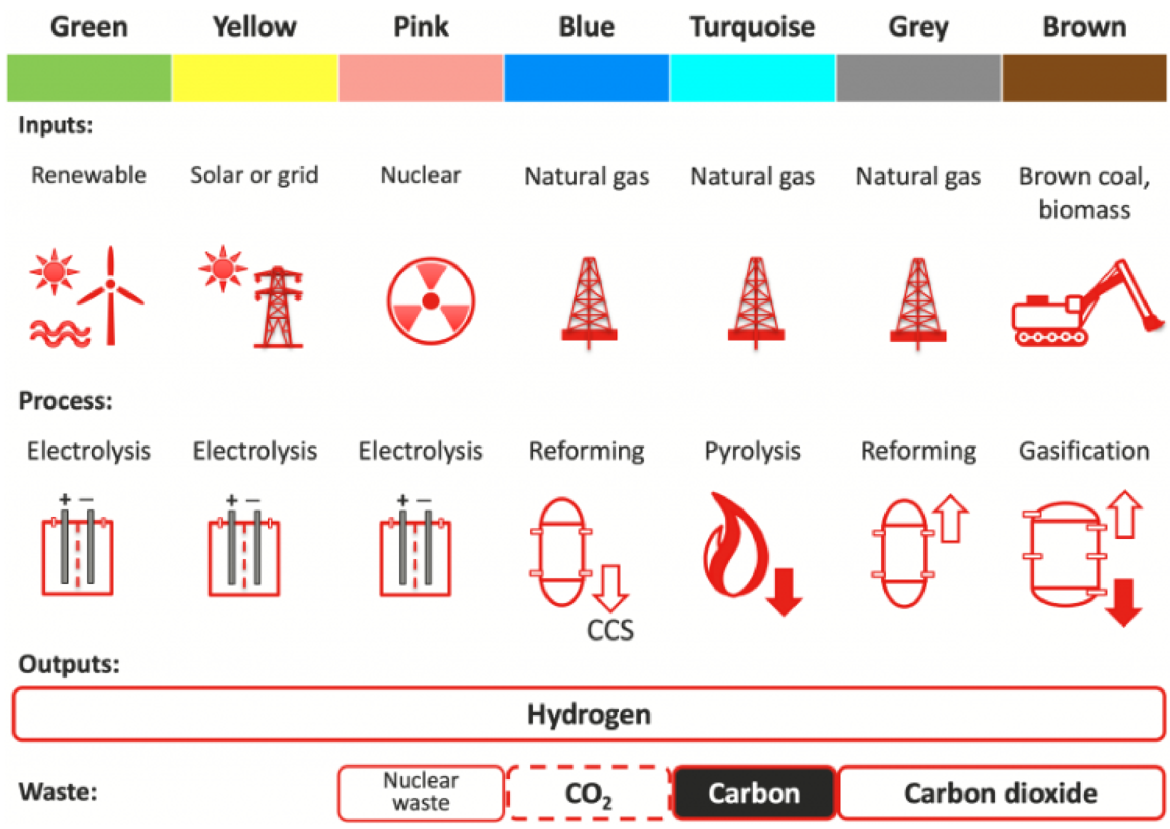
2 THEORETICAL BACKGROUND

2.1 Hydrogen Production

To make a TEA on hydrogen using ammonia as a carrier, it is important to understand the different ways hydrogen can be produced for proper comparison. Firstly, because production methods need to be filtered considering the most sustainable ones, as the whole point of a hydrogen economy is to reduce carbon emissions. Secondly, each production method entails distinct costs, efficiencies, and potential for large-scale replication. Thus, they influence LCOH and need to be taken into account.

Dincer and Acar (2015) summarized the materials used for hydrogen production in three different types: fossil fuels, water and biomass. The most common hydrogen production methods in 2022 were all derived from fossil fuels: natural gas (62%), coal (21%) and by-product (16%), which refers to hydrogen produced during refinery and conversion processes at refineries and in the petrochemical industry (International Energy Agency, 2023a). There is also a color spectrum that categorizes different hydrogen production methods, as shown in Figure 4. All of them will be discussed in sequence.

Figure 4: Hydrogen Color Spectrum

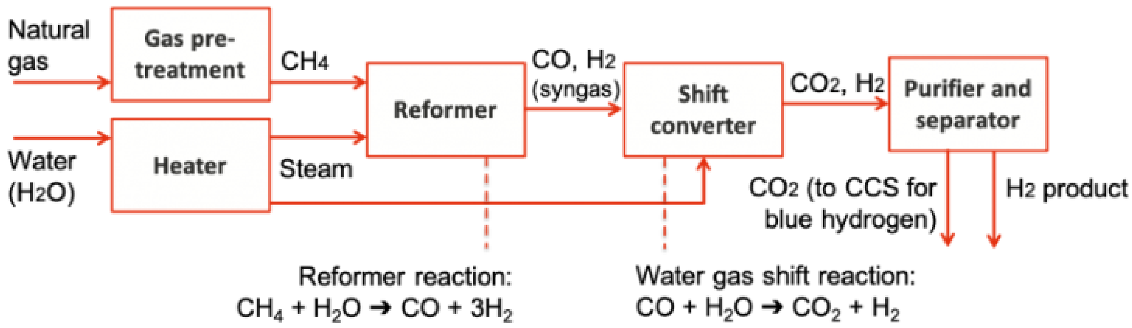


Source: Broadleaf (2023)

2.1.1 Fossil Fuel Based Methods

Fossil fuel reforming is the main method for hydrogen production. Reforming processes consist of a set of chemical processes that convert hydrocarbons into hydrogen and carbon oxides. The three main reforming technologies are steam reforming, partial oxidation and auto-thermal reforming. In terms of color classification, only natural gas reforming is labeled, due to its representativeness. Those colors are grey and blue, with the difference between them being the existence of carbon capture and storage (CCS) technologies, which is true for the latter. Both process outlooks can be depicted in Figure 5, which represents steam-methane reforming (SMR) as a use case example. Still, other fuels can be used, such as gasoline, diesel and propane. In these cases, desulfurization might be necessary because these fuels often contain sulfur compounds that can cause environmental pollution and damage equipment (Holladay et al., 2009).

Figure 5: Steam-Methane Reforming Process (Grey and Blue)



Source: Broadleaf (2023)

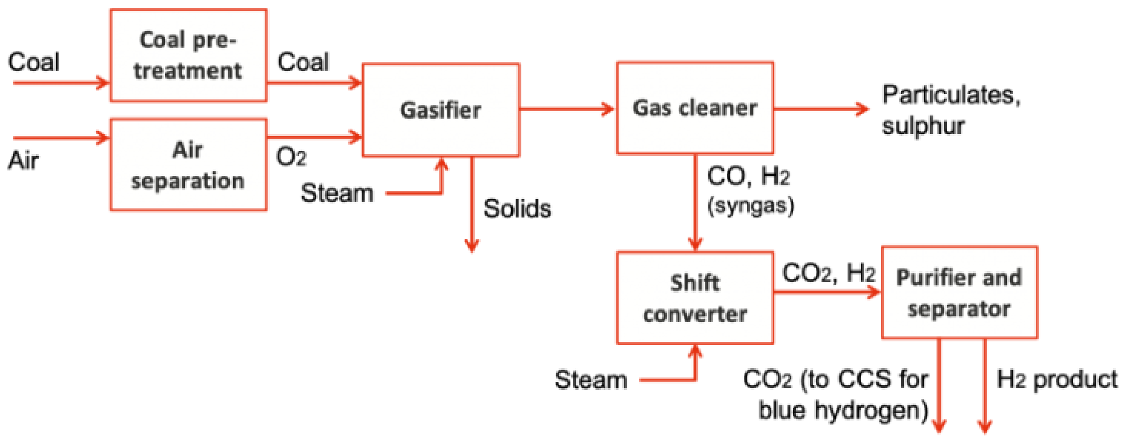
Steam is the most popular out of the three reforming methods, as it does not requires oxygen, provides the best H_2/CO ratio and is the cheapest. On the other hand, it also emits the highest amount of pollutants due to its endothermic nature, meaning it requires an external heat source. The hydrogen produced through SMR often has a high H_2/CO ratio, but this ratio may not always be ideal for certain industrial applications. To ensure that, the water-gas shift (WGS) reaction can be used as a key step that follows reforming to increase hydrogen yield by converting carbon monoxide (CO) and water (H_2O) into additional hydrogen (H_2) and carbon dioxide (CO_2). In terms of fuels, natural gas is the most popular one, as it is the most developed process and cheapest among all types of hydrogen production. Yet, other fuels such as liquefied petroleum gas (LPG), naphtha, kerosene and methane are also possible (El-Shafie; Kambara; Hayakawa, 2019).

Partial oxidation (POX) reforming consists in transforming a hydrocarbon into a carbon oxide by using a high quantity of pure oxygen and more heat than the other two methods, which makes this method more expensive. In addition to this, POX shows less efficiency and H_2/CO ratio than steam reforming, which contributes to its low popularity. POX is more suitable for heavier hydrocarbons such as diesel, justifying its commercial use in automobile fuel cells (El-Shafie; Kambara; Hayakawa, 2019). Finally, the least popular reforming method is auto-thermal. It also requires oxygen or air, although less temperature for combustion than POX, but has the least commercial applications among the three methods, despite presenting greater flexibility than the other two methods.

One final reforming technology is plasma reforming, which is similar to conventional methods but utilize energy and free radicals generated by plasma. The plasma is typically created using electricity or heat, and it produces highly reactive species like H, OH, and O radicals that facilitate both reductive and oxidative reactions. Benefits of plasma reforming include the lack of need of catalysts and desulfurization, being able to operate at a lower bulk operating temperature than traditional methods. However, challenges such as high electrical requirements and electrode erosion at elevated pressures are problematic for this sort of technology (Holladay et al., 2009).

Besides reforming, which is favourable for liquid and gas states, gasification is another common method for hydrogen production, which is used mostly for coal, but can be also used for biomass. In gasification, coal is partially oxidized with steam and oxygen in a high-temperature and high-pressure reactor, generating hydrogen, carbon monoxide and carbon dioxide mixed with steam (syngas). This method is economically and technically practical due to coal availability, maturity and high carbon content, however, it also emits the most amount of CO_2 compared to other methods (Holladay et al., 2009). That is why it is classified as black or brown hydrogen, depending on whether black coal or lignite was used in production, respectively. Therefore, CCS technologies are required to address this problem.

Figure 6: Gasification Process



Source: Broadleaf (2023)

Hydrogen can also be produced with hydrocarbons through pyrolysis, which is a thermal decomposition process that takes place in the absence of oxygen and with high temperatures, which depends on the material that is being decomposed and can be reduced by the presence of catalysts. Even though it is a simple process, it requires a high energy consumption to maintain high temperatures. In the case of methane, the decomposition reaction does not produce GHG emissions, only hydrogen and co-products that can even be used to generate extra income for the plant (Michaut, 2022).

Because of this, pyrolysis using natural gas has been considered as an alternative of low CO_2 emission, if powered with renewable energy sources, which awarded a spot in the color scale between blue and green - turquoise hydrogen. Methane pyrolysis has an energy efficiency of about 55%, being comparable to steam reforming with CCS technologies (Mendes; Nascimento, 2022), and can also be categorized in three main types: thermal, catalytic and plasma. Comparison among these three types are shown in Table 1.

Table 1: Turquoise Hydrogen Pyrolysis Processes Comparison

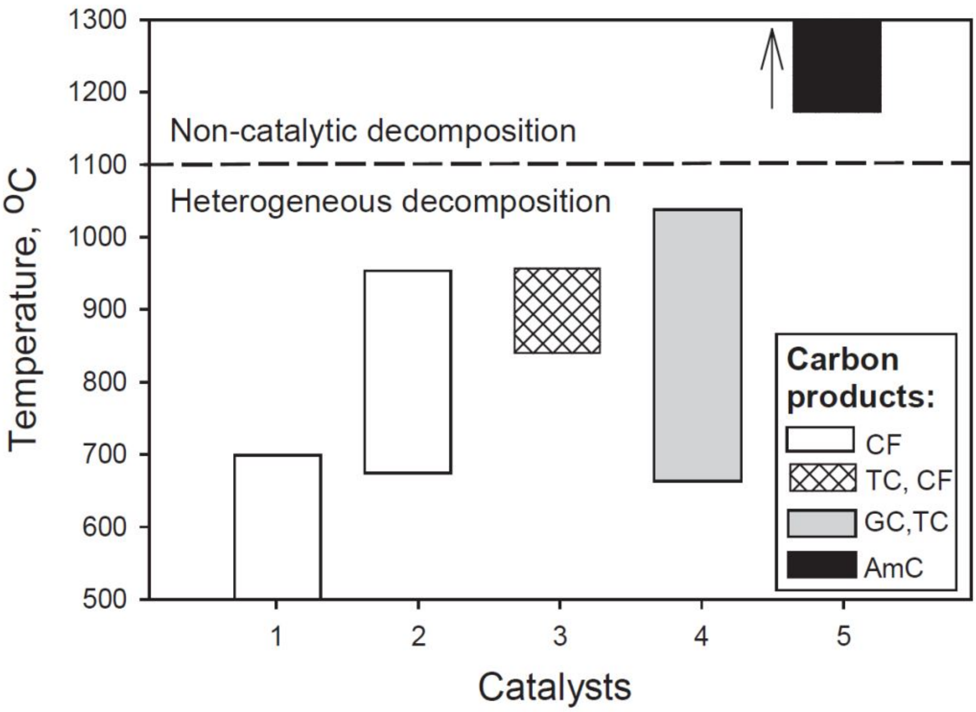
Pyrolysis Type	Advantages	Disadvantages	Carbon
Thermal	- No catalyst deactivation; - Pure carbon.	- High temperatures; - Lack of homogeneity; - High temperatures limit the choice of construction materials.	Tires
Catalytic	- Low temperature; - Scalability.	- Low carbon purity; - Catalyst deactivation; - Catalyst cost.	Carbon black
Plasma	- Flexible reactors - Known technology; - No catalyst deactivation.	- Low energy efficiency; - Limited scalability; - Variability in carbon quality.	Carbon black

Source: Mendes and Nascimento (2022)

Thermal decomposition process takes place inside furnaces that are heated at approximately 1200 °C and maintained at pressures slightly above atmospheric. It has the advantage of producing pure carbon that can generate extra income, although having the disadvantages of a high-temperature system, which requires specific materials for construction and high energy consumption (Mendes; Nascimento, 2022).

Catalytic decomposition utilizes a catalyst to enable chemical reactions at lower temperatures. Most common catalysts are nickel, carbon, noble metal and iron. This method was introduced in the early 1900s, however, lost significance due to the industrial scale that the steam reforming process obtained. Its drawbacks are catalysts' rapid deactivation because of carbon accumulation on their surfaces and the low purity carbon obtained in the process, which can, however, be transformed into carbon with advanced morphology, such as nanofibers and nanotubes (Korányi et al., 2022), being also capable of generating extra income to the plant. Figure 7 shows ranges of temperatures for different catalysts and expected by-products (groups 1-4), also comparing with non-catalytic decomposition (group 5).

Figure 7: Temperature Ranges and Carbon Products for Different Catalysts in Methane Decomposition



Catalysts: 1-Ni-based, 2-Fe-based, 3-carbon-based, 4-summary of data related to Co, Ni, Fe, Pd, Pt, Cr, Ru, Mo, W catalysts, 5-non-catalytic decomposition. Carbon products: CF-carbon filaments, TC-turbostratic carbon, GC-graphitic carbon, AmC-amorphous carbon. Source: Korányi et al. (2022)

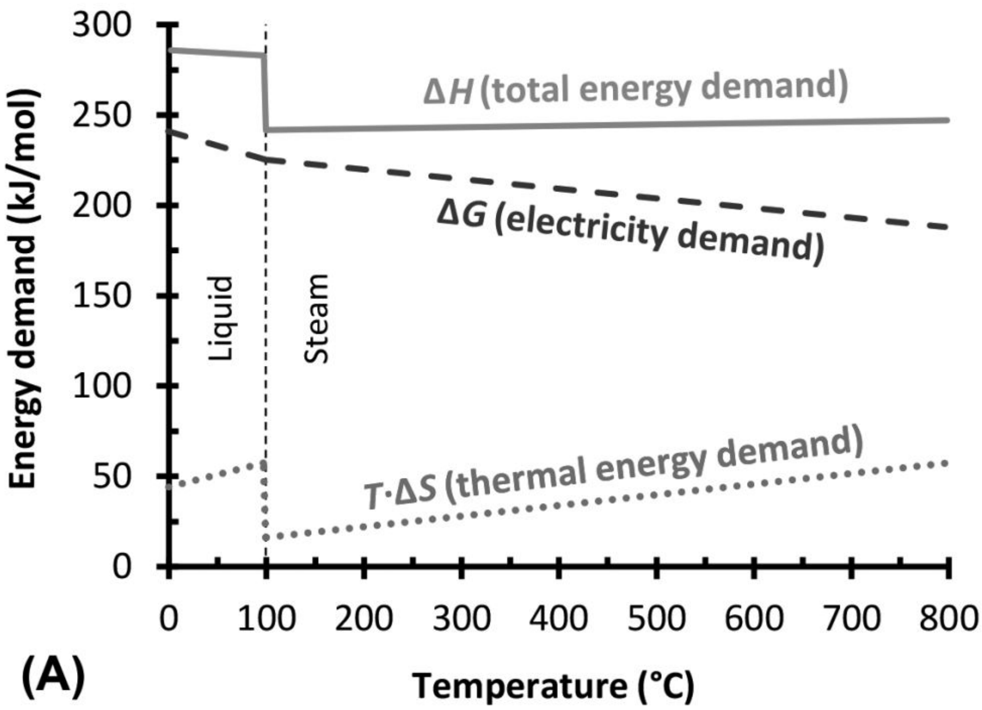
Lastly, there is pyrolysis backed by plasma technology. Plasma is the fourth state of matter, which is an ionized gas, which can conduct electricity, unlike conventional gas. Plasma technology can be separated in thermal or non-thermal, based on operating temperature, and that usually means temperatures higher or under 700 °C, respectively. Non-thermal plasma seems to be more suitable for natural gas, as it shows better efficiency and lower energy needed for cooling (Mendes; Nascimento, 2022). Another benefit is that catalysts are not necessary. However, its technological maturity is still below what is necessary for commercial use, given the efficiency and scalability issues.

2.1.2 Water Based Methods

Another popular hydrogen production method is water electrolysis. Even though it accounted for just 0,1% of the global hydrogen production in 2022, International Energy Agency (2023a) points out to interesting trends: a 35% growth compared to the previous year and 600 projects announced since the previous report to increase global installed water electrolyzer capacity. Therefore, its significance is expected to increase in the future.

Water electrolysis is a basic industrial process that uses an electrical circuit to split water into hydrogen and oxygen, that appear in the cathode and anode, respectively. It is an endothermic reaction that requires an external energy supply to be triggered, which can be in the form of electricity or heat. In reality, the total energy demanded for electrolysis has a thermal portion (in the form of entropy) and an electric portion - the higher the temperature, the lower the electricity demand, with a sweet spot at 100 °C due to water vaporization, as showed in Figure 8 (Dutta; Hussain, 2020). This means that vaporized water is the most energy efficient state for electrolysis.

Figure 8: Influence of Temperature on Theromdynamic Parameters in Water Electrolysis

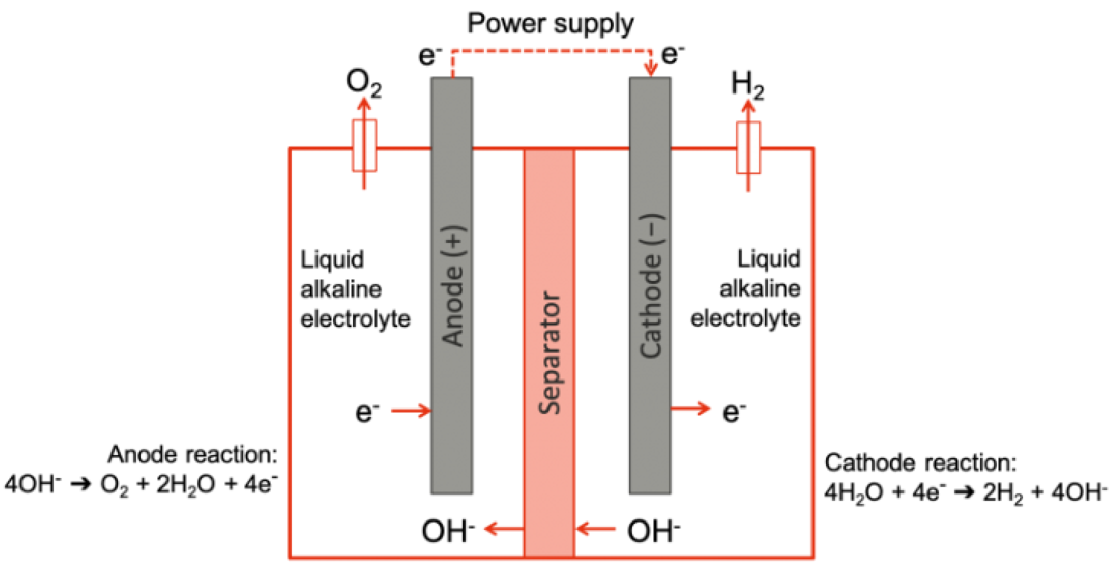


Source: Dutta and Hussain (2020)

As the process itself is carbon-free, the environmental impact of electrolysis is dictated by the type of electricity that powers the electrolyzing system. If electricity is used from the grid, which is powered mostly by fossil fuels, then it is considered yellow hydrogen. In case of electricity from renewable sources, then that hydrogen is classified in the color spectrum as green.

The three common electrolysis technologies are alkaline, proton exchange membrane (PEM), and solid oxide electrolysis cells (SOEC). In alkaline electrolysis, the electrodes are submerged in a liquid alkaline electrolyte (often an aqueous solution of KOH or NaOH) and separated by a porous material called diaphragm, that serves as a filter of gas, isolating hydrogen and nitrogen that are formed and only allowing ions to flow, maintaining the oxidation-reduction reaction (Dutta; Hussain, 2020). The process is shown in Figure 9. However, alkaline systems face several challenges. Firstly, it operates more efficiently at low loads (below 40% capacity), which gives overall less volume of hydrogen produced. Secondly, the diaphragm operates at low pressures, meaning more occupied space and need to compress hydrogen in further processes (Carmo et al., 2013).

Figure 9: Alkaline Electrolysis

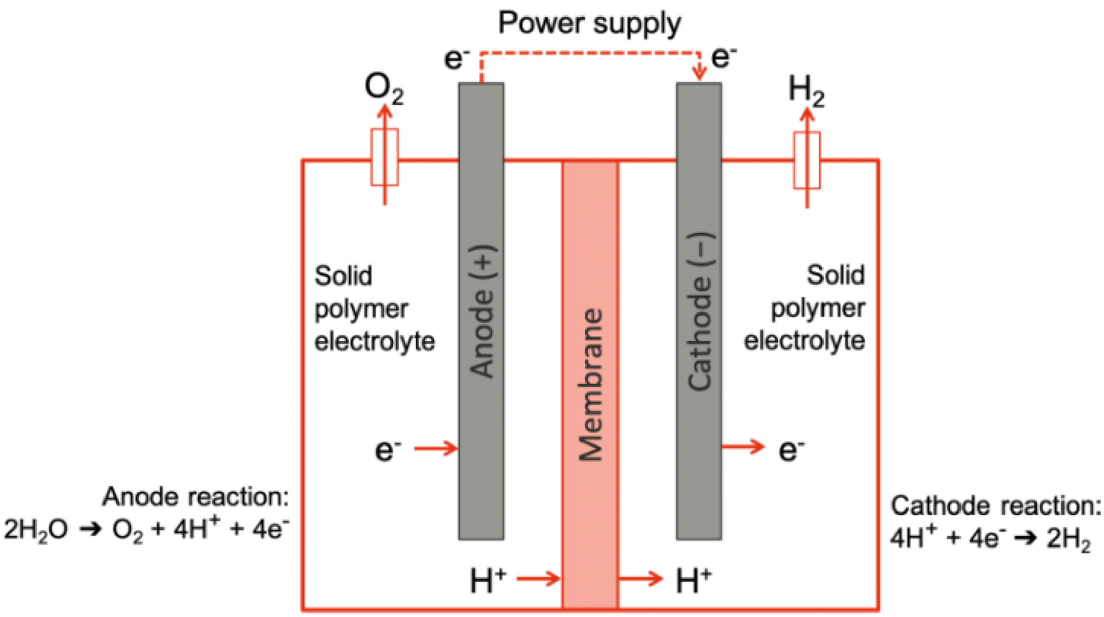


Source: Broadleaf (2023)

PEM electrolysis follows a similar structure, but the membrane itself serves as the electrolyte, conducting protons and isolating the gases. PEM systems also require catalysts, typically noble metals, which contribute to higher costs. Despite these costs, PEM electrolyzers are more efficient than alkaline ones and offer advantages such as high gas purity, compact system design and optimized operation even with lower load ranges.

However, they still face technological challenges related to the cost and durability of the components, as well as scale issues to enable commercialization (Carmo et al., 2013). The process is shown in Figure 10.

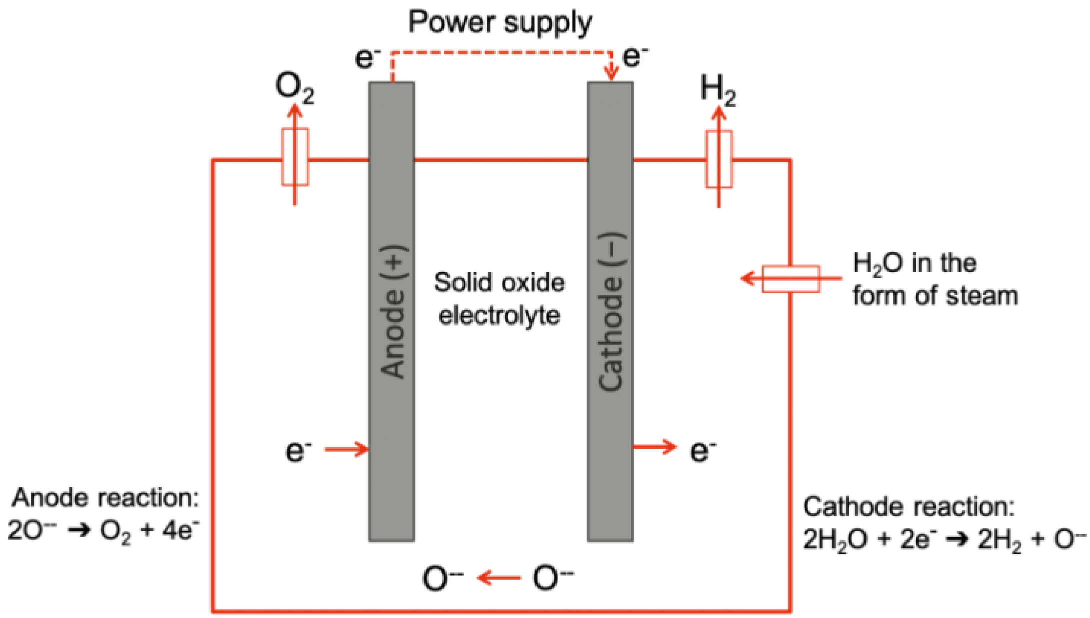
Figure 10: Proton Exchange Membrane (PEM) Electrolysis



Source: Broadleaf (2023)

SOEC technology, which also uses a solid electrolyte, stands out due to its high operating temperatures (800-1000 °C against less than 100 °C for the other technologies), increasing the share of thermal energy relative to electrical energy in the electrolysis process. SOECs can convert electrical energy into chemical energy, producing hydrogen with high efficiency (Carmo et al., 2013), as expected from the behavior of energy according to system temperature from Figure 8. This makes SOECs a promising technology for future large-scale hydrogen production. However, this technology is still in laboratory stage and faces significant challenges regarding corrosion, seals, thermal cycling and chrome migration (Holladay et al., 2009). Addressing these issues is crucial for the commercialization of SOECs, as well as having preliminary cost estimates to assess economic viability. The process is shown in Figure 11.

Figure 11: SOEC Electrolysis



Source: Broadleaf (2023)

When comparing all three technologies, alkaline systems are the most mature, presenting the lowest cost and highest lifetime, despite requiring hydrogen purification and having the lowest efficiency (Dutta; Hussain, 2020). SOEC technology offers the highest efficiency but is the least developed, requiring significant advancements in the durability of ceramic materials under high temperatures for long-term operation. PEM electrolyzers offer balance between the two, offering higher efficiency than alkaline systems without the corrosion and sealing issues that SOECs present, though at a higher cost due to the use of noble metals. Advantages and disadvantages from each electrolysis technology are shown in Table 2.

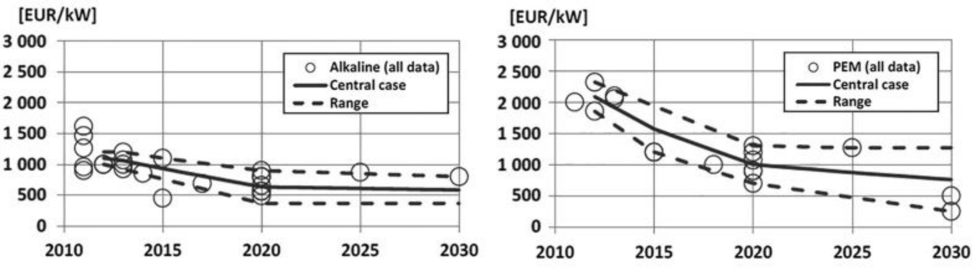
Table 2: Advantages and Disadvantages of Each Type of Electrolysis

Aspect	**Alkaline**	**PEM**	**SOEC**
Advantages	Well established technology Non noble catalysts Long-term stability Relative low cost	High voltage efficiency Good partial load range Rapid system response Compact system design High gas purity	High efficiency Non noble catalysts High pressure operation
Disadvantages	Crossover of gases (degree of purity) Low partial load range Low operational pressures Corrosive liquid electrolyte	High cost of components Acidic corrosive environment Possibly low durability Commercialization	Laboratory stage Bulky system design Durability (brittle ceramics) No dependable cost information

Source: Carmo et al. (2013)

For large-scale production of hydrogen, a crucial factor is the economic viability of technologies. As discussed, SOEC electrolysis is out of this discussion for now, as there is little data on the literature for this asssessment. On the other hand, PEM electrolysis systems have showed a descending trend of power consumption since 2010, which makes prospects for this technology very favourable (Dutta; Hussain, 2020). Cost perspectives for both alkaline and PEM systems were calculated based on suppliers and manufacturers data on CAPEX and OPEX (in EUR) in relation to installed power (in kW), leading to a cost per kW metric that shows competitiveness of these technologies. Results are shown in Figure 12, with PEM electrolysis presenting a higher cost descent on recent years, but also higher variability in the future.

Figure 12: Alkaline and PEM Electrolysers Projected Costs



Source: Dutta and Hussain (2020)

Electrolysis is not the only hydrogen production method from water, even though it is the most popular. Thermochemical water splitting is a method that uses high temperatures to break water into hydrogen and oxygen. This process typically occurs in multiple chemical steps involving metal oxides or other chemical intermediates that react with water at high temperatures to release hydrogen. One of the major advantages of thermochemical water splitting is that it can be highly efficienct by using heat, which is often a byproduct of other processes. Therefore, it can be combined with other process flows to "recycle" energy. In addition to that, there is also the possibility of integrating with renewable heat sources, such as solar power, which makes it a promising method for sustainable hydrogen production. However, the thermochemical water splitting also has significant disadvantages. The need for very high temperatures (often over 1000 °C) can lead to material degradation and the need for specialized, durable reactor materials that can be quite expensive (Holladay et al., 2009).

One final method to be discussed on water-based technologies is photoelectrolysis. This involves using sunlight to split water, through a process driven by light-absorbing semiconductor materials. When exposed to sunlight, these materials generate electrical charges that facilitate the chemical reactions needed to break the water molecules apart. One of the main advantages of photoelectrolysis is its potential for high efficiency, as it directly converts solar energy into chemical energy, without any intermediate steps in between. Another advantage is the fact that it eliminates the need for external electricity, which can significantly reduce operational costs in regions with abundant solar irradiation. However, the technology is still highly inefficient when comparing to others, as semiconductor materials that can withstand prolonged exposure to sunlight and water without degrading are still being developed. Moreover, current photoelectrolysis systems present high costs. These factors make this technology less competitive to other hydrogen production methods. In a nutshell, while promising, photoelectrolysis is still in the research and development stage, requiring significant technological maturity and advancements before it can be widely adopted. Another similar method is direct photolysis, which is also based in water splitting powered by sunlight, but relies on algae or cyanobacteria instead of semiconductors. This method shows similar challenges when comparing to photoelectrolysis.

2.1.3 Other Methods

To close the discussion on hydrogen production technologies, there are methods that have low economic relevance, but are worth considering. Nuclear powered hydrogen is another low-carbon method, though not renewable, which is classified as pink hydrogen. It is the same principle of green hydrogen, as an electrolyser is also used for hydrogen production, the only difference is the power source. Nuclear power relies on finite resources, usually uranium or thorium, and was first conceived as an alternative of electric power generation source. In spite of that, several severe accidents have been responsible for a greater concern in terms of this type of power. Not only that, but also the environmental challenges regarding nuclear waste management. Fernández-Arias et al. (2024) found an increase in the number of publications referring to pink hydrogen, which demonstrates a growing interest in this technology, but still with low techonological readiness level (TRL). Also, a lack of a unique global strategy for nuclear power makes research unclear and challenging.

Another section of hydrogen production technologies are biological processes. These methods leverage microorganisms to produce hydrogen, and often are explored in research for their renewable potential (using organic materials and sunlight, for example), but are still very immature in terms of scalability and efficiency. Two methods can be highlighted here: as a first, dark fermentation uses anaerobic bacteria to break down organic material in the absence of light, producing hydrogen, though its yield is limited and requires additional waste treatment.; the other is photo-fermentative processes, which involve bacteria converting organic acids into hydrogen with sunlight, but slow enzyme activity limits its efficiency (Holladay et al., 2009).

Dincer and Acar (2015) compared every hydrogen production technology considering specific criteria: environmental impact, social impact, financial cost and efficiency. Fossil fuel based methods presented the most environmental and social impacts, least financial cost and highest efficiency. Water electrolysis, on the other hand, showed medium levels of efficiency and cost, and would also present low environmental and social impact if the electricity used was based on renewable sources. Therefore, data shows that hydrogen production relies on a fossil-fuel-based infrastructure that is cost competitive.

2.2 Hydrogen Carriers

Hydrogen carriers are crucial for addressing the challenges associated with transporting hydrogen directly. One of the main issues is that hydrogen is highly flammable, possibly leading to dangerous accidents. To prevent this, pressurization or liquefaction is required for transport, both of which involve high costs and energy consumption. On the other hand, hydrogen carriers such as ammonia, methanol, or liquid organic hydrogen carriers (LOHCs) promote a safer and more efficient alternative for hydrogen transport.

This is because one of the main advantages of a hydrogen carrier is leveraging existing infrastructure, especially in maritime transport. When discussing worldwide clean energy utilization, there are countries that cannot produce sustainable hydrogen domestically - due to climate conditions or even technological advancement. In this scenario, importing hydrogen in the form of carriers is a practical solution, as it utilizes the current port and shipping infrastructure, which is already set up for transporting chemicals like ammonia or methanol, which require less or no energy for liquefaction. This eliminates the need for high pressurization on transport, which accounts for high costs. In this scenario, countries can import large quantities of renewable energy stored in hydrogen carriers, promoting the global transition to sustainable energy.

Multiple substances have been analyzed to serve the purpose of a hydrogen carrier, solving infrastructure, cost and safety issues. Ammonia is one of the options of interest. It enables liquid-phase storage of hydrogen, making it easier to transport (Lamb; Dolan; Kennedy, 2019), and also can be converted to hydrogen at a large scale process, minimizing substance loss (Dincer; Acar, 2015). In addition, ammonia is a widely used chemical in world economy, meaning that the current infrastructure is sufficient overall. Finally, gravimetric content is higher than pure hydrogen and liquefaction conditions require less energy (Kanaan et al., 2023). Although ammonia is a toxic substance, as dangerous health effects can be caused due to human inhalation, safe handling procedures for NH_3 are well established worldwide.

Another contender to play the role of carrier is methanol. Even though it has slightly less gravimetric hydrogen contents than ammonia, it is still a good option because of its low volatility at ambient conditions of temperature and pressure. It also has an existing infrastructure for transportation and storage, as it is a widely used chemical in the economy. However, methanol utilization produces CO_2, which requires a carbon capture technique to prevent environmental impacts or a CO_2-free production method. Some reactions might also produce CO, which poisons most of the catalysts used in fuel cells, making their life time shorter (Aziz; TriWijayanta; Nandiyanto, 2020). Comparison among different hydrogen storage options can be seen in Table 3.

Table 3: Hydrogen Storage Methods

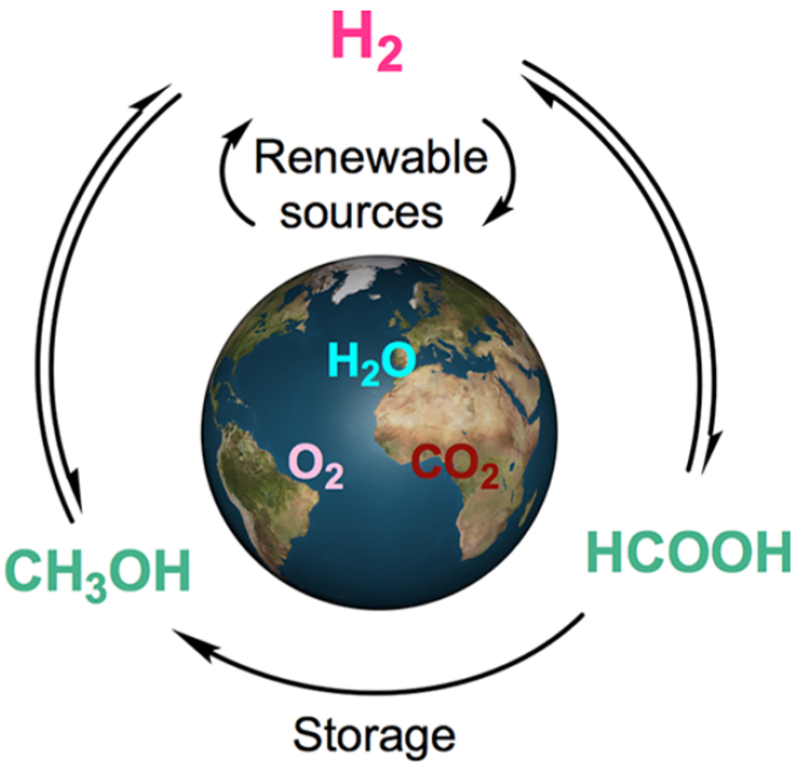
Properties	Unit	Compressed Hydrogen	Liquid Hydrogen	Methanol	Liquid Ammonia
Storage method	-	Compression	Liquefaction	Ambient	Liquefaction
Temperature	°C	25 (room)	-252.9	25 (room)	25 (room)
Storage pressure	MPa	69	0.1	0.1	0.99
Density	kg/m^3	39	70.8	792	600
Explosive limit in air	%vol	4-75	4-75	6.7-36	15-28
Gravimetric energy density (LHV)	MJ/kg	120	120	20.1	18.6
Volumetric energy density (LHV)	MJ/L	4.5	8.49	15.8	12.7
Gravimetric hydrogen content	wt%	100	100	12.5	17.8
Volumetric hydrogen content	kg-H_2/m^3	42.2	70.8	99	121
Hydrogen release	-	Pressure release	Evaporation	Above 200°C	Above 400°C
Energy to extract hydrogen	kJ/mol-H_2	-	0.907	16.3	30.6

Source: Aziz, TriWijayanta and Nandiyanto (2020)

Methanol is an example of a broader category of hydrogen carrier possibilities, which are synthetic hydrocarbons, as categorized by Salmon and Bañares-Alcántara (2021). Their main limitation is in terms of sustainability, as their production is energy and carbon-intensive. Carbon could be obtained by direct air capture, creating a renewable loop of energy utilization, as showed in Figure 13. However, this technology is currently limited to be applied at a small scale, which makes the scenario of using fossil fuels for production more likely, which is not sustainable. Another group analyzed by Salmon and

Bañares-Alcántara (2021) is liquid organic hydrogen carriers (LOHCs), which includes toluene or dibenzyltoluene, for example. As ammonia, they share the benefit of being easy to transport at ambient conditions and current infrastructure due to their liquid state. However, LOHCs loses relevance to ammonia because of low volumetric hydrogen density and requirement of energy-intensive processes for hydrogenation and dehydrogenation, generating low levels of efficiency overall.

Figure 13: Renewable Energy Cycle Using Formic Acid and Alcohols



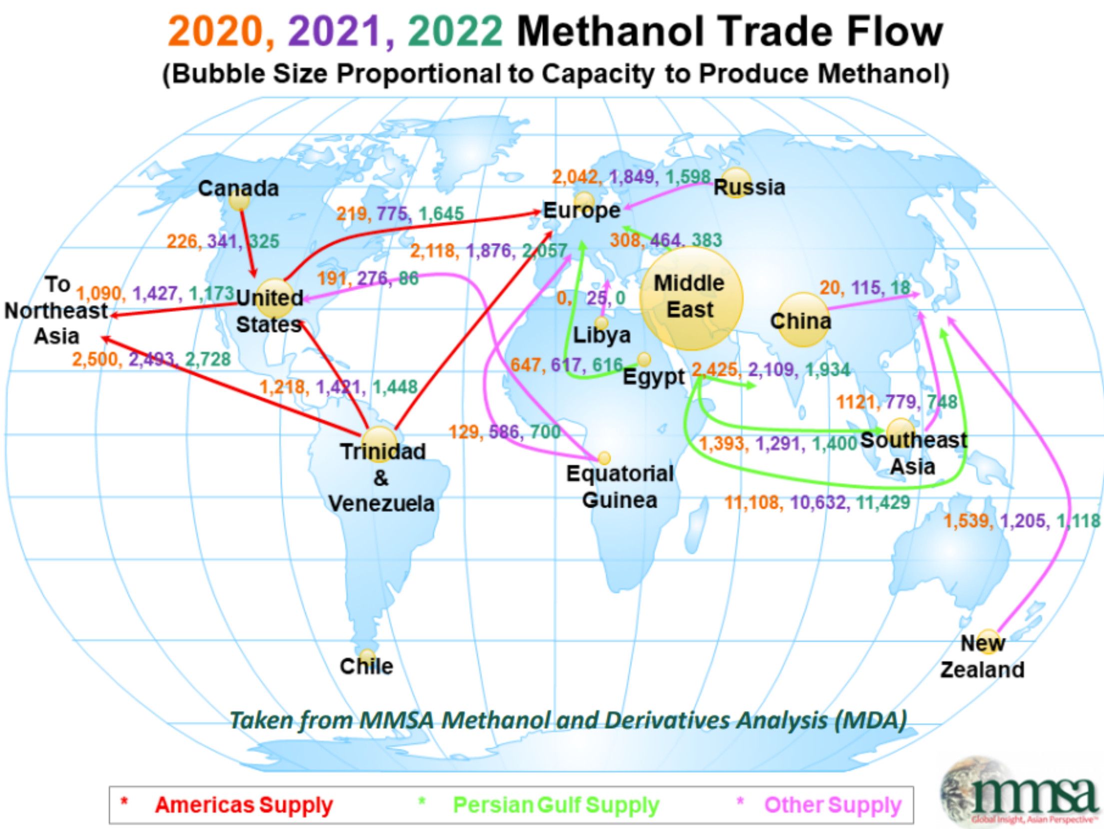
Fonte: Sordakis et al. (2018)

Among the possible hydrogen carriers, ammonia and methanol have caught attention of the literature, so it is important to grasp how hydrogen can be produced from these carriers.

2.2.1 Methanol

Methanol is produced by combining hydrogen with carbon dioxide through well-established industrial processes and benefits from existing massive scale infrastructure of around 110 million tonnes per year (as shown in Figure 14), with use cases mainly from the transportation and chemical sectors (Berggren, 2023). Methanol also has broad applications such as feedstock for producing fuels like gasoline and dimethyl ether (DME).

Figure 14: Methanol Trade Flow Worldwide



Fonte: Berggren (2023)

Methanol dehydrogenation can be done in three different ways. It can produce only one hydrogen molecule and formaldehyde; two hydrogen molecules and carbon monoxide; or three molecules of hydrogen and carbon dioxide, if water is present in the reaction. All chemical reactions are described in Table 4 and all are endothermic, meaning they require energy input to occur. Steam reforming is the most common method, as it has the highest efficiency and well-established technology. It takes place between 200-300 ^{o}C and requires heterogeneous catalysts, being copper-based catalysts the top performers. As discussed by (Sordakis et al., 2018), aqueous phase reforming (APR) can be applied to prevent CO generation and maximize hydrogen, allowing production to happen at the lower end of temperature ranges (200 °C).

Table 4: Methanol Dehydrogenation: Possible Chemical Reactions

Reaction	ΔH° **(kJ mol^{-1})**	ΔS° **(J mol^{-1} K^{-1})**	ΔG° **(kJ mol^{-1})**
$CH_3OH(l) \rightarrow HCHO(g) + H_2(g)$	+129,8	+222	+63,5
$CH_3OH(g) \rightarrow CO(g) + 2H_2(g)$	+94,6	+219,1	+29,3
$CH_3OH(l) \rightarrow CO(g) + 2H_2(g)$	+127,9	+332	+29,0
$CH_3OH(g) + H_2O(g) \rightarrow 3H_2(g) + CO_2(g)$	+53,3	+176,8	+0,6
$CH_3OH(l) + H_2O(l) \rightarrow 3H_2(g) + CO_2(g)$	+130,7	+408,7	+8,9

Source: Sordakis et al. (2018)

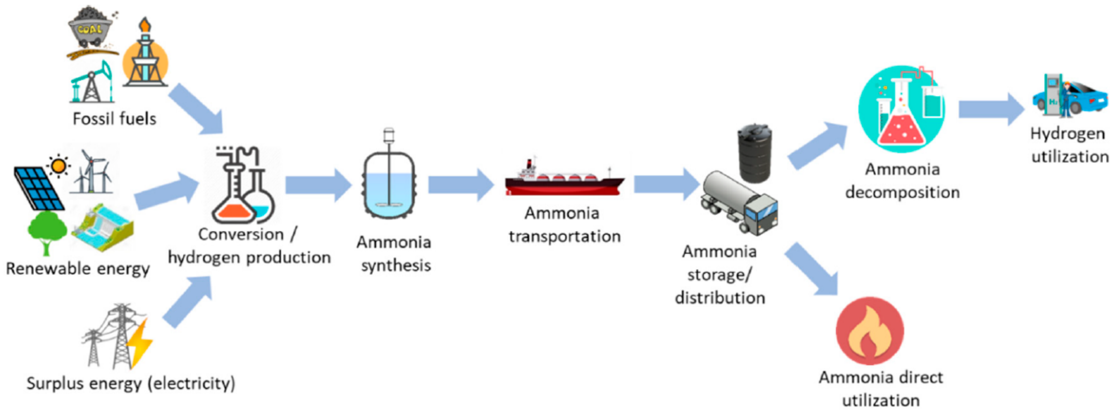
One significant disadvantage of methanol in the context of hydrogen carriers is the need for CO_2 in its production. While CO_2 can be sourced from renewable processes like direct air capture or reutilized from industrial emissions, its availability and cost affects the overall competitiveness of methanol as a hydrogen carrier. Direct air capture solutions are still very incipient, being necessary more technological development for actual use (Daggash et al., 2018). In terms of costs, recent studies suggest that renewable methanol could be priced between 400 and 600 U$D/ton when CO_2 is priced around 100 U$D/ton (Schorn et al., 2021).

Even though methanol is a notorious option to serve the purpose of a hydrogen carrier, this TEA study will only focus on ammonia, which is expected to be more promising out of all the hydrogen carriers. A deep dive on ammonia will be made in sequence.

2.2.2 Ammonia

Ammonia has acquired relevance as a hydrogen carrier due to multiple factors. As a starter, there is a lot of knowledge in terms of handling this substance, due to an existing ammonia fertilizer supply chain of 180 million tons per year (Cesaro et al., 2021). Its liquid form at mild conditions (-33 °C at atmospheric pressure or ambient temperature at approximately 10 bar) and high volumetric energy density (as compared in Table 3) make it an interesting carrier for hydrogen. Also, its liquid state enables pipeline utilization, resulting in reduced costs (Salmon; Bañares-Alcántara, 2021). An overview of ammonia as a hydrogen carrier is displayed in Figure 15

Figure 15: Ammonia as a Carrier Economy Overview



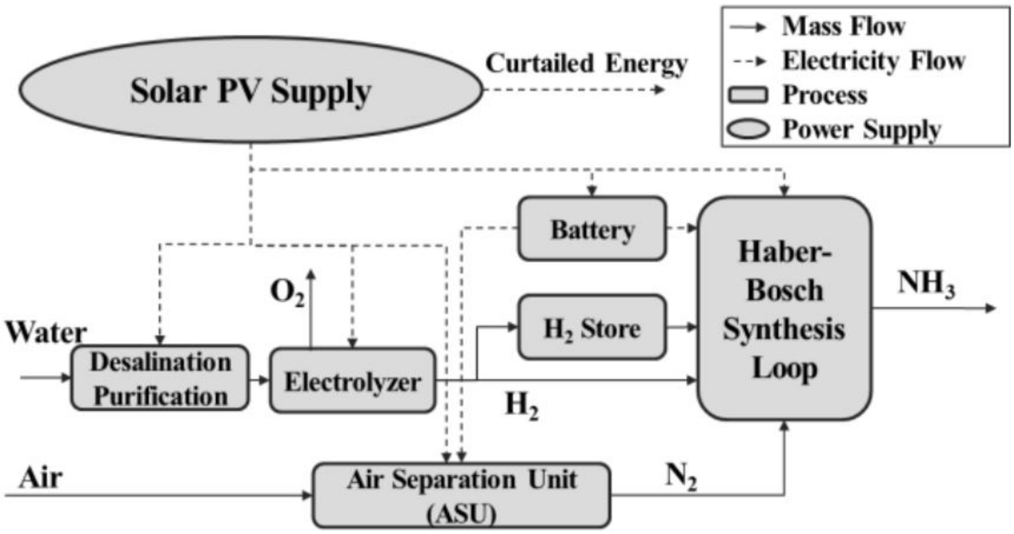
Fonte: Aziz, TriWijayanta and Nandiyanto (2020)

In the context of decarbonization, a global supply chain of green ammonia is also gaining interest. Not only to decarbonize the existing ammonia fertilizer supply chain, but also other industries, such as shipping transport (DNV GL, 2019). Cesaro et al. (2021) analyzed that, as a result of this trend, industrial-scale production of green ammonia is being assessed in terms of feasibility in multiple locations across the world, such as Chile, New Zealand, Australia, Norway and Saudi Arabia.

Ammonia's most popular production method is via Haber-Bosch synthesis, which uses an iron-based catalyst to produce ammonia from nitrogen and hydrogen mixtures. Currently, around 96% of worldwide hydrogen production for ammonia is derived from fossil resources, with the methods discussed in the previous chapter (Mayer et al., 2023). Therefore, even when thinking about a hydrogen economy driven by ammonia as a carrier, the sustainability of hydrogen production methods are still relevant. As a derivation from the hydrogen color scale, ammonia can also be classified in grey, blue or green, according to its hydrogen production type. Mayer et al. (2023) made a techno-economic assessment of blue and green production methods and found out that blue ammonia is more cost-competitive currently, if methane leakage and carbon capture challenges are mitigated (so that blue and green are comparable in terms of environmental impact). This is especially true if co-generation is utilized in blue ammonia production, and this means that gases from the ammonia synthesis loop that are rich in methane and hydrogen are used to generate heat and power, decreasing overall energy demand and making the cost of ammonia ballpark at around $400/ton with a 25% net margin.

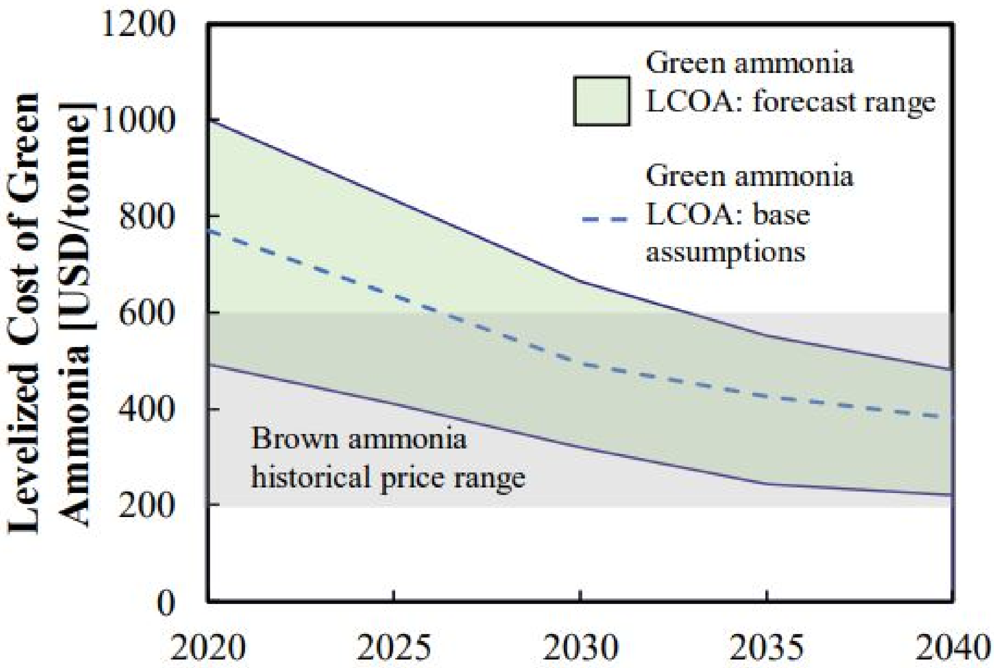
Cesaro et al. (2021) also developed a novel methodology for calculating the levelized cost of green ammonia (LCOA), based on a solar photovoltaic system with night-time battery storage integration, displayed in Figure 16, encountering values for LCOA under $400/t by 2040, inside the range of brown ammonia production, as showed in Figure 17. This is promising because decarbonizing all ammonia-based supply chains while maintaining cost-competitiveness will leverage a green hydrogen economy.

Figure 16: Scheme of Green Ammonia Synthesis



Source: Cesaro et al. (2021)

Figure 17: Forecasted Cost of Green Ammonia by 2040



Source: Cesaro et al. (2021)

A case study from (Makhloufi; Li, 2019) assessed the economic feasibility of different hydrogen carriers, including liquid hydrogen (LH_2), ammonia (NH_3), liquid synthetic natural gas (LSNG) and dibenzyl toluene (DBT). The study analyzed the LCOE from each carrier, produced using renewable electricity from three cities in Morocco, and included production, storage, conditioning, long-distance transportation and terminalling costs that were forecasted for 2030, 2040 and 2050. The conclusions where that NH_3 and LH_2 where the most promising forms of hydrogen transport when analyzing cost-effectiveness. When comparing the two in terms of drawbacks, LH_2 has the logistical problems related to hydrogen-handling, namely the need of high pressurization with appropriate equipment and risks of flammability and leakage, while the efficiency of NH_3's decomposition to hydrogen in scale is a question mark that makes it uncertain.

Ammonia can also be used directly to generate electricity: Cesaro et al. (2021) demonstrated that a combined cycle gas turbine system can deliver an LCOE at scale comparable to fossil-fuel-based plants with carbon capture strategies by 2040. However, even though there is research suggesting direct ammonia fuel cells are comparable to hydrogen fuel cells in durability and efficiency (Wan et al., 2021), their usage is limited and cost of ammonia fuel cells are not known (Salmon; Bañares-Alcántara, 2021). Further research in the literature is needed in order to make a techno-economic assessment of direct ammonia cells.

The conversion of ammonia to hydrogen can be done in multiple ways: thermal decomposition using multiple types of reactors, electrolysis and photocatalysis. The level of advancement of these technologies can be described in terms of a measurement system called Technology Readiness Level (TRL), which was developed by NASA in the 1970s for space missions and further incorporated for research and innovation projects by the International Organization for Standardization (ISO). A scale is provided to describe different levels of technology readiness, and the definition for each level is described on Table 5. Thermal decomposition using a fixed bed reactor is the most developed technology (TRL 9), while the other technologies are far from achieving a state-of-the-art technological maturity (TRL below 4) (Kanaan et al., 2023).

Table 5: Technology Readiness Level Scale (EU)

TRL Level	Level Description
TRL 1	Basic principles observed
TRL 2	Technology concept formulated
TRL 3	Experimental proof of concept
TRL 4	Technology validated in lab
TRL 5	Technology validated in relevant environment
TRL 6	Technology demonstrated in relevant environment
TRL 7	System prototype demonstration in operational environment
TRL 8	System complete and qualified
TRL 9	Actual system proven in operational environment

Source: Horizon Europe NCP Portal (2022)

Thermal decomposition is the chemical process that splits ammonia into H_2 and N_2. It is an endothermic reaction that requires high temperatures. Catalysts can be used to reduce the amount of heat needed for the reaction to occur (but still above at least 450 °C). Literature shows that the most common reactors are fixed bed and membrane reactors, both using ruthenium (Ru) or aluminum oxide (Al_2O_3) as catalyst and in temperature ranges close to 850 °C (Kanaan et al., 2023). After decomposition, the hydrogen and nitrogen mixture is separated in a pressure-swing adsorption (PSA) unit.

Plasma can once again be used for ammonia decomposition with a membrane reactor, usually made of palladium-copper alloys, that allows hydrogen to flow through one side of the reactor, remaining isolated from nitrogen and with high purity. Its benefits include lower operating temperatures, lack of need of a catalyst and purity of hydrogen produced.

On the other hand, there are challenges regarding energy consumption, as plasma requires significant electrical power, and membrane durability.

Ammonia can be also be decomposed into hydrogen and nitrogen through electrolysis, which uses electricity in an energy-intensive though effective mechanism; and photocatalysis, which uses sunlight and semiconductors in an inefficient though sustainable way.

2.3 Levelized Cost of Hydrogen (LCOH)

2.3.1 Definitions

Levelized Cost of Energy (LCOE) is a metric used to compare the cost-effectiveness of different technologies, considering how much energy it produces. It tells us the total cost of generating energy per unit of energy produced. In terms of costs, the present value of every component of building and operating an energy plant is put into account, such as capital expenditures (CAPEX), operating and maintenance (O&M), fuel, financing and others. To calculate the actual energy generated, a capacity factor is multiplied by potential output, which considers a plant operating at full capacity. Both costs and production calculations take into account the operational lifespan of the plant, which varies between different energy-generating technologies. LCOE is a key metric in comparing various energy sources, as it shows a standardized per-unit cost of energy generation. This way, decisions regarding investments, policy making, financing and energy planning are made possible with a number that is easy to understand (Chentouf et al., 2021). The mathematical formulation is expressed in equation 2.1, where C_t is the total cost in year t, E_t is the total energy produced in year t, and r is the discount rate.

$$\text{LCOE} = \frac{\sum_{t=1}^{T} \frac{C_t}{(1+r)^t}}{\sum_{t=1}^{T} \frac{E_t}{(1+r)^t}} \tag{2.1}$$

As hydrogen has increased in popularity as a sustainable alternative to energy production, as described earlier, a similar metric has been used for evaluating the cost-effectiveness of different hydrogen production technologies: the Levelized Cost of Hydrogen (LCOH). When analyzing the difference between types of costs in both metrics, LCOH requires the same inputs overall, but also feedstock costs, which refer to the cost of raw materials and other inputs, such as natural gas, water or electricity (for electrolysis). Besides that, the indicator presents cost per kilogram of hydrogen instead of an energy measurement. In a nutshell, LCOH's calculation is tailor-made for hydrogen production

(Lazard, 2023). LCOH is expressed mathematically by equation 2.2, where C_t is the total cost in year t, H_t is the total hydrogen produced in year t, and r is the discount rate.

$$\mathrm{LCOH} = \frac{\sum_{t=1}^{T} \frac{C_t}{(1+r)^t}}{\sum_{t=1}^{T} \frac{H_t}{(1+r)^t}} \tag{2.2}$$

It is worth noting that LCOH should be understood economically as the minimum selling price of hydrogen, considering a project with a positive net present value at a given discount rate (Industry; Umlaut, 2023). The actual price of hydrogen will depend on market and project-specific conditions. Figure 18 gives a better understanding of different cost or price metrics for hydrogen and its uses.

Figure 18: Hydrogen Financial Metrics and Uses

Metric	Users	Use	Data sources
Hydrogen price	Sellers and buyers	Market transactions	Commercial
Realised project cost*	Project developers, investors	Making site-specific projects within regional context bankable**	Commercial, confidential
Simple levelised cost of hydrogen	Policy makers	High-level analyses at pre-feasibility level	Publicly accessible, traceable

Source: Industry and Umlaut (2023)

2.3.2 Modelling

2.3.2.1 Variables

Calculating LCOH is fundamental for decision-making among several stakeholders, yet some studies found inconsistencies in calculations in the literature. Frieder (2024) found differnt ranges of values according to geographical and timeframe variations, which is expected. However, Industry and Umlaut (2023) examined several studies to find out that some crucial cost components where not detailed enough to ensure correct calculation, or had different classifications between studies, penalizing clarity. Thus, Industry and Umlaut (2023) proposed a pragmatic approach to calculating LCOH for electrolyzer plants, which is shown in Figure 19.

