



Dual Technical and Environmental Assessment of the Transition from Grey to Green Hydrogen in the Haber–Bosch Process: A Modelling and Simulation Approach [†]

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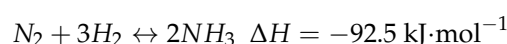
Abstract

This work evaluates the transition from grey to green hydrogen in the Haber–Bosch process through a case study of the Fertial ammonia plant. An integrated assessment per ton of NH₃ was conducted using coupled process simulation with system-level mass, energy, and emission accounting, which link the electrolyser dynamics with ammonia loop operation under variable renewable conditions. The results show an electrical demand of 8.9 MWh/t NH₃ and significant water consumption potential of 27–34 m³/t NH₃. Compared with grey ammonia produced via SMR hydrogen (3.65–4.63 t CO₂/t NH₃), renewable electrolysis reduces total emissions by up to 64% and fossil resource use by approximately 71% (case of 100% PV), depending on electricity carbon intensity. While renewable electricity enables ammonia decarbonization, high water consumption potential represents a challenge. Additionally, hydrogen purity fluctuations and intermittent electrolyser output affect loop conversion and process stability, highlighting the need for heat integration and storage strategies to maintain steady operation.

Keywords: ammonia; grey hydrogen; green hydrogen; simulation; carbon footprint; transition

1. Introduction

Ammonia is a key chemical product for fertilizer production with increasing importance for agriculture and global food security. It is also gaining attention as a potential energy carrier and long-term energy storage vector for renewable energy systems, which could further increase its future demand [1]. Current global production exceeds 176–180 Mt per year [2], with more than 96% of ammonia being produced through the Haber–Bosch process (HB) coupled with natural gas-based hydrogen production via steam methane reforming (SMR) [1]. In this process, nitrogen from the atmosphere reacts with hydrogen under high temperature and pressure in the presence of an iron-based catalyst to produce ammonia [3]. The reaction is exothermic and is expressed as:



However, ammonia synthesis is highly energy-intensive, consuming approximately 2% of total global energy production and 3–5% of the world's natural gas supply [4,5].



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Nearly 40% of this energy input is used as feedstock for hydrogen production, while the remainder is consumed as process energy, mainly for heat generation [2].

In conventional ammonia plants, hydrogen is first produced via SMR, which represent the most energy- and carbon-intensive stage of the process. Therefore, ammonia production generates approximately 450 Mt of direct carbon dioxide (CO₂) emissions annually and about 170 Mt of indirect emissions, contributing roughly 1.8% of global CO₂ emissions [2]. As a result, ammonia is considered one of the most carbon-intensive processes in the chemical industry and is identified as one of the four major industrial sectors requiring deep decarbonization in order to achieve the net zero carbon emissions target by 2050 [5]. In response to these challenges, alternative production pathways are being explored, particularly green ammonia production based on hydrogen generated using water electrolysis powered by renewable electricity. This approach has the potential to significantly reduce the carbon footprint of ammonia synthesis. However, several challenges remain, particularly regarding the integration of electrolytic hydrogen with intermittent renewable energy sources such as solar and wind [6].

In Algeria, international climate commitments and the global transition toward low-carbon energy systems are increasing pressure on energy-intensive industrial sectors to reduce their environmental impact. Within this context, the ammonia production facility of Fertial, which currently produces ammonia using hydrogen derived from natural gas through SMR, resulting in significant CO₂ emissions, represents a strategic candidate for industrial decarbonization. One promising pathway involves the production of green ammonia based on hydrogen generated via proton exchange membrane (PEM) water electrolysis powered by renewable electricity. However, the overall environmental performance of this transition remains uncertain due to potential trade-offs associated with electricity supply, resource consumption, and infrastructure requirements.

To address these issues, this study applies a life cycle assessment (LCA) to ammonia production at the Fertial plant, where the existing grey ammonia process is compared with alternative scenarios based on green hydrogen produced via electrolysis under different electricity supply mixes. The objective is to evaluate the environmental viability of this transition, focusing on climate change impact, fossil resource use, and water consumption while identifying key environmental hotspots and analysing the influence of electricity supply on the overall life cycle performance of green ammonia scenarios.

2. Methodology

2.1. LCA Methodological Frameworks

The environmental assessment was performed following an attributional life cycle assessment (A-LCA) approach in accordance with ISO14040 and ISO 14044 standards [7,8]. All simulations were conducted using Activity Browser software version 2.11.2 coupled with the ecoinvent database version 3.11 [9,10]. The modelling approach is process chain- and inventory-based, ensuring consistency between foreground operational data and background life cycle datasets.

2.2. Goal and Scope Definition

The goal of the present study is to evaluate and compare the environmental performance of conventional grey ammonia and green ammonia produced via proton exchange membrane (PEM) water electrolysis under different electricity supply compositions. The assessment aims to quantify the influence of the photovoltaic-grid electricity mix on the sustainability of green ammonia production.

The functional unit is 1 ton of anhydrous ammonia (t NH₃) produced with 99.9% purity at the plant gate. The study follows a cradle-to-gate system boundary and includes

feedstock extraction and processing, hydrogen production (via SMR in grey ammonia, and PEM electrolysis in green ammonia), nitrogen production through cryogenic air separation (green ammonia), ammonia synthesis (HB loop), and upstream energy supply chains. The LCA system boundaries are shown in Figure A1.

The case study is based on a real fertilizer complex situated in Annaba, Algeria, with a production capacity of 1000 tons NH_3 per day, and motivated by the plant's decarbonization strategy.

2.3. Life Cycle Inventory

The life cycle inventories of the two processes combine real industrial data and literature-based modelling within the ecoinvent 3.11 database. The foreground system is modelled based on operational data from the Fertial plant for the grey process, whereas green ammonia configuration was developed by adding cryogenic air separation for nitrogen production and replacing hydrogen from SMR with PEM water electrolysis. Inventories for hydrogen production via PEM water electrolysis are adapted from Wei et al. 2024 [11]. Process mass and energy balances are maintained consistent with the integrated simulation framework. The background system consists of electricity mix, natural gas supply, industrial gases and chemicals, and materials and fuels; it is modelled using ecoinvent version 3.11, allocation, cut-off by classification [9].

The real industrial case of the grey ammonia plant uses actual operating conditions, including efficiency losses and operational variability, which enables comparison with the nominal design case. For the green scenarios, hydrogen was produced via PEM electrolysis powered by photovoltaic electricity and/or grid electricity depending on the scenario and accounting for seasonal solar irradiation conditions.

2.4. PV–Grid Mix Modelling

The electricity supply of the hydrogen production via PEM electrolysis in the green process was evaluated under several scenarios derived from local solar availability. The PV–grid fractions were calculated based on the global horizontal irradiation profile of the city of Annaba over one year (2023), where the year was divided into four seasons. For each season, PV electricity production was first estimated using the minimum seasonal GHI obtained from the PVGIS solar database [12]. The specific PV yield was calculated, then the required PV surface was determined from the plant electricity demand as detailed in Table 1. Seasonal PV electricity was calculated using this fixed surface. When PV production was lower than the electrolyser demand, the deficit was supplied by the grid; when it exceeded demand, the case was modelled as 100% PV.

Table 1. Main hypotheses and equations for PV–grid mix modelling.

Parameter	Value/Expression	Unit	Description of Parameters and Assumptions
Plant electricity demand for PEM electrolysis	$E_{plant} = m_{H_2} \times SE_{PEM} \times P_{NH_3}$	$\text{MWh} \cdot \text{d}^{-1}$	E_{plant} : daily electricity demand of the ammonia plant; m_{H_2} : hydrogen requirement per tonne of NH_3 ; SE_{PEM} : specific electricity consumption of the PEM electrolyzer ($\text{MWh} \cdot \text{t}^{-1} \text{H}_2$); P_{NH_3} : ammonia production capacity at Fertial ($1000 \text{ t NH}_3 \cdot \text{d}^{-1}$). Calculated assuming full plant capacity and a PEM electrolyzer efficiency (η_{PEM}) of 66%.
Minimum monthly global horizontal irradiation (GHI)	0.12642	$\text{MWh} \cdot \text{m}^{-2} \cdot \text{month}^{-1}$	GHI: global horizontal irradiation. Minimum monthly value obtained from PVGIS [12].
Daily PV electricity per area	$E_{PV} = \frac{GHI_{min} \times \eta_{PV}}{30}$	$\text{MWh} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$	E_{PV} : daily photovoltaic electricity generated per unit area; GHI_{min} : minimum monthly global horizontal irradiation; η_{PV} : photovoltaic efficiency (21%). GHI data obtained from PVGIS [12].

Table 1. *Cont.*

Parameter	Value/Expression	Unit	Description of Parameters and Assumptions
Required PV surface	$S_{PV} = \frac{E_{plant}}{E_{PV}}$	m ²	S_{PV} : photovoltaic surface area required to satisfy the plant electricity demand for PEM electrolysis.
Seasonal electricity production by PV	$E_{PV,season} = GHI_{season} \times S_{PV} \times \eta_{PV}$	MWh·d ^{−1}	$E_{PV,season}$: seasonal photovoltaic electricity production; GHI_{season} : average seasonal global horizontal irradiation; S_{PV} : required PV surface area; η_{PV} : photovoltaic efficiency. Calculated using seasonal irradiation data from PVGIS [12].

2.5. Life Cycle Impact Assessment (LCIA)

The LCIA was performed using three impact indicators and different impact assessment methods, as presented in Table 2. Life cycle impact assessment results are reported per functional unit and analysed through contribution analysis at elementary flows and process levels.

Table 2. Impact indicators and impact assessment methods used in the study.

Indicator	Impact Method	Unit
Climate change	IPCC 2021, global warming potential (GWP100) [13]	kg CO ₂ -Eq
Fossil energy resources	CML v4.8 2016, energy resources: non-renewable, abiotic depletion potential (ADP): fossil fuels [14]	MJ
Water consumption potential	ReCiPe 2016 v1.03, midpoint (H), water use, water consumption potential (WCP) [15]	m ³

3. Results and Discussion

3.1. PV–Grid Mix for Green Hydrogen

As shown in Table 3, three scenarios were evaluated in this study, based on the minimum global horizontal irradiation (GHI) of each season and a calculated PV surface of approximately 10 km². It is clear that the increase in the PV fraction during periods with high irradiations reduces the dependence on grid electricity. Consequently, the carbon intensity of electricity decreases according to the PV share. However, during low solar seasons, the grid share increases and thus limits the environmental benefits of green hydrogen production. Spring and summer seasons were able to fully satisfy the electrolyser demand, which were therefore considered as one scenario working with 100% PV, thus confirming the technical feasibility of green hydrogen production under favourable solar conditions. However, the intermittency of solar energy remains the main operational challenge, given that fluctuations in irradiation can lead to power deficits or surpluses relative to the continuous demand of the electrolyser and the HB loop, even when PV potential is sufficient. Therefore, periods of excess generation may result in renewable curtailment, which require energy storage or grid export to maintain process stability.

Table 3. PV–grid fractions of each scenario.

Season	March–August	September–November	December–February
Scenario	1	2	3
PV fraction	100%	62.862%	48.806%
Grid fraction	0%	37.138%	51.194%

3.2. Climate Change Impact

The climate change impact was assessed using the global warming potential (GWP100), which quantifies the cumulative radiative forcing of greenhouse gas emissions relative to

CO₂ over a 100-year time horizon [16]. Figure 1a compares the climate change GWP100 results for the two cases of grey ammonia and green ammonia under different electricity supply scenarios.

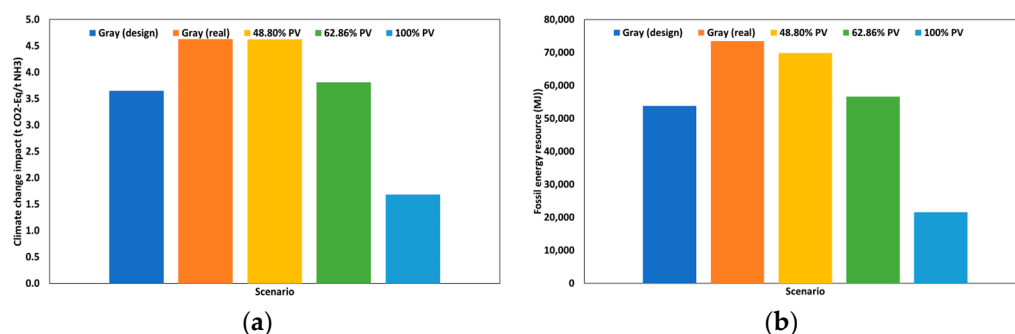


Figure 1. LCA results: (a) climate change impact; (b) fossil energy resource.

The results show strong sensitivity to both process efficiency and electricity carbon intensity. For the grey process, the real industrial case exhibits a higher GWP (4.63 t CO₂-eq) compared with the design case (3.65 t CO₂-eq). This increase is mainly due to the overconsumption of natural gas as fuel for process heating, particularly in the SMR section. Process contribution analysis confirms that SMR is the dominant contributor. Heat generation from natural gas furnaces contributes 43.2% of GWP while steam production accounts for about 14.9% of GWP, with upstream natural gas venting adding 7–8% in the real case. The main emissions released are both fossil CO₂, which dominates the impact (90–91%), while fossil methane contributes by 9–9.6%. Methane emissions are mainly fugitive CH₄, originating from upstream leakage and venting, with additional releases during other stages of the natural gas supply chain and minor emissions related to process losses within the plant. These results are largely linked to the CH₄ leakage rates assumed in the ecoinvent natural gas datasets, which represent approximately 1.2% for natural gas venting and about 0.1% for distribution [9]. However, it is important to mention that the Algerian “market for natural gas, high pressure” dataset used in this study accounts only for distribution losses, while upstream emissions from extraction, processing, and transport (including venting and flaring) are included via linked production datasets based on extrapolated data from other regions [17,18], introducing uncertainty in the estimation of total methane leakage.

The performance gap between the design and real case of grey ammonia can be explained by several operational factors. The first one is the catalyst aging, which significantly reduces SMR efficiency and increases the specific heat demand, resulting in much higher natural gas consumption as fuel. The second factor is the unplanned production shutdowns and the higher fuel demand during repeated start-up phases, mainly due to the plant aging. Another factor may be the suboptimal operating conditions in the real plant compared with the design assumptions.

For the green process, electricity generation becomes the primary driver of climate change impact across the three scenarios summarized in Table 3. Both scenarios S2 and S3 show higher impacts than S1. In these two scenarios, the electricity demand of electrolysis dominates by 75% in S2 and 79% in S3, with the scenario of higher PV fraction showing lower impact, which demonstrates the strong sensitivity of green ammonia performance to the electricity mix. The 100% PV scenario achieves a 63.71% reduction in GWP relative to the real grey process (1.68 t CO₂-eq vs. 4.63 t CO₂-eq), thus confirming the environmental benefits of the transition toward renewable solar electricity. In this scenario, electricity requirement for hydrogen production via PEM electrolysis is the largest contributor of emissions, followed by electricity for cryogenic air separation and then electricity for

compression. A detailed contribution analysis of the electrolysis subsystem reveals that 42.4% of the impact originates from the construction of the photovoltaic power plant, as shown in Figure 2a, with PV modules and the mounting system production identified as the main hotspots. However, the impacts associated with electricity generation from fossil fuels remain significantly higher than those from the PV supply chain, as shown in S2 and S3, which both exhibit higher impacts than S1 due to the higher carbon intensity of the grid electricity.

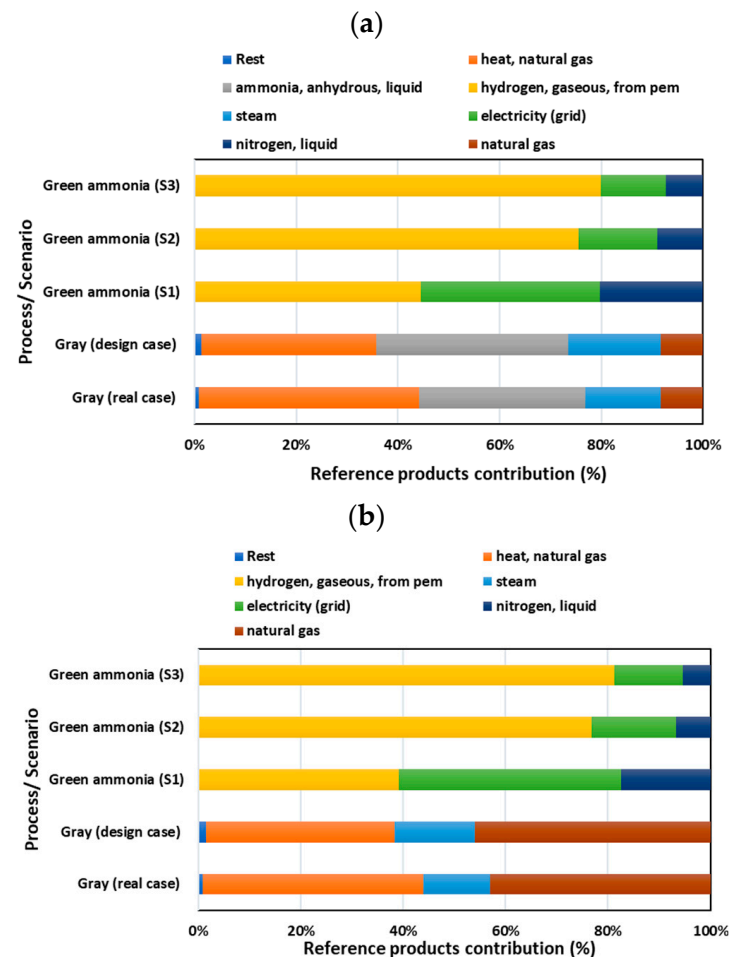


Figure 2. First tier (Ft) contributions: (a) climate change impact; (b) fossil energy resource.

3.3. Fossil Energy Resources

Fossil resource use was evaluated using the abiotic depletion potential for fossil fuels (ADP-fossil). This metric quantifies the depletion of non-renewable fossil energy carriers such as natural gas, crude oil, and coal based on their global use-to-availability ratio [19].

The results presented in Figure 1b show a clear contrast in fossil energy resources between grey and green ammonia processes, mainly driven by natural gas consumption and electricity mix composition. Grey ammonia shows the highest impacts, with the real case reaching the highest value of 7.35×10^4 MJ. Natural gas represents the dominant contributor (90–93%) due to its high consumption as both feedstock and fuel, with the remainder originating mainly from the grid electricity used in steam production.

The lowest fossil resource use is observed for the green process under the 100% PV scenario (S1), with 2.15×10^4 MJ representing a 71% reduction compared with grey ammonia and a 33.43% decrease in natural gas contribution. However, the relative contributions of hard coal, crude oil, and brown coal become more visible due to the manufacturing stage

of PV system components, which require substantial energy input. These results align well with those reported by Chisalita et al. 2020 [20].

In the PV-grid scenarios (S2 and S3), fossil depletion remains significant due to the high fraction of the fossil-based grid electricity in the electricity mixes. Natural gas contribution also remains significant, representing 85–88% of fossil energy use, while hydrogen production via PEM electrolysis becomes the dominant process contributor (77–81%) as shown in Figure 2b, due to its high electricity demand.

Overall, the transition to green ammonia significantly reduces fossil resource use under the different electricity supply scenarios, particularly when using full renewable electricity. However, this reduction strongly depends on the share of renewable electricity in the system.

3.4. Water Consumption Potential

The results of the water consumption potential are illustrated in Figure 3. Grey ammonia production shows the lowest water demand (2.12–2.62 m³/t NH₃). The water demand increases significantly in the fully renewable green ammonia scenario, which exhibits the highest value of 34.1 m³/t NH₃.

