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Techno-Economic Analysis of Power to Ammonia Production

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Abstract. This study introduces a novel methodology for conducting a techno-economic analysis of green ammonia production using mathematical models that meticulously parameterize plant units and technical specifications. The approach involves two key steps: first, identifying and modeling the essential components of green ammonia production, such as electrolyzers, ammonia synthesis units, and plant configurations; second, developing a non-linear optimization model to minimize the levelized cost of ammonia, payback period, internal rate of return, and return on investment. The model also incorporates constraints like maintaining minimum plant unit loads and optimizing electricity costs. By leveraging renewable energy through power purchase agreements, the study ensures a stable energy supply and carbon neutrality across the ammonia value chain. Two scenarios are examined: one with a user-defined electrolyzer configuration and another with an optimized configuration. In the latter, electricity consumption drops to 10 MWh per ton of ammonia produced, saving 60 GWh of energy annually, along with reductions in capital costs by 53% and operating costs by 10% compared to the first scenario.

Keywords. Ammonia production, power-to-x, techno-economic analysis, green hydrogen.

1 Introduction

In a world thirsty for energy, dependence and overreliance on fossil fuels, has taken a tone on our planet with potent drawbacks as global warming and the depletion of natural resources [1-5]. The growing policy drives from major world climate change actors such as the United Nations Climate Summit or the African Climate Summit are initiatives that raises the need for higher integration of renewable energies [6-11]. According the world energy transition outlook in 2023, renewable energies accounted for 28% of the shares in electricity generations with an expected growth to 91% by 2050 to achieve carbon neutrality [12]. Such growth requires strong strategies notably to foster a smooth integration of greener technologies into hard to abate industries such as transportations and manufacturing thereby extending the use of renewable energies to the economy scale. However, the dilemma raised by conventional renewable energy technologies lies on their intermittency as solar panels are unable to produce energy during nighttime and wind turbine are almost non-functional in absence of wind. This challenge can be resolved by providing an innovative solution to conventional green technology limitations by converting renewable energy electricity into energy careers and further, convert these later into monetizable products. This process is called power to X, literally meaning the conversion of power generated from a renewable source into usable electricity or any other form of energy.

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This study will focus particularly on power conversion into ammonia, a product with a wide range of application ranging from fertilizers, industrial chemicals, refrigerant, Ammonia market is estimated to reach USD 313.21 billion by 2030 [13]. Furthermore, Ammonia conventional manufacturing is highly energy intensive as it represents on a yearly basis about 1.8% of the global energy output for a carbon footprint reaching approximately 500 million tons of CO_2 [14]. These emissions are primarily due to the use of natural gas such as methane as principal feedstock during the conventional synthesis of ammonia [15]. Thus, in alignment with the growing need to achieve carbon neutrality, this study will investigate an alternative manufacturing process to produce green ammonia and thus propose an efficient strategy for decarbonization in the agricultural industry, thereby fostering the larger integration of renewable technologies.

Several models have been proposed while designing and optimizing the green ammonia production, such as the one suggested by Guerra et al. [16] where a technical and economic study of the production of ammonia using hydrogen by means of electrolysis has been performed by taking into consideration a set of parameters such as capital expenditures (CAPEX) and operational expenditures (OPEX), and results showed that the hydrogen production in Chile and its transportation to Japan using ammonia as an energy carrier would be a technically viable and profitable solution along with its environmental benefits however it showed a couple of limitations such as the fact that it does not consider the ammonia market volume availability to introduce the ammonia produced in that facility. Lee et al. [17] electrolysis technologies as it is a key component in the configuration of power to ammonia production, the comparison was based on the learning rate and cost-effectiveness of the electrolysis process improve over time and concluded that solid oxide electrolyzer cell as the most promising water electrolysis technology owing to its high energy efficiency. Additionally, Nayak-Luke and Bañares-Alcántara [18] and AlZahrani and Dincer [19] have highlighted the potential of the solid oxide electrolysis cells as the new generation of electrolyzers due to the matching ability with ammonia synthesis expressed through the possibility of heat integration which enhances the overall process energy-efficiency. However, as opposed to alkaline electrolyzers and proton exchange membrane electrolyzers, the solid oxide electrolyzer cell technology is yet at the laboratory stage and thus, have a low maturity level. Furthermore, while some studies like Ikäheimo et al. [20], Blanco et al. [21], and Pawar et al. [22] have analyzed e-fuels potential using aggregate data and energy system-based modelling and offered valuable insights into the broader economic potential of these fuels, but they do not fully address the cost variability at the individual plant level. This gap is critical, as the economic feasibility of Ammonia production infrastructure depends on localized factors such as energy prices, operational scales, and the integration capabilities within existing industrial infrastructures. In addition to mentioning this, Grahn et al. [23] have also highlighted the problematic that electricity supply is assumed to be fixed alike operations costs which represents an oversimplification of e-fuel plants given the fluctuation of electricity cost and availability abiding to a realistic scenario and focused their research primarily on variable electricity supply and on the dynamics of the system. However, plant cost reduction generally relies on expanding plant flexibility, reducing energy price and the use of a mix of renewable energy sources. These alternatives are extensively costly in real life as they require additional infusion of capital investments. Therefore, to fully assess these challenges along with the viability of these emerging technologies, it is crucial to undertake more detailed, plant-specific analyses. This would provide a clearer understanding of the micro-economic factors that significantly influence the competitiveness of these innovative systems in practical, real-world contexts.

As revealed by the literature review, the electrolyzer unit presents a significant hurdle in scaling up the adoption of green ammonia engineering processes on a large scale, aiming to serve as a zero-carbon emission alternative to grey and blue ammonia production methods.

However, there is a lack of comprehensive research comparing the outcomes of optimized electrolyzer sizing for varying levels of ammonia demand and assessing potential cost reductions achieved by utilizing different profiles tailored to different demand levels. Most existing research mainly outlines the advantages or challenges associated with different electrolyzer technologies while assuming fixed parameterizations for these systems. That is why the research objective of this paper is to address this gap by parameterizing a typical power-to-ammonia plant to design an optimization model tailored to a specific ammonia demand. The model is developed with the primary objective of analyzing a range of technical and financial parameters that are critical to the operation and economic performance of the plant. These parameters include the power rating, which determines the scale of energy input, and the unit percentage of capital expenditure (CAPEX), which reflects the cost structure of the plant. The analysis also focuses on calculating the levelized cost of green ammonia production, which serves as a key indicator of the plant's economic efficiency over its lifetime. Moreover, the study delves into assessing the economic viability of the plant by examining essential financial metrics such as net present value (NPV), return on investment (ROI), and payback period. By integrating these technical and financial analyses, this investigation aims to offer a new comprehensive evaluation of the feasibility and sustainability of implementing power-to-ammonia technology on a practical scale.

2 Methodology

This section explores in detail the mathematical model used to optimize the production of green ammonia through non-linear optimization. The model involves a comprehensive designing of various plant units in accordance with their technical specifications, ensuring a realistic and practical approach to optimization. The key components considered include the electrolyzer unit, which converts water into hydrogen and oxygen using renewable electricity, with parameters like the different types of Ammonia, the air separation unit (ASU), the electrolysis different units, and the set of processes involved. Furthermore, it delves into the formulation of parameters and constraints of the non-linear optimization that is used with an aim of minimizing the overall cost of both capital investment and operational expenses while meeting a predetermined annual production target for ammonia.

2.1 System components: selection and modelling

2.1.1 Selection of ammonia type

Conventional ammonia, often referred to as grey ammonia, is produced using methane as a feedstock. This process is named for the significant CO_2 emissions generated during synthesis. However, with growing environmental concerns, it is essential to also explore and understand alternative types of ammonia, such as blue and green ammonia, which offer more sustainable production methods and lower carbon footprints. With this being said, this section will explore those three types of ammonia and their chemical reactions modeling trough equations along with the different methods used in manufacturing each one of them starting with the conventional one and is produced through the following two methods:

Firstly, the steam methane reforming (SMR) process which represents about 70% of the World Ammonia production [24]. The steam methane reforming process involves the use of hydrocarbons such as Natural gas or naphtha as feedstock to synthetize Hydrogen while the required Nitrogen is sourced from ambient air. The process involves the production of syngas which is a mixture of Hydrogen, Carbon Monoxide, Carbon Dioxide, Methane and Water as follows:

$$CH_4 + H_2O \rightarrow CO + 3H_2 \quad (1)$$

The second process and that more complex than the steam methane reforming is named Auto-Thermal Reforming (ATR) and that involves the combination of partial oxidation and steam reforming in one single reactor. This process also involves the production of syngas following this chemical reaction:

$$CH_4 + \frac{1}{2}O_2 + H_2O \rightarrow CO + 3H_2 \quad (2)$$

In both manufacturing processes of conventional ammonia, the Syngas is conveyed to a shift converter that oxidizes carbon monoxide to carbon dioxide. Fig.1 depicts the schematic of grey ammonia production. When carbon capture, utilization, and storage (CCS) technology is applied to the production of grey ammonia, the result is blue ammonia, a less polluting alternative. This approach significantly reduces the carbon emissions typically associated with conventional ammonia production by capturing and repurposing the CO_2 that would otherwise be released into the atmosphere. The carbon capture, utilization, and storage technology enables the captured CO_2 to be stored safely or utilized in other industrial processes, thereby enhancing the overall efficiency and sustainability of ammonia production. Carbon Capture can be described in simple terms as the capture of CO_2 gas using special solvents and further trough the methanation process as follows:

$$\mathrm{CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O} \quad (3)$$

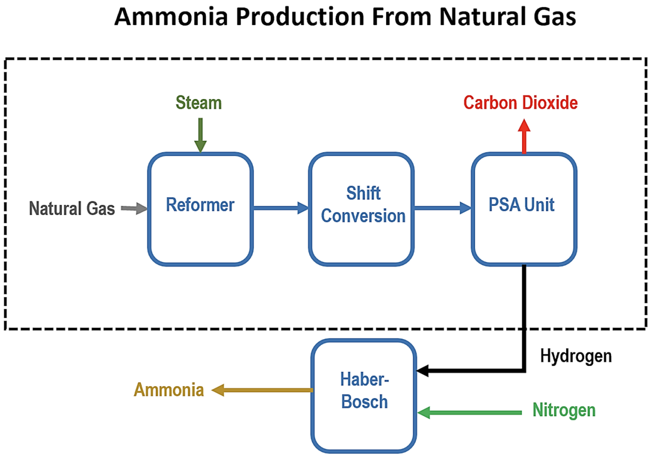

Fig. 1. Conventional Ammonia Production Process

Green ammonia on the other hand is the ammonia that is obtained using renewable energy sources. It results in a net zero emission of greenhouse gas emissions as its production process does not involve any fossil fuel-based feedstock. The hydrogen and Nitrogen feedstock required for green ammonia synthesis are respectively produced using electrolysis unit and an air separation unit (ASU), both powered using electricity from renewable sources. The feedstock is then compressed using a compressor before being conveyed to the Haber-Bosch unit which synthesizes ammonia. This green ammonia synthesis process is modelled using the schematic shown in Fig. 2.

Finally, and based on the different types of ammonia presented before, the green ammonia has been chosen in the current as study as it is the type with the lowest greenhouse gas emissions and would fit the best in the optimization.

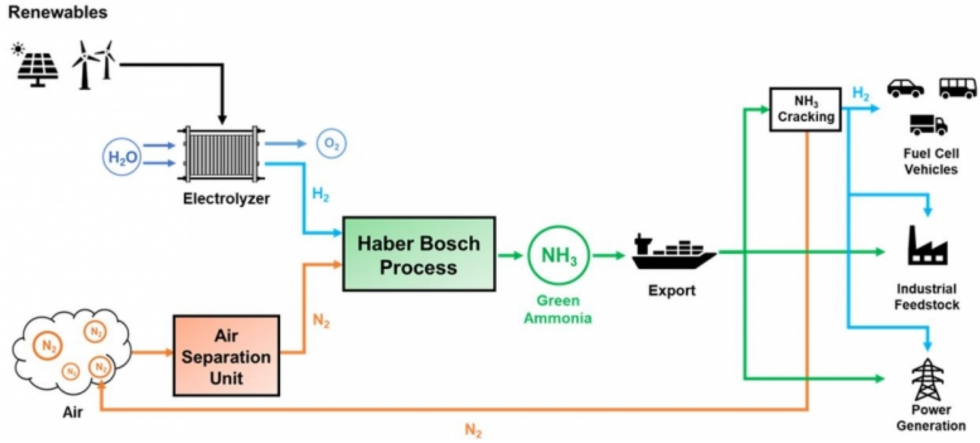

Fig. 2. Green Ammonia Production Process

2.1.2 Selection of the electrolyzer unit

An Electrolyzer, in the framework of green-ammonia synthesis is an industrial unit that electrochemically splits water molecules H_2O into two hydrogen (H_2) moles and one mole of Oxygen (O_2) based on the following chemical equation:

$$2H_2O \rightarrow 2H_2 + O_2 \qquad (4)$$

Based on the literature review, there has been found that there currently exist three types of electrolyzers notably alkaline electrolyzers, proton exchange membrane electrolyzers, and solid oxide electrolyzer cells. Even though the inputs and output of these electrolyzers is the same in nature, their underlying engineering process used for splitting water varies significantly, impacting unit efficiency, energy load, and capital cost of investment. That is why, a comparison of the three types has been made in order to appropriately choose the best unit to model in the current study.

Starting with the alkaline electrolyzer unit which represents the earliest form of electrolyze. In these systems, two metal electrodes are immersed in a water-based solution and separated by a porous diaphragm that selectively allows the passage of negatively charged ions. When an electric current is applied across the electrodes, hydrogen is liberated at the cathode, while oxygen is released at the anode in the form of bubbles. These electrolyzers use an aqueous electrolyte solution, typically containing minerals like potassium hydroxide (KOH) or sodium hydroxide (NaOH). These minerals dissociate in water to release ions, facilitating ion transport within the electrolyte. However, KOH electrolytes are generally preferred mainly due their higher ionic conductivity and lower CO_2 solubility. In fact, NaOH electrolytes can easily dissolve the CO_2 present in the air and thus form CO_3^{2-} carbonate ions thereby reducing ionic conductivity. At the cathode: Water molecules (H_2O) are reduced to hydrogen ions (H+) and hydroxide ions (OH-) in the presence of electrons (e-) supplied by an external electric circuit following the chemical reaction:

$$2H_2O\,(l) + 2e^- \rightleftharpoons H_2(g) + 2OH^- \qquad (5)$$

At the anode: Hydroxide ions (OH-) from the electrolyte are oxidized, producing oxygen gas (O_2) and releasing electrons (e-) to the external circuit as modelled below:

$$2OH\_(aq) \leftrightharpoons \frac{1}{2}O_2\,(g) + H_2O\,(l) + 2\,e^- \qquad (6)$$

At an industrial scale, efficiency of hydrogen production using these electrolyzers is enhanced by having several cells combined in series within a stack which creates a compact layout operated on a larger voltage.

The second type of unit that could be used is the proton exchange membrane electrolyzer in which a solid specialized plastic material serves as the electrolyte. At the anode, water undergoes a reaction to produce oxygen and positively charged hydrogen ions (protons) as follows:

$$2H_2O \rightarrow O_2 + 4H+ + 4e^- \qquad (7)$$

Subsequently, electrons flow through an external circuit, while the hydrogen ions selectively migrate across the proton exchange membrane electrolyzer to reach the cathode. Upon reaching the cathode, the hydrogen ions combine with electrons from the external circuit, resulting in the formation of hydrogen gas as follows:

$$4\,H^+ + 4\,e^- \rightarrow 2\,H_2 \qquad (8)$$

Finally, the third type of electrolyzers is the solid oxide electrolyzers which utilize a solid ceramic material as the electrolyte and selectively conducts negatively charged oxide ions (O^{2-}) at high temperatures. This process of electrolysis generates hydrogen in a slightly different manner. At the cathode, steam combines with electrons from the external circuit to produce hydrogen gas and negatively charged oxygen ions as follows:

$$H_2O + 2e^- \rightarrow H_2 + O^{2-} \qquad (9)$$

The oxide ions thus traverse the solid ceramic membrane to reach the anode, where they follow an oxygen evolution reaction to generate oxygen gas and produce electrons for the external circuit as follows:

$$2O^{2-} \rightarrow O_2 + 4e^- \qquad (10)$$

Solid oxide electrolyzer necessitate operating temperatures sufficiently high to ensure proper functioning of the solid oxide membranes, typically around 700°–800°C. This contrasts with PEM electrolyzers, which operate at 70°–90°C, and commercial alkaline electrolyzers, which typically operate at less than 100°C.

Al last, the alkaline electrolyzer was selected due to the high maturity level of the technology and the several financial benefits such as low levelized cost of energy (LCOE), low levelized cost of ammonia (LCOA), and low unit electricity price.

2.1.3 Air separation unit

An ASU or air separation unit, in ammonia synthesis is responsible for the production of the required nitrogen feedstock. The implementation of specific air separation technologies is essential for realizing the air separation process. Various technologies exist today, each designed to exploit different characteristics of the constituent air gases' physical properties. Essentially, air separation technologies leverage the distinct physical properties of air's fundamental components, including differences in molecule sizes, diffusion rates through materials, adsorption preferences of specific materials for atmospheric gases, and variations in boiling temperatures. When nitrogen is produced using an air separation unit, a cryogenic method is used. Cryogenic air separation technology operates on the principle that the individual gases composing air possess distinct boiling points. By adjusting the temperature and pressure conditions of the surrounding environment, the air can be effectively divided into its constituent elements. Finally, the air separation process is modelled as given in Fig. 3.

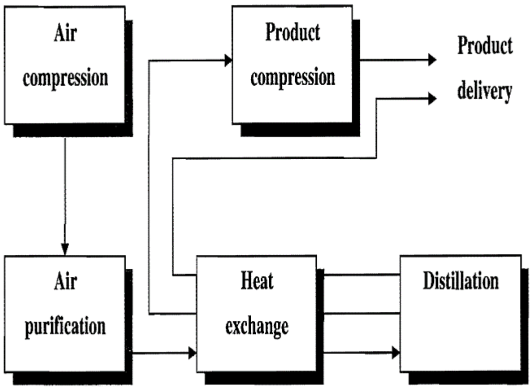

Fig. 3. Air Separation Unit Flow Process [25]

2.1.4 Haber-Bosch process modelling

After having modelled all the different components of the ammonia production system, there comes the final process and that encompasses both the produced nitrogen from the air separation unit and pressurized hydrogen which is called the Haber-Bosch engineering process. This process involves combining nitrogen from the air with hydrogen primarily derived from natural gas into ammonia. This reaction is reversible and exothermic as it yields a negative change in enthalpy during the reaction and is given as follows:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g) \quad \Delta H_f^{\circ} = -92.5\ kJ \qquad (11)$$

With ΔH_f° being the standard enthalpy change of formation of ammonia (NH_3).

2.2 Optimization parameters and constraints

2.2.1 Parameters modeling

A key parameter of this parametric optimization is the electricity degradation index. It accounts for the fact that due to potential internal deficiencies (electrolytes contamination, electrochemical corrosion, coking and Hydrogen and Nitrogen poisoning etc.) the units within the production line of ammonia may require higher energy input as per the stated power consumption from state-of-the art. The impact of this parameter in the energy consumption is modelled as follows [26]:

$$E_p = E_0 \times \left(1 + \frac{d_{ip}}{100}\right)^p \quad (12)$$

Where dip (% p.a) is the electricity consumption degradation index in a period p, E_p is the electricity consumption in period p and E_0 is the initial electricity consumption at the start (when $p = 0$).

In the optimization of ammonia production aimed at cost reduction, a crucial aspect to address in formulating an optimization model pertains to the replacement of stacks within the Electrolyzer unit and the catalysts within the Haber-Bosch unit. These structural elements possess finite lifespans, thereby necessitating their replacement during the operational lifespan. Consequently, the costs associated with replacing these components must be factored into the evaluation of capital expenditure for both the electrolyzer and Haber-Bosch units. The timing of replacement primarily hinges upon the lifespan predetermined by design specifications or prevailing state-of-the-art reliability standards [27]. To account for such variability, the following parameters are used in the model as a built-in algorithm aimed at valuing the additional CAPEX required for the Electrolyzer and Haber-Bosch units throughout the project's duration and were divided as follows:

The Accumulated Hours in Period p for the:

- Plant: $Ah_p\ (hours) = Ah_{p-1} + Oh_p\ \forall p \in n$ (13)
- Haber-Bosch unit: $Ah'_p\ (hours) = Ah'_{p-1} + Oh_p\ \forall p \in n, p \in [1, n]$ (14)

Where $\mathrm{Ah_p}$ and $\mathrm{Ah'_p}$ are the operating hours accumulated of the plant and the Haber Bosch unit respectively and helps track the total usage of the equipment along with its lifespan. Finally, $\mathrm{Oh_p}$ is the plant operating hours per year.

The Closing balance for the:

- Plant: $Cb_p = (Oph_p + Hu_p) - LR_p\ \forall p \in n$ (15)
- Haber-Bosch unit: $Cb'_p = (Oph'_p + Hu'_p) - LR'_p\ \forall p \in n$ (16)

Where $\mathrm{Cb_p}$ and $\mathrm{Cb'_p}$ refer to the closing balance in period of the plant and the Haber Bosch unit respectively and help track the total usage of the equipment along with its lifespan. Also, $\mathrm{LR_p}$ and $\mathrm{LR'_p}$are the lifetime reset in period that the components are designed to operate before needing replacement (h), and $\mathrm{Hu_p}$, $\mathrm{Hu'_p}$ the hours used.

Furthermore, as the current model aims to determine the optimal electrolyzer profile out of the 18 configurations present in the literature from current and mature technology variants, including alkaline electrolyzer and proton exchange membrane electrolyzer. This configuration selection is tailored to the demand level for ammonia, and the following parameters are instrumental in this endeavor. These parameters include a definition of the Electrolyzers' profile and configuration set as follows.

$$\forall u \in U, u \in [1{,}18] \quad (17)$$

$$\mathrm{I}\ \forall i \in I, i \in [1{,}6] \quad (18)$$

Where "U" represents the different electrolyzer configurations that the current model considers when determining the best setup for this hydrogen production, while "I" represents the set of profiles with respect to the different performance characteristics of each electrolyzer such as efficiency, capacity, or operating conditions.

2.2.2 Constraints modeling

In order to optimize the ammonia production, it is essential to set constraints allowing both the electrolyzer and the Haber-Bosch units to operate while aligning with their technical and operational limits. These constraints account for factors such as the permissible range of hydrogen production, the accumulated operating hours leading to equipment replacement, and the degradation of equipment efficiency over time. Hence, the current study incorporated a set factors to insure having the best configurations and profiles for the units, while achieving the goal of reducing costs and maintaining efficiency and reliability of the system. Among which the following.

In addition to the accumulated operating hours, all the initial conditions have to be set to zero at the beginning of the project period (p), as illustrated in (19). Additionally, another constraint in (20) is put in place in order to make sure the unit operates within its capacity based on the load factor. Finally, the assumption in (21) is that the total operating hours of the electrolyzer and Haber-Bosch units are equal to their total available hours, implying there is no downtime or idle periods.

$$Ah_{(p=0)} = 0, Cb_{(p=0)} = 0, Oh_{p=0} = 0, Hu_{p=0} = 0 \quad (19)$$

$$Oh_p = load \times 8760\ \forall p \in n \quad (20)$$

$$Hu_p = Oh_p \forall p \in n \quad (21)$$

Another significant constraint examined in this study involves the indicators for stack and catalyst replacements. These indicators ensure that both components are replaced only when their accumulated operating hours exceed their designed lifespan, thereby mitigating unnecessary replacement costs.

$$SR_p = \begin{cases} 1 \ \ if \left(Oph_p + Hu_p\right) > SL_u \\ 0, \ \ otherwise \end{cases} \forall p \in n \quad (22)$$

$$CR_p = \begin{cases} 1 \ \ if \left(Oph'_p + Hu'_p\right) > CL \\ 0, \ \ otherwise \end{cases} \forall p \in n \quad (23)$$

These constraints are vital because they govern the core operational aspects of the Electrolyzer and Haber-Bosch units. They ensure that the model remains realistic by accounting for equipment degradation, replacement needs, and operational limits. Including these constraints allows the model to optimize costs effectively while maintaining the reliability and efficiency of the production process. However, and in order to get a reliable configuration that is both economical and technically feasible. Defining technical constraints is also important and was done in this study in the following manner.

As previously noted, incorporating the degradation index is essential in this type of optimization. Therefore, (24) and (25) have been introduced to represent the decline in equipment efficiency over time, impacting both energy consumption and operational costs. By monitoring this index, the model can account for the rising energy demands caused by equipment wear and tear.

$$d_{i(p=0)} = d_{ip} \quad (24)$$

$$d_{i(p=1)} = 1 + d_{ip} \quad (25)$$

Where $d_{i(p=0)}$ represents the starting point of the degradation index and $d_{i(p=1)}$ the subsequent degradation index represents a constant increase of the electricity degradation of the period of time p describing how the efficiency of the equipment degrades over time as it operates.

To prevent anomalies during the optimization process, two key constraints must be considered. The first in (26) is the constraint for the electrolyzer configuration selection, which ensures that only one specific electrolyzer configuration is chosen for each optimization run, prohibiting the simultaneous selection of multiple configurations.

$$\sum_{u=1}^{18} y_u = 1 \ \forall u \in U \ (26)$$

The second constraint, outlined in (27), limits hydrogen production to feasible existing levels, ensuring that production remains within realistic and attainable boundaries, thereby preventing it from dropping below or exceeding achievable limits. $MinH$ and $MaxH$ are the minimum and maximum hydrogen production level respectively $\mathrm{H_{prod}}$ the hydrogen production level.

$$\mathrm{MinH} \leq \mathrm{H_{prod}} \leq \mathrm{MaxH} \ \ (27)$$

Finally, an electrolyzer profile range check is important as is it ensure that this profile is capable of producing hydrogen within the specified range, validating the feasibility of the production levels for each profile.

$$\mathrm{PrCheck_i} = \begin{cases} 1, MinH_i \leq Hy_{prod} \leq MaxH_i \\ 0, otherwise \end{cases} \quad (28)$$

In the current study, and for in order to test all the 18 configurations those profile range checks were divided as follows:

$$\begin{Bmatrix} \forall u \in [1,2,3], y_u \leq PrCheck1 \\ \forall u \in [4,5,6], y_u \leq PrCheck2 \\ \forall u \in [7,8,9], y_u \leq PrCheck3 \\ \forall u \in [10,11,12], y_u \leq PrCheck4 \\ \forall u \in [13,14,15], y_u \leq PrCheck5 \\ \forall u \in [16,17,18], y_u \leq PrCheck6 \end{Bmatrix} \quad (29)$$

2.3 Data acquisition

Now that all the parameters and constraints have been explored, a data gathering is needed before digging into the optimization model. This data was mainly gathered from official reports of the International Energy Agency datasets and LAZARD assumption on hydrogen-based studies and they cover specification of the most common electrolyzer units. These inputs are clustered into 3 main categories: technical, operational, and financial inputs. Table 1 is summarizing the inputs along with their units and considered values.

Table 1. Optimization Model Input Values

Input Name	**Unit**	**Value**
Project Lifetime	years	25
Learning Rate	% p.a.	1
Weighted Average Cost of Capital	%	9.7
Power Purchase Agreement	USD/MWh	21
Ammonia Plant Load	%	96
Electrolyzer Plant OPEX % of CAPEX	% p.a.	1.5
Electrolyzer Water Requirement	L/kg.H_2	11
Depreciation Expense	% p.a.	4
Degradation Index	% p.a.	1
Compression Power Requirement	MWh/Tn.NH_3 p.a.	1
Compression Sizing Cost	$/kW	235.09
Air Separation Unitary CAPEX	USD/Ton.N_2	22
Air Separation Unit Power requirement	MWh/Tn.NH_3 p.a.	0.9
Haber-Bosch OPEX as % of CAPEX	% p.a.	1.5%

Haber-Bosch Unitary Sizing CAPEX	USD/kWe	487
Haber-Bosch Unit Power requirement	MWh/ton of NH_3	0.64
Catalyst Replacement Cost % of CAPEX	% p.a.	30
Haber-Bosch Unit Catalyst Lifetime	hours	80,000
Ammonia Demand	Kton p.a.	84
Inflation Rate	% p.a.	2

2.4 Optimization

2.4.1 Optimization tool

Based on the literature review, several solving methods and algorithms have been used to optimize the ammonia production such as sequential quadratic programming using packages such as Optima, MATLAB, and LSGRG packages. However, and due to the powerfulness of this tool in similar optimization studies, the current study utilized the generalized reduced gradient non-linear optimization technique. This method scans the slope or the gradient of the objective function as the decision variables are changed to decide on the optimality of the solution when the partial derivatives equal to zero. As the study aims at comparing two optimization scenarios, this technique is suitable and allows for a first layer optimization of the model to provide insight regarding the methodology used in assessing the viability of green ammonia.

2.4.2 Optimization model

As explained earlier, the goal of the optimization is to minimize the levelized cost of ammonia, which represents the comprehensive expense involved in producing a defined quantity of ammonia, typically measured per ton in this study. It encompasses the total outlay associated with generating the necessary feedstock for ammonia synthesis T_{COST} , as well as the operational and acquisition costs linked to the Haber-Bosch unit, $Hb_{Cx_{recovery}}$, divided by the amount of ammonia produced by the plant in tons, A_{prod}.

$$Objective\ Function:\ Min\left(LCOA=\left(\frac{T_{COST}+Hb_{Cx_{recovery}}}{A_{prod}}\right)\right)\ (30)$$

This minimization requires the analysis of each feedstock and associated costs individually. Firstly, hydrogen that stands as a primary feedstock for ammonia synthesis. Its cost of production is intricately tied to the plant's hydrogen production and its levelized cost as in (31).

$$LCOH=\left(\frac{Ox_{recovery}+S_{recovery}+Cx_{recovery}}{HyProd}\right)\quad(31)$$

Secondly, another essential feedstock is nitrogen and the cost calculus for it hinges on relationship between the plant's nitrogen production, and the levelized cost of air separation as represented in (32). Additionally, compression plays a pivotal role in the synthesis process and is illustrated in (33).

$$LCAS=\left(\frac{As_{Tcost}}{N_{prod}}\right)\ (32)$$

$$LCOC = \left(\frac{C_{EXP}+CompCx_{recovery}}{A_{prod}}\right) \quad (33)$$

Where C_{EXP} is the Compression Power Expense, $CompCx_{recovery}$ is the compression CAPEX recovery, and A_{prod} is the ammonia production. Furthermore, the Electrolyzer, the compressor, the air separation, and the Haber-Bosch process units levelized cost all depends respectively on each unit sizing. It is important to notice also that all units' sizing within the ammonia production line are dependent on electrolyzer sizing as can be observed.

$$EOC = \left(\frac{Eef_u \times A_{prod}}{Oh_p \times 5.6}\right) \quad (34)$$

$$Comp_C = C_{Preq} * \left(\frac{EOC \times 5.6}{Eef_u}\right) \quad (35)$$

$$As_c = As_{Preq} * \left(\frac{EOC \times 5.6 \times Oh_p}{Eef_u}\right) \quad (36)$$

$$Hb_C = \left(\frac{EOC \times 5.6 \times Hb_{Preq}}{Eef_u}\right) \quad (37)$$

Where EOC is the electrolyzer capacity/sizing, $Comp_C$ is the compressor CAPEX, As_c air separation unit CAPEX and Eef_u is the electrolyzer efficiency using configuration compression power expense.

To summarize, the data used in this study are uniquely the plant input values of the model as explained before. They are composed of general operational and financial considerations of the ammonia plant such as the electricity pricing, operational power requirements, units' efficiencies, plant load, water cost, inflation rate, depreciation rate, learning rate, units' sizing CAPEX, units' OPEX percentage of CAPEX etc.…These data are the only non-user defined inputs for the model. In this paper, they represent the 3rd order of input data after the Electrolyzer profiling configuration which is optimally selected by the optimization model and the ammonia demand which, represents a user-defined input as can be observed in Fig. 4. Upon definition of inputs, the model follows a built-in algorithm for power scheduling based on each operating year degradation index, stack replacement scheduling based on the selected optimal Electrolyzer configuration lifespan of the stack and catalyst replacement scheduling based on Haber-Bosch catalyst defined lifespan. This schedule allows to determine total replacement capital expenditure and an adjusted electricity demand. The model uses these simple algorithms in addition of the 1st and 3rd input orders to optimize the Electrolyzer profiling configuration (2nd order input), and units' sizing (model's variables in Fig. 4) thereby minimizing the levelized of cost of ammonia under the presented constraints.

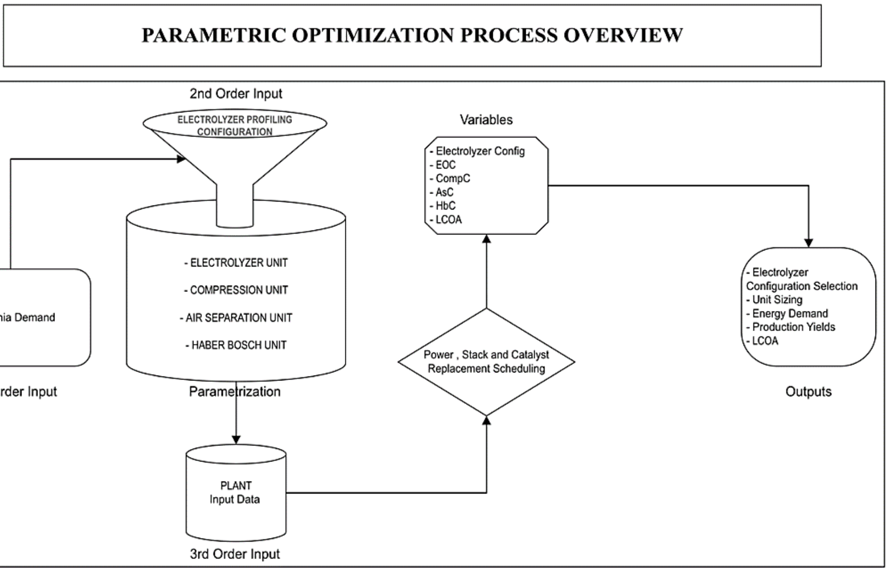

Fig. 4. Optimization Process Overview

Finally, this study is divided into two main scenarios while studying the feasibility of green ammonia production. The first scenario entails optimizing the configuration through user defined Electrolyzer parameters. Alternatively, the second scenario involves the optimization model selecting an Electrolyzer configuration profile tailored to the ammonia demand level as shown in Table 2 and explained in the following section.

Table 2. Summary of characteristics of the presented scenarios.

Scenario	Characteristics
1	User-defined Electrolyzer Parameters
2	Optimal Electrolyzer Profiling

3 Results

This paper will base the simulation on the sections discussed in the methodology to generate the results that are divided into two main sections: Section 1 will present the technical results and the plant electricity consumption; Section 2 provides an economic assessment based on the output of the model's output.

3.1 Technical analysis

3.1.1 Custom electrolyzer plant: sizing & power consumption

Assuming an ammonia demand of 84 kton representing the plant yearly production, running the optimization model allows to determine an optimal unit sizing with specific power rating respectively for each of the electrolyzer, compression, air-separation, and Haber-Bosch unit as presented in Table 3. The analysis of these data clearly shows the dominance of electrolyzer in terms of power rating.

Table 3. Optimized Unit Sizing with NEL Electrolyzer

Component	**Power rating (MW)**
Electrolyzer	82,14
Compression	10
Air Separation Unit	9,00
Haber-Bosch Unit	6,4

With the current user defined electrolyzer (referred to as SCN1), the model enabled to determine a total plant's electricity consumption of 904.392 MWh subdivided as shown in Fig. 5 into 690.788 MWh, 84.096 MWh, 75.686 MWh, and 53.821 MWh respectively for the Electrolyzer, compression, air-separation, and Haber-Bosch units.

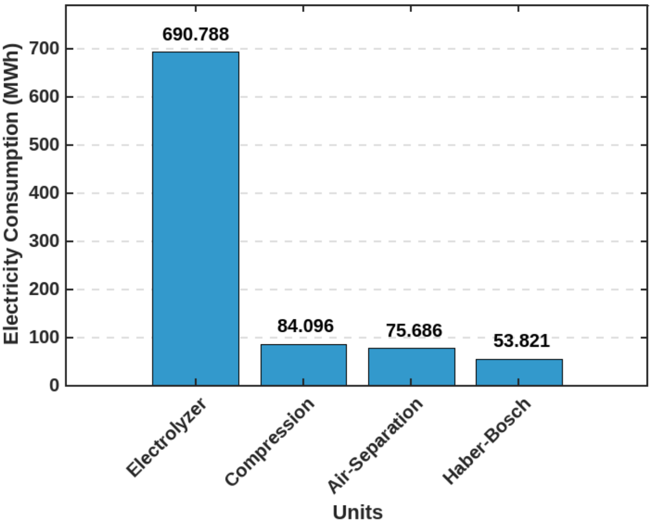

Fig. 5. Electricity Consumption per Plant's Unit (Scenario 1)

3.1.2 Sizing & consumption with optimal electrolyzer profiling

In this section, results of the same optimization model will be examined but with an inclusion of further constraints to account for variability in electrolyzer profiling and configurations according to LAZARD [28]. It is worth mentioning that the demand for green ammonia and feedstock production levels are identical.

Running the optimization model enabled to determine as optimal unit sizing: 75 MW, 10 MW, 9 MW, and 6.4 MW respectively for the electrolyzer, compression, air-separation, and Haber-Bosch units. A downsizing is observed at the level of the electrolyzer and the other units' parameterizations are kept identical. Thus, the current optimal electrolyzer configuration enable a downsizing of the electrolyzer power rating compared to a user defined one. These results are presented in Table 4.

Table 4. Optimized Electrolyzer Unit Sizing using Optimal Profiling

Component	Power rating (MW)
Electrolyzer	75,00
Compression	10
Air Separation Unit	9
Haber-Bosch Unit	6,4

With the current optimized electrolyzer in Scenario 2, the model enabled to determine a total plant's electricity consumption of 844.324 MWh subdivided as shown in Fig. 6. Similarly, to the sizing results, it can be seen that using an optimal electrolyzer allows a reduction in the total electricity consumption of the plant too.

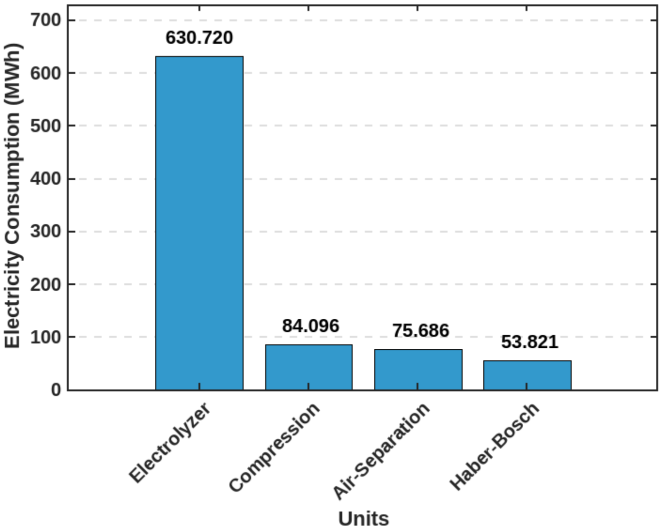

Fig. 6. Electricity Consumption per Unit (Scenario 2)

3.2 Plant economic assessment

In the subsequent section, an exploration of the economic feasibility of green ammonia across two distinct scenarios will take place. As explained earlier, the first scenario entails optimizing the levelized cost of ammonia through user defined electrolyzer parameters. Alternatively, the second scenario involves the optimization model selecting an Electrolyzer configuration profile tailored to the ammonia demand level, thereby optimizing its levelized cost. For both scenarios, detailed insights into capital expenditure (CAPEX) and operational expenditure (OPEX) will be provided along with a financial assessment of the plant, using a reference ammonia selling price of 540 USD/ton [29]. Finally, a comparative financial analysis will be conducted in section for both scenarios to enable the assessment of the plant's profitability through both methodologies by employing key financial metrics, including net present value, anticipated return on investment, internal rate of return, payback period, break-even period, and the levelized cost of ammonia

3.2.1 Plant CAPEX and OPEX

Assuming that the plant will be operated over period 25 years with a user defined electrolyzer parameterization, the optimization model yields the following results:

- Total CAPEX: 74,462,962 USD
- Total OPEX: 152,459,591 USD

The CAPEX represents the cost of acquisition and installation of the various plant units while the OPEX represent the cost associated with operating the facility. These results clearly show the dominance of the operating cost (water, power expenses etc.). In Fig. 7, is represented the plant yearly capital expenditure or CAPEX, highlighting the ratio of participation of each unit to the total CAPEX. An analysis of this chart reveals that indeed as mentioned in the literature review, the Electrolyzer represents the most significant cost in the synthesis process of green ammonia as it represents alone about 90% of the total CAPEX, followed by the Haber-Bosch Unit with 5%, the compression unit with 3% and the Air Separation Unit with 2%.

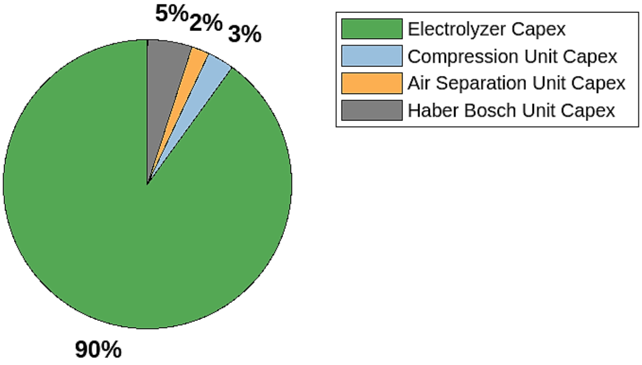

Fig. 7. CAPEX of Green Ammonia Plant (Scenario 1)

The individual plant's unit participation level with respect to the total OPEX is represented in Fig. 8. This graph shows that the Electrolyzer unit contributes significantly to the cost of operating the plant as it represents alone 97% of the total OPEX with compression, air separation and Haber-Bosch unit representing each about 1% of the total OPEX.

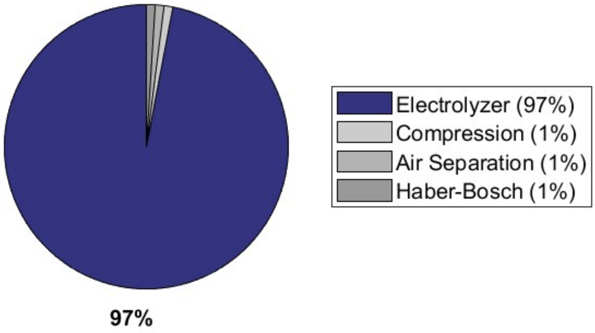

Fig. 8. Yearly OPEX of Green Ammonia Plant (Scenario 1)

Under the same operating conditions as in Scenario 1, an optimized selection of the electrolyzer profiling configuration yields the following results:

- Total CAPEX: 38,870,782 USD
- Total OPEX: 139,243,720 USD

After optimizing the Electrolyzer, these results clearly show again the dominance of the operating cost as in Fig. 9. An analysis of these results reveals that the Electrolyzer still represents the most significant cost in the synthesis process of green ammonia.

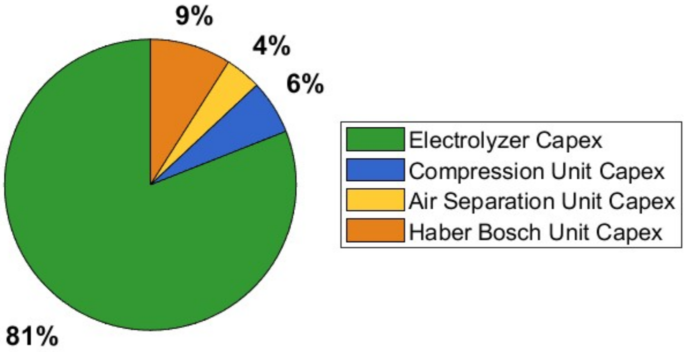

Fig. 9. CAPEX in Green Ammonia Plant (Scenario 2)

However, the OPEX remain distributed among the plant units in the same proportions as seen in Scenario 1. This distribution continues to reflect the dominance of the Electrolyzer unit, which retains a significant share of the overall costs.

3.2.2 Financial results

Based on the optimized plant's sizing, a comprehensive financial analysis has been drowned to assess the financial viability of Green Ammonia considering the time value of money, a weighted cost of capital of 9.7%, an inflation rate of 2%, a depreciation expense of about 4%, and a tax rate of 25% [28]. Analysis shows that an optimized plant sizing for ammonia may indeed be profitable over a period of 25 years (Table 5).

Table 5. Green Ammonia Plant Financial Metrics (Scenario 1)

NPV	$78.904.569
Payback Period (in Years)	4
ROI	16%
IRR	22%

In fact, the optimization model portrays a net present value of 78,904,569 UDS with a payback period estimated for 4 years, a return on investment (ROI) of about 16%, an internal rate of return (IRR) of 22%, and a break-even point (BEP) achieved in year 5 (Fig. 10). Additionally, the model found respectively for the levelized cost of Hydrogen (LCOH), the levelized cost of compression (LCOC), the levelized cost of air-separation (LCOAS) and the levelized cost of ammonia (LCOA): 1.58 USD/Kg$_{H2}$, 24.13 USD/Tn$_{NH3}$, 25.47 USD/Tn$_{NH3}$, and 346.15 USD/Tn$_{NH3}$.

