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Techno-economic optimization of a decentralized, small-scale electrochemical haber-bosch process for green ammonia production

Yeşil amonyak üretimi için merkezi olmayan, küçük ölçekli elektrokimyasal haber-bosch sürecinin teknolojik-ekonomik optimizasyonu

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Techno-Economic Optimization Of A Decentralized, Small-Scale Electrochemical Haber-Bosch Process For Green Ammonia Production

Highlights

- *Reactor pressure affects conversion efficiency and residence time.*
- *High pressure increases conversion rate and reduces reactor volume.*
- *LCOA and OPEX values decrease as electrolyzer efficiency increases.*
- *Increased production scale significantly reduces unit costs.*
- *High capacity factor spreads fixed costs over more production.*

Graphical Abstract

This study examines the technical and economic feasibility of green ammonia production via the electrochemical Haber-Bosch (eHB) process, showing that reactor pressure, electrolyzer efficiency, and large-scale low-cost electricity make it competitive with conventional methods.

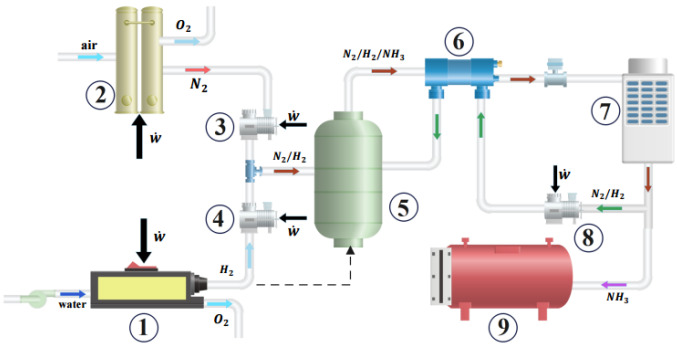

Figure 1. System schematics

Aim

This study aims to evaluate the technical and economic feasibility of the electrochemical Haber-Bosch (eHB) process for green ammonia production and provides a detailed analysis of the effects of process parameters on costs.

Design & Methodology

The design and methodology of the study are based on modelling and parameter optimization for the technical and economic analysis of green ammonia production using the electrochemical Haber-Bosch (eHB) process.

Originality

This study is unique in its comprehensive technical and economic assessment of green ammonia production using the high-pressure electrochemical Haber-Bosch (eHB) process and presents an innovative approach for decentralized production.

Findings

This study has revealed the decisive effects of scale, electricity cost and capacity factor on the economic feasibility of green ammonia production. The findings indicate that, at production scales above 25 tones/day and with low electricity prices, the eHB process could be cost-competitive for decentralized production.

Conclusion

The results indicate that the economic viability of the electrochemical Haber-Bosch (eHB) process depends on the balanced optimization of scale, electricity cost and capacity factor. Under suitable conditions, the eHB process offers a competitive alternative to conventional methods for decentralized green ammonia production.

Declaration of Ethical Standards

The author(s) of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

Techno-Economic Optimization Of A Decentralized, Small-Scale Electrochemical Haber-Bosch Process For Green Ammonia Production

Araştırma Makalesi / Research Article

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ABSTRACT

Ammonia has become a strategic compound for sustainable energy systems due to its carbon-free structure, high hydrogen density and compatibility with existing infrastructures. In this study, the technical and economic feasibility of green ammonia production based on the electrochemical Haber-Bosch (eHB) process is analysed in detail. Modelling results show that reactor pressure and electrolyser efficiency have decisive effects on the levelized cost of ammonia (LCOA) and operating expenses (OPEX). Under pressures above 9000 kPa, the conversion efficiency and the residence time in the reactor decreases, decreasing the conversion efficiency but resulting in a smaller reactor volume, thus reducing reactor costs. Especially at electricity prices as low as 30 USD/MWh, LCOA has been observed to be competitive with conventional methods at scales above 25 tonnes/day. Furthermore, increases in capacity factor and production scale improve economic performance by spreading capital and fixed operating costs over a larger production volume The results demonstrate that high-pressure eHB systems supported by renewable sources offer an industrially viable and competitive option for decentralised green ammonia production across various sectors, from the fertiliser industry to hydrogen carrier applications.

Keywords: CAPEX/OPEX, green ammonia production, Haber-Bosch process, levelized cost of ammonia, techno economic assessment.

Yeşil Amonyak Üretimi İçin Merkezi Olmayan, Küçük Ölçekli Elektrokimyasal Haber-Bosch Sürecinin Teknolojik-Ekonomik Optimizasyonu

ÖZ

Amonyak, karbon içermeyen yapısı, yüksek hidrojen yoğunluğu ve mevcut altyapılarla uyumluluğu nedeniyle sürdürülebilir enerji sistemleri için stratejik bir bileşik haline gelmiştir. Bu çalışmada, elektrokimyasal Haber-Bosch (eHB) sürecine dayalı yeşil amonyak üretiminin teknik ve ekonomik fizibilitesi ayrıntılı olarak analiz edilmiştir. Modelleme sonuçları, reaktör basıncı ve elektrolizör verimliliğinin amonyağın seviyelendirilmiş maliyetine (LCOA) ve işletme giderlerine (OPEX) belirleyici etkileri olduğunu göstermektedir. 9000 kPa'nın üzerindeki basınçlarda, dönüşüm verimliliği ve reaktördeki kalma süresi azalır, bu da dönüşüm verimliliğini düşürür ancak reaktör hacminin küçülmesine ve dolayısıyla reaktör maliyetlerinin azalmasına neden olur. Özellikle 30 USD/MWh gibi düşük elektrik fiyatlarında, LCOA'nın 25 ton/gün üzerindeki ölçeklerde geleneksel yöntemlerle rekabet edebileceği gözlemlenmiştir. Ayrıca, kapasite faktörü ve üretim ölçeğindeki artışlar, sermaye ve sabit işletme maliyetlerini daha büyük bir üretim hacmine yayarak ekonomik performansı iyileştirir. Sonuçlar, yenilenebilir kaynaklarla desteklenen yüksek basınçlı eHB sistemlerinin, gübre endüstrisinden hidrojen taşıyıcı uygulamalarına kadar çeşitli sektörlerde merkezi olmayan yeşil amonyak üretimi için endüstriyel olarak uygulanabilir ve rekabetçi bir seçenek sunduğunu göstermektedir.

Anahtar Kelimeler: CAPEX/OPEX, yeşil amonyak üretimi, Haber-Bosch prosesi, amonyağın seviyelendirilmiş maliyeti, tekno-ekonomik değerlendirme.

1. INTRODUCTION

Ammonia has received further interest since global concerns on climate change accelerate, due to its high hydrogen content, energy density, and compatibility with existing infrastructure. Once primarily known as a fertilizer feedstock, ammonia is now increasingly recognized as a promising carbon-free energy carrier as well [1,2]. A comprehensive assessment of its potential in the sustainable energy transition has become critical. Traditionally, approximately 80% of the ammonia produced worldwide is used in the production of nitrogen-containing fertilizers [1]. However, its utility in energy systems is gaining further interest. Ammonia contains 17.6% hydrogen by weight and can be liquefied at room temperature under a relatively low pressure of 10 bar, making it a promising hydrogen carrier for storage and transportation [2,3]. Due to its carbon-free combustion, ammonia is a potential fuel for power generation, marine propulsion, and direct use in fuel cells [4,5]. Also, it can be synthesized using green hydrogen

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by producing from the electrolysis of water powered by renewable sources, offering a pathway to decarbonize energy-intensive sectors [6]. As summarized in Table 1, ammonia strikes an optimal balance among hydrogen carriers in terms of hydrogen content, energy density, and ease of storage.

Table 1. Comparison of Hydrogen Carriers in Terms of Energy Density, Heating Value, and Storage Conditions

Carrier	H2 Content (wt%)	LHV (MJ/kg)	Volumetric Energy Density (MJ/L)	Typical Storage Conditions	Reference
Ammonia	17.6	18.6	11.5	10 bar, 20 °C (liquid)	[2]
Liquid Hydrogen	100	120	8.5	–253 °C, 1 atm	[3]
Methanol	12.5	19.9	15.6	Ambient	[4]
LOHC (e.g., DBT)	6.2–7.2	~11–13	9.3	150–300 °C (release phase)	[5]
Compressed H2	100	120	~5.6 (at 700 bar)	700 bar, 20 °C	[6]

The Haber–Bosch (HB) process, developed in the early 20th century, remains the industrial standard for ammonia production. Operating at high pressures (~100 bar) and high temperatures (~700 K), the process typically uses hydrogen from methane steam reforming and nitrogen from cryogenic air separation. While highly efficient at scale, the HB process is responsible for approximately 1.2% of global CO_2 emissions and nearly 2% of total energy consumption [3,7]. Moreover, the infrastructure required is capital-intensive, making the process viable only in large-scale centralized facilities. This limits its application in decentralized or modular setups. To address the environmental and economic drawbacks of the conventional HB process, researchers have investigated alternative ammonia synthesis routes that operate under more moderate conditions and incorporate renewable resources. Among these, the electrochemical Haber–Bosch (eHB) process has emerged as a leading contender.

The term “electrochemical Haber–Bosch (eHB)” used in this study does not imply that direct electrochemical nitrogen reduction occurs within the reactor. The process represents an electrification-supported Haber–Bosch configuration in which the classical Haber–Bosch synthesis cycle is preserved, the hydrogen source is provided by water electrolysis, and the system energy is supplied by electricity-based inputs. Therefore, the term eHB is used here to describe a process that, unlike the direct electrochemical ammonia synthesis (NRR) systems in the literature, is based on the thermocatalytic Haber–Bosch process in terms of reaction mechanism but has an electrified hydrogen production and energy supply infrastructure. This distinction is important to emphasize that the modeling and economic assessments conducted within the scope of this study focus solely on examining the effects of the hydrogen production method and energy integration.

In this study, the eHB configuration refers to a conventional thermocatalytic Haber-Bosch synthesis loop supplied by electrolytic hydrogen rather than a direct electrochemical nitrogen reduction reactor. This hydrogen is then reacted with nitrogen gas to form ammonia, eliminating the need for fossil-based hydrogen sources. While this route significantly reduces greenhouse gas emissions, it remains hindered by high electricity demands. Electrolysis is an energy-intensive process, and the cost of electricity remains the primary obstacle to widespread economic deployment [7,8]. The scalability of eHB systems is closely tied to reductions in electricity price, improvements in electrolyzer efficiency, and expansion of renewable energy access. Moreover, the strong triple bond of nitrogen molecule makes it chemically inert, highly selective and efficient catalysts. In eHB systems, the electrolysis stage accounts for the majority of total energy input, consuming approximately 50–55 kWh/kg H2 [7]. Depending on local electricity rates, this translates to hydrogen costs ranging from $1.5 to $3.5/kg [3,7,8]. Studies on the energy and exergy performance of green hydrogen production processes show that production efficiency is strongly dependent on operating conditions and that system integration plays a decisive role in overall energy efficiency. In particular, thermodynamic analyses reveal that hydrogen production processes are one of the critical steps in the energy conversion chain [9].

Another promising approach is the Direct Nitrogen Reduction Reaction (DNRR), which directly reduces atmospheric nitrogen to ammonia using renewable electricity. DNRR operates at ambient temperature and pressure, offering a highly sustainable alternative. However, the process suffers from extremely low yields and slow kinetics due to the robust N≡N bond. Compounding this issue is the competing hydrogen evolution reaction (HER), which diverts electrons toward H2 production instead of ammonia. This severely limits Faraday efficiency and the economic viability of the process [10]. The NOx Reduction Reaction (NOxRR) provides another electrochemical pathway for ammonia production by converting nitrogen oxides (NO and NO2)—air pollutants—into ammonia. While this offers a dual benefit of pollutant mitigation and NH3 production, it remains at an early development stage. Selectivity remains low, and catalyst design is critical. Faraday efficiency is typically limited, and side reactions contribute to energy losses [1,7]. The decisive effect of reactor and electrode structure on reaction efficiency in electrochemical energy conversion systems is also frequently emphasized in the literature. It has been demonstrated that electrode surface properties and electron transfer mechanisms directly affect system performance, highlighting the importance of the electrochemical approach in modeling electrification-supported chemical production processes [11].

Deploying modular eHB units at localized sites presents a transformative opportunity, especially in off-grid or remote regions. These systems, powered by solar or wind energy, can facilitate on-site fertilizer or fuel production, eliminating the need for expansive transport infrastructure [6]. In recent years, there has been a rapid increase in academic studies on the role of hydrogen and hydrogen-derived fuels in sustainable energy systems. Bibliometric analyses conducted specifically for Turkey reveal that hydrogen production, ammonia, and thermodynamic energy conversion processes are among the new research trends, emphasizing the strategic position of these fuels in the energy infrastructure of the future [12]. However, smaller system sizes often operate at reduced capacity, resulting in higher capital cost per unit of product (CAPEX). Economic analyses reveal that as system size and current density decrease, the levelized cost of ammonia (LCOA) rises steeply [7,10/7,13]. Despite these limitations, integrating green hydrogen production with localized ammonia synthesis could revolutionize energy and agricultural infrastructure. Ammonia can serve not only as a zero-carbon fuel and hydrogen carrier, it can also provide flexible energy storage medium compatible with existing logistics [4-6].

Multiple studies have analysed the techno-economics of green ammonia production. Hochman et al. and Fernandez and Hatzell reported LCOA values between \$800 and \$1000/ton NH_3, mainly due to high CAPEX, low capacity factors, and variable electricity costs [7,10]. Izelaar et al. examined three electrochemical synthesis routes—direct, indirect, and lithium-mediated. Their study concluded that for economic viability, Faraday efficiency must exceed 80%, current density must surpass 300 mA/cm², and electricity costs must remain below \$0.024/kWh [14]. Zhang et al. obtained the highest system efficiency (~74%) in power-to-ammonia processes, but noted long capital payback times [15]. Mersch et al. (2024) emphasized that green ammonia is still 70% to 150% more expensive than blue ammonia in countries like Germany and Saudi Arabia [16]. Olabi et al. noted that a 164 MW electrolyzer system may cost over €144 million, with a payback period exceeding seven years [17]. Li et al. emphasized that electrochemical systems currently operate above the theoretical energy limit (~26 MWh/ton NH_3) and that achieving commercial viability requires minimum Faraday efficiencies of 50% and current densities over 300 mA/cm² [18]. Morgan et al. (2023) assessed offshore wind-powered systems in the U.S., estimating an LCOA of \$1224/ton NH_3 [19]. This value is marginally competitive compared to conventional ammonia prices from the 2010s but reflects challenges in cost reduction. Alshehhi evaluated solar-powered systems in the Middle East, reporting LCOA values between \$1040 and \$1170/ton NH_3, with about 80% of this cost attributable to electrolyzer-related expenses. In the same study, the levelized cost of hydrogen (LCOH) was reported at \$2.5/kg [20]. Ahmed et al. reported that electrochemical methods could achieve LCOA values around \$951/ton NH_3—approaching parity with traditional HB processes under certain assumptions [21]. Ghavam et al. found that ammonia production via electrolysis consumes approximately 12,000 kWh/ton NH_3 and 1588 kg of water [22]. These values underscore the substantial energy and resource demands of green synthesis pathways.

Lowering LCOA to below \$1000/ton NH_3 from renewables demands not only major advances in system efficiency, materials, and design but also policy interventions and substantial reductions in electricity prices [7,17]. A comprehensive approach encompassing technology, economics, and regulatory frameworks will be essential to unlock the full potential of green ammonia as a sustainable and scalable energy carrier. This study examines in detail the impact of multidimensional parameters such as reactor pressure, electrolyzer efficiency, production scale and capacity factor on LCOA in green ammonia production based on the electrochemical Haber-Bosch process. Through model-based analyses, the key technical and economic interactions shaping the process performance are revealed and system-level optimization opportunities are evaluated under different scenarios. Thus, it is questioned whether eHB systems can be a decentralized and economically viable alternative in sustainable energy infrastructure, and an original contribution to the limited number of holistic analyses in the literature is presented.

2. METHODOLOGY

The schematic in Figure 1 illustrates the process flow of the eHB system designed for green ammonia production. The process begins with an electrolyzer (1) powered by a renewable energy source producing H_2 from water. Simultaneously, the air separation unit (ASU) (2) obtains N_2 from atmospheric air. These two gases are then compressed to reactor pressure via the N_2 (3) and H_2 (4) compressors, respectively, and subsequently fed into the Haber–Bosch reactor (5). In this reactor, ammonia synthesis occurs under medium-temperature and high-pressure conditions. The hot gas stream exiting the reactor passes through a regenerator (6), where heat is recovered to increase the overall efficiency of the system, and then reaches the condenser (7) unit, where the ammonia is condensed and separated. The unreacted gases are fed back into the reactor via a recycling compressor (8). Finally, the ammonia obtained is stored in an NH_3 storage tank (9).

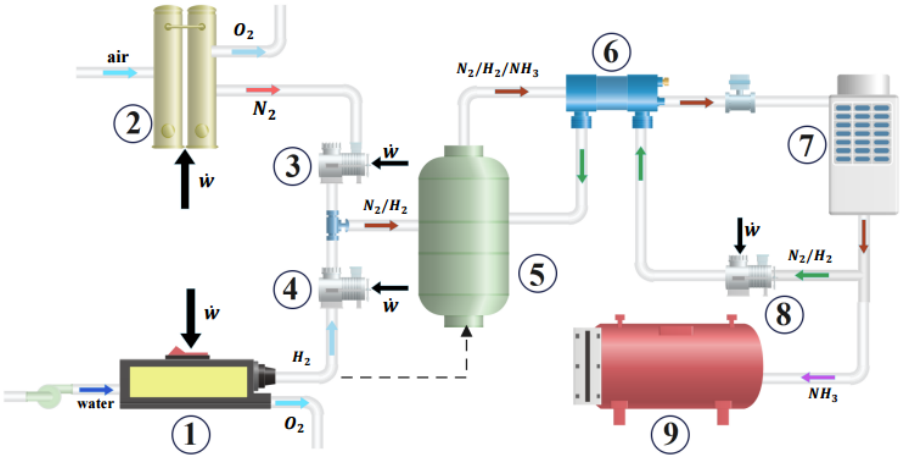

Figure 1. System schematics

A simplified thermal and economic model was developed to assess the feasibility of green ammonia production using a small-scale electrochemical Haber–Bosch (eHB) system. The model focuses on key physical and economic components, enabling a rapid evaluation of system performance under various operating conditions. Ammonia production for the plant is achieved through the following series of reactions [23].

$$H_2O \rightarrow H_2 + 1/2O_2 \quad \Delta H = 286\ kJ/mol \tag{1}$$

$$N_2 + 3H_2 \rightarrow 2NH_3 \quad \Delta H = -92.4\ kJ/mol \tag{2}$$

The molar flow rate of ammonia for the specified tone/day scale is obtained by dividing the target production quantity by its molecular mass. The required amounts of hydrogen and nitrogen are calculated according to the stoichiometric ratio. In this context, two-thirds of the molar flow rate of NH_3 per hour is hydrogen, and half is nitrogen. The power values required for the electrolyzer and air separation unit (ASU) are given below:

$$W_{el} = \frac{\left(m_{H_2} + m_{H_{2heating}}\right) * HHV_{H_2}}{\eta_{el}} \tag{3}$$

$$W_{ASU} = \frac{0.6 m_{N_2}}{24} \tag{4}$$

Where $m_{H_{2heating}}$ expression defines the amount of hydrogen required to maintain the temperature of the HB reactor at the desired level, HHV_{H_2} represents the high heating value of hydrogen, while η_{el} indicates the efficiency of the electrolyzer. The hydrogen requirement is calculated taking into account the additional heat demand based on the reactor's operating conditions:

$$Q_{heat} = m_{mix} * c_{p_{avg}} * \left(T_R - T_{avg}\right) \tag{5}$$

Here, m_{mix} , $c_{p_{avg}}$, T_{avg} and T_R are the mass flow rate of the N2 and H2 mixture, the average specific heat of the mixture, the average temperature of the gases at the compressor outlet, and the operating temperature of the reactor, respectively. These parameters enable the calculation of the additional hydrogen quantity required for the heating process.

Although the Haber-Bosch reaction is exothermic, additional heat input is required to heat the return flows to the reaction temperature and to compensate for thermal losses in the system. In this study, the heat requirement in question was represented using the lower heating value of the hydrogen available within the process, without modelling an external fuel system. This approach is a simplified energy balance assumption used for small-scale, electrification-based systems, and the calculated hydrogen quantity is included in the economic analysis solely to ensure temperature sustainability.

During the modelling process, it was assumed that the electrolyser efficiency is independent of the selected electrolyser type. The power requirements of the compressors were determined based on fundamental polytropic equations; the outlet conditions were evaluated considering the pressure ratio required to reach the HB reactor pressure. Furthermore, for the purpose of simplifying the model, the ammonia conversion rate has been defined as a function of the HB reactor temperature and pressure; it has been assumed that temperature is a function of pressure under the ideal gas assumption. [24]:

$$Y = \frac{-1.2804 + 0.4457\left(\frac{P_R}{100}\right) - 0.00149\left(\frac{P_R}{100}\right)^2 + 0.2223T_R - 0.000396T_R^2}{100} \tag{6}$$

Here Y is the ammonia conversion rate, and PR is HB reactor pressure. The ammonia conversion rate is considered a critical parameter in determining the recycling rate and sizing the post-reactor equipment. The reactor volume is related to the scaling cost and is essentially dependent on the residence time of the gas in the system.

In the Haber–Bosch synthesis, ammonia formation does not depend solely on pressure but occurs under the combined influence of parameters such as temperature, equilibrium constant, and recirculation rate. Therefore, the conversion relationship used in this study is not treated as a direct kinetic model but as a simplified approach representing the equilibrium behavior reported in the literature within the relevant temperature and pressure range. The expression used was chosen to enable a comparative analysis of the economic effects of process parameters without increasing the computational load, and it represents an equilibrium representation of the actual system behavior.

This relationship is also defined by the Arrhenius-type expression given below [25]:

$$\tau = 5.96 * 10^{-7} e^{\frac{12027.9}{T_R + 273.15}} \quad (7)$$

Finally, the reactor volume is determined with the existing gases in the reactor and their required residence time at the existing reactor conditions:

$$V_R = (v_{mix} m_{mix} + Y * v_{NH_3} * m_{NH_3} + (1 - Y)(v_{mix} m_{rec})) * \tau \quad (8)$$

The residence time approach used in reactor sizing represents a design range determined for comparative system analysis rather than actual kinetic design. In this context, the selected residence time values have been limited to be consistent with the typical gas contact times reported in the literature for Haber–Bosch reactors [26−28]. Thus, the model has been treated as a scalable representation for comparing the economic effects of process parameters rather than absolute reactor design.

The gas flow exiting the reactor is first cooled by passing through a regenerative heat exchanger, during which the heat released is transferred to the return flow. The flow is then expanded to storage pressure (20 bar), ammonia is condensed and separated from the gas phase and stored in the NH_3 storage tank. The gases in the recycling line are compressed back to reactor pressure by a recycling compressor, and the energy consumption of this process is evaluated in a similar manner to other compressors. The heat exchanger area is calculated using the logarithmic mean temperature difference (LMTD) method, and the heat load of the condenser is determined based on the enthalpy of vaporisation of ammonia. This simplified mass and energy balance model allows for the calculation of the dimensions of the basic system components to be used in cost estimation.

Total hourly power consumption of the process, corresponding Power-to-X efficiency and specific energy consumption is as follows:

$$W_{total_{HB}} = W_{el} + W_{ASU} + W_{comps} + W_{aux} \quad (9)$$

$$\eta_{HB} = \frac{6.25 * Scale * \frac{1000}{24}}{W_{total_{HB}}}, W_{spec,HB} = \frac{6.25}{\eta_{HB}} \quad (10)$$

Where, W_{aux} represents the auxiliary power requirement arising from electronic conversion processes and is assumed to be approximately 5% of the total power consumption. η_{HB} represents the ammonia production efficiency of the system, while W_{spec} indicates the specific power consumption expended per unit mass (kg) of ammonia produced.

Capital investment costs are estimated using log-based cost correlations developed for the electrolyser, compressors, reactor, heat exchangers, condenser, storage tank, and ASU unit. These values are updated taking into account scale factors and CEPCI indices, and the final equipment costs are adjusted accordingly. The general calculation form for equipment purchase costs is presented below [29]:

$$C_p = C_0 + a \cdot log_{10} X + b \cdot (log_{10} X)^2 \quad (11)$$

Here C_p is the purchase cost, C_0 is the reference cost, and a and b are constants related to each component and X is the component specific size such as area, power consumption, volume etc. Table 2 tabulates these constants for each major component of the system. The module and system factors for the electrolysis system are:

$$F_m = 5.7676 \cdot W_{el}^{-0.156} \quad (12)$$

$$F_s = 2.0642 \cdot W_{el}^{-0.063} \quad (13)$$

These regulations have been implemented with the aim of reducing impacts in large-scale systems and relatively increasing them in very small-scale applications. For components other than electrolysers, the bare module factor (F_{BM}) is used, depending on the selected material [30]. The bare module cost (C_{BM}) for each component is presented along with the relevant material, module, and system factors; additionally, in some cases, a pressure factor is applied for processes operating at high pressure, and the details are shown in Table 3.

Additionally, the correlations in [31] were scaled using the Chemical Engineering Plant Cost Index (CEPCI) and a value of 2.01 was taken as the basis. Equipment costs have been adjusted to the current cost level using the CEPCI index based on reference year values provided in the literature. The cost approach used is at the conceptual design level and is an order-of-magnitude estimate. In such early-stage process designs, the typical uncertainty range for investment cost calculations is approximately ±30–50%. Therefore, the results obtained have been interpreted to comparatively evaluate the relative

economic effects of the parameters rather than to represent the absolute investment cost [31]. The total bare module cost of each component is referred to as C_{BM} and the CAPEX for each system is calculated according to the equation given below:

$$CAPEX = \sum_{i=1}^{n} C_{BM} \cdot F_{MSCE} \quad (14)$$

It is assumed that F_MSCE accounts for approximately 30% of the total CBM, this ratio covers maintenance, site provision, engineering and construction-related expenses. The OPEX calculation takes into account a 20-year operating period, a capacity factor in the range of 0.3 to 0.8, and the levelized cost of electricity (LCOE):

$$OPEX = 8760 \cdot W_{total} \cdot LCOE \cdot Capacity \cdot Life \quad (15)$$

Here, 8760 represents the total number of hours in a year, and OPEX only covers expenses related to power consumption. As the study focuses on small-scale businesses, labour, other operating consumables, waste management, and interest rate-related costs have not been included. Finally, the levelled cost of ammonia (LCOA) is given as follows:

$$LCOA = \frac{CAPEX + OPEX}{Scale \cdot 365 \cdot Capacity \cdot Life} \quad (16)$$

In this study, electricity consumption is considered the dominant component of operating expenses. However, non-electricity expenses such as maintenance, labour, water consumption, and auxiliary consumables also contribute to the total operating costs in small-scale ammonia production facilities. These expenses have not been modelled in detail and have been evaluated as secondary effects representing fixed operating expenses. Therefore, the results have been interpreted to show comparative economic trends where electricity costs are the determining factor.

Table 2. Constants for purchase cost correlation given in (Eq. 11)

Component	C_0	A	b	X	Unit
Air separation unit	2736.63	-1099.26	140.68	Power consumed	kWh
Electrolyzer	4403.56	-1811.57	256	Power consumed	kWh
Compressors	4473.61	-1666.33	192.32	Power Consumed	kWh
Regenerator	2241.02	-730.6	71.37	HEX area	m2
Condenser	1799.48	-672.99	99.88	HEX area	m2
HB Reactor	112342	-55459	11462	Volume	m3
Storage Tank	67837	-139663	119986	Volume	m3

Power-to-ammonia efficiency (η_{P2A}) is defined as the ratio of the chemical energy content of the ammonia produced to the total electrical energy supplied to the system. This parameter is widely used to evaluate the efficiency of converting electrical energy into a chemical energy carrier [32]. In this study, the efficiency was calculated using the following equation:

$$\eta_{P2A} = \frac{\dot{m}_{NH_3} \cdot LHV_{NH_3}}{P_{elc}} \quad (17)$$

Here, $\dot{m}_{NH_3}$ represents the mass flow rate of ammonia production (kg/s), LHV_{NH_3} represents the lower heating value of ammonia (MJ/kg), and P_{elc} represents the total electrical power consumed by the system (kW). This definition is consistent with the standard energy efficiency definition used to comparatively evaluate the performance of power-to-fuel conversion systems.

Table 3. Bare module cost equations for system components

Component	Bare module cost equation	Factor
Electrolyser	$C_{BM} = C_p \cdot X \cdot F_M \cdot F_S$	Eqs. 12 and 13
Compressors	$C_{BM} = C_p \cdot X \cdot F_{BM} \cdot CEPCI$	$F_{BM} = 4.5$
HB Reactor*	$C_{BM} = C_p \cdot X \cdot F_{BM} \cdot F_P \cdot CEPCI + C_{p_{cat}}$	$F_{BM} = 6, F_P = 1.2$ $C_{p_{cat}} = 180000 \cdot V_{reactor}$
Regenerator	$C_{BM} = C_p \cdot X \cdot F_{BM} \cdot CEPCI$	$F_{BM} = 3.5$
Condenser	$C_{BM} = C_p \cdot X \cdot F_{BM} \cdot CEPCI$	$F_{BM} = 3.5$
Storage Tank	$C_{BM} = C_p \cdot F_{BM}$	$F_{BM} = 3.5$
* $C_{p_{cat}}$ represents the loading cost of the catalyst and this value is directly related to the reactor volume.		

This study uses a system model based on steady-state principles. The time-dependent production variability of renewable energy sources has not been directly modelled dynamically. Instead, intermittent operating conditions have been indirectly represented using different capacity factor values. Thus, the model aims to comparatively evaluate the effects of renewable source variability on

annual production and economic performance rather than simulating real-time operating behaviour.

The fundamental thermophysical properties of the streams used in the system analysis have been evaluated based on the process conditions. The reactor inlet stream consists of a mixture of N_2 and H_2 under high pressure and is considered to be in the gas phase. At the reactor outlet, the NH_3 formed is converted to the liquid phase in the condensation unit, while the recirculation gases remain in the gas phase. Density, specific heat, and phase behaviour were determined in the calculations using the ideal gas approximation and the ammonia condensation conditions given in the literature.

3. RESULTS AND DISCUSSION

Figure 2a presents the variation of ammonia conversion and reactor residence time with respect to reactor pressure, based on the developed pressure- and temperature-dependent conversion model. In line with Le Chatelier's principle, an increase in pressure favours the formation of ammonia due to the reduction in the number of gas-phase molecules, which tends to shift the equilibrium toward the product side (Le Chatelier, 1884). Although higher temperatures which are coupled with pressure in the model, thermodynamically reduce the equilibrium conversion rate due to the exothermic nature of the synthesis reaction. This limitation is partially mitigated by the beneficial effect of increased pressure. Moreover, elevated temperatures accelerate the reaction kinetics via the Arrhenius relation, significantly decreasing the reactor residence time. This kinetic advantage outweighs the thermodynamic drawback within the scope of the model, which is steady-state and does not explicitly simulate equilibrium behaviour. As a result, pressure increase yields a net positive impact on system performance, simultaneously reducing residence time and supporting conversion, thereby contributing to improved process economics. These results emphasize the trade-off between conversion efficiency and reactor sizing, underlining the necessity of optimizing operating conditions to achieve a balance between productivity and system compactness. Figure 2b shows that power-to-ammonia efficiency decreases with increasing reactor pressure across all electrolyzer efficiencies. Higher electrolyzer efficiency significantly improves overall system performance, reaching up to ~0.61 at 80% efficiency. However, even at high efficiency of electrolyzer, increasing pressure slightly reduces the efficiency due to additional compression energy demand and decreased ammonia-conversion.

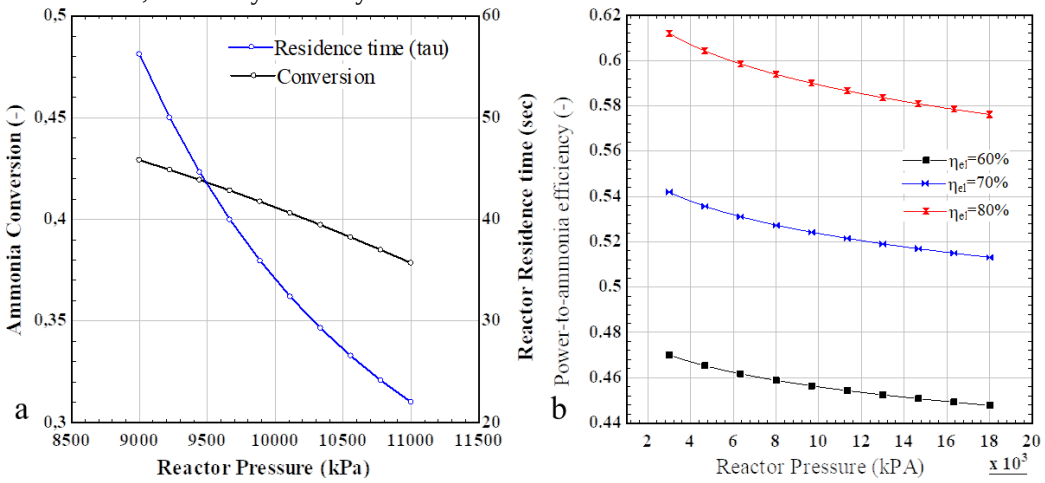

Figure 2. (a) Effect of Reactor Pressure on Ammonia Conversion and Residence Time. (b) Effect of reactor pressure and electrolyser efficiency on power-to-ammonia efficiency.

Figure 3a illustrates the impact of reactor pressure and production scale on the Levelized Cost of Ammonia (LCOA) for two different electricity prices (10 and 50 USD/MWh), under a fixed capacity factor of 0.3. As expected, the LCOA decreases significantly with increasing production scale, primarily due to the economies of scale in both capital and operational costs. Additionally, higher reactor pressures (e.g., 11000 kPa) result in slightly lower LCOA values compared to lower pressures (7000 kPa), due to improved conversion efficiency and reduced recycle loads, which reduce the required reactor volume and related investment. Notably, at an electricity cost of 10 USD/MWh, the LCOA drops below 1000 USD/ton for scales above approximately 25 ton/day, particularly under higher-pressure operation. This threshold is commonly regarded as the cost competitiveness point with conventional Haber–Bosch processes. Thus, the results suggest that small-scale electrochemical ammonia production can become economically viable if powered by very low-cost renewable electricity sources, especially when operated at elevated pressures and moderate-to-large scales. The obtained cost values were evaluated alongside the conventional and renewable ammonia production cost ranges reported in the literature [33,34]. This allowed the system's competitiveness to be interpreted not only in terms of low electricity prices but also within the context of the typical cost bands of existing production technologies.

Figure 3b compares the capital expenditure (CAPEX) and operational expenditure (OPEX) as a function of plant scale for three reactor pressures (7000, 9000, and 11000 kPa) under a fixed LCOE of 50 USD/MWh and capacity factor of 0.3. CAPEX increases nearly linearly with scale, yet at a decreasing marginal cost when moving from lower to higher pressures, suggesting more efficient utilization of reactor volume and auxiliary systems. On the other hand, OPEX grows moderately and shows stronger sensitivity to reactor pressure. Higher pressure operations (e.g., 11000 kPa) consistently lead to lower OPEX, driven by reduced hydrogen recycle requirements and improved energy integration. These dual reductions in CAPEX and OPEX under elevated pressures provide strategic guidance for minimizing total system cost, particularly at medium-to-large production scales.

The effect of electrolyzer efficiency (η_{el}) on both LCOA and OPEX under different reactor pressures is examined in Figure 3c. In this scenario, where the LCOE is fixed at 50 USD/MWh and the capacity factor is 0.3, both OPEX and LCOA decrease significantly as η_{el} increases from 0.6 to 0.8. This reduction is due to the lower electricity consumption per unit of ammonia production at higher efficiency. The trend is particularly sharp in the lower efficiency range, indicating a strong nonlinear dependence of the system on this parameter. Among the pressures compared, the high pressure of 11000 kPa stands out, achieving the lowest LCOA and OPEX values across the entire efficiency range. This demonstrates that high electrolyzer efficiency combined with high pressure provides a synergistic advantage. In conclusion, where renewable electricity supply is limited or cost is a concern, the use of advanced electrolyzer technologies combined with pressure optimization is a critical strategy for economically competitive ammonia production.

Reactor temperature is also an important parameter determining conversion efficiency. Although high temperature accelerates reaction kinetics, it can limit equilibrium conversion. Therefore, the economic optimum is determined not only by pressure but also by the temperature-pressure balance. Although a constant temperature assumption was used in the study, the effect of temperature variation on system performance should be evaluated as a design parameter.

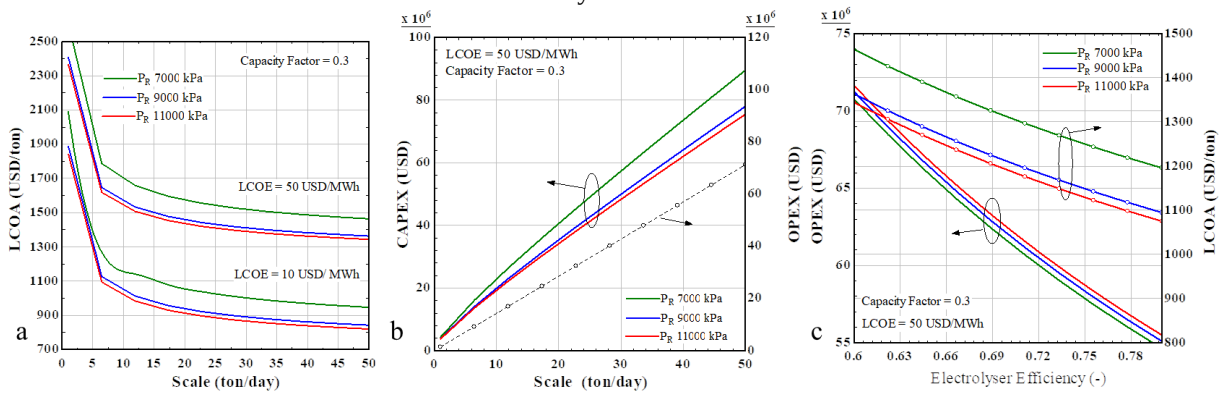

Figure 3. (a) Influence of Reactor Pressure and Plant Scale on LCOA for Different Electricity Prices **(b)** CAPEX and OPEX Trends with Scale for Different Reactor Pressures **(c)** Effect of Electrolyzer Efficiency on LCOA and OPEX

Figure 4a illustrates the effect of capacity factor (CAP) on the Levelized Cost of Ammonia (LCOA) and operational expenditure (OPEX) for three reactor pressure levels (7000, 9000, and 11000 kPa), under fixed electrolyzer efficiency (η_{el} = 0.6) and electricity cost (LCOE = 50 USD/MWh). The results show that OPEX exhibits a strong linear relationship with the capacity factor across all pressures, increasing proportionally as CAP rises. The increase in the capacity factor naturally leads to higher annual operating expenses because it increases total energy consumption. However, the increased value here represents total expenditure and does not indicate the unit product cost. As production volume increases, fixed costs are spread over more products, resulting in a decrease in cost per ton. Therefore, the economic impact of the capacity factor should be evaluated from the perspective of unit production cost rather than total cost. This is due to the fact that higher capacity operation leads to increased total energy consumption, despite spreading fixed costs over more production. In contrast, LCOA displays a distinctly nonlinear (parabolic) decrease with increasing CAP, emphasizing the role of capacity utilization in amortizing capital and fixed operational costs. Higher reactor pressures again demonstrate lower overall LCOA and OPEX, particularly evident at higher capacity factors.

These results confirm that maximizing plant utilization is crucial for improving economic performance, and this effect is amplified when operating at elevated pressures due to their inherently higher conversion efficiencies and lower recycle burdens. The three-dimensional link between reactor pressure (kPa), capacity factor (%) and the Levelized Cost of Ammonia is shown in Figure 4b. The graph shows how these two factors interact significantly to determine whether ammonia production is economically viable. As can be seen, LCOA decreases as reactor pressure increases, indicating that higher pressures result in more efficient ammonia synthesis and hence lower ammonia production costs per ton. At the same time, a decrease in LCOA is associated with an increase in capacity factor, highlighting the financial advantage of optimizing plant uptime. The color gradient

further highlights the varying costs under diverse conditions, as warmer colors (indicating higher LCOA values) occur at lower capacity factors and reactor pressures, and cooler colors (indicating lower LCOA values) occur at higher pressures and capacity factors. These findings are particularly valuable in optimizing ammonia production processes, as they provide clear guidance on how adjusting reactor pressure and operational efficiency can lower production costs. The results shown in this figure offer important insights into the key factors influencing LCOA, supporting the optimization strategies discussed throughout this study.

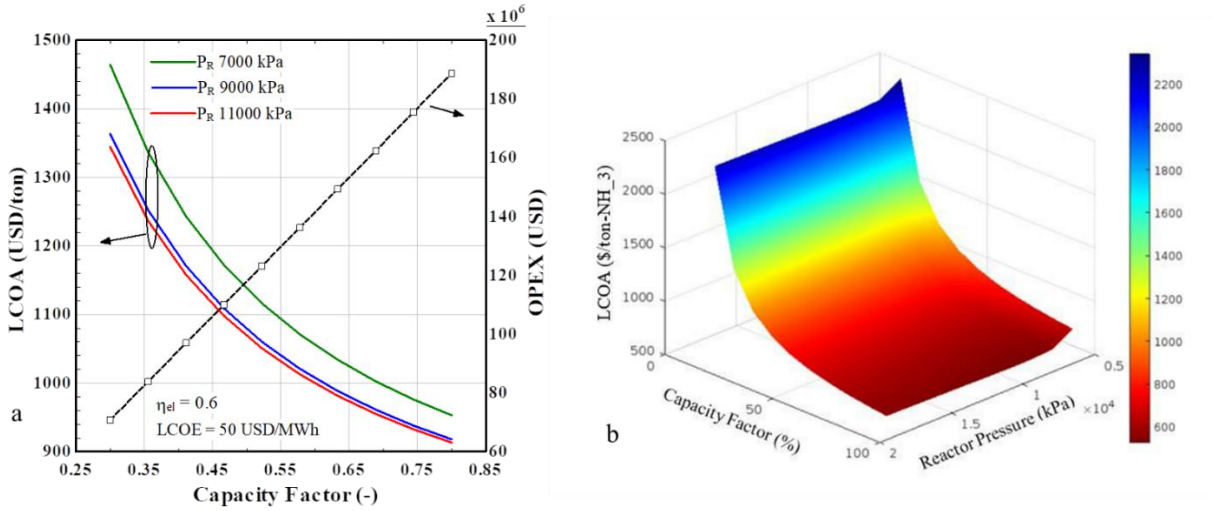

Figure 4. (a) Influence of Capacity Factor on LCOA and lifetime OPEX at Different Reactor Pressures (b) Effect of Reactor Pressure and Capacity Factor on the Levelized Cost of Ammonia (LCOA)

Figure 5 shows the variation of CAPEX for the main equipment in the eHB system depending on the production scale (1–50 tonnes/day) and the corresponding LCOA. The analysis was carried out under the assumptions of a low electricity price of 10 USD/MWh, reactor pressure of 7000 kPa, and a capacity factor of 0.3. These conditions represent systems operating intermittently with renewable energy sources. At all scales, the CAPEX component of the electrolyzer ($CAPEX_{el}$) accounts for the largest share of the investment cost, exceeding 39 million USD at 50 tonnes/day. The costs of other equipment such as the reactor ($CAPEX_{HB}$), compressors, air separation unit (ASU), heat exchanger, and tank increase with scale but remain relatively lower compared to the electrolyzer. As the production scale increases, total investment costs grow in absolute terms. For example, while the total CAPEX is about 4 million USD for a 1 tonne/day capacity system, this value increases to approximately 11.7 million USD at 10 tonnes/day and 39 million USD at 50 tonnes/day. However, despite this increase, the cost per unit of production (LCOA) significantly decreases as the system operates more efficiently. LCOA, which is 1912 USD/tonne at 1 tonne/day, decreases to 832.2 USD/tonne at 10 tonnes/day and further to 714.3 USD/tonne at 50 tonnes/day. This trend clearly demonstrates the depreciation effect of CAPEX on unit cost through economies of scale. Especially from 20 tonnes/day and above, the LCOA drops below 800 USD/tonne, approaching the range of conventional Haber-Bosch (cHB) processes. Although eHB systems are still more expensive, this narrowing gap highlights their growing commercial potential, especially if electrolyzer costs can be reduced, capacity factors improved, and system integration optimized.

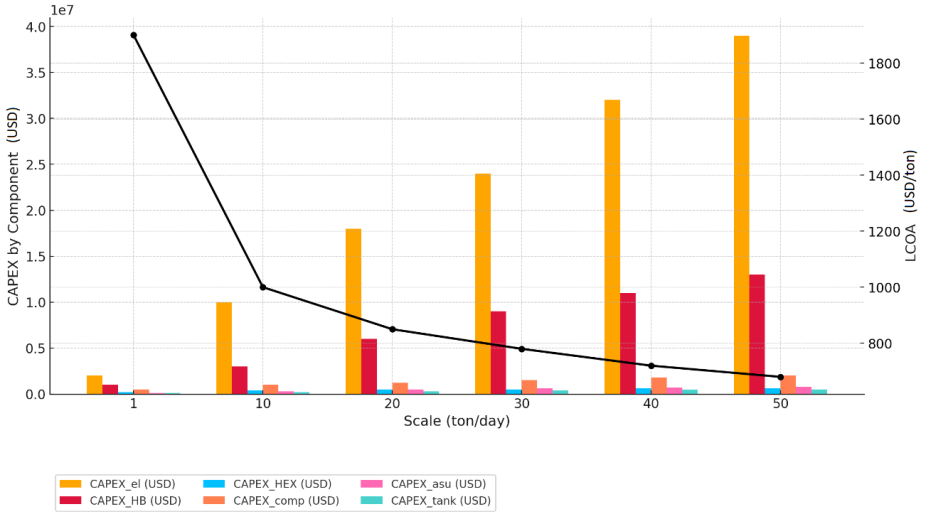

Figure 5. CAPEX breakdown and its impact on LCOA across production scales.

4. CONCLUSION

This study is devoted to an integrated techno-economic model to investigate the effect of thermal and cost parameters on electrical Haber-Bosch process at scale. While operational conditions are critical for a better performing and cost- effective system, scale, cost of electricity from renewables and capacity are the major decision makers to its economic feasibility. Assuming compatible ammonia production costs are below USD 1000 per tons, size of the decentralized plant should be over 25 tons/day, capacity range should not be below 35% and LCOE needs to stay lower than USD 50 per MWh. The global market costs for methane-based ammonia fluctuates based on global dynamics, however, it is still below USD 500 / ton, and economically viable. Here, eHB process can serve as a very good alternative for regions lack of natural gas resources, inland locations that need to pay more for transportation and to liberate from fluctuating and fast evolving global dynamics. e-HB remains with some disadvantages of the conventional Haber-Bosch process, particularly its limited compatibility with intermittent renewable energy sources due to high thermal inertia and continuous operation requirements. This makes it less adaptable to the fluctuating nature of renewable energy sources like solar and wind, thereby posing challenges for dynamic load-following and energy matching. Hybridized grids and increased renewable capacity should solve the two major problems; matching with renewable electricity and the latter is the decreased cost. The main findings of this study are summarized below:

- Increasing reactor pressure significantly reduced ammonia production costs, with the lowest cost achieved under high-pressure conditions.
- The capacity factor is one of the most critical parameters determining economic performance, and its increase significantly reduced the unit production cost.
- Improvements in electrolyzer efficiency have shown a linear and strong effect on LCOA.
- Electricity cost is the dominant factor determining system economics, and the system becomes competitive in low-cost renewable energy scenarios.
- The economic viability of small-scale eHB systems is strongly dependent on high capacity factor and low electricity cost conditions.

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DECLARATION OF ETHICAL STANDARDS

The author(s) of this article declare that the materials and methods used in this study do not require ethical committee permission and/or legal-special permission.

AUTHOR'S CONTRIBUTION

Ahmed Emin KILIÇ: Methodology, Investigation, Data Curation, Writing-Original Draft, Writing-Review & Editing

Senanur TEKİN: Conceptualization, Methodology, Investigation, Data Curation

Hasan ÖZCAN: Conceptualization, Writing-Original Draft, Writing-Review & Editing, Supervision, Project Administration, Funding Acquisition

Selahattin ÇELİK: Writing-Original Draft, Writing-Review & Editing, Supervision, Project Administration, Funding Acquisition

CONFLICT OF INTEREST

There is no conflict of interest in this study.

NOMENCLATURE

Abbreviations

ASU	Air separation unit
CAP	Capacity factor
CAPEX	Component-level capital expenses
CEPCI	Chemical engineering plant cost index
DNRR	Electrochemical nitrogen reduction reaction
cHB	Conventional Haber-Bosch
eHB	Electrochemical Haber-Bosch
HB	Haber-Bosch
HER	Hydrogen evaluation reaction
HEX	Heat exchanger
HHV	Higher heating value
LCOA	Levelized cost of ammonia
LCOE	Levelized cost of electricity
LCOH	Levelized cost of hydrogen
LMTD	Logarithmic mean temperature difference
LOHC	Liquid organic hydrogen carrier
NOxRR	NOx reduction reaction
OPEX	Operational expenses

Symbols

c_p	Specific heat
T	Temperature
Y	Ammonia conversion rate
P_R	Haber-Bosch reactor pressure
W	Power
V	Volume
I	Current
C	Cost
F	Factor
V	Voltage
η	efficiency

Subscripts

el	electrolysis
ASU	air separation unit
mix	mixture
avg	average
R	reactor
aux	auxiliary
rec	recycle
$comps$	compressor
$spec$	specific
p	purchase
m	module
s	system
BM	bare module
$MSCE$	maintenance, site purchase, engineering and construction
0	reference
cat	catalyst

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