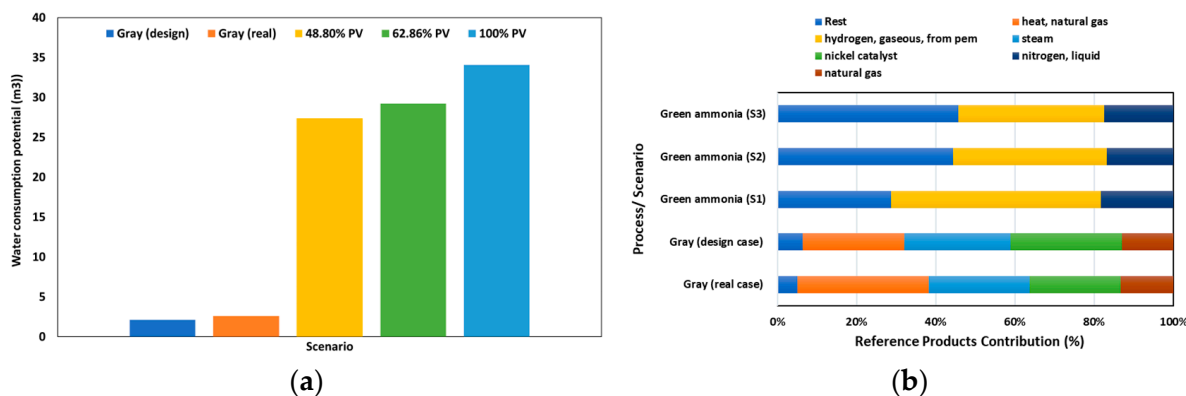


Figure 3. Water consumption potential. (a) LCA results; (b) first tier (Ft) contributions.

For the grey process, the real case shows a higher water consumption than the design case, which can be explained by higher utility demand and operational inefficiencies. In both cases, direct impacts are mainly driven by steam generation for SMR and cooling requirements, while indirect contributions arise from upstream electricity and natural gas supply. In contrast, the green ammonia process, particularly under the 100% PV scenario, is largely driven by indirect water demand associated with the green hydrogen production chain. Although PEM electrolysis requires about 1.6 m³ of deionized water per ton of NH₃, the dominant hotspot is PV infrastructure manufacturing (24.4 m³), particularly multi-silicon production for photovoltaic cells and wafer, which represents more than 70% of the total water demand. This is consistent with previous studies reporting that most water use in PV systems occurs during upstream manufacturing processes, particularly during silicon purification and multi-crystalline silicon production, which require large volumes of deionized water for wafer cleaning and cooling operations [21,22]. Polysilicon production is widely identified as the most water-intensive stage of the PV value chain due to the significant water demand associated with silicon purification and wafer manufacturing [23]. Although several studies have quantified water consumption in PV manufacturing and supply chains, assessments of water consumption associated with PV-based electricity in green ammonia production systems remain very limited in the literature.

Additionally, cryogenic air separation contributes by $8.5 \text{ m}^3/\text{t NH}_3$, which accounts for 25% of total water consumption. For S2 and S3, water demand remains significantly higher than in the grey process but lower than in the fully renewable scenario, with a slight increase observed as the PV share rises. These results reveal that while electrification with renewable energy significantly reduces climate impacts, it shifts part of the environmental burden toward upstream water-intensive PV infrastructure.

It should be noted that the required PV surface area was kept constant across all electricity supply scenarios. The PV area was sized using the minimum seasonal irradiation value to guarantee sufficient electricity production under the most conservative operating conditions. Therefore, the higher water consumption observed in Scenario 1 (100% PV) is not associated with a larger photovoltaic installation, but rather with the greater contribution of PV electricity within the life cycle inventory.