Figure 19: LCOH Input Variables to be Considered (Electrolysis)

Parameter	Notes
Electrolyser CAPEX	Account for CAPEX scaling influence.
Discount rate	Also known as Weighted Average Cost of Capital (WACC).
Electricity price	Should include all charges.
Electrolyser efficiency	Specific energy consumption including auxiliary power [kWh/kgH_2].
Electrolyser system lifetime	Major cost driver due to distribution of CAPEX.
Stack lifetime & replacement	Costs for stack replacement to be included in the CAPEX.
Stack degradation	Considered through average specific energy consumption.
Engineering, Procurement, Construction	Contains usually detailed planning and control, purchasing, execution of construction, installation work, and commissioning.
Buildings	Reflect cost difference between greenfield / brownfield.
Balance of Plant (BoP)	BoP typically includes power supply, water conditioning, and process utilities like pumps, process-value-measuring devices, and heat exchangers.
OPEX	Typically in the range of 1.5%–5% of CAPEX.
Compression	Consider compression costs for system output below reference pressure.
Hydrogen quality	Identified as a minor cost driver. Nevertheless, it is recommended to calculate with a 5.0 quality to ensure that there are no technical issues.
Water supply	Costs are to be considered if a seawater desalination plant is required.
Electrical grid	Assumption of an existing grid.
Contingency	Not taken into account in most studies.
Funding	Funding programmes strongly influenced by political conditions and vary over time.
Properties	Vary significantly between countries as well as urban and rural areas.
Hydrogen transport & storage	Multiplicity of further possible applications.
By-product revenues	Omit revenues from by-products (waste-heat, oxygen).

to be considered   individual decision   not to be considered

Fonte: Industry and Umlaut (2023)

Variables to model LCOH can be organized in four different categories: plant expenditures, production, distribution and financial variables. Plant expenditures encompasses all costs related to construction, operation and maintenance of the plant; production variables account for process modelling inputs; distribution includes infrastructure or adjustment costs for distributing hydrogen; and financial variables relate to market conditions and project funding.

Among plant expenditures, these can be divided in two big groups: capital expenditures (CAPEX) and operational expenditures (OPEX). CAPEX relates to long term investments in property, plant and equipment (PP&E), while OPEX refers to short term investments that are necessary to keep the plant operational. OPEX is further divided in variable and fixed OPEX, which accounts for costs that depend on how much is produced or not, respectively. In the literature, fixed OPEX is often modelled as a percentage of CAPEX per year, typically between 1.5%-5% (Industry; Umlaut, 2023), while variable

OPEX should be calculated according to process specifics. CAPEX also has key components that should be modeled and analyzed individually, and depend on production methods. For electrolysis, for example, not only cost of acquiring electrolyzers should be accounted, but also stack degradation and replacement. Creating a connection with the electrical grid should also be accounted for, if this infrastructure is not developed yet. Common CAPEX elements among all production methods are properties, buildings, balance of plant (BoP) and engineering, procurement, construction (EPC).

Properties vary between countries and rural or urban areas, so its value can range widely, although with low impact on LCOH, which is why Industry and Umlaut (2023) recommends not considering it on analysis. Buildings refer to the amount of basic infrastructure required onsite for greenfield projects, which are developed in land that has never been used previously, or revitalization and other adjustments required for brownfield projects, which are developed on previously used land for other purposes. Brownfield projects might benefit economically from existing infrastructure, such as roads and other utilities that might already be in place. Even though the buildings component can also differ significantly between regions, it is recommended to include in LCOH calculation due to its simple data gathering. The BoP component, though a quite generic term, is a major cost driver when referring specifically to power supply, water conditioning and process utilities such as pumps, process-value-measuring devices and heat exchangers (Industry; Umlaut, 2023). Finally, EPC also accounts for a major cost driver, and it encompasses all activities from planning to construction of the project, usually operated as turnkey contracts - a type of agreement where the contractor agrees to fully complete a project (in this case, building a facility) for immediate use by the client.

Another crucial category to analyze is production variables. In this group, there are multiple process-specific inputs that depend on the chosen production method. Nonetheless, universal variables can be discussed. First of all, there are raw material prices, that can be of great impact in the final LCOH, as some raw materials are more costly than others, and all of them fluctuate according to market conditions. Examples can be natural gas, ammonia or water. Energy prices are also relevant and work similarly. Secondly, there is system efficiency, which shows the amount of output energy produced given the amount of energy required in the process. The less efficient a system is, the more energy it requires to operate, which translates to more costs and potentially more GHG emissions or other environmental impacts. System efficiencies are normally expected to improve over the years, due to increasing research investments for technological advancements, and also vary significantly between production methods, as explored in the previous section. Thirdly, the system lifetime is a key component to be analyzed, as it determines how much hydrogen can be produced, and thus how diluted CAPEX will be. Finally, when possible, by-product revenues, such as carbon black on turquoise hydrogen production, can be taken into account to boost sales and improve financial margins (Mendes; Nascimento, 2022).

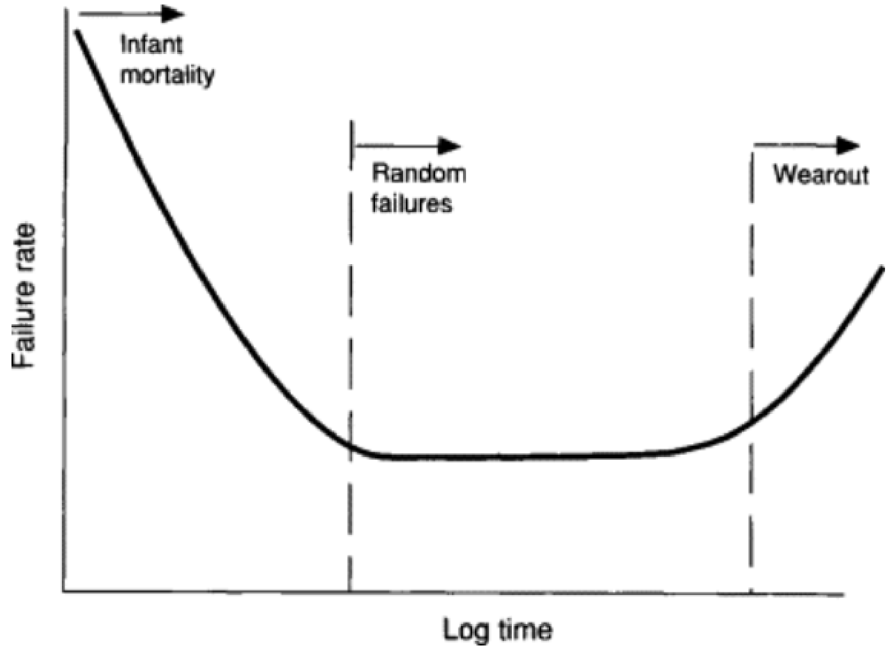
The distribution category includes compression, hydrogen quality adjustments, transport and storage costs. Compression might be necessary if output hydrogen is below reference pressure of 30 bar, which is possible when electrolyzers operate below that number, for example. Hydrogen quality adjustments might also be necessary for selling to the market, as some chemical processes generate hydrogen at low purity levels. However, purification is a minor cost driver (Industry; Umlaut, 2023). Transport and storage costs depend on specific applications and can range drastically. This type of disparity has also been found in other studies for other compounds, such as the work from Salmon and Bañares-Alcántara (2021) on the Levelized Cost of Ammonia (LCOA). To preserve the purpose of comparability, Industry and Umlaut (2023) propose drawing system boundaries that restrict analysis of distribution for onsite production, being acceptable to disregard all distribution components for a more pragmatic and consistent calculation of LCOH. This is in line with NREL's analysis for the U.S. Department of Energy (DOE) (Ramsden; Steward; Zuboy, 2009).

The last category to be discussed is the financial, which is simpler to grasp. This group includes the discount rate, which is very influential in output results due to the long-term nature of projects. Discount rates are also highly sensitive to market fluctuations and region-specific, despite correlation between regions. Other financial variables include funding programs, through government incentives, for example, and project contingencies. However, these tend to be very project-specific, which is why Industry and Umlaut (2023) recommends ignoring these components for a more precise calculation of LCOH across projects.

During the first years of plant operation, an operational ramp-up can occur, meaning there is a steady gain of efficiency, shown as a reduction in (O&M) costs over time. Due to the nature of a long-term project with heavy machinery involved, the pattern of the bathtub curve is also expected. The bathtub curve indicates a cost profile for O&M, according to maintenance demands. In the beginning, there may be higher maintenance needs due to initial equipment failures or adjustments, followed by a long period of steady, low-maintenance operation. Towards the end of the plant's lifetime, increasing failure rates are expected due to wear-outs and equipment aging, making O&M costs rise again

(Ohring, 1995). The bathtub behavior can be seen in Figure 20. These fluctuations in maintenance needs and operational efficiency can impact the O&M of a plant and influence LCOH.

Figure 20: The Bathtub Curve



Source: Ohring (1995)

Besides efficiency and maintenance, several variables involved in calculating LCOH are inherently uncertain due to fluctuating market conditions, geopolitical shifts, climate change and the evolving state of technology. These include variables such as CAPEX, O&M, raw material prices, energy prices, plant capacity and the discount rate, which can drastically affect the total cost of hydrogen production. As examples, energy prices can fluctuate based on renewable energy availability; the discount rate can vary due to macroeconomic conditions and interest rates; and technological breakthroughs such as the development of more effective catalysts for hydrogen conversion can significantly enhance efficiency. Given these uncertainties, Monte Carlo simulations are a valuable tool for analyzing LCOH (Andrade et al., 2024). By running multiple scenarios with a specified probability distribution for these variables, Monte Carlo simulations provide a range of costs instead of relying on a single deterministic estimate. This approach, which will be used in this study, is beneficial because it enables a proper risk assessment.

2.3.2.2 H2FAST Model

H2FAST is a project executed by the National Renewable Energy Laboratory (NREL) and funded by the U.S. Department of Energy (DOE) that aims to evaluate business cases and risk of investments in hydrogen systems through a financial model. It is a reference in hydrogen analysis, as it is provided by a government agency, and it has contributions and validations of multiple renowned people and institutions, such as the Investment and Finance Working Group (IFWG), Welford Energy, Energy Independence Now and others, which makes it reliable. It was designed for retail station owners that want to evaluate project ideas, governments and policymakers that need to determine how much incentives are required for infrastructure development, equity investors that seek financial returns or debt investors that aim to evaluate risk, and also academic institutions and other national laboratories that conduct research on the topic. Uses of the model in the literature is scarce, but existent (Marzouk (2023), for example).

The model requires diverse user inputs to be functional. This list includes plant capacity and utilization; capital costs and construction timeline; incentives; maintenance, labor and other fixed costs; feedstock consumption and prices, for example, regarding electricity and raw material prices, and also their escalation through the years; and financial parameters, such as depreciation schedules, interest rates, debt types, expected returns, among others.

As an output, the model generates the three main financial statements: income, cash flow and balance sheet statements, designed in a way that it is possible to visualize data considering both accounting standards: Generally Accepted Accounting Principles (GAAP) or the International Financial Reporting Standards (IFRS). The first one is primarily used in the United States and it is based on clear rules for maximizing precision, with the burden of a rigid structure that limits adaptability. IFRS, on the other hand, is based on principles, which enables greater flexibility, making it easier to compare across borders. Even though IFRS may provoke inconsistencies due to the openness of interpretation, it is more appropriated when discussing global economic viability of hydrogen production, as it is the most widely used across the globe.

The model spills outputs such as financial performance parameters, which include net present value (NPV), internal rate of return (IRR), payback period, break-even price and others; time series charts for all parameters; per-kilogram cash flows breakdown for assessing the influence of each component financially; and uncertainty distributions for risk analysis. For this type of assessment, it is possible to assign uniform distributions to any variable and run Monte Carlo Simulations (MCS) to evaluate risk, which will be further explained in depth.

Powerful analyses can be made through the H2FAST model by using the Goal Seek Excel native function, which allows the user to set a desired value for a cell ("goal") by changing the value of another cell. For example, if returns for a given hydrogen plant are not interesting for investors, policymakers can determine the amount of an incentive by using the Goal Seek function with the IRR cell and an incentive cell. This can be made for any type of "what-if" analysis, given an output cell and an input cell. There are also tools for assessing relevance of each parameter in the model in terms of LCOH, such as pareto and tornado charts.

A range of Excel spreadsheets are available at NREL's website to assist in calculating LCOH. Historically, each production method — whether through electrolysis, natural gas reforming, or other pathways — was represented by its own individual spreadsheet. These spreadsheets included specific data for each process, such as cost figures, efficiency rates, and various other modeling parameters. Recently, NREL introduced H2ALite, a consolidated spreadsheet tool that integrates multiple hydrogen production pathways into a single, clear and organized interface. H2ALite simplifies the modeling process by allowing users to switch between different production methods within the same file, making it easier to compare scenarios and analyze costs across a range of technologies. This all-in-one format not only improves user experience by eliminating the need for multiple documents but also improves modeling flexibility, clarity and transparency.

2.4 Cost Estimation for Chemical Processes

For a proper techno-economic assessment, adequate cost estimation techniques are necessary to ensure the validity of the analysis. Depending on the type of variable, cost estimation is rather straightforward, as a calculation based on price and volume according to market information and process modeling, respectively. This is usually the case for variables that are classified as variable OPEX.

However, CAPEX and some fixed OPEX cost lines are somewhat harder to estimate, as information about machinery and plant costs are not widely known, being usually quoted by suppliers and tailored to each client use case. Due to this, there are different strategies for modeling these costs. In the literature, there are two references that are most commonly used: Turton et al. (2018) and Peters, Timmerhaus and West (2003). In both of them, there are specific equations to estimate the cost of equipment, and other cost lines are derived from this main cost, based on tabulated factors. Examples of usage of these frameworks in the literature are the works of Devkota et al. (2024) and Avilez (2023) for Peters, Timmerhaus and West (2003) and Turton et al. (2018), respectively.

In the case of Turton et al. (2018), the base cost of equipment is defined by equation 2.3

$$C^0_{BM,i} = \exp\left(K_1 + K_2 \log_{10}(A) + K_3 \left[\log_{10}(A)\right]^2\right) \tag{2.3}$$

where K_1, K_2 and K_3 are constants for each type of equipment, A is a capacity parameter that is also specific to each equipment. The base cost of each equipment is then adjusted to inflation based on the Chemical Engineering Plant Cost Index (CEPCI), which is necessary because base equipment cost were modeled considering reference data for 2001, and is tabulated for every given year. Cost (C) is adjusted according to equation 2.4.

$$C_{\text{new}} = C_{\text{ref}} \times \frac{\text{CEPCI}_{\text{new}}}{\text{CEPCI}_{\text{ref}}} \tag{2.4}$$

Based on this inflation-adjusted base cost, the bare module cost can be calculated by multiplying the base cost to a factor (equation 2.5), which is then given by equations 2.6 and 2.7, in which B_1, B_2, C_1, C_2 and C_3 are constants specific for each type of equipment, F_m is a tabulated factor that varies based on the type of construction material and P is the equipment's operating pressure.

$$C_{BM,i} = C^0_{BM,i} F_{BM} \tag{2.5}$$

$$F_{BM} = B_1 + B_2 F_p F_m \tag{2.6}$$

$$F_p = \exp\left(C_1 + C_2 \log_{10}(P) + C_3 \left[\log_{10}(P)\right]^2\right) \tag{2.7}$$

With the bare module cost for each equipment, all of them are summed for a grouped value. Based on this value, other cost lines can be derived, such as grass-roots, administrative and other fixed expenses.

On the other hand, Peters, Timmerhaus and West (2003) provide a different approach, which is rather easier to grasp, with a high-level calculations. They provide tabulated costs for each type of equipment based on a given capacity. In the same way that Turton et al. (2018) indicates, these base costs should be adjusted by CEPCI, based on equation 2.4. These inflation-adjusted base costs are then adjusted by scale, described by equation 2.8.

$$C_{\text{base}} = C_{\text{ref}} \left(\frac{A}{A_{\text{ref}}} \right)^n \tag{2.8}$$

where C_{base} is the estimated cost for the desired capacity A, C_{ref} is the known cost for a reference capacity A_{ref}, and n is the scaling exponent, typically between 0,6 and 0,8, but depends on the type of equipment. Finally, based on the sum of the cost of each equipment, other indirect costs such as project contingencies, service facilities, piping and other cost lines can be calculated based on tabulated factors, that are different for different types of processing in a given plant (solid, solid-fluid and fluid). Though high-level estimations, the method proposed by Peters, Timmerhaus and West (2003) is usually preferred for early-phase feasibility studies, due to its flexibility, and often used in studies, such as Devkota et al. (2024).

On a final note, it is often the case that authors use a rule of thumb rather than proper cost estimation techniques. This is the case, for example, of a similar study on LCOH made by Kanaan et al. (2023). Even though it is preferred a more precise framework for a more detailed techno-economic assessment, it may sometimes be helpful to use such rules of thumb, in scenarios in which CAPEX costs are not the most relevant in the overall estimation.

2.5 Monte Carlo Simulations

Monte Carlo Simulations (MCS) are a type of computational algorithms that is widely used on problems that deal with uncertainty. The theoretical basis of MCS is probability theory and statistics, as its algorithm models any given outcome as a function of various uncertain parameters that have their own probability distributions. The essence of the algorithm is running multiple simulations and obtaining a distribution of potential outcomes. This approach is especially useful for estimating the probability distribution of complex systems, such as estimating LCOH, as it depends on technology, prices and economical parameters that are not analytically predictable (Rubinstein; Kroese, 2016).

For example, in a hydrogen production cost model, variables such as feedstock price, energy cost, and discount rate may each follow their own distributions. During each simulation, random samples are drawn from these distributions to calculate the corresponding LCOH. This process is repeated for every trial, n times, where n is sufficiently large to ensure the results capture the full range of possible outcomes.

Mathematically, this means that MCS is primarily used to estimate the expected value of a random output variable Y, with an unknown probability distribution. In this sense, the Monte Carlo estimate of the expected value of Y is given by equation 2.9

$$E[Y] \approx \frac{1}{n}\sum_{i=1}^{n} Y(X_{1,i}, X_{2,i}, \ldots, X_{k,i}) \tag{2.9}$$

in which n is the number of simulations, and $X_{1,i}, X_{2,i}, \ldots, X_{k,i}$ are the sampled input variables for the i-th simulation (Rubinstein; Kroese, 2016). This approximation is only true if the law of large numbers is considered, meaning that as the number of simulations approach infinity, the average result of the outcome converges to the expected value of that random variable X, which is described in equation 2.10 (DeGroot; Schervish, 2012).

$$\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} g(X_i) = E[g(X)] \tag{2.10}$$

This convergence is also seen when analyzing the standard error (SE) of the random output variable Y, as described in equation 2.11. As n tends to infinity, SE is expected to go to zero, converging with the expected value of Y.

$$SE = \sqrt{\frac{\mathrm{Var}(Y)}{n}} \tag{2.11}$$

MCS are more powerfully used when summarized as a probability distribution. This way, the decision-maker is able to understand the variability and risks associated with the complex system at hand, rather than just an approximation of the expected value of the output variable. That is why it will be used for assessing uncertainty and risk in this LCOH analysis.

2.6 Value at Risk (VaR)

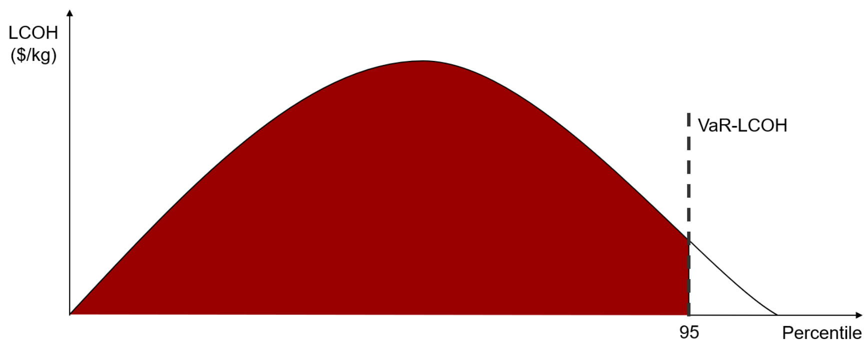
Value at Risk (VaR) is a well-established indicator for managing risk in a portfolio. It was introduced as a regulatory metric in 1994 at a G-30 conference, as a tail risk measure (Barrosa, 2015). It expresses the expected maximum loss of a portfolio, asset or variable that is subject to volatility, given a specific timeframe and a confidence level. Loss can be defined either as an absolute value or a percentage. Its biggest advantage is summarizing risk in a single number that is easy to understand, in the same unit of measurement of the target metric.

In its most general form, VaR can be calculated by integrating the probability distribution of a given outcome so that the probability of exceeding the worst possible value W is the confidence level c, as proposed by Jorion (2007) and described in equation 2.12.

$$1 - c = \int_{-\infty}^{W} f(w)dw = P(w \leq W) = p \tag{2.12}$$

The objective is to use a derived metric called VaR-LCOH, which is basically applying the VaR concept to an LCOH probability distribution, as done before by Andrade et al. (2024). A more intuitive way is to depict it as a tail's threshold, as exposed in Figure 21.

Figure 21: VaR-LCOH



Source: Own elaboration

There are multiple ways to determine VaR. A first approach is called the parametric method, which uses a defined probability distribution, mean and standard deviation as assumptions. This method is accurate, but it requires a known probability distribution that is suitable for the context and can be approximated to a normal distribution. Other methods do not require using the above equation, as VaR can be obtained by simply organizing data in order. A popular approach is taking historical data, ordering it and checking the value of the n-th percentile that corresponds to the requested confidence level. This is a much simpler method, and while it accounts for randomness of events that happened in the past, this can also lead to a biased VaR if there is not enough historical data available.

The Monte Carlo Simulation (MCS) method is a bridge between the two previously mentioned approaches. It starts out with a known probability distribution and defined mean and standard deviation, as does the parametric method. However, instead of calculating VaR deterministically, MCS is deployed for generating random values. Then, similarly with the historical method, these values are ordered and VaR is obtained for a determined confidence level. As pointed out by Jorion (2007), this method is the most powerful, as it is flexible and accounts for a wide range of exposures and risks. The more simulations, the more accurate the model tends to be, trading off with computational load.

This study will use an MCS approach for calculating VaR-LCOH, in order to assess the risk in green hydrogen investments in Brazil. Therefore, the results can be analyzed considering also what could happen in pessimistic scenarios.

3 METHODOLOGY

This study's objective is to make a techno-economic assessment of hydrogen produced by thermocatalytic decomposition of ammonia, using a fixed bed reactor, which is the most common method for producing hydrogen from ammonia (Rizi; Shin, 2022). The analysis will be modeled using NREL's H2A Lite Excel Model for reliable and flexible calculation (NREL, 2020).

The first step is to define process specification. This study will be based on a project being made by the Chemical Institute of the University of Sao Paulo (IQ-USP) on the same topic. This project, developed by Leonardo Avilez and coordinated by Prof. Dr. Rita Alves, models the same process of thermocatalytic decomposition of ammonia, using a fixed-bed reactor heated by a furnace (Alves; Avilez; Mereguete, 2024). The chemical modeling of the process has already been completed and validated by the team. However, the authors are in the process of publishing an academic article on the topic, with no definitive completion date. Even though the authors have agreed to share process data for use in this study, it will not be fully disclosed in respect of their ongoing work.

The work done by Alves, Avilez and Mereguete (2024) will not be the only basis for the modeling in this study. Additional references from academic articles will also be used. Firstly, the report from Industry and Umlaut (2023), which provides a guide for a more consistent and reliable LCOH calculation, will be used in the selection of relevant variables to include in the model. Although this report was developed considering hydrogen production via electrolysis, some basic principles of variable prioritization can be adapted for this study. To complement this, other academic articles that calculate the LCOH for the same thermocatalytic decomposition of ammonia using a fixed-bed reactor will also be taken into account. Finally, classic references on cost modeling in the chemical industry, such as Peters, Timmerhaus and West (2003) and Turton et al. (2018), will be deployed for deriving cost lines from CAPEX and OPEX.

Based on these sources, values will be assumed for all of the input variables of the H2A Lite Excel Model, which will be run for a deterministic result of LCOH of hydrogen produced by thermocatalytic decomposition of ammonia using a fixed-bed reactor. In addition to the this result, a sensitivity analysis will be conducted to understand the impact of each input variable on LCOH, the output variable. With these results, it will be possible to compare the modeled project with other academic studies that follow the same methodology.

In the second phase, variables with high uncertainty will be deemed as random, being assigned to probability distributions, particularly triangular distributions, based on literature data. Several experimental simulations will be run, where the baseline value of each random variable will be altered (the probability distribution is maintained constant) to assess the impact of this variability on hydrogen levelized cost. Finally, the VaR-LCOH will be calculated, following the methodology provided in Andrade et al. (2024). Based on these analyses, this study will evaluate the economic feasibility with embedded risk analysis of using green ammonia for large-scale hydrogen production.

3.1 Process Modelling and Assumptions

As previously mentioned, NREL's H2A Lite model requires various process inputs to calculate LCOH. The model includes specific inputs for straightforward costs, such as capacity, inflation rate, installation cost, among others. However, it remains flexible enough to accommodate user-defined costs, whether they are one-off costs like CAPEX, fixed costs determined on an annual basis, or variable costs defined per kilogram of hydrogen produced, as in the case of using ammonia as a feedstock.

Firstly, process modeling variables will be discussed, which include capacity, utilization, system lifetime, energy consumption (considering electricity and cooling water), and ammonia consumption per kilogram of hydrogen. These variables, having been modeled in the project conducted by Alves, Avilez and Mereguete (2024), are strongly based on the data provided by the authors. The process modeling data is presented in Table 6.

Table 6: Process and Plant Parameters

Process Parameters	**Value**	**Reference Unit**	**Source**
Capacity	751.997	kg/day	Alves, Avilez and Mereguete (2024)
System Lifetime	15	years	Alves, Avilez and Mereguete (2024)
Utilization	91,3	%	Alves, Avilez and Mereguete (2024)
Energy Consumption (Electricity + Cooling Water)	2,22	kWh/kg H_2	Alves, Avilez and Mereguete (2024)
Ammonia Consumption	8,11	kg/kg H_2	Alves, Avilez and Mereguete (2024)

Source: Own elaboration

Secondly, cost estimation parameters will be discussed, starting with CAPEX. The first step was to identify what are the relevant CAPEX lines to be included in this study. As mentioned before, this decision-making was based on the report from Industry and Umlaut (2023) and other similar studies that calculate LCOH based on ammonia decomposition. Variables that were considered impactful were the cost of equipment, installation cost, cost of buildings, BoP, service facilities and EPC. These are all cost components that are estimated in similar studies, such as Devkota et al. (2024). Other CAPEX variables such as properties and project contingency were deprioritized, following the reasoning on Figure 19 (Industry; Umlaut, 2023).

With the variables defined, cost estimations were based on Peters, Timmerhaus and West (2003), which provides a guide for deriving several cost lines based on the cost of equipment, through a reference table that shows different costs and their respective factors, specifically for industrial plants that processes fluids. To estimate the cost of equipment itself, Alves, Avilez and Mereguete (2024) employed an empirical formula created by Turton et al. (2018), based on reference constants for each equipment type and capacity parameters for scaling adaptation. The calculated cost of equipment and other CAPEX lines, along with their own factors, are displayed in Table 7.

Table 7: CAPEX Parameters

Cost Line	Factor (%)	Value ($)	Source
Cost of Equipment	100	78.013.900	Alves, Avilez and Mereguete (2024), Turton et al. (2018)
Installation cost	47	36.666.533	Peters, Timmerhaus and West (2003)
Buildings	18	14.042.502	Peters, Timmerhaus and West (2003)
BoP (Instrumentation, Piping, Electrical)	95	74.113.205	Peters, Timmerhaus and West (2003)
Service Facilities	70	54.609.730	Peters, Timmerhaus and West (2003)
EPC (Engineering, Procurement, Construction)	74	57.730.286	Peters, Timmerhaus and West (2003)

Source: Own elaboration

In sequence, fixed OPEX values were analyzed. For this set of costs, the framework provided by Industry and Umlaut (2023) is not the most appropriate, as it provides only a range of estimates based on CAPEX, without the required level of granularity for this study. Therefore, to define important OPEX cost lines, this study referred to other similar studies that calculate LCOH based on an ammonia decomposition process, such as Devkota et al. (2024) and Kanaan et al. (2023), alongside textbook references from Peters, Timmerhaus and West (2003) and specific data from Alves, Avilez and Mereguete (2024).

The variables that were deemed as relevant for OPEX were catalyst replacement, labor, supervision, maintenance and working capital costs. The former two were calculated by Alves, Avilez and Mereguete (2024), while the latter three were estimated given the factors from Peters, Timmerhaus and West (2003) of 15% of operating labor cost, 6% of CAPEX and 15% of CAPEX, respectively. Catalyst replacement was assumed to be needed every 5 years, a common assumption on related studies (Kanaan et al., 2023), resulting in an annual cost of $3.351.807, except for the first year, when the full value of $16.759.037 should be considered. Fixed OPEX cost lines are shown in Table 8.

Table 8: Fixed OPEX Parameters

Cost Line	Value ($/year)	Source
Catalyst Replacement*	3.351.807	Alves, Avilez and Mereguete (2024), Kanaan et al. (2023)
Labor	1.000.481	Alves, Avilez and Mereguete (2024)
Supervision	150.072	Peters, Timmerhaus and West (2003)
Maintenance	18.910.569	Peters, Timmerhaus and West (2003)
Working Capital	55.619.322	Peters, Timmerhaus and West (2003)

Source: Own elaboration

*Note: For the first year, 100% of catalyst cost is considered

Another side of OPEX is variable costs, which are defined per amount of hydrogen produced. The amount of feedstock to produce one kilogram of hydrogen was considered a process parameter, defined in Table 6. However, to determine the cost itself, a price should be estimated for each feedstock. Power prices were determined based on a study from KPMG (2022) that assessed parameters for evaluating the cost of the green hydrogen business case and found that a range of 0,05-0,07$/kWh was the most appropriate for the european context, which is why the deterministic estimate was assumed to be 0,06$/kWh. The price of green ammonia was also determined based on estimate ranges from two different studies that converge to an average of 0,64$/kg (Lee et al., 2023), (Cesaro et al., 2021). Prices for each feedstock are displayed in Table 9.

Table 9 also presents two financial parameters applied in this study. The first one is the income tax rate, which was used for the Netherlands (PwC, 2024). The second is the discount rate: this variable is less dependent on the specific hydrogen use case, as it reflects the broader economic environment and represents the cost of capital itself, given macroeconomic conditions, alternative investment opportunities and investor risk tolerance. For this estimate, multiple European studies that made an economic assessment of capital-intensive industry projects were taken into consideration. In the collected sample, the lowest value encountered was 8% from Kanaan et al. (2023) and Pozo and Cloete (2022), while the highest was 12% (Frowijn; Sark, 2021). Market reports from KPMG

(2023) found a 8,1% discount rate for the industrial manufacturing sector in Europe in 2023. For this study, a more conservative discount rate of 10% will be used, given that no debt structure will be analyzed. Nonetheless, different values for the discount rate will be further analyzed to understand the impact of this variable in LCOH.

Table 9: Financial Parameters

Financial Parameters	**Value**	**Reference Unit**	**Source**
Energy Cost	0,06	$/kWh	KPMG (2022)
Ammonia Cost	0,64	$/kg	Lee et al. (2023), Cesaro et al. (2021)
Discount Rate	10	%	Similar studies, KPMG (2023)
Income Tax Rate	25,8	%	PwC (2024)

Source: Own elaboration

One final parameter to assess in the model are the cost escalation rates. Considering that this is a project with a 15-year operational lifetime, it is assured that the deterministic costs should change overtime. For most of them, the general inflation rate of 2% was applied. However, there is one parameter that is expected to have a descending trend due to technological advancements, which is the cost of green ammonia. Based on the projection made by Cesaro et al. (2021), the LCOA is expected to decrease at a -3,3% rate annually until 2040. However, for a more conservative approach, the escalation rate of ammonia cost in this study will be set to -1,5%.

3.2 Random Variables

One of the innovations this study aims to introduce to the scientific community is incorporating the variability of some key variables in the LCOH calculation, when considering ammonia as a carrier. This approach, which introduces a notion of risk in the final cost by running multiple simulations with different ranges of values, was used similarly in the work of Andrade et al. (2024). Therefore, the selection of which variables will be considered random will now be discussed.

All of the random variables will be modeled as a triangular distribution, for simplicity purposes, requiring a minimum, maximum and mode values. This is done because NREL's H2A Lite Excel Model can only process triangular probability distributions for its embedded risk analysis using MCS. This can be seen as limitant factor, however, the decision-making of a probability distribution to some of the variables that will be considered random could be content for one whole article. Since the purpose of this study is mostly based on cost, it was considerate appropriate to use this simplification that the deployed model permits.

The first variable to be discussed in this context is the discount rate, as previously mentioned. In many studies that assess the time value of money, it is common to conduct some form of sensitivity analysis (Brealey; Myers; Allen, 2020). This is done for two main reasons. Firstly, the determination of a discount rate is not strictly deterministic — while renowned economic models can assist with this, such as the model by Modigliani and Miller, who developed the Weighted-Average Capital Cost (WACC) formula based on the cost of equity and the cost of debt, the definitions rely on concepts like the risk-free rate, risk premium, and beta, which are conceptual and often approximate. In investment decisions, it is quite common to base the discount rate on similar past projects (Brealey; Myers; Allen, 2020). The second reason is that the discount rate frequently emerges as a highly impactful variable within investment analyses. Therefore, given its significance and moderate precision, it is crucial to run simulations using different discount rates to capture the range of potential outcomes.

To decide on minimum and maximum values for the discount rate, similar European studies were evaluated. As mentioned before, the lowest rates encountered were 8%, while the highest were 12%. Apart from similar studies in the literature, market sources were also consulted, such as the also previously cited report from KPMG (2023). In this sense, the discount rate was considered to range ±20% from its base value of 10%.

The second variable to be classified as random was the cost of ammonia. Following the same reasoning from the discount rate, the variability of this cost is also relevant because of the impact in LCOH and expected variability in the upcoming years. In terms of impact, the effect of this lever is quite obvious, as most studies show that ammonia is the biggest cost when producing hydrogen through thermocatalytic decomposition (Kanaan et al., 2023), (Makhloufi; Kezibri, 2021). In regards to expected variability, it can be argued that the cost of green ammonia is expected to decrease in the following years, as projected by Cesaro et al. (2021). However, as a commodity, its prices can vary according to market cycles or geopolitical events, as has happened in 2021, when prices surged in the fertilizer industry (Wongpiyabovorn; Hart, 2024). Therefore, setting a probability distribution for the cost of ammonia is essential.

The definition of lower and upper values were based on the work of Cesaro et al. (2021) on LCOA projection until 2040, shown in Figure 17. In most years, the cost of ammonia ranges ±20% from its base value (dotted blue line). Due to this, this is the variability that can be expected from the cost of ammonia and will be considered in this study.

The last variable to be considered random is the energy cost. Reasoning behind this decision is the fact that, although not commonly the most impactful, it also presents variability from market oscillations. The basis for this definition was the report from KPMG (2022) on cost evaluation of hydrogen business cases, which dedicated a section for power prices. The variability presented in this report was from 0,05$/kWh to 0,07$/kWh, accounting for an approximate ±15% range, which will be used in this study.

As for the other variables, no other was considered random as there is no strong evidence of expected variability: most process and other cost parameters are defined considering known technologies and equipment. All of the random variables and their respective variability are shown in Table 10.

Table 10: Random Variables

Random Variable	**Variability**	**Minimum Value**	**Maximum Value**	**Source**
Energy Cost	±15%	0,05	0,07	KPMG (2022)
Ammonia Cost	±20%	0,51	0,77	Cesaro et al. (2021)
Discount Rate	±20%	8%	12%	Similar studies, KPMG (2023)

Source: Own elaboration

4 RESULTS

4.1 Deterministic Analysis

The model was run for the deterministic scenario, assuming the base case values for all variables. The obtained value of LCOH was $5,46/kg, considering an internal rate of return (IRR) of 10%. The net present value (NPV) was zero, as the model was set to calculate the LCOH that would breakeven the specified IRR. Finally, the nominal payback was 11 years - this means that in absolute values, without discounting cash flows, the investors receive their money back after 11 years. This is different from the discounted payback, that is equal to the system lifetime, considering the assumed IRR of 10%. The deterministic results are shown in Table 11.

Table 11: Deterministic Results

Metric	Results	Reference Unit
Levelized Cost of Hydrogen (LCOH)	5,46	$/kg
Internal Rate of Return (IRR)	10	%
Net Present Value (NPV)	0	$
Payback	11	years

Source: Own elaboration

Comparing these results with other studies from the literature is important to elucidate key learnings and potential breakthroughs. However, for proper comparison, the studies should be reasonably similar. For this purpose, this study will be compared to the works of Makhloufi and Kezibri (2021) and Kanaan et al. (2023), which both present LCOH results for a large scale plant located in Europe that uses green ammonia decomposition to produce hydrogen. The high-level comparison of both studies is shown in Table 12.

Table 12: Results Comparison

Study	LCOH ($/kg)	Ammonia Price ($/kg)	Discount Rate (%)	Lifetime (years)
Makhloufi and Kezibri (2021)*	5,16	0,48	10%	30
Kanaan et al. (2023)	8,00	1,00	8%	30
This study	5,46	0,64*	10%	15

Source: Own elaboration

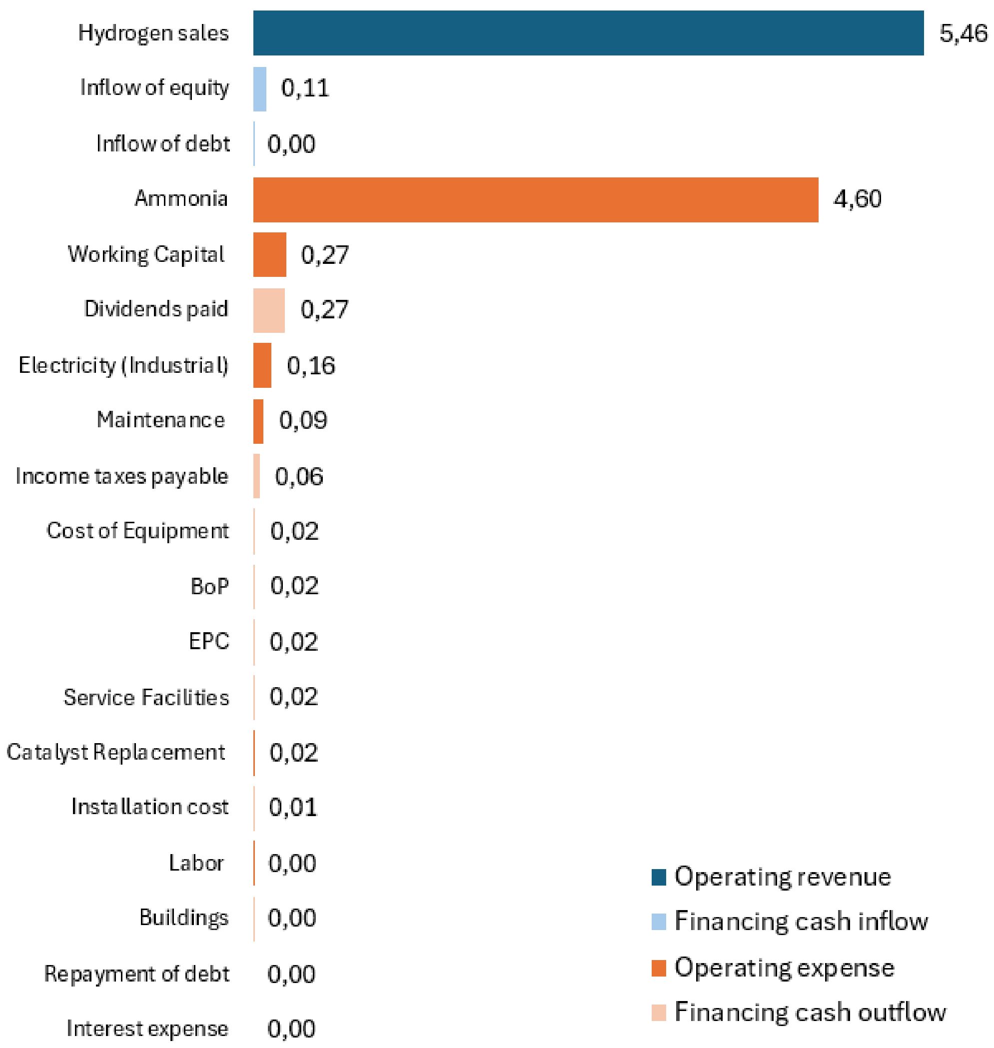
*Note: Values from Makhloufi and Kezibri (2021) were converted from euros to US dollars using a 1,07 exchange rate; the price of ammonia in this study decreased 1,5% annually

The obtained value of $5,46/kg resonates with the $5,16/kg (converted from euros to dollars using a 1,07 exchange rate) achieved in Makhloufi and Kezibri (2021). This is mainly due to the lower price of ammonia considered, at approximately $0,48/kg. In the sensitivity analysis presented in that study, the price of $0,6/kg would lead to an LCOH around $6/kg, which is close to the $5,94/kg from this analysis if ammonia cost is assumed the same for the whole period (in the base case, a de-escalation rate of -1,5% is considered).

On the other hand, the obtained LCOH for this study was much lower than the one from Kanaan et al. (2023), at $8/kg. Once again, what explains the difference is the cost of ammonia, assumed to be $1/kg in that study. If the model of this study is adjusted for this fixed price of ammonia, then the new LCOH encountered is $8,86/kg, with the new difference being due to a higher discount rate and also cost of equipment, which translates to higher CAPEX, maintenance and working capital costs. Therefore, it can be said that the results obtained in this study verse with other similar work from the literature.

When analyzing the breakdown of costs and revenue, the model provides a detailed view of each component, which is shown in Figure 22. In terms of operating components, the only source of revenue is assumed to be hydrogen sales itself, while the largest cost driver is ammonia, representing $4,6/kg or about 84% of the total LCOH. This reflects the significant influence of this specific feedstock, as expected and seen in other studies from the literature (Kanaan et al., 2023), (Lee et al., 2019) (Lim et al., 2021), (Makhloufi; Kezibri, 2021). Other expenses, such as working capital and energy, also contribute to the operating expenses but to a much smaller extent when compared to ammonia.

Figure 22: LCOH Breakdown

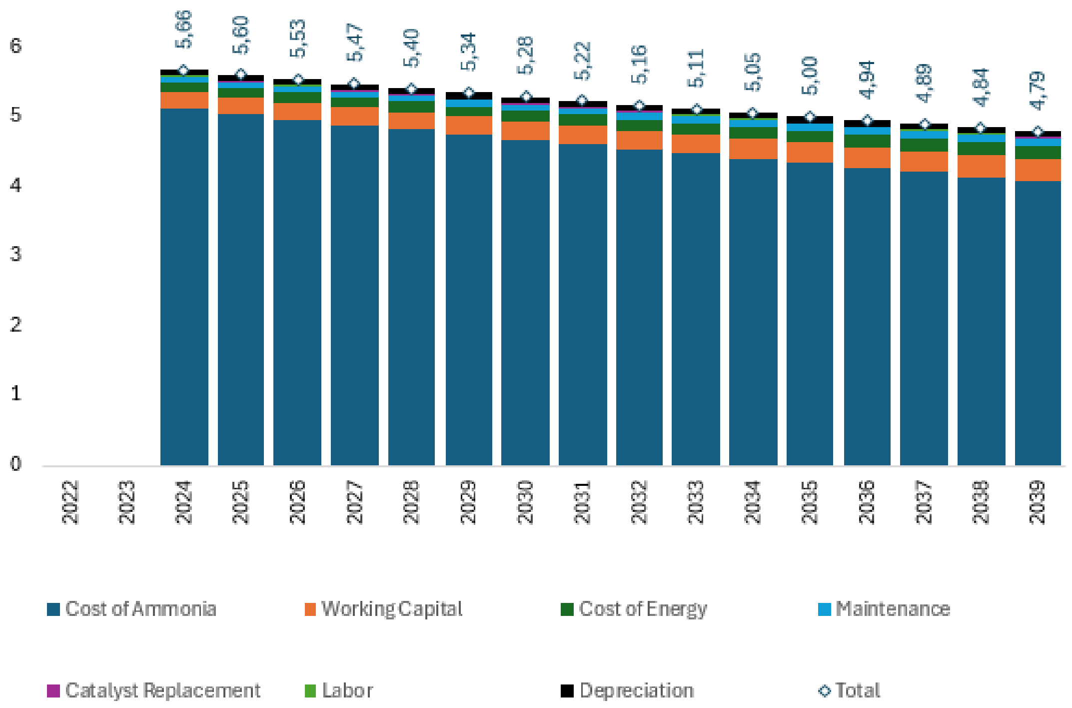


Source: H2A Lite Model with own data

The project financing is assumed to be entirely equity-based, which is why all of the financing cash inflow is equity. Dividends paid are shown as financing cash outflow, which represents the return to those equity investors based on an assumed 10% IRR.

Even though green ammonia is the biggest cost lever, its price is expected to decrease in the future, which translates in the model to a -1,5% annual de-escalation rate. Therefore, it is relevant to analyze the impact of ammonia along the lifetime years, as other costs increase with inflation rate and ammonia goes in the other direction. As depicted in Figure 23, even though there is a clear decrease in the component that represents ammonia, with a slight increase in working capital and cost of energy representativeness, ammonia remains by far the largest portion of operating costs.

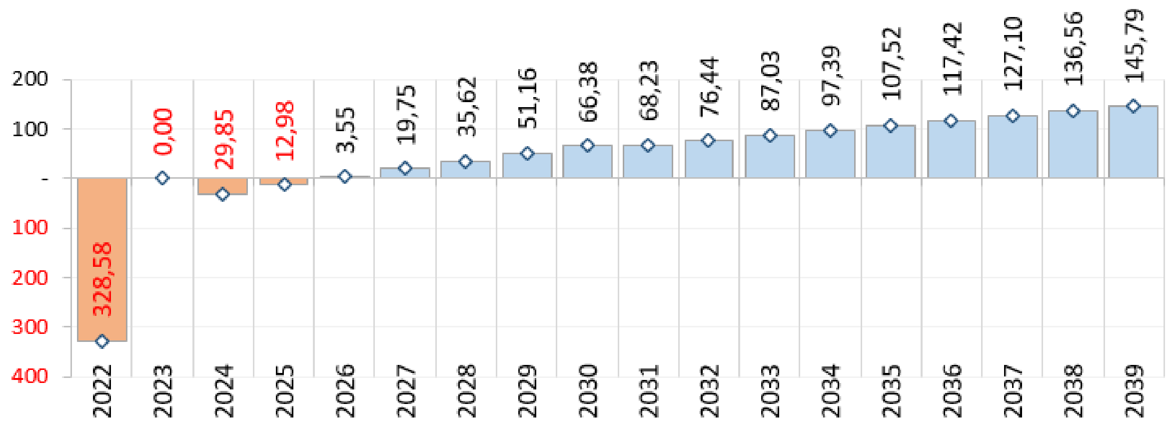
Figure 23: Evolution of Operating Costs



Source: H2A Lite Model with own data

Looking further into financial information, it is possible to analyze cash flows from an investor's point of view. Figure 24 shows exactly how a large amount of cash is required at the start of the project to cover all of the CAPEX. NREL built the model in a way that construction takes place a year before actual plant startup, which is why 2023 appears with no cash flow movement - the injection of capital is configured to occur on the last day of 2022. Actual sales start only in 2024, with a negative cash flow that soon turns positive on the third year of operation (2026), and increasingly positive until the last year of operation, due to the assumed constant hydrogen demand and decrease in costs depicted in Figure 23.

Figure 24: Investor Cash Flow ($Millions)



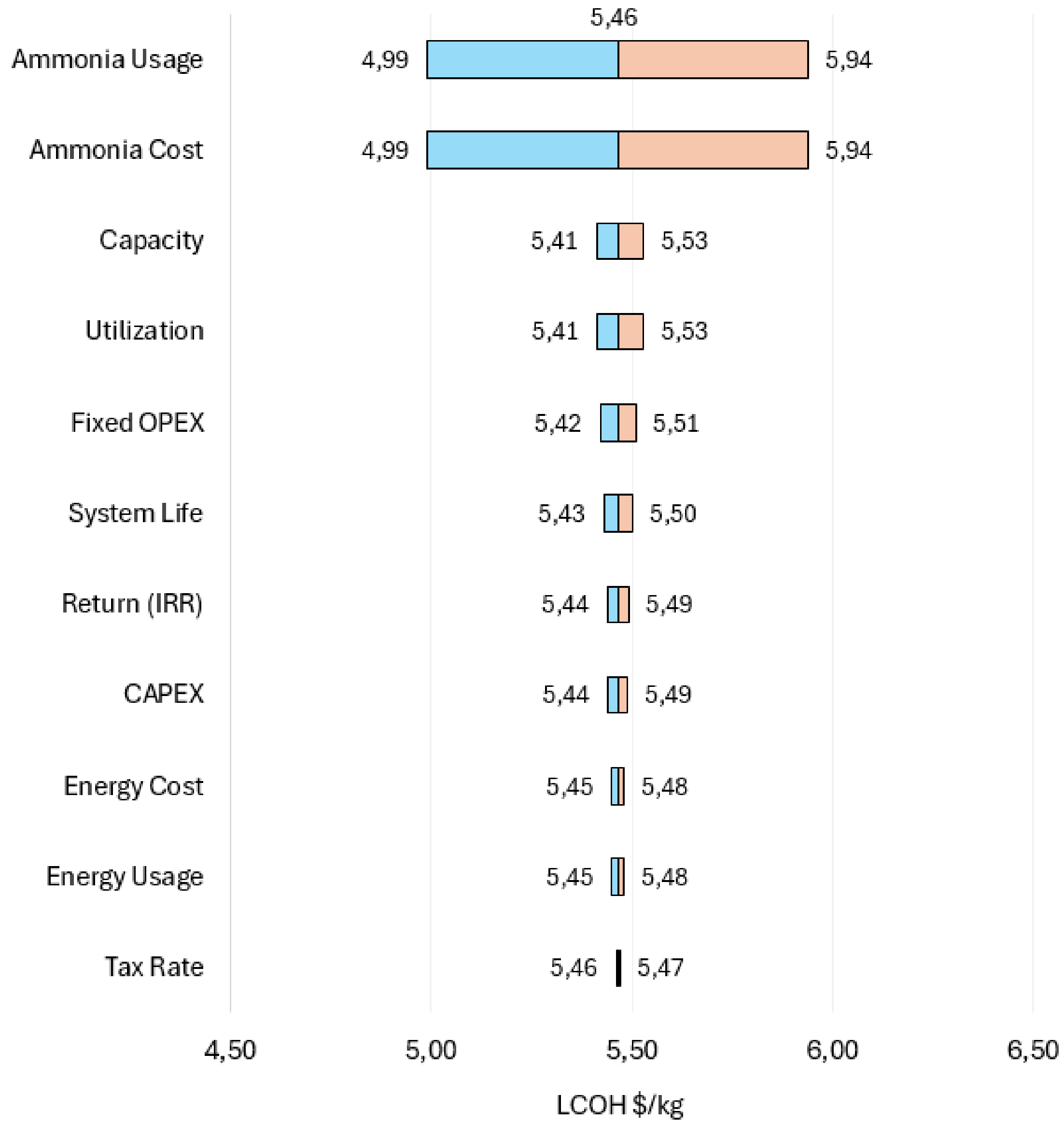
Source: H2A Lite Model with own data

4.2 Sensitivity Analysis

The deterministic scenario is useful for the definition of a base case, so that it can be used as reference and be compared to other scenarios. However, it does not provide enough information about which variables are the most influential in the model. In terms of costs, the breakdown exposed in Figure 22 provides insight into this question. However, there are many other variables that were used in the model that are not cost lines, and thus it is equally relevant to understand the impact of these variables to the final LCOH.

To provide a clear picture on this topic, a sensitivity analysis will be performed. The method behind this type of analysis is modifying one variable at a time, keeping all others constant, to see what is the impact on LCOH. All modifications are proportional, so that there is no bias for different types of variables. In this exercise, a baseline variation of ±10% was used, and fixed OPEX costs and CAPEX costs were aggregated in to one single variable so that the greater impact is clearer. The results of the sensitivity analysis are shown in Figure 25.

Figure 25: Sensitivity Analysis



Source: H2A Lite Model with own data

Once again, it is shown that ammonia usage and cost are the most impactful variables in the model. An increase 10% in either of them would raise LCOH to \$5,94/kg, 8,7% higher than the base case. They are equally influential, as they are directly proportional. In sequence, the variables with greater influence are capacity and utilization, which link directly to hydrogen sales, the only source of revenue, which also makes sense in terms of impact. The system lifetime's impact appears for the first time in this analysis, as it is a variable that determines revenue indirectly and the depreciation curve, or in other words, it is a proxy for asset optimization. If the lifetime would be of 30 years, then it means that the same equipment could generate the same amount of hydrogen for more years, which translates to a lower LCOH. This behavior of being inversely proportional to LCOH also is true for capacity and utilization - the higher these values are, the more efficient the system is and the lower the final cost. Finally, other variables that appear with a minor impact are fixed OPEX, CAPEX, IRR and energy cost and usage, which are expected as they are directly linked to specific costs.

When comparing the obtained hierarchy with the comparable studies, the highlighted variables are in agreement. Makhloufi and Kezibri (2021) restricts its sensitivity analysis to ammonia, energy and catalyst costs, finding ammonia to be the most sensible. On the other hand, Kanaan et al. (2023) performs a quite similar sensitivity analysis in a tornado chart format, finding the same hierarchy between ammonia, capacity, utilization and energy cost. The difference is that capacity is broken down into specific equipment efficiencies, which is not possible in this study, as this type of data was not disclosed from Alves, Avilez and Mereguete (2024). Nonetheless, the level of sensibility is quite similar as a whole.

4.3 Uncertainty Analysis

In this section, uncertainty will be incorporated into the LCOH calculation. This is the central point of innovation in this work compared to other studies in the literature on LCOH considering ammonia. The purpose of adding uncertainty to this analysis is understanding the risk embedded in the deterministic scenario. As an investment, green hydrogen plants based on ammonia should also be evaluated based on returns and risk. In this sense, triangular probability distributions will be assigned to three variables: the discount rate, the cost of ammonia, and the cost of energy. The defined variation and the reasoning for each of these variables are presented in Table 10.

For this analysis, 5000 MCS interactions were performed, generating 5000 LCOH values. To do this, NREL's H2A Lite Model was run five different times, since it only allows for 1000 simulations at a time. Each of them had their own unique values, and the data was later consolidated in to one single database of 5000 observations. The statistics for the simulations are shown in Table 13.

Table 13: MCS Statistics

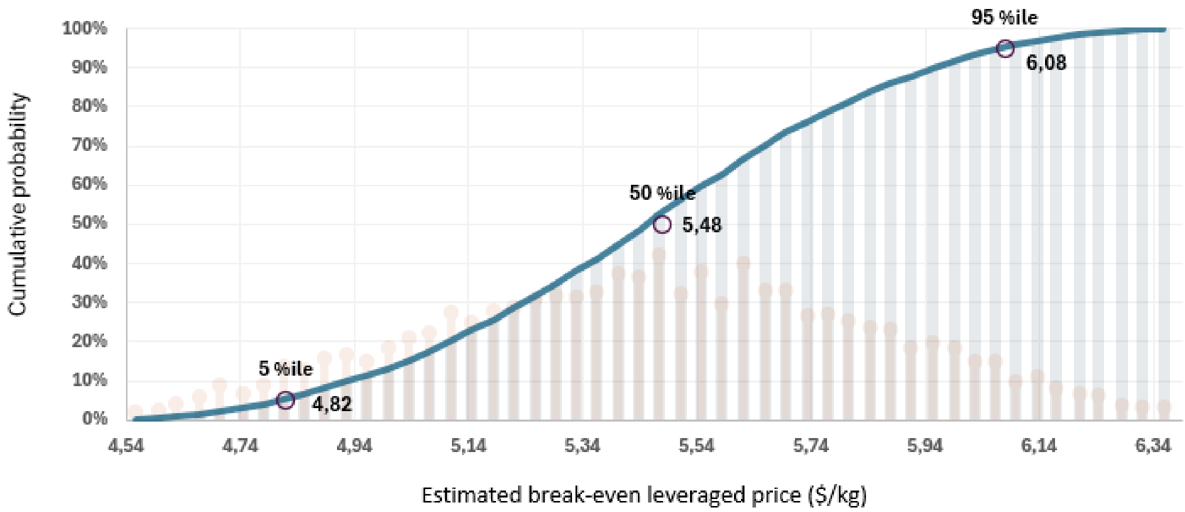
MCS Statistics	LCOH Values
Trials	5000
Base Case	5,46
Mean	5,47
Median	5,48
Standard Deviation	0,53
Variance	0,28
Skewness	0,00*
Kurtosis	1,81
Coefficient of Variation	0,10
Minimum	4,54
Maximum	6,34
Range Width	1,80
Mean Standard Error	0,01

Source: Own elaboration

*Note: Skewness is not exactly zero, but it rounds up to 0 with two decimal places

Looking at the results, it is clear that the range of LCOH is quite wide, from $4,54/kg to $6,43/kg, showing how impactful the random variables are to the model. The median and the mean were quite close to the the deterministic results, at $5,47/kg and $5,48/kg, respectively, which implies a higher level of confidence on the base case scenario. However, it can also be said that this is the case because of a symmetric distribution, revealed by a close to zero skewness, implying that the assumed probability distributions are quite balanced - which they are, as triangular distributions with equal maximum and minimum variation in absolute terms. This aspect of the designed probability distributions are also likely to explain the low mean standard error (MSE) and low kurtosis value of 1,81, indicating a platykurtic distribution, which mean it's flatter (few peaks) than a normal distribution with light tails. These values and implications are consistent with the cumulative probability distribution and embedded histogram of LCOH in Figure 26.

Figure 26: Cumulative Probability Distribution of LCOH



Source: H2A Lite Model with own data

Analyzing the cumulative probability distribution in Figure 26, it is possible to grasp what the VaR-LCOH would be with a 95% confidence interval by looking at the 95th percentile of \$6,08/kg. This means that there is only a 5% chance that LCOH would be greater than \$6,08/kg, about 11% higher than the base case. As a best-case scenario, the 5th percentile, LCOH would be about \$4,82/kg.

After including uncertainty into the analysis, it is now possible to compare hydrogen produced via ammonia to other production technologies costs, as explicit in Table 14. Among renewable production methods, ammonia outperforms all other energy types, according to costs provided by Center on Global Energy Policy at Columbia University (2021) for the US. However, it is important to note that the cost of these technologies is expected to decrease with technological advancements to come, and they might out perform ammonia in the near future. Despite all of that, all renewable energy types are at least twice as expensive as SMR methods, which still shows a big gap between the current standard and the renewable technologies.

Table 14: Hydrogen Production Costs by Method

Hydrogen production method	**Best Case ($/kg)**	**Base Case ($/kg)**	**Worst Case ($/kg)**
SMR without CCS	1,05	1,29	1,50
SMR with CCS (89% capture)	1,71	1,93	2,15
Wind energy	6,02	6,64	7,25
Solar energy	6,70	7,50	8,30
Hydropower	4,80	5,57	6,34
Ammonia (this study)	4,82	5,46	6,08

Source: Own elaboration based on Center on Global Energy Policy at Columbia University (2021)

SMR with CCS technologies provide the best relation between cost and environmental impact, even though it uses a fossil fuel as feedstock and does not work with net carbon emissions. In this scenario, literature research should aim to evaluate possible cost optimizations in renewable production technologies, considering that electrolyzer CAPEX and electricity costs are the main cost-reduction levers (Clean Hydrogen Observatory, 2024). At the same time, incremental cost and emissions optimizations in CCS tecnologies should be investigated, seeking to provide sustainable hydrogen at a reasonable cost.

5 CONCLUSIONS AND FUTURE PERSPECTIVES

This study provided an in-depth review of hydrogen production technologies, including fossil fuels, water, biological and nuclear processes. It also discussed the role of hydrogen carriers like ammonia and methanol in an economy powered by hydrogen, addressing safety, storage and transport issues. Economic viability of the most common hydrogen production method via ammonia, the thermocatalytic decomposition, was assessed using data from Alves, Avilez and Mereguete (2024) to calculate LCOH in NREL's H2A Lite Model in Excel based on deterministic and stochastic approaches, that enabled the incorporation of uncertainty and a sensitivity analysis of key variables affecting LCOH.

The results demonstrated that an LCOH of \$5,46/kg is the base case scenario, with ammonia as the major cost driver representing 84% of LCOH, which is generally aligned to the values reported in the comparable studies of Makhloufi and Kezibri (2021) and Kanaan et al. (2023). Sensitivity analysis confirmed that ammonia cost is the most influential variable in the model, as well as highlighted the relative importance of capacity and utilization variables in determining LCOH, which is also aligned to the mentioned studies. This consistency with literature values reinforces confidence in the results obtained using the NREL's H2A Lite Model, setting a reliability stamp to this tool which should ease the process of LCOH evaluation, given the flexibility of the model. Not only that, but proximate results provide a benchmark for assessing ammonia decomposition's competitiveness relative to other hydrogen production methods.

The base case value is expected to range from \$4.54/kg to \$6.34/kg, considering 5000 randomly simulated scenarios, with mean and median values close to the base case, as a consequence from symmetric triangular probability distributions that were assigned. From these simulations, it was possible to derive the VaR-LCOH with a 95% confidence interval of \$6,08/kg, which can be used by investors to evaluate the risk of a project of such type, along with expected returns to determine investment allocation. This can also be used by policymakers to set eventual subsidies or tax credits that are realistic based on the expected scenarios.

This range of values puts ammonia in the lower-cost-tier of renewable hydrogen production technologies, according to data from Center on Global Energy Policy at Columbia University (2021). While this does not mean that ammonia will continue to be one of the most cost-competitive, as all of the renewable production methods are expected to become more efficient in a 10-20 year horizon, it does put ammonia in a promising place among its peers. An implication of this statement is that, in a green hydrogen economy, ammonia could be the most suitable hydrogen carrier to regions with limited renewable resources, as it is fully integrated in the global supply chain due to the use of fertilizers.

Still, the obtained values are between two to three times the current costs for the most popular fossil-fuel-based method, which is SMR, even when considering CCS technologies. This has a few implications. As a first, future research should focus on analyzing cost-reduction levers in renewable production methods, in order to set the stage for an economically viable green hydrogen powered economy. In the meantime, research should also be made regarding optimizing CCS technologies in order to achieve net zero carbon emission in SMR. This would allow for a zero-carbon hydrogen production method at a reasonable price. Though not ideal, as it is fossil-fuel based, its cost is in a range that government incentives could make it the most competitive. Exploring this alternative makes sense because using the so-called blue hydrogen can be more feasible than green hydrogen, given economic and environmental matters.

Considering the case of ammonia, cost is expected to decrease at a higher rate than it was considered in this study, as elaborated by Cesaro et al. (2021). Studies of this nature should continue in the upcoming years, as to confirm the rate of this descending trend. Furthermore, a deep-dive in the expected probability distributions of key variables, such as ammonia and energy prices, would be beneficial for a more refined risk assessment than the one provided in this study. With these next steps, ammonia's potential as a cost-effective hydrogen carrier can be better understood and optimized, to support a sustainable and economically competitive green hydrogen economy.

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