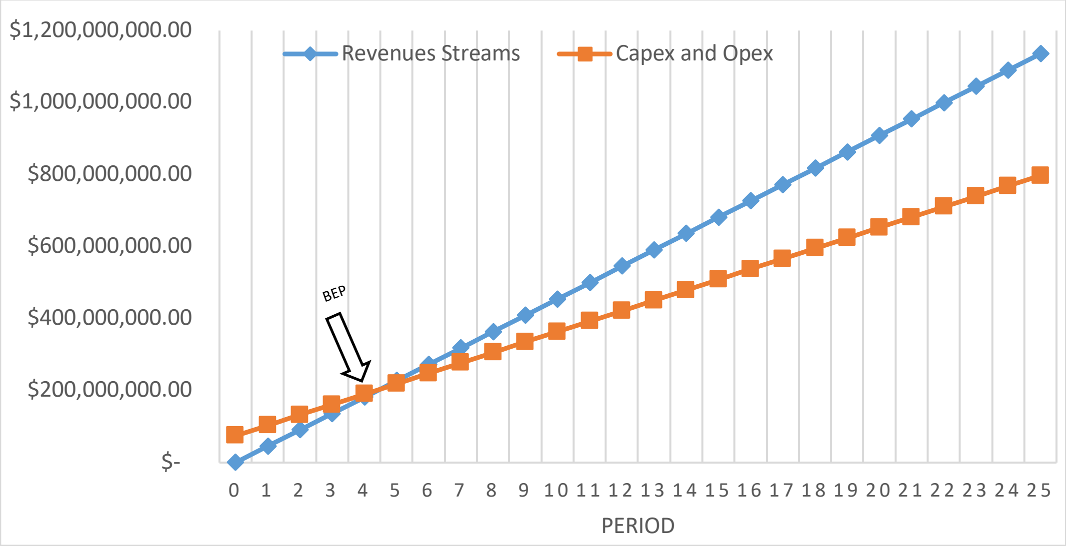

Fig. 10. Break Even Chart (Scenario 1)

Furthermore, in Fig. 11 representing the net cash flow diagram, it can observed that the plant requires an initial investment of 74,462,962 USD while generating a yearly net profit after tax deduction of 16,507,924 USD.

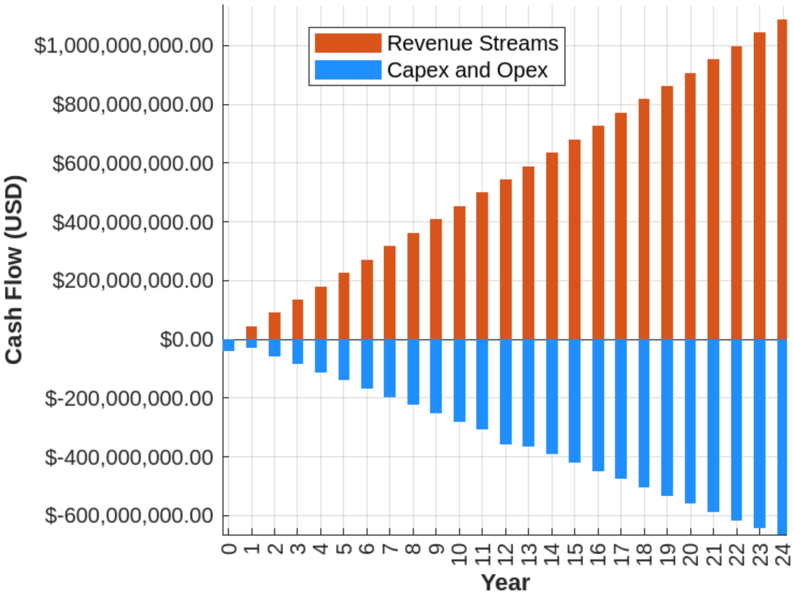

Fig. 11. Cash Flow Diagram of Green Ammonia Plant (Scenario 1)

Using identical financial parameter assumptions as in Scenario 1, an analysis shows in Table 6 that an optimized plant sizing for ammonia may indeed be profitable over a period of 25 years and further, yields costs reduction potentials when using an optimal electrolyzer profiling.

Table 6. Green Ammonia Plant Financial Metrics (Scenario 2)

NPV	$123,528,654
Payback Period (in Years)	2
ROI	30%
IRR	45%

The current optimization model portrays a net present value of 123,528,654 USD with a payback period estimated for 2 years, a return on investment (ROI) of about 30%, an internal rate of return (IRR) of 45%, and break-even point (BEP) achieved around year 3 (Fig. 12). Additionally, for the levelized cost of Hydrogen (LCOH), the levelized cost of Compression (LCOC), the levelized cost Air-Separation (LCOAS) and the levelized cost of ammonia (LCOA), the model found respectively 1.22 USD/Kg-H_2, 24.13 USD/Tn_{NH3}, 25.47 USD/Tn_{NH3}, and 281.52 USD/Tn_{NH3}.

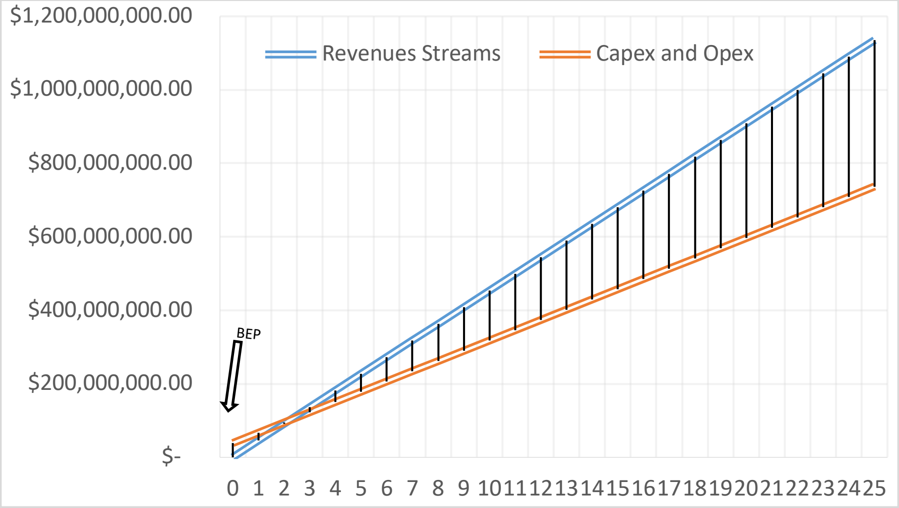

Fig. 12. Break Even Chart (Scenario 2)

Additionally, the current scenario shows a significant decrease in the plant an initial investment required that is 38,870,782 USD while an increase in the generated yearly net profit after tax deduction of 17,480,085 USD, as shown in Fig. 13.

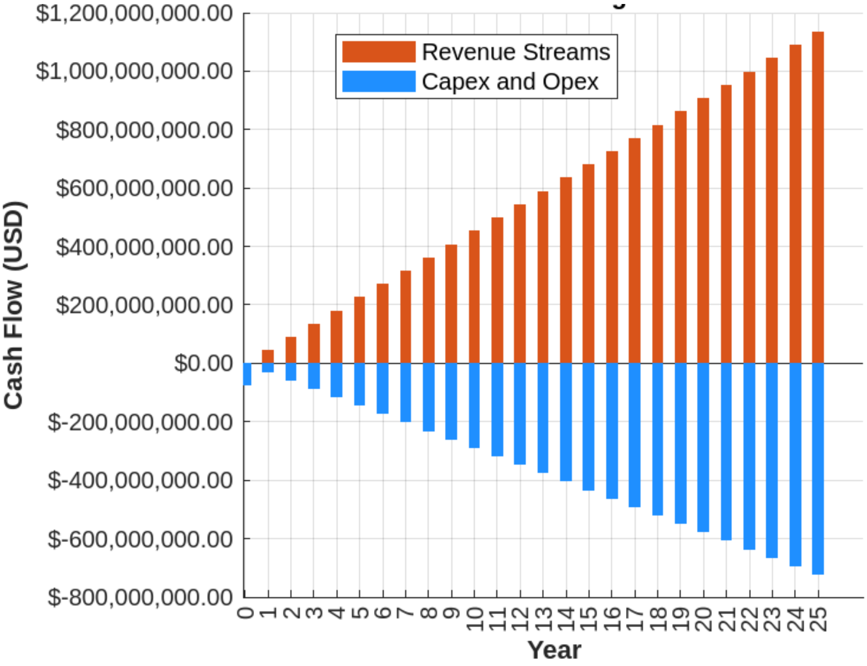

Fig. 13. Green Ammonia Plant Net Cash Flow Diagram (Scenario 2)

4 Discussion

The results obtained from the optimization analysis provide valuable insights into the economic and technical aspects of green ammonia production. Through a detailed examination of the results, the current study was able to assess the effectiveness of different optimization approaches used to optimize the cost of ammonia production. Furthermore, by comparing these results with industry and forecasts, an ascertaining of the competitiveness and prospects of green ammonia production can be done. Concerning technical and economic aspect, two distinct optimization scenarios were explored in this work: user defined Electrolyzer parameters and optimal Electrolyzer configuration profiling. These scenarios led to significant differences in power rating, capital expenditure (CAPEX), and operational expenditure (OPEX) across different plant units.

In the first scenario, where Electrolyzer parameters were user-defined, the power rating remained relatively high, with an overall electricity consumption per ton of ammonia produced of about 10,8 MWh/ton. This remains closer to current green ammonia production requirements as mentioned by Wang et al. [30]. However, a substantial reduction in CAPEX was achieved, indicating potential cost savings in the initial investment. On the other hand, the second scenario, employing optimal Electrolyzer configuration profiling, demonstrated a notable decrease in Electrolyzer power rating translated by a downsizing of the electrolyzer from 82 to 75 MW resulting in further reductions in both CAPEX and OPEX respectively by 53% and 10%. Indeed, when the electrolyzer is optimized, the electricity consumption per ton of ammonia produced drops to 10 MWh/ton with a total energy saving of the plant of 60 GWh per year.

Furthermore, the financial analysis conducted for both optimization scenarios revealed promising outcomes in terms of net present value, payback period, return on investment, and internal rate of return. Comparing the results, the optimized scenario exhibited substantial improvements across all metrics, indicating enhanced profitability and financial feasibility. Indeed, in the scenario of the optimized electrolyzer, the NPV increased by 57%, the payback period decreased by 2 years, the return on investment (ROI) increased by 14% and the internal rate of return (IRR) significantly increased by 23%.

To contextualize these findings within the broader industry landscape, comparisons were made with existing research and industry forecasts. Cesaro et al. [31] for instance, have worked on the levelized cost of electricity from green ammonia and provided valuable insights into future pricing trends and industry expectations. It concluded based on forecasting that a levelized cost of Ammonia below 400$/ton is achievable by 2040, with the potential to reach pricing levels below 300 USD if the electrolyzer is optimally calibrated to achieve efficient cost reduction. Considering the time value of money considered in this work and the levelized cost of ammonia obtained in both scenario 1 and 2, it can be concluded that the results obtained are relevant to the industry and further that the optimization model is realistic and accurate. Given an LCOA in scenario 2 of 281.5 USD/Tn(NH3) , it was shown that green ammonia can achieve competitiveness in the market as compared to traditional grey ammonia, particularly amidst increasing carbon taxation.

5 Conclusion

Throughout this paper, the study presented a pioneering approach to optimizing green ammonia production using mathematical models and Generalized Reduced gradient non-linear optimization technique the results have been illustrated and analyzed. The simulation encompassed two different scenarios, one focusing on a commonly used user defined electrolyzer and its parameters present in the literature. The second involves the optimization of the configuration profile of the electrolyzer along with its parameters and is tailored to the ammonia demand level. The analysis is done from both technical and financial aspects and the results show a great potential and feasibility in real life. Furthermore, the proposed methodology has not only addressed the environmental challenges posed by conventional ammonia production but also demonstrates significant potential in reducing both capital investments and operational expenses. By ensuring a stable energy supply through renewable sources and optimizing plant operations, the model offered a viable path toward economically sustainable and carbon-neutral ammonia production. The insights gained from this work contribute valuable knowledge to the ongoing efforts in sustainable energy transitions, providing a solid foundation for future advancements in green ammonia production.

However, the current work presented some limitations. Such as the plant's electricity supply that was considered under assumptions of being constantly supplied via a power purchase agreement. However, in real life such assumptions might not held as a power purchase agreement especially and exclusively based on green electricity accounts for a further agreement upon service level inherently to the intermittent nature of conventional green electricity technology such as wind and solar. Accounting for such variability in the electricity supply has several direct implications for the plant such as the need for electricity storage and feedstock storage capability in order to ensure a buffering capability to the plant while meeting some predefined production levels. Such variability further depends on forecasting based on weather data inputs and raises the concern about power scheduling and storage sizing optimization to ultimately lower the levelized cost of ammonia. This further implies assumptions that the optimization technique will have perfect foresight to allow the determination of operating conditions and schedules that will indeed optimize the cost of both building and operating the plant. For future works, these aspects of green ammonia might be explored with other optimization techniques to improve the results obtained in this study and ultimately promote the adoption of green ammonia by industrials as a sustainable substitute to grey and blue ammonia.

NOMENCLATURE

Abbreviation	**Meaning**
LCOH	Levelized Cost of Hydrogen
Capex	Capital Expenditure
Opex	Operational Expenditure
$S_{recovery}$	Electrolyzer Stack Recovery
$Ox_{recovery}$	Electrolyzer Opex Recovery
$Cx_{recovery}$	Electrolyzer Capex Recovery
Hy_{prod}	Hydrogen Production
LCOC	Levelized Cost of Compression
C_{PEXP}	Compression Power Expense
$CompCx_{recovery}$	Compression Capex Recovery
A_{prod}	Ammonia Production
LCAS	Levelized Cost of Air Separation
AS_{Tcost}	Air Separation Total Cost
N_{prod}	Nitrogen Production
LCOA	Levelized Cost of Ammonia
T_{COST}	Total Cost of Maintenance and Operation
$T_{E_{Ox}}$	Total Electrolyzer Opex
$E_{PExp_{NPV}}$	Electrolyzer Power Expense Net Present value
W_{Exp}	Water Expense
E_{Ox}	Electrolyzer Operational Expenditure
Sr_{NPV}	Stack Replacement Net Present Value
$Comp_{Cx}$	Compressor Capex
As_{Tcost}	Air Separation Unit Total Cost
$AS_{Cx_{recovery}}$	Air Separation Unit Capex Recovery
$AS_{P_{Exp}}$	Air Separation Power Expense

Hb_{Ox}	Haber-Bosch Unit Opex
$Hb_{P_{Exp}}$	Haber-Bosch Unit Power Expense
Hy_{Cost}	Hydrogen Production Cost
N_{Cost}	Nitrogen Production Cost
$Comp_{Cost}$	Compression Process Cost
$Hb_{Cx_{recovery}}$	Haber-Bosch Unit Capex Recovery
$Cat_{R_{Cx_{NPV}}}$	Catalyst Replacement Capex Recovery
Hb_{Cx}	Haber-Bosch Unit Capex

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