4. Conclusions

This study evaluated the transition from grey to green ammonia production at the Fertial plant using life cycle assessment. Grey ammonia showed the highest GWP and fossil use impacts, while green ammonia achieved significant GWP reduction at the cost of increased water use. Electricity carbon intensity from PEM electrolysis was the main driver. The PV–grid mix improved reliability but added fossil burden, while the 100% PV enabled approximately 64% CO₂ reduction and the lowest fossil use, with the highest water demand. Renewable electricity can support deep decarbonization, but water management, operational stability, and strategies such as energy storage and effective heat integration are critical to ensure stable and efficient operation. Future work should explore blue hydrogen pathways and industrial deployment.

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Abbreviations

The following abbreviations are used in this manuscript:

HB	Haber–Bosch
SMR	Steam methane reforming
LCA	Life cycle assessment
PEM	Proton exchange membrane
PV	Photovoltaic
GWP	Global warming potential
GHI	Global horizontal irradiation

Appendix A

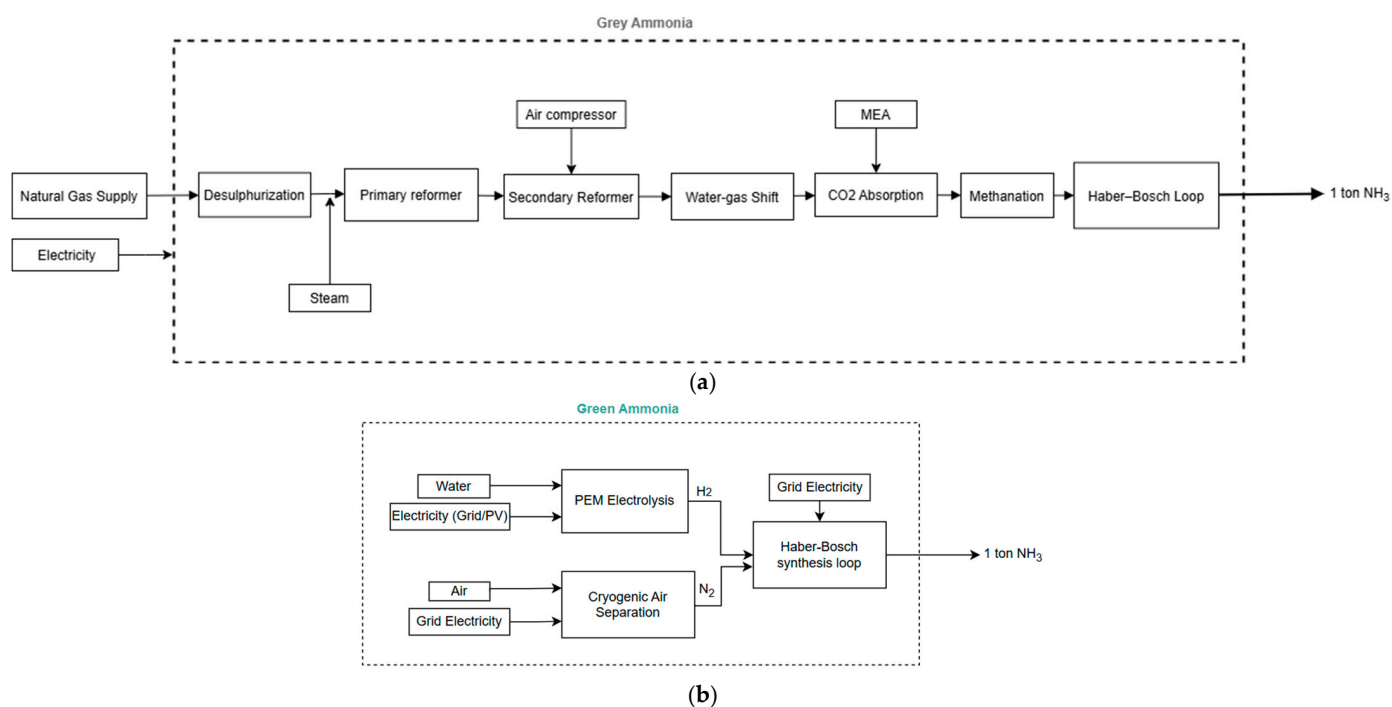


Figure A1. System boundaries for: (a) grey ammonia process; (b) green ammonia process.

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