

Techno-economic Study of an Electrolysis-Based Green Ammonia Production Plant

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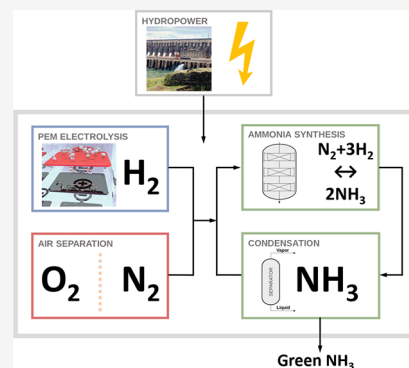


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ABSTRACT: This paper presents an investigation of a storage option of green hydrogen (H_2) in the form of ammonia (NH_3) based on system simulations considering detailed technical properties. Experimental data from a 1 MW PEM electrolyzer is used to develop an electrolyzer model and downstream a kinetic reactor for NH_3 synthesis. Exemplarily, the electricity is supposed to be supplied by a hydropower plant in Norway. An economical evaluation of the plant is performed for optimized process parameters. The costs of H_2 and NH_3 are calculated based on electrolyzer investment costs published for deployment between 2020 and 2030 and several electricity cost scenarios. From the results, a broad economic optimum of the operating range of the electrolyzer in the entire plant is obtained. This work provides a basis for the future evaluation of complex plants with electrolyzers for the production of green ammonia as well as strategies for the reduction of costs of green NH_3 in the future.



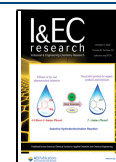
INTRODUCTION

The synthesis of ammonia (NH_3) from nitrogen (N_2) and hydrogen (H_2) with iron catalysts, known as the Haber–Bosch process, is considered to be one of the most important industrial chemical processes. For the theoretical and practical development of this process and its industrialization, the German chemists Fritz Haber and Carl Bosch were awarded the Nobel Prize in Chemistry in 1918 and 1931, respectively.¹ This process provided the world-scale production of NH_3 fertilizers, increasing agricultural productivity in a large part of the planet. As a result, the survival of more than a quarter of the world's population during the 20th century was assured.¹ The importance of these fertilizers has increased in recent years. It is estimated that currently approximately half of humanity has its food subsistence associated with this process. Globally, 235 million metric tons of NH_3 was synthesized in 2019, being the second highest produced chemical commodity in the world after sulfuric acid.² About 80% of the NH_3 produced is used as a fertilizer and the remaining 20% is used in a variety of industrial applications.³ The benefits of ammonia, however, are offset by a series of harmful effects on the environment. NH_3 itself is carbon-free and the decarbonization of its production is very much dependent on the source of H_2 , which can be synthesized via a complete carbon-free process (Figure 1). However, H_2 used for the NH_3 production, today, is predominantly produced via steam reforming of fossil fuels, e.g., natural gas, coal, or oil entailing a high carbon footprint; actually, 90% of carbon emissions within the ammonia synthesis process are assigned to the production of H_2 . Typically, for each metric ton of NH_3 produced, 2.16 metric tons of CO_2 is emitted.² As an example,

in 2010, 409 million metric tons (MT) of CO_2 were emitted by the worldwide synthesis of NH_3 , which accounts for approximately 1% of the global CO_2 emissions, making it the largest carbon dioxide emitting industrial chemical-making reaction and consuming about 1% of the world's total energy production.⁴ As the demand for N_2 fertilizers is expected to increase, scientists and engineers around the world are currently working to develop more efficient and sustainable ways to support agriculture and growing population.

A simple power to NH_3 concept is shown in Figure 1. To produce green NH_3 , H_2 must be produced through the electrolysis of water, which is already a commercial technology, using renewable sources of energy. N_2 is obtained through the separation of air. NH_3 is then produced combining H_2 and N_2 via the Haber–Bosch process. The main challenge for this technology is the higher costs due to the fact that electricity is more expensive than natural gas or coal in most countries worldwide. In fact, the electrolysis section is the main consumer of the electricity. In this respect, it is of paramount importance that renewable power technologies have undergone dramatic cost reductions in the last decade, making them cost-competitive with both fossil fuels and nuclear sources in certain regions around the world. According to the International Renewable Energy Agency, renewables are becoming the

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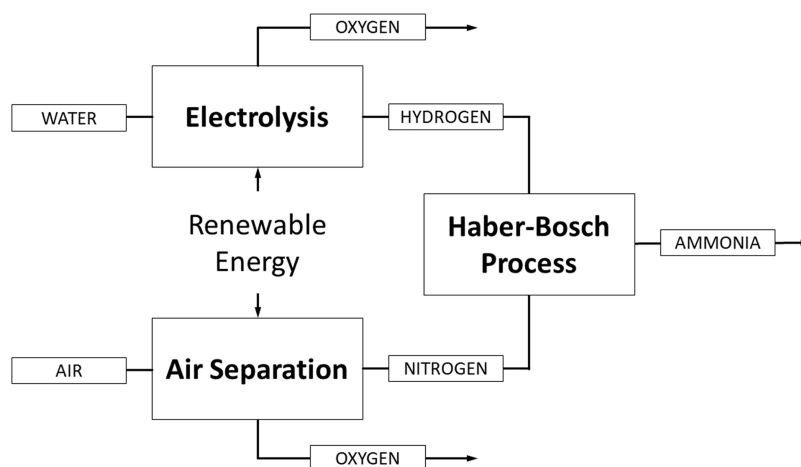


Figure 1. Schematic of green NH_3 production based on hydrogen production from water electrolysis.

cheapest source of electricity worldwide, with potential for a continued decline.⁵ Especially interesting are the winning bids for solar and wind energies in resource-rich countries: A solar photovoltaic auction in Saudi Arabia yielded 1.50 €cent/kWh, and similar prices have been achieved in the UAE (2.03 €cent/kWh) or Chile (2.44 €cent/kWh).⁶ In August 2020, a record of 1.10 €cent/kWh was settled in Portugal.⁷ This indicates that water electrolysis might already be at a competitive price point with methane steam reforming with carbon capture and storage (blue H_2) in regions with favorable renewable energy conditions.⁸ Though, the indicated price levels for blue hydrogen range between 1.43 and 2.27 \$/kg while green hydrogen prices range between 5 and 6 \$/kg.⁹ Notably, the overall progress and economical investment in the area of renewable energies positively affects the economics of water electrolysis, resulting in additional cost reductions. On the one hand, more advanced technology with higher efficiencies reduce the operational costs (OPEX), and on the other hand, advances in production technology increase the quality and reduce the investment costs of water electrolysis (CAPEX). Electrolyzers are the key facility to convert renewable power and water to green H_2 and oxygen (O_2). Two electrolysis technologies are particularly suitable for the implementation of green H_2 : alkaline water electrolysis (AEL) and the proton exchange membrane water electrolysis (PEMEL).¹⁰ Regardless of their market availability and maturity, PEMEL and AEL are still considered highly expensive in terms of investment and operational costs, compared to conventional fossil fuel-based H_2 production.⁵ The system investment costs of PEMEL are 50–60% higher than AEL, which is an extra obstacle to market penetration.⁵ Though, PEMEL is believed to bear a higher efficiency improvement potential (> 80%) over the next three decades compared to AEL (> 70%),⁵ which could relativize the effect of higher CAPEX through reduced OPEX. Both technologies are considered to have significant potential for cost reduction and to eventually become competitive against conventional hydrogen production technologies when considering economies of scale, automation, technological innovations (e.g., reduction in expensive materials for PEMEL), an increase in availability of components, and market penetration and deployment for energy storage.^{5,11} Compared to AEL, which requires potassium hydroxide (KOH), PEMEL is run on pure water. It can be expected that once PEMEL reaches the development maturity of AEL, the absence of highly corrosive

media and its advantages in volumetric power density outweigh today's lag in investment costs. Therefore, the process simulation in this study is focused on PEM electrolyzer technology.

Besides the established industrial use, ammonia has the potential to serve as a fuel. At the end of 2020, the global renewable electricity generation capacity added up to 2799 GW with hydropower accounting for the predominant share (1211 GW).¹² Due to the intermittence in electricity production from renewable sources, energy storage systems will play a decisive role in solving the imbalance between energy supply and demand, compensating for the surplus or deficit of electricity in the power grid.¹³ Chemical energy storage is the only flexible mechanism permitting abundant amounts of energy to be stored over long periods of time. The need for an energy vector with near-zero CO_2 emissions became a major concern with H_2 , proving to be a great alternative.¹⁴ Nevertheless, after decades of research into the development of a H_2 economy, H_2 is still not a commonly used transportation or stationary fuel. Physical characteristics of H_2 , such as low energy density, embrittlement of metals, difficulty in storage and transportation, and inflammability are obstacles to its implementation. Hence, NH_3 that contains 17.65 wt % H_2 is being considered as a chemical hydrogen carrier, as it may provide similar environmental benefits while mitigating the barriers to the implementation and deployment of H_2 . Some advantages of liquid NH_3 over liquid H_2 are its 71% higher energy density, the lower cost per unit of stored energy, its lower vapor pressure that facilitates the design of storage tanks, its higher distribution capacity, and better commercial feasibility. NH_3 can be easily liquified and stored at room temperature and can be produced locally from renewable energy sources. Being the second most common chemical produced worldwide, a reliable infrastructure is already established for its storage and distribution (including pipeline, rail, road, ship).^{14–16}

NH_3 can also be used as a transport fuel: when reacting with O_2 in a fuel cell, electricity to power a motor can be produced, or by direct combustion in an especially designed engine.^{9,17} In fact, green NH_3 has long been considered as one of the most promising alternative marine fuels to reduce greenhouse gas emissions within the shipping industry, which is in line with the International Maritime Organization strategy to reduce CO_2 emission by 2050.¹⁸

electrolysis and the Haber–Bosch process, producing 30 kg of NH_3 per day, and the energy is stored as NH_3 and converted back to electricity. The goal is to show the viability and round-trip efficiency through synthesis, storage, and combustion of green NH_3 . In Denmark, Skovgaard Invest has initiated a partnership with Vestas and Haldor-Topsøe to build the first commercial-scale green NH_3 plant in the world by 2022. An on-site wind and solar plants will supply the electrical power necessary to an electrolyzer. The production plant will have 10 MW of capacity and is expected to produce a total of 5000 MT of NH_3 annually, leading to a reduction of 8200 MT of CO_2 per year.¹⁹ In Norway, the joint initiative HEGRA between Yara, Aker Clean Hydrogen, and Statkraft has the goal to electrify the NH_3 plant of Heroya; hence, a reduction of 725,748 MT of CO_2 per year will be achieved. This will be the first large-scale production facility for zero-emission fertilizer.²⁰ In Louisiana, USA, thyssenkrupp and CF Industries scheduled the production start of a 20 MW electrolyzer for the production of green ammonia by 2023. A production of 20,000 MT of NH_3 per year is expected.²¹ Moreover, new demonstration plants were announced in Japan, Australia, Morocco, and the Netherlands.¹⁵ A collective effort is being made to build green NH_3 plants, impacting the transition to a carbon-free network.

In this work, a techno-economical evaluation of a 30 MW green ammonia plant is performed. The power-to-ammonia process is simulated in Aspen Plus. The technological process is divided in three sections: H_2 generation with a physical model based on experimental work from a 1 MW PEM electrolyzer, air separation unit, and NH_3 synthesis, considering a kinetic approach for the Haber–Bosch loop. We assume that the plant is installed in Bergen, Norway, and the electrical power necessary is supplied by a hydroelectric power plant. As a novelty, a realistic refrigeration cycle and phase change condensation in the synthesis loop are simulated, assuming sea water as cooling/heating medium. With ammonia as the coolant of the condensation, loop temperatures of $-10\text{ }^\circ\text{C}$ are achieved. The process is optimized based on process parameter variation. Further to this, an economical evaluation of the plant is carried out. The optimized current density operation of the electrolyzer is determined based on several economic assumptions. Finally, strategies for reducing costs of green ammonia are presented. To our knowledge, no study has considered these details in the techno-economical model.

■ PROCESS SIMULATION AND DESCRIPTION

The overall process of power to NH_3 downstream the electrolyzer flowsheet is given in Figure 2. The process is divided into three main sections: H_2 generation (H), air separation (A) and NH_3 synthesis (N). In the diagram, all the process streams are identified by the section letter followed by a number. The characterization of each stream is shown in Tables S4–S7 of the Supporting Information. In the following subchapters, each of the sections will be presented in more detail. Within the physical simulation, an Aspen Plus Block “Multiplier” is used to represent a 30 MW plant as a modular composition of 1 MW units. It is assumed that the plant is installed in Norway. Norway has the highest share of renewable electricity in Europe, with 1690 hydropower plants that account for approximately 88% of Norwegian production capacity, the remainder being wind and thermal power with 10 and 2%, respectively.²² This is the basis for assuming the hydrogen production to be truly green. The electricity used

will be sourced from hydro power, making it carbon neutral. Electricity costs of 0,04 €/kWh are considered for Norway.^{23,24}

Sea water is used as the cooling medium for the heat exchangers. Though being costly due to corrosion issues, sea water heat exchangers are common worldwide because sea water is a free heat-transfer medium that does not produce emissions. However, cooled/heated seawater discharged back to the sea could affect marine life and general sea water quality. Thus, most jurisdictions limit the temperature change to 10 K.²⁵ Since sea water temperature changes during the year, the water flow will need to be adapted depending on the current sea water temperature (see the Supporting Information). For simulation purposes, an average value of $10.6\text{ }^\circ\text{C}$ was assumed that corresponds to the average temperature in 2020 in the Norwegian city of Bergen.²⁶

Hydrogen Production. H_2 is chosen to be generated from purified water via PEM electrolysis. Great development opportunities have arisen with the PEM technology because of its versatility; thus, many companies are developing and producing PEM electrolyzers in significant power ranges (MW range).²⁷ Comparing to other commercial or near-commercial technologies, PEMEL offers a compact system design, high operating pressure, variable operating range potential, the ability to reach high current densities, high power densities, and high voltage efficiencies. It is therefore interesting if these properties lead to a specific techno-economical optimized system. Furthermore, with PEMEL, there is a fast response of system components allowing dynamic operation, operation at a lower dynamic range without showing negative impacts on H_2 purity and short cold-start times as well as energy-efficient stand-by operation that are requirements for electrolyzers that operate with intermittent power sources.^{28,29} Industry is considering PEMEL as more efficient for automated production and therefore better suited for large-scale plants.^{30,31}

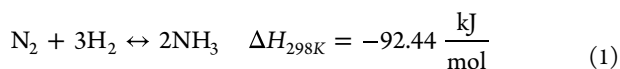
The experimental work has been performed with a PEM electrolyzer provided by Hydrogenics, and the results can be seen in the Supporting Information.³² The electrolysis stack is assembled from 212 cells with a membrane area of 1500 cm^2 . At the nominal electrical power input of 1 MW, a H_2 production rate of $290\text{ Nm}^3/\text{h}$ is reached. The operation pressure is kept constant at 30 bar, and the operation temperature ranges from 50 to $80\text{ }^\circ\text{C}$. During the experimental trials, the stack was operated between 0.5 and 2.3 A/cm^2 . In this range, a stack efficiency of 0.76 at 0.5 A/cm^2 to 0.69 at 2.3 A/cm^2 is recorded. Due to the balance of the plant, which is including water deionization, system control, and downstream gas conditioning, the real-life efficiency is slightly below this number ranging from 0.71 to 0.68 within the tested current density range. The I – V characteristics show an almost linear behavior within the tested current density range when the water temperature is controlled to an almost constant value of $65\text{ }^\circ\text{C}$.

The implementation of the electrolyzer has been performed using the model developed by Lettenmeier.³³ The model is written as a Fortran90 code with an interface to exchange data with AspenPlus. The electrolyzer is represented as a “User2” block, a user-defined block that offers free programming of a block unit. The electrochemical model is zero dimensional and requires input of temperature, pressure, and current density. From this, the cell voltage, the amount of O_2 and H_2 , and the required electrical power as well as the off-heat are determined. The equations and details for the electrochemical model can

be found in the [Supporting Information](#). Water, which is not consumed inside the electrolyzer, is being recycled in a loop. As the gases originate from a liquid water atmosphere, they exit the electrolyzer in saturated conditions. The amount of water that is driven out of the system via O₂ and H₂ depends on temperature and pressure. This is implemented in this model as it gives insight into the necessity of H₂ purification especially in the context of subsequent processing to NH₃. The amount of water consumed for electrolysis and the loss via vapor in the gases is fed from an external source and hydraulically pumped to operation pressure. In the real system, a water purification unit is implemented upstream the electrolyzer. This is not represented in the simulation except for a pressure drop inside the water cycle. The water cycle is driven by a second pump. The water flow inside the loop determines the temperature spread between the electrolyzer inlet and outlet. Increased operation temperatures improve the performance of the electrolysis; therefore, a low temperature increase over the stack is preferred. There is a pressure drop inside the water loop at the radiator, pump, piping, valves, and water pretreatment. Thus, the power requirement for water cycling increases, which is compensating for the benefit of an equal temperature distribution within the electrolyzer. An optimum flow is determined as a function of current density. This is implemented in the process control within the simulation.

Nitrogen Generation. The second necessary reactant for the Haber–Bosch process is N₂, which can be obtained from air. Three alternatives to achieving the required N₂ are considered: separation via pressure swing adsorption (PSA), a membrane system, or Linde’s double column. According to a review performed by Sanchez *et al.*, membrane permeation is more adequate to small-scale systems (<1 MW), PSA is preferred for intermediate scales (1–100 MW), and cryogenic distillation is the best method for large-scale plants.³⁴ We simulate a basic air separation unit, by simply modeling a compressor, a heat exchanger, and a separator.

Ammonia Synthesis. NH₃ production takes place in a synthesis loop in a process known as the Haber–Bosch process where H₂ gas reacts with N₂ gas at a molar ratio of 3:1, at high temperature and pressure, conventionally over an iron catalyst, to form NH₃ according to eq 1. The technology with which H₂ is obtained makes the distinction of different NH₃ processes.



The NH₃ synthesis reactor was modeled as a plug flow reactor by “RPLUG” in Aspen Plus, and the kinetics have been implemented by a user kinetics subroutine. The kinetics expression proposed by Anders Nielsen (1968) was used to model the NH₃ synthesis.³⁵ The rate expression is expressed as kmol_{NH₃} produced per m³ catalyst bed per hour, and it can be formulated as given in eq 2:

$$r = \left[\frac{k_2^0 \left(a_{\text{N}_2} K_a^2 - \frac{a_{\text{NH}_3}^2}{a_{\text{H}_2}^3} \right)}{\left(1 + K_3 \frac{a_{\text{NH}_3}}{a_{\text{H}_2}} \right)^{2\alpha}} \right] \left[\frac{\text{kg mol}}{\text{m}^3 \text{ h}} \right] \quad (2)$$

where a_i variables are the activities of each component, K_a is the equilibrium constant, k_{20} is the specific rate constant, K_3 is the adsorption equilibrium constant, and α and w are parameters that take values of 0.604 and 1.564, respectively. The equations are available in the [Supporting Information](#).

The reactor rate equations for the reactants are determined using the stoichiometry of the Haber–Bosch reaction, as follows:

$$r_{\text{NH}_3} = -2r_{\text{N}_2} = -\frac{2}{3}r_{\text{H}_2} \quad (3)$$

The reversible equilibrium type of the Haber–Bosch reaction makes it into a complex reaction. High inlet temperatures to achieve high reaction rates are necessary; however, a low outlet temperature is also necessary to achieve high equilibrium conversion.³⁶ High temperatures resulting in fast kinetics affect the conversion at equilibrium; while low temperatures favor equilibrium, it affects the reaction kinetics, compromising NH₃ yield.³⁷ A compromise between kinetics and equilibrium is accomplished through the use of temperatures between 320 and 500 °C and pressures between 150 and 300 bar.^{36,39} Furthermore, the use of several catalyst beds in series with an intercooling system is an approach used in the chemical industry to dispatch this problem. Among multibed reactor systems, studies suggested that using a three-bed system is the most efficient and cost-effective solution.³⁶

Published data by Nielsen *et al.* concerning commercial triply promoted iron catalysts was the base for the calculations and simulation for the three-catalytic bed NH₃ converter in Aspen Plus: surface area of 8.57 m²/g, particle size with an equivalent diameter of 4.6 mm, and particle density of 2200 kg/m³ are considered.^{38,39} It is assumed that the catalyst accounts for 70% of the total volume of the reactor and a void fraction of 0.3.

The NH₃ synthesis flow diagram is illustrated with a green color in [Figure 2](#). H₂ from the H₂ generation section and N₂ from the Air separation section are compressed to 150 bar (N-1 and N-2, respectively) and then mixed (N-3). The pure gas is introduced into the synthesis loop and mixed with the recycle stream (N-21) that contains unreacted H₂ and N₂ and a small amount of NH₃ that was not condensed in the liquid–vapor separator (N-4); N-3 is cooled down with the help of N-21 before entering the reaction section. The N-4 stream is then divided into two: the main stream (N-5) and the quench stream (N-6), that is again divided into two streams (N-6 and N-7). The complete NH₃ synthesis reactor was simulated as three separate reactors, each representing one single bed. A calculator was set up in the simulation to calculate the pressure drop over each reactor bed. The pressure drop along the length of a packed bed is determined through the Ergun model, given the velocity, packing size, viscosity, and density, according to eq S15 in the [Supporting Information](#).⁴⁰ N-5 flows through the heat exchanger (HX-N1), and the temperature increases before entering Bed 1. In each bed, the reaction increases the temperature and the NH₃ concentration in the exiting gas mixture. After exiting Beds 1 and 2, the streams are cooled down with the help of the quench streams N-8 and N-7, respectively, before entering the subsequent bed. After leaving the multibed reactor (N-15), the stream goes through the refrigeration cycle before entering the vapor–liquid separator (SEP-N1). At the start of the thermodynamic cycle, the refrigerant (NH₃, N-26) enters the compressor at low temperature and pressure, leaving at higher temperature and pressure (N-27). The hot gas then passes through the condenser (N-24) as it cools and condenses completely, using sea water as a cooling stream. The cooler high-pressure liquid passes through the expansion valve (N-25), which reduces the pressure causing the temperature to drop abruptly.

The cold low-pressure mixture of liquid and vapor goes through the evaporator, where it vaporizes completely as it accepts heat from the NH₃ synthesis stream (N-15) before returning to the compressor to continue the cycle. The vapor–liquid separator is used to separate NH₃ products (N-17) and the unreacted gaseous reactants (N-18). The NH₃ product with 98% purity leaves the process as a liquid stream. Since all of the NH₃ is not condensed at a time, there is a remainder of NH₃ that is recycled back to the reaction section with the unreacted gases. A small flow is purged from the recycle stream to prevent the accumulation of undesired material in the synthesis loop. Note that the sea water stream N-23 is used as the cooling medium in the refrigeration cycle and later serves as the heating medium for the recycle stream (N-20).

Economical Evaluation. After the simulation in Aspen Plus, an economic analysis of the electrolysis-based NH₃ production was performed. The capital and operating costs were approximated based on the correlation given by Turton *et al.*, who developed a general engineering approach to estimate costs.⁴¹ These correlations predict the cost of equipment based on the simulation results, i.e., mass flow rates, heat duties, operating pressures, and material of construction. Although all equipment is dimensioned according to standard material, carbon steel, a material conversion factor was applied in the end. Considering the composition of the process streams of the installation, stainless steel was used. Finally, to account for the effects of inflation it was necessary to update the costs provided by the correlations, based on the CEPCI economic index, according to eq 4, where cost index year 2000 and 2019 take the values of 394 and 634, respectively.^{37,41}

$$\text{cost}_{2019} = \text{cost}_{2000} \times \left(\frac{I_{2019}}{I_{2000}} \right) \quad (4)$$

Equation 5 is used to calculate the bare module cost for each piece of equipment (C_{BM}), where F_{BM} is the bare module cost factor and C_p^0 is the purchase cost for base conditions.

$$C_{\text{BM}} = C_p^0 \left(\frac{I_{2019}}{I_{2000}} \right) F_{\text{BM}} \quad (5)$$

The purchased cost of equipment at ambient pressure and using carbon steel construction (base conditions) is calculated according to eq 6, where A is the capacity of the equipment that was obtained from simulation, and K_1 , K_2 , and K_3 are values provided by Turton *et al.*⁴¹

$$\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2 \quad (6)$$

By incorporating material and pressure factor, F_M and F_p , the bare module cost is determined with eq 7, with B_1 and B_2 being provided by Turton *et al.*⁴¹

$$C_{\text{BM}} = C_p^0 \left(\frac{I_{2019}}{I_{2000}} \right) (B_1 + B_2 F_M F_p) \quad (7)$$

Together with the bare module costs, other costs associated with capital costs, such as contingency fees, auxiliary facilities, and miscellaneous costs, are taken into consideration with eq 8, to calculate the grassroot costs, also known as fixed capital investments.

$$\text{FCI} = 1.18 \sum_{i=1}^n C_{\text{BM},i} + 0.50 \sum_{i=1}^n C_{\text{BM},i}^0 \quad (8)$$

The total capital investment (TCI) is calculated by the sum of the fixed capital investment (FCI), with the working capital (WC), that corresponds to 15% of the fixed capital investments.

To evaluate the feasibility associated with the operation of a chemical plant, the costs associated with the day-to-day operation need to be estimated. In accordance with eq 9, the manufacturing costs (COM) are divided into three categories: direct manufacturing costs (DMC) that correspond to operating expenses that vary with the production rate (raw materials, waste treatment, utilities, operating labor etc.); fixed manufacturing costs (FMC) that are independent of changes in production rate (depreciation, local taxes, and insurance); and general expenses (GE) that represent an overhead burden that is necessary to carry out business functions (administration costs, distribution and selling costs, R&D).⁴¹

$$\text{COM} = \text{DMC} + \text{FMC} + \text{GE} \quad (9)$$

COM can be estimated knowing the fixed capital investments (FCI), cost of operating labor (COL), cost of utilities (CUT), and cost of raw materials (CRM), based on eq 10.

$$\text{COM} = 0.280\text{FCI} + 2.73C_{\text{OL}} + 1.23(\text{CUT} + \text{CRM}) \quad (10)$$

With the purpose of analyzing the profitability of the project, economic indicators such as the internal rate of return (IRR), net present value (NPV), and the payback period were calculated, assuming a period of amortization of 20 years. For the evaluation, we highlight the importance of the capital investment, the annual operation costs, and the revenues. The IRR represents the profitability generated from an investment, and the payback period is the time required to recoup the investment cost. The NPV is the difference between the inflows and outflows of operating cash flows discounted to the present, minus the investment costs. If NPV is positive, the investment is viable. Finally, the levelized cost of NH₃ (LCOA) represented by eq 11 is also calculated. The LCOA corresponds to the sum of the net present value of the capital and operating costs divided by the overall NH₃ production over the lifetime of the project, where r is the discount rate, P_t is the production rate, and n_{ifc} is the plant lifetime.³⁷

$$\text{LCOA} = \frac{\text{TCI} + \sum_{t=1}^{n_{\text{ifc}}} \frac{\text{COM}}{(1+r)^t}}{\sum_{t=1}^{n_{\text{ifc}}} \frac{P_t}{(1+r)^t}} \quad (11)$$

The last step of the economic balance is the analysis financial sensitivity of the project. When evaluating an investment, it is important to know how sensitive the feasibility indicators are to certain key variables in the analysis. Hence, it is usual to establish various scenarios, optimistic and pessimistic, in which positive and negative variations in costs are simulated.

RESULTS AND DISCUSSION

In this section, results are presented and commented. No plant operates without shutdown; these are indispensable for example for maintenance, inspection, or equipment cleaning. For most chemical processes, the plant works generally between 90 and 95% of the total hours in a year (8760 h).⁴² For calculations purposes, this plant is assumed to be working 92% of the time, corresponding to 8088 h per year or 28 days of off-time. Please note that in this paper, all data in US dollars retrieved from other sources as well as the bare modules costs

of plant equipment were converted to Euros, assuming 0.84 €/€ (consulted on September, 2021).

Hydrogen Production. The NH_3 plant was optimized for a fixed hydrogen flow of 0.08 kmol/s resulting from a 30 MW electrolyzer operated at a mean current density of 1.7 A/cm². In order to analyze the effect of current density variation, the number of cells is varied to keep the H_2 flow constant. With this approach, a conclusion of whether it is better to reduce capital costs by increasing current density or cutting operational costs by increasing efficiency can be drawn. According to data available in the literature regarding the development of water electrolyzers in the EU, electrolyzer system investment costs in 2020 are around 1000 €/kW, reaching 760 €/kW in 2030, based on stakeholder consultation.⁴³ It is assumed that the values retrieved from Buttler and Spliethoff¹¹ and Bertuccioli et al.⁴³ and illustrated in Figure 3 correspond to

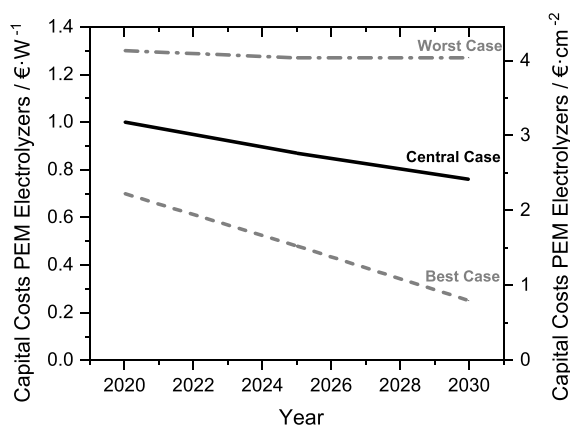


Figure 3. System cost for PEM electrolyzers between 2020 and 2030, generated with data from Bertuccioli et al.⁴³ System costs include stack, power supply, system control, and gas drying (purity above 99.4%) but exclude grid connection, external compression, external purification, and H_2 storage.

an electrolyzer stack with an active area of 318,750 cm² (@ 1.7 A/cm²). The unit €/kW is not a precise basis for system comparison as the corresponding current density between manufacturer companies may vary. Finally, the price per cm² is estimated and the capital cost of electrolyzers for different current densities is calculated. As an example, the 1 MW

electrolyzer with the investment cost of 1000 €/kW corresponds to 3.14 €/cm².

The number of cells required for each value of current density to produce the same amount of H_2 (0.08 kmol/s) and corresponding electrolyzer price is shown in Figure 4a, assuming 3.14 €/cm² as the standard price. Figure 4b shows the efficiency and power requirement for each value of current density. The results indicate that the efficiency is maximized at lower current densities, but so are the capital costs. On the other hand, the power requirements increase with rising current density, meaning higher operational costs.

In the next sections, the trade-off between efficiency and cost will be discussed. The current density is varied to understand if due to increased cell voltage (low efficiency), operational costs are exceeding the effect of investment costs as well as to identify the current density value that translates into an optimum value between investment and capital costs.

Ammonia Synthesis. The complete NH_3 synthesis reactor was simulated as three separate adiabatic reactors, each representing a single bed. After exiting each bed, the stream is cooled down before entering the following bed. Bed 1, bed 2, and bed 3 show lengths of 0.5, 0.9, and 1.1 m, respectively. The reactor diameter is constant and equals to 0.6 m. The pressure drop in each of the reactors beds is calculated according to the Ergun equation. The total pressure drop in the reactor beds is equal to 0.8 bar and will show an effect on the compression of the synthesis loop (approx. 6 kW).

To determine the conversion, N_2 is chosen as the basis of the calculation according to eq 12, where y_0 represents the mole fraction of NH_3 in the beginning of bed and y_i represents the mole fraction along the length of the reactor.

$$x_{\text{N}_2} = \frac{2(y_{0,\text{NH}_3} - y_{i,\text{NH}_3})}{(1 + y_{0,\text{NH}_3})(-y_{0,\text{NH}_3})} \quad (12)$$

Figure 5a represents the changes of NH_3 mole fraction along the three beds. At the end of the first and second bed, the NH_3 mole fraction drops because the streams leaving the bed being diluted by the quench streams. Slopes in Figure 5 can be regarded as the rate of NH_3 production; slopes are decreasing from bed to bed due to higher concentration of educts. The overall conversion of N_2 is 26%; the conversion achieved in the first bed is 50% of the overall conversion, 31% in the second bed, and 19% in the last bed. Even though the reactor length

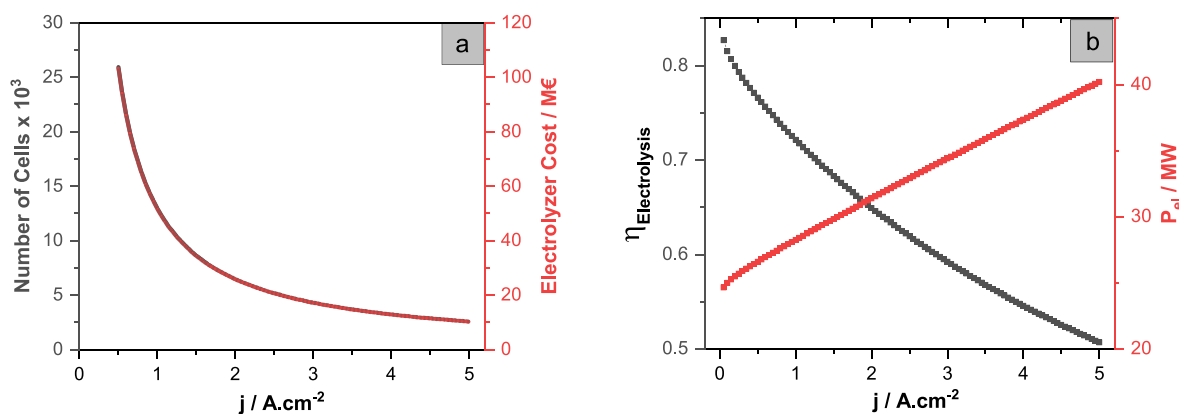


Figure 4. (a) Number of cells required to produce 0.08 kmol/s of H_2 in the PEMEL for different current densities, assuming a cell area of 1500 cm². The respective cost of the PEM electrolysis unit is calculated, assuming a specific electrolyzer cost of 3.14 €/cm²; (b) electrolyzer efficiency and system electric power consumption over current density at constant H_2 production.

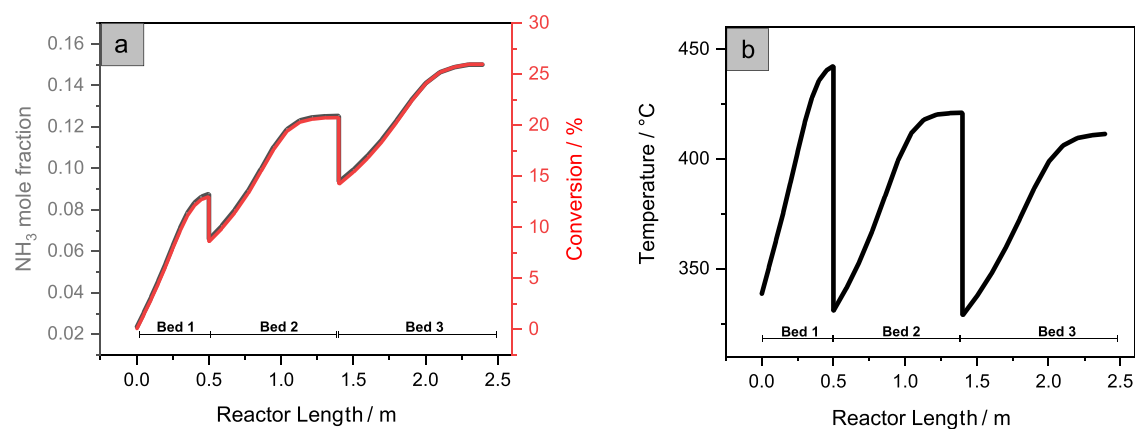


Figure 5. (a) Ammonia mole fraction and conversion of nitrogen along the beds; (b) temperature profile along the reactor beds.

increases in the second and third beds, the NH₃ concentration and feed flow rate are higher; thus, NH₃ partial pressure is increasing in the beds and the production rate is more controlled by the reverse reaction. The gas mixture enters the first bed with 2 mol % NH₃ due to limited vapor–liquid separation via condensation. Figure 5b illustrates the temperature change along the beds. In the first bed, the concentration of NH₃ is low, the reaction rate is high, and the temperature is increasing along the bed, approaching equilibrium limitation at its end. After the first and second bed, the gas is cooled down by the quench streams, resulting in decreased conversion due to kinetic limitation until it also reaches the equilibrium limitation.

Energy Analysis of the System. The typical NH₃ production is energy-consuming as a result of the considerable compression work necessary for the synthesis loop (to be efficient, the Haber–Bosch reaction must be carried out at high pressures) as well as the vapor–liquid separation at the end of the reaction loop.³⁷ The energy consumption is calculated based on the power requirements of the system, with data retrieved from the simulation in Aspen Plus. For this analysis, the three sections introduced in the beginning of this chapter are considered: H₂ generation, air separation, and NH₃ synthesis. The overall energy efficiency of the system is defined with eq 13, where η_{NH_3} is the number of moles of liquid NH₃ (stream N-17) in mol/s, LHV_{NH_3} is the lower heating value of NH₃ that corresponds to 318 kJ/mol, and $P_{\text{el,total}}$ refers to the total power requirements of the system in kW.

$$\eta_{\text{NH}_3} = \frac{\dot{n}_{\text{NH}_3} \times \text{LHV}_{\text{NH}_3}}{P_{\text{el,total}}} \times 100 \quad (13)$$

The total energy consumption of the system is 10.98 kWh/kg_{NH₃}, with an energy efficiency of about 45%. Simulation results show this optimum efficiency when the mixture is cooled down until −10 °C before the vapor–liquid separation (see the Supporting Information). An overview of the electricity consumption distribution within the system is shown in Table 1 and Figure 6.

The H₂ generation section represents the energy consumed by the electrolyzer and the pumps. In the air separation section, the compressor and pump are the equipment consuming energy. Last but not least, the NH₃ section is divided into three: the feed compression that comprises the compressors C-N1 and C-N2 necessary to increase the pressure of the H₂ and N₂ streams required for the synthesis

Table 1. Energy Consumption of the H₂ Generation, Air Separation, and NH₃ Synthesis Sections, in Percentage

	energy consumption/%
H ₂ generation	88.5
air separation	1.3
NH ₃ synthesis	10.2

loop; the recycle compression (C-N3) and the refrigeration cycle that are represented in the power to NH₃ flowsheet with dotted lines. Note that the sea water pump P-N1 is also considered in the refrigeration cycle. These results show that the H₂ production is by far the main one responsible for energy consumption followed by the NH₃ synthesis and ending with the air separation section.

Comparing our results with the ones published for conventional NH₃, a total energy consumption of about 8.89 kWh/kg_{NH₃} with an overall energy efficiency of 78% is reported.³⁷ Green NH₃ production consumes about 2 kWh/kg_{NH₃} more than the conventional SMR production. Comparing the efficiency of the conventional process with the NH₃ production via electrolysis, the enthalpy difference between the different educts CH₄ and H₂O must be considered. However, conventional NH₃ data takes advantage of the economy of scale, whereas in this study, a 30 MW plant is considered. Several studies show that the energy consumption of green NH₃ plants can be improved with expanded production capacity.^{37,44} Furthermore, technological innovation in PEMEL is still needed to further improve its efficiency that will additionally reduce the energy consumption of green NH₃ production.

Economic Analysis of the PEM Electrolysis. Figure 7 shows a detailed cost structure for the green H₂ production over a 10 year period. The cost is defined by the investment costs (account for the electrolyzer system and additional costs that include shipping, transportation, and installation that are approximately 10% of the investment costs), operation and management costs (O&M, include planned and unplanned maintenance and correspond to 5% of capex per year), and production costs (electricity and water costs).¹¹ Results from Figure 7 show that the production costs are responsible for 82% of the total green H₂ costs, investment costs for 17%, and O&M for 1%. The cost of renewable energy necessary to power the electrolyzer has the major impact on green H₂ costs; consequently, low electricity costs are a requisite for producing

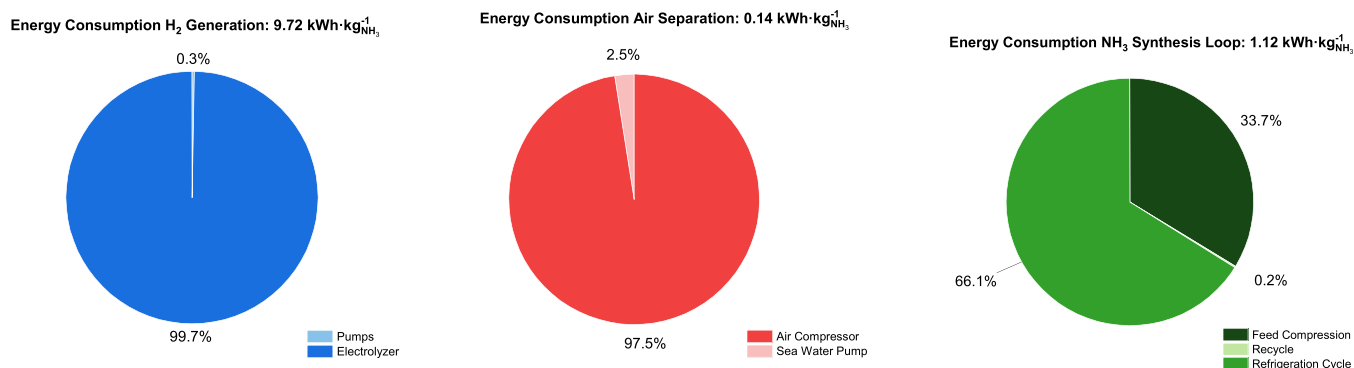


Figure 6. Energy consumption in each section of the power to the ammonia plant. The first pie (left) shows the energy consumption in the H₂ generation section, the second pie (middle) shows the energy consumption in the air separation section, and the third pie (right) shows the energy consumption in the ammonia synthesis loop.

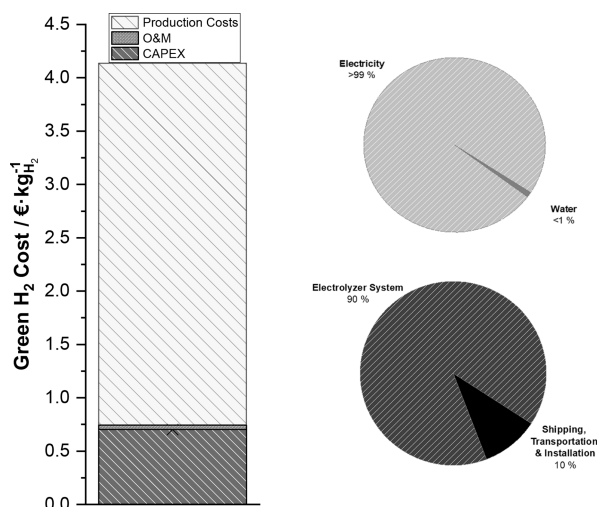


Figure 7. Green H₂ generation cost structure. Assuming $j = 1.7$ A/cm², electricity cost = 0.06 €/kWh, electrolyzer cost = 1000 €/kW, and an interest rate of 2.5%.

H₂ with competitive prices. Electrolyzer system costs are the second main driver of green H₂ costs.

Figure 8 shows a promising decrease in green H₂ costs between 2020 and 2030, based on the electrolyzer deployment costs shown in Figure 3, assuming three different electricity costs: 0.02, 0.04, and 0.06 €/kWh. Throughout the analysis, these three values will be the base for the calculations and discussion to investigate its impact on H₂ and NH₃ costs; 0.04 €/kWh is chosen as an approximation of the current price in Norway and 0.06 and 0.02 €/kWh as more pessimistic and optimistic values, respectively. Electricity prices around 0.02 €/kWh can already be found in resource-rich countries.^{6,7} Results from Figure 8 suggest that electrolyzer cost reductions are not enough for competitiveness if electricity costs do not decrease as well. IRENA reports a blue H₂, i.e., produced from SMR with carbon capture and storage, cost range between 1.06 and 2.12 €/kg_{H₂}.⁵ In fact, results show that green H₂ can be competitive with blue H₂ if electricity cost is 0.02 €/kWh, keeping in mind the difference in size between SMR and the presented 30 MW electrolysis plant.

In Figure 10b, the optimized operation points of the electrolyzer for different electricity scenarios are determined. The results demonstrate that for lower electricity costs, the optimum operation point is at higher current densities. At

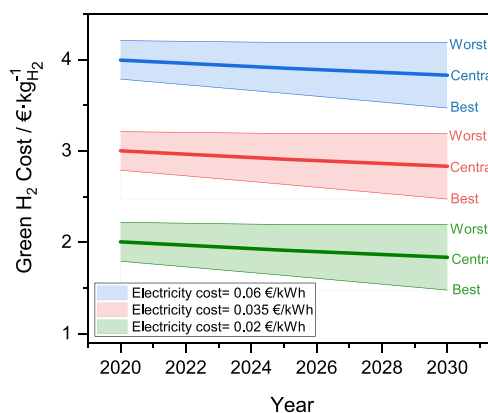


Figure 8. Green H₂ generation costs. Assuming $j = 1.7$ A/cm², electricity costs of 0.02, 0.04, and 0.06 €/kWh, electrolyzer costs in 2020 are varying between 700 and 1300 €/kW, 480 and 1270 €/kW in 2025, and between 250 and 1270 €/kW. We assume a stack lifetime of 80,000 h and an interest rate of 2.5%.

higher current densities, the effect of operational costs, i.e., electricity, is more pronounced. That is much more visible for the black line in the graph, corresponding to the higher electricity costs. Thus, it can be concluded that if the electricity cost corresponds to 0.06 €/kWh, the electrolyzer in the beginning of life (BoL) should operate at 2.4 A/cm², for 0.04 €/kWh at 3.2 A/cm², and for 0.02 €/kWh at 4.4 A/cm².

To evaluate the economics of PEMEL, the pay-off time of the electrolyzer is estimated based on the profit (difference between revenue from H₂ sales and production costs), investment cost, and interest rate. The revenues correspond to the money earned from the sale of H₂, that is dependent on the market. H₂ selling prices are varying from 4 to 10 €/kg_{H₂}.⁴⁵ In the present case, the H₂ production rate is constant for all current densities; this implies that the revenues remain constant, varying only with the H₂ market selling price. On the one hand, operational costs increase with rising current density, suggesting that the higher the current density, the lower the profits. On the other hand, the lower the current density, the higher the investment costs because more cells are required in the stack. Taking this into consideration, the pay-off time is calculated (Figure 9a).

Figure 9 helps to better understand what is the best current density depending on the electricity costs and H₂ market price. Results show that it is mostly more profitable to work at higher current densities as the pay-off times are inferior. In other

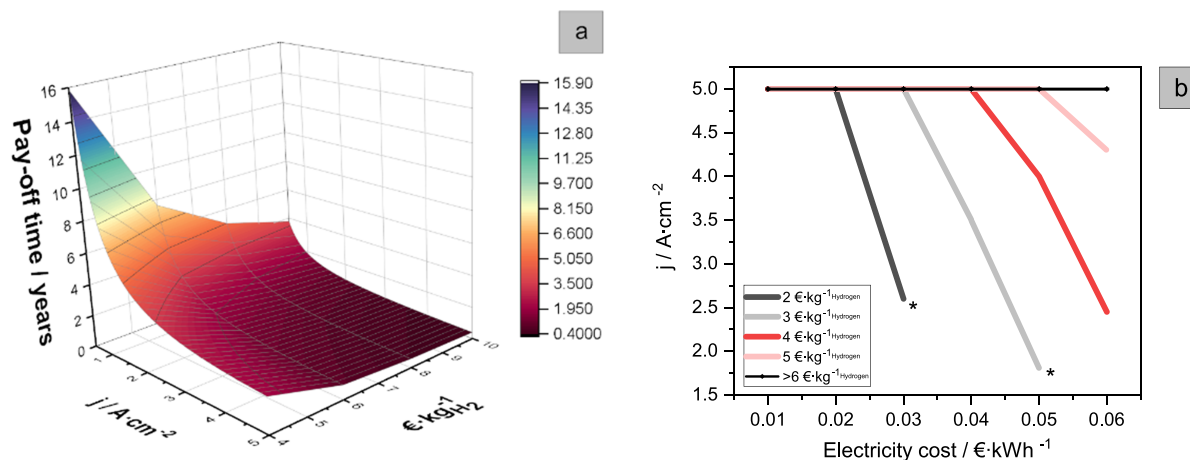


Figure 9. (a) Pay-off time as a function of H₂ price and current density, electricity = 0.04 €/kWh; electrolyzer cost = 3.14 €/cm²; (b) optimized current density over electricity cost (based on pay-off time data), varying selling price of H₂. *If the H₂ selling price is 2 €/kg, it will only be profitable if electricity cost is ≤0.03 €/kWh. If the H₂ selling price is 3 €/kg, the electricity cost must be ≤0.05 €/kWh.

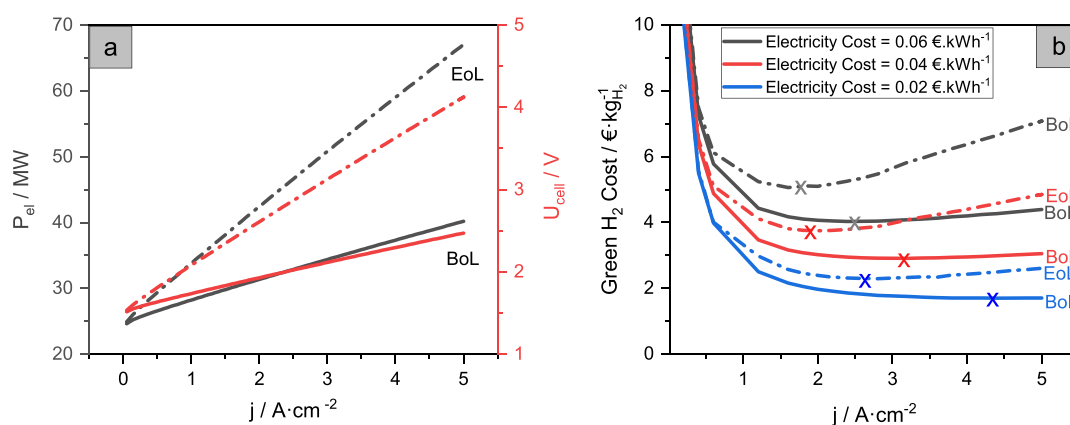


Figure 10. (a) Difference in power consumption and cell voltage between beginning of life (BoL) and end of life (EoL) taking PEMEL degradation into consideration. EoL corresponds to a time period of 100,000 h of operation. Operation limit of the electrolyzer cell voltage is set to 2.5 V; (b) sensitivity analysis of the cost of green H₂ for different electricity costs and optimized point of operation for each scenario (compact line). The dashed dotted line represents the effect of degradation after 100,000 h in the green H₂ cost. The cross, ×, represents the optimum point of operation, i.e., where the lowest green H₂ production costs are achieved.

words, this means that it is better to sacrifice the electrolyzer efficiency in favor of lower investment costs. However, that is very much dependent on electricity and H₂ market prices. Findings suggest that when facing a situation where high electricity costs are combined with low H₂ selling prices, then it will be more beneficial to working at lower current densities.

According to the information shared by the FCHJU website,⁴⁵ in Europe, most of the H₂ is being sold at prices higher than 6€/kg. As can be seen in Figure 9b marked with an asterisk, if the H₂ selling price is 2 €/kg, then it will only be profitable if the electricity cost is equal or below 0.03 €/kWh; similarly, if the H₂ market price is 3 €/kg then electricity cost must not be higher than 0.06 €/kWh in order to make profit. Note that these two situations are not considered in Figure 9a because of negative profit results. As previously stated, the combination of two factors, H₂ selling price and electricity cost, will determine the optimum operational point for the electrolyzer. Taking for example the red curve (4 €/kg_{H₂}), it is more favorable to operate the electrolyzer at current densities higher than 5 A/cm² as long as the electricity costs are below 0.04 €/kWh, whereas if the electricity cost is 0.05 €/kWh, it is

more advantageous to operate the electrolyzer at a current density below 4 A/cm², and so on.

One issue of commercial electrolyzer systems is degradation. Continued operation leads to degradation by deteriorating the physical and chemical stability of the cell components, reducing its performance and lifetime.⁴⁶ Electrolyzer manufacturers report lifetimes between 60,000 and 100,000 h, with voltage degradation rates below 4–8 μV/h.¹¹ It is assumed that 6 μV/h corresponds to the degradation rate at 1.7 A/cm² and a degradation-based resistance, that increases with higher current density is added to the electrolyzer model in the simulation. The effect of degradation on power requirement and cell voltage as well as on H₂ production cost is shown in Figure 10a, represented with a short dashed dotted line. The electrolyzer operation time is assumed to be 100,000 h (EoL). Degradation results in higher cell voltage, hence increased power requirement and decreased efficiency. In Figure 10b, a comparison between BoL and EoL is depicted: when taking degradation into consideration, the optimum current density is lower as a result of the increase of electricity requirement that shifts the optimum to the left side of the graph. It is important to highlight that from a technical point of

view operation above 2.5 V cell voltage is not recommendable due to severe degradation. However, more research needs to be conducted in electrolyzer degradation, especially for higher current densities so that it is possible to have more accurate data for this analysis.

Economical Evaluation of the Power to the Ammonia Process. Based on the simulation results, investment and operational costs are calculated and discussed in this section. In the following, the reference case is the following: current density of 1.7 A/cm², electrolyzer investment cost of 1000 €/kW, an interest rate of 2.5%, and plant lifetime of 20 years with operational time of 8088 h per year. The plant produces approx. 25,000 metric tons of NH₃ annually, corresponding to approximately 3 metric tons of NH₃ per hour.

Investment Costs. Cost estimation was performed for the equipment used in the NH₃ synthesis downstream an electrolyzer process. Allman *et al.* reported a fixed installed capacity cost of a PSA unit producing 12.5 kg_{N₂}/h to be 27,333 €. ³⁸ Using the rule of the six-tenths, the approximate cost of a unit (C_B) can be calculated if the cost of a similar unit (C_A) of a different capacity (S_A) is known, according to eq 14. With 2832 kg_{N₂}/h required to fully convert the hydrogen produced to ammonia, the PSA unit cost is determined to be 710,116 €.

$$C_B = C_A \left(\frac{S_B}{S_A} \right) \quad (14)$$

The calculation of the bare module costs is based on the use of equations and values provided by Turton *et al.*, as previously described. Bare module costs consider the purchased cost of equipment and material and pressure factors. Since we are dealing with NH₃, stainless steel is assumed to be the construction material for all equipment in the plant. In Table 2, a distribution of the costs per section of the flowsheet is

Table 2. Total Bare Module Costs by Section of the NH₃ Green Plant

	bare module cost/M€	total cost/%
hydrogen generation	30.54	77.64
air separation	1.09	2.78
ammonia synthesis	7.70	19.58
total	39.33	100

presented. The total bare module cost is about 39.3 M€. The percentage that each piece of equipment represents in the overall total cost is given in Figure S9 in the Supporting Information. The H₂ generation section shows the highest capital investment, with the electrolyzer representing 76% of the total costs followed by the 19% of compressors (Figure S9). The remaining costs of the fixed capital investment are estimated based on the bare module costs, according to eq 5. The fixed capital investment costs are 51.8 M€, and the working capital is 7.7 M€. Hence, the total investment capital (TCI) is 59.6 M€.

Operating Costs. Operating cost are estimated considering variable and fixed costs. Variable costs include costs that vary with the production rate such as raw materials, utilities, and operating labor. On the other hand, fixed costs are independent of changes in the production rate and include administrative costs, taxes, insurances, and maintenance, among others. The total annual operating costs (COM) are calculated according to eq 9, by the sum of the direct

manufacturing costs (DMC), fixed manufacturing costs (FMC), and general manufacturing costs (GMC). These costs are estimated based on values of fixed capital investments, utilities and raw materials costs, and operating labor costs. Labor costs are predicted based on the total annual production of the plant; for the analysis, 25 employees with average salaries of 2700 € gross are assumed. ⁴⁷ Utilities correspond 100% to electricity costs that are required for each unit. Raw materials include water for electrolysis (0.005 €/kg_{H₂O}, not considering costs for deionization), the refrigerant NH₃ for the refrigeration cycle, and the iron-based catalyst for the reactor, with the cost of 5 €/kg, changed once per year. ⁴⁸ From this, DMC, FMC, and GMC are calculated (Table 3),

Table 3. Operating Costs

	operating costs/M€	total cost/%
direct manufacturing costs	16.51	60.35
fixed manufacturing costs	6.92	25.29
general manufacturing costs	3.93	14.36
total	27.36	100

giving a total operating cost of 27.36 M€ per year. The direct manufacturing costs are the main contributors to the operating costs, and this is due to high electricity costs of the system.

Financial Feasibility Analysis. To analyze the profitability of the process, indicators such as the internal rate of profitability (IRR), the return on investment (Payback-Time), and the current value were used (NPV), considering a time horizon of 20 years. For the economic evaluation, all the costs previously characterized were considered with special attention to the investment and production costs as well as annual revenues. The revenue of the plant is entirely obtained through the sale of the product for which the industrial unit is intended, NH₃, as well as O₂ produced via the electrolysis of water and in the air separation unit. However, revenues will not only be influenced by the amount produced but also by the value of the products in different markets. Overall, a total amount of 5719 kg/h of O₂ is generated in the plant: 4876 kg/h via electrolysis and 843 kg/h during air separation. It is assumed that O₂ will be sold locally for medical use for the avoidance of extra costs of transportation, in 54 storage tanks with a capacity of 682 L each, that can afterward be sold at 105 €/tank. ³⁷ It is estimated that approx. 24 M€/year is spent in tanks and that the income from selling the O₂ is 46 M€, resulting in a profit of 22 M€/year. For the O₂, the profit is assumed to be constant. The NH₃ market price is very unstable; for instance, between July 2020 and July 2021, the bNH₃ price increased by 53%, from 409€/MT (continuous lines in the Figure 11) to 627€/MT (dotted lines in Figure 11). ⁴⁹ Calculations were performed considering a tax rate of 22%. ⁵⁰ Figure 11 displays the evolution of the accumulated cash flows over the years, assuming the three different electricity costs scenarios.

In this analysis, the variation in electrolyzer cost was not considered. Observing Figure 11, it can be concluded that with the sales of NH₃ and O₂, the plant would be profitable for all different scenarios with the payback period strongly depending on electricity costs and achievable NH₃ price. As an example, when facing a case like the one represented with the dotted blue line, in 5 years, the plant would start having profit. Overall, this is a profitable process. However, if the revenue of the plant would come exclusively from selling NH₃, the plant

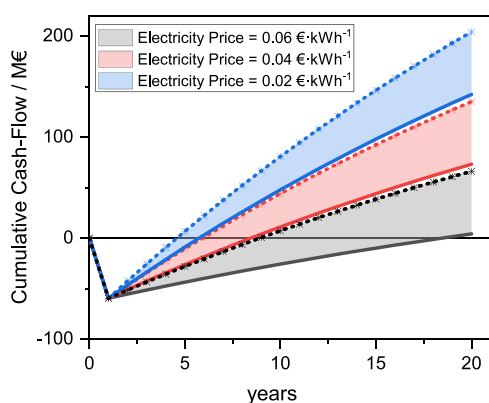


Figure 11. Cumulative cash-flow over 20 years, tax of 22%, interest rate of 2.5%, electrolyzer cost 1000 of €/kW and ammonia market prices between 409 and 627 €/MT.

would only be profitable in the case where the market price of NH_3 is around 1000 \$/MT and the electricity is 0.02 €/kWh.

Levelized Cost of Ammonia. The levelized cost of NH_3 is calculated knowing the total capital investment (TCI), total operating costs (COM), and the annual production rate, according to eq 11. It is to be noted that the impact of electrolyzer degradation is not considered in the calculation of costs due to the lack of reliable data.

Variables having the highest impact on NH_3 cost were electricity and electrolyzer investment costs. A sensitivity analysis of the LCOA to electricity and electrolyzer costs is performed. For this, electricity costs between 0 and 0.06 €/kWh are presumed, as renewable energy is becoming cheaper with technological evolution. For the system cost of PEMEL, data between 2020 and 2030 from Figure 3 is considered; the central and best cases are chosen for this analysis. The results of the sensitivity analysis can be seen in Figure 12 and are compared with conventional NH_3 costs. These values were calculated for a constant current density value of 1.7 A/cm²; later on, an evaluation considering the

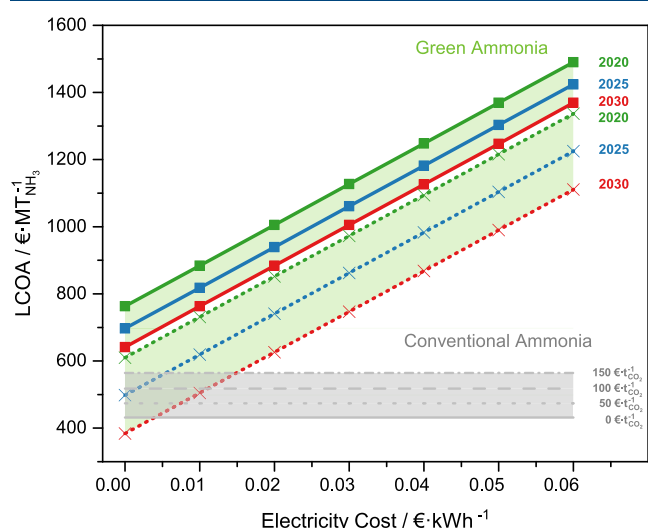


Figure 12. Sensitivity analysis of LCOA to electricity costs, for different values of electrolyzer costs between 2020 and 2030 (the dotted lines correspond to the best case, and the straight lines to the central case illustrated in Figure 3). These results correspond to an electrolyzer operation point at 1.7 A/cm².

optimized operational point of current density for different scenarios of electricity and electrolyzer variation will be performed. 420 €/MT was assumed for a typical SMR plant, and to this value, a CO_2 emission penalty cost is added.⁴⁹ A growing number of countries are making commitments to achieve net zero carbon emissions within the next few decades. A typical SMR plant produces 2 tons of CO_2 per tons of NH_3 ; thus, if a CO_2 tax of 21–63 €/tons of NH_3 is assumed, the CO_2 penalty cost will be in the range of 42 to 126 € per metric ton of NH_3 .⁵¹

Results from the sensitivity analysis indicate that the LCOA decreases if electricity and electrolyzer system costs decrease. Nevertheless, the values are still not competitive with typical NH_3 plants except for the situation where the green and the gray zones overlap (e.g., electrolyzer cost is 480 €/kW (2025) and 0.005 €/kWh). Still, the difference in scale between the two technologies, which is disadvantaging electrolysis, has to be considered.

Assuming electricity cost of 0.04 €/kWh, LCOA is estimated to be 1248 €/MT, whereas Lin *et al.* reported a conventional NH_3 plant LCOA to be 441 €/MT, about 3 times cheaper.³⁷ The severe cost decrease is predominantly due to high energy consumption and capital costs for the H_2 production. In the same paper, a LCOA of 908 €/MT for a similar green NH_3 process is stated; the difference is mostly due to the fact that alkaline electrolysis (AEL) is used, with the cost 288 €/kW, while in this study, PEMEL is chosen, which still is more expensive.

The optimized current density operation point for the NH_3 production is determined, based on different scenarios. In Figure 13a, the optimized values for an electrolyzer system cost ranging between 50 and 1000 €/kW are presented, varying the electricity costs. An extremely optimistic scenario is investigated: it is supposed that in the future, values between 50 and 200 €/kW will be realistic for PEMEL as well as electricity costs below 0.02 €/kWh. Actually, researchers are working to find cheaper materials for PEMEL which, if successful, will result in a dramatic cost drop.

The results demonstrate different optimum points of operation depending on the electrolyzer and electricity costs. Findings reveal that for lower electricity costs, it is preferable to operate the electrolyzer at higher current densities. An increase of electricity costs has a strong impact on operating costs; therefore, it is recommended to work in the middle range of current densities where there is a compromise between capital and operational costs. Analyzing the results on the effect of the electrolyzer costs, one can conclude that once the system cost decreases, then operation at lower current densities is advantageous from an economical point of view. Lower current density operation also means higher electrolyzer capital costs (Figure 4a); however, these results prove that if the electrolyzer capital costs decrease in the near future, it will be no longer necessary to operate the electrolyzer at higher current densities and compromise its efficiency as the main setback from working at lower current densities, high capital costs, will be reduced.

Knowing the optimized value considering the two variables, electricity and PEMEL cost, the LCOA was calculated as shown in Figure 13b. The graph is divided into three scenarios: very optimistic (electrolyzer range between 5 and 200 €/kW), optimistic scenario (Figure 3, “best case” line), and base scenario (Figure 3, “base” line). Conventional NH_3 cost and its correspondent CO_2 penalty are considered in the analysis. The

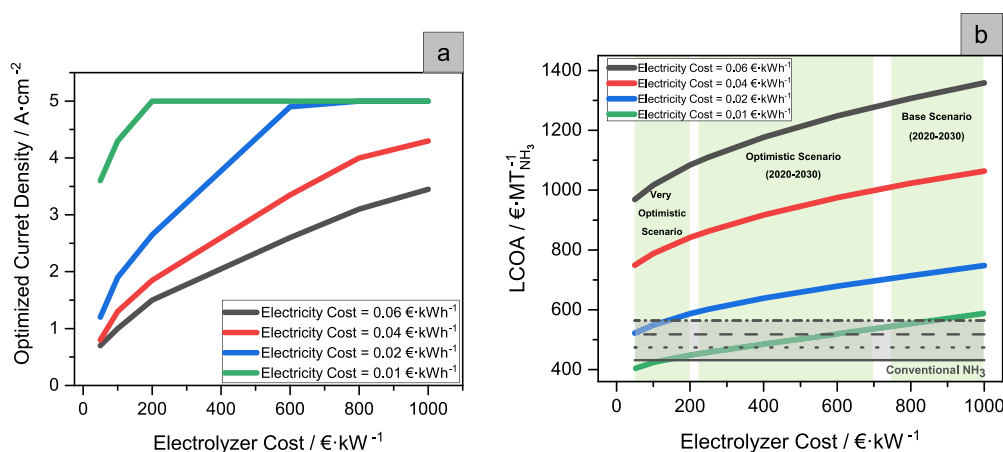


Figure 13. (a) Optimized current density as a function of electrolyzer and electricity costs. (b) LCOA for different scenarios of electrolyzer and electricity costs and comparison with conventional ammonia costs including CO₂ taxes.

results indicate that if electricity costs decrease to values of 0.01 €/kWh, then green NH₃ will be competitive with conventional NH₃ as long as the electrolyzer costs are below 900 €/kW and that the maximum CO₂ tax (126 €/MT_{NH₃}) is applied.

The results show that green NH₃ still is uncompetitive on the global fertilizer market. The authors conclude green NH₃ produced in a 30 MW plant to be competitive in the time frame between 2020 and 2030. CO₂ penalties must increase and that plants must be located in favorable geographical conditions where continuous supply of electricity from renewable energy resources is available at the lowest possible cost. However, it should be pointed out that conventional NH₃ cost takes advantage of economy of scale. Actually, a typical large-scale SMR plant produces about 1500 MT/day whereas the 30 MW green NH₃ plant produces around 83 MT/day, 18 times less production.² We emphasize the fact that the plant will only benefit from economy of scale: the larger the production scale, the lower the average costs; concerning the ammonia synthesis and air separation section, this is in accordance with the six-tenths rule (eq 14) by which it is more favorable to produce green NH₃ in a large-scale plant. Additionally, with increasing production size, energy consumption can be reduced. Concerning the electrolysis, it is expected that due to increasing volume production (standardizing manufacture and design allows industrialization and scale-up), supply chain development, and technology innovation, the investment costs of PEMEL will decrease. Improvement of efficiency results in the reduction of the electricity consumption. Lowering the noble metal content of the electrodes reduces the capital costs of PEMEL, and the increase of the durability prolongs the equipment lifetime.^{5,11} Increasing stack production to automated production in the GW scale manufacturing facilities can achieve a step-change cost reduction.⁵ Continuous R&D on the efficiency, performance, and cost of PEMEL is crucial to further reduce costs with green NH₃. To complement the idea of increasing carbon taxes, the solution can also come from governments that can offer incentives to green H₂ and NH₃ producers by establishing manufacturing targets, tax exceptions, and incentives by providing cheaper electricity fees to support energy storage technologies.¹⁵ In this way, the production of green NH₃ would become more attractive to future investors.

CONCLUSIONS

The aim of this study is to create results that can be used for the evaluation of H₂ conversion options. Power to fuel is discussed as an important element in a future renewable energy system. In this context, the main goal of this project was to develop a system simulation to study the possibility of using NH₃ as an energy carrier using green H₂ produced by means of PEM electrolysis. Data from the 1 MW electrolyzer from Hydrogenics was used for the simulation. The high pressure and temperature Haber–Bosch synthesis loop were simulated using an adiabatic reactor with triple catalyst beds and quench cooling in between. The design uses a refrigeration cycle that operates with NH₃ as the refrigerant and a vapor–liquid separator to separate liquid NH₃. Through the optimization of the operational parameters, e.g., within the refrigerant cycle and the ammonia synthesis process, the system efficiency could be increased to some extent, which could be part of future research. The plant exemplarily is supposed to be installed in Norway to take advantage of present hydropower resources, and seawater is used as cooling/heating medium in the heat exchangers. Around 25,000 metric tons of green NH₃ are produced annually. In a future study, the size of the plant could be increased to allow for better comparison with existing NH₃ production plants based on SMR. An economical evaluation of PEMEL with the determination of the payoff time for this technology, based on several economic assumptions, was performed; the optimum operation points of the electrolyzer with and without degradation effects were estimated.

On a general green NH₃ plant perspective, the total installed cost of the plant was found to be 59.6 M€, whereas the operational costs are 27.36 M€. These values are achieved assuming an electrolyzer cost in 2020 of 1000 €/kW and electricity cost of 0.04 €/kWh, which is a good approximation of the current electricity cost in Norway. Assuming that the PEMEL operates at 1.7 A/cm², the levelized cost of NH₃ (LCOA) was calculated for the aforementioned conditions and correspond to 1248 €/MT_{NH₃}, being off from conventional NH₃ production by the factor of 3. Results unanimously show that electricity costs are the main cost driver of green NH₃ followed by electrolysis investment costs. Sensitivity analysis on the LCOA were performed varying the electrolyzer and electricity cost, and the optimized operational current density for each situation was determined. Results suggest that small-scale NH₃ generation based on hydropower is still

uncompetitive with conventional NH_3 . It is concluded that the cost is very much depending on the geographical conditions and must be installed in countries with very low electricity costs in order to be profitable. However, the financial situation for green NH_3 is projected to improve in the future, not only because of the expected decay in renewable electricity costs but also the reduction in PEMEL costs due to research, development, and mass production. Efforts are being made by scientists and engineers worldwide into the decarbonization of NH_3 production to meet the zero carbon targets. Government incentives such as the implementation/increasing of CO_2 penalties, establishment of emission restrictions, and subsidization could play a key role as it would assist the progress and make the green NH_3 industry more attractive to investors.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.iecr.2c00383>.

Experimental work of the 1 MW PEM electrolysis plant; electrochemical model implemented in Aspen Plus; reactor kinetics model implemented in Aspen Plus; pressure drop in the reactor; sensitivity analysis of the effect of pressure and temperature in the mole fraction of NH_3 ; sea water as cooling/heating medium and condenser (HX-N2) requirements; effect of temperature of the vapor–liquid separation process on the overall system efficiency; stream table results; estimation of equipment costs; financial feasibility analysis; leveled cost of ammonia; effect of interest rate variation on LCOA results (PDF)

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Notes

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