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Research article

Assessing climate change impact of blue ammonia via carbon capture and utilization in life cycle modelling

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ABSTRACT

Ammonia production represents a fundamental aspect of the global chemical industry. It is a significant contributor to carbon dioxide (CO_2) emissions, and it is necessary that innovative methods be developed to reduce its climate impact. This study assesses the environmental impact of blue ammonia production incorporating carbon capture and utilization (CCU) through a novel Life Cycle Assessment (LCA) approach, based on the latest guidelines from the Together for Sustainability (TfS) initiative. This analysis is centred on three systems: grey ammonia (System A), blue ammonia with in-process carbon capture (System B), and blue ammonia utilizing system expansion via direct air capture (DAC) (System C). The results demonstrate that the production of grey ammonia in Germany generates 3.12 $kgCO_{2eq}$ per kg of ammonia, predominantly due to emissions from steam methane reforming (SMR). The incorporation of in-process CO_2 capture in blue ammonia (System B) results in a climate impact of 1.79 $kgCO_{2eq}$ for the functional unit of 1 kg ammonia plus 1.85 kg of succesfully captured CO_2. The implementation of system expansion via DAC (System C), as recommended by the TfS guidelines, results in a further reduction of ammonia emissions to 2.64 $kgCO_{2eq}$, in comparison to System A. This approach also yields a net negative impact of −0.85 $kgCO_{2eq}$ for the captured CO_2 co-product, enabling the realization of the shared incentivization objective articulated in the suggested guideline. The regional scenarios convincingly demonstrate that the proposed approach achieves varying levels of success, often leading to more polarized incentivization. The future scenario will significantly enhance the benefits of CCU and the utilization of CO_2 as a co-product. However, this will be at the expense of incentivizing the production of blue ammonia. This work advances the methodologies for LCA of multi-functional CCU systems, demonstrating the potential for shared incentives in the transition to a new ammonia generation system as a prime example. Nonetheless, it also highlights limitations in regions where the energy source is dominated by fossil fuels or where the energy source is fully renewable. The current TfS framework methodology proposition is therefore a short-term solution to promote the sustainable production of blue ammonia with CCU applications.

1. Introduction

Ammonia plays a pivotal role in global chemical production, extending its significance beyond its essential contribution to global agriculture through fertilizers. It demonstrates remarkable versatility in various chemical reactions, easily converting into a range of chemical intermediates. Furthermore, it shows significant potential for fostering sustainable production practices, particularly when utilizing hydrogen with low emission potential (IEA, 2021). As the global population grows, the demand for ammonia is poised to increase significantly, making it important to develop and deploy defossilized ammonia production technologies to meet the goals of the Paris Agreement, which aims to restrict global warming to well below 2 °C. Ammonia production today accounts for approximately 2 % of the total energy demand and 1.3 % of carbon dioxide (CO_2) emissions globally, with an overwhelming share (approximately 95 %) of the energy stemming from fossil-based sources like natural gas and coal (Morlane et al., 2021). This positions ammonia as one of the most emission-intensive commodities produced by heavy industry and prompts the need for an environmentally friendlier alternative (IEA, 2021).

The Haber-Bosch (H-B) process is the most widely used and commercially viable method for producing ammonia on a large scale (Amhamed et al., 2022). It is a chemical process that combines nitrogen and hydrogen to produce ammonia and is categorized as an energy

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intensive process (Rafiqul et al., 2005). In a bid to reduce the overall CO_2 emissions tied with ammonia production, heavy focus was placed on analyzing alternative hydrogen production methods, ultimately leading to products such as 'blue ammonia' and 'green ammonia' (Ishaq et al., 2022).

In up-to-date research navigating the different technology developments for ammonia production and its potential application as a sustainable fuel of the future, MacFarlane et al. (2020) highlighted three distinctive generations of ammonia production.

- Generation One (Gen 1) involves the use of carbon sequestration or offsets to achieve net-zero carbon emissions in ammonia production. The existing H-B technology is used, but with the addition of a carbon capture and storage (CCS) system in the conventional fossil-based hydrogen production step. This generation is seen as a transitional solution to establish a market for ammonia beyond fertilizer and chemical industries. This type of ammonia produced is often referred to as 'blue ammonia' (El-Shafie and Kambara, 2023).
- Generation Two (Gen 2) encompasses the production of ammonia using hydrogen produced through renewable energy instead of fossil fuel-based resources. Electrolysis-based ammonia production plants powered by renewable energy are emerging globally. Multi-megawatt and gigawatt projects are in various stages of planning and operation, aiming to provide adequate green hydrogen feedstock for large-scale ammonia production (Rouwenhorst, 2023).
- Generation Three (Gen 3) represents the future potential of ammonia production at a large scale using advanced technologies. The use of water as a hydrogen source employs electrochemical nitrogen reduction reactions to produce ammonia. In such advanced electrochemical technologies, the H-B process is no longer required.

Several research endeavors discussed the environmental impact of ammonia production through Life Cycle Assessment (LCA). One study, highlighted the significance of examining diverse hydrogen production pathways for ammonia synthesis and their environmental implications, compared various production methods, including SMR, coal gasification, partial oxidation of heavy oils, and electrolysis powered by nuclear energy (Bicer et al., 2017). The common denominator in this assessment was the commercially proven H-B process for ammonia synthesis. The results unequivocally demonstrate that nuclear electrolysis-based ammonia production generates the lowest greenhouse gas (GHG) emissions, while coal-based methods pose significantly higher environmental concerns. For China, one study highlighted lower GHG emissions of natural gas-based grey ammonia compared to coal and coke oven-based brown ammonia on a nation-wide scale (Zhang et al., 2022). In a more recent case study solar energy-based green ammonia vs. CCS-based blue ammonia was examined in the context of production in Saudi Arabia, where blue ammonia production has a higher environmental impact than green ammonia production in terms of climate change and cumulative energy demand (CED) due to the CCS process energy demand and the potential for natural gas leakage (Mayer et al., 2023). All published research supports the view that green ammonia is an environmentally superior option compared to blue ammonia and other production methods. However, blue ammonia is currently considered as the most accessible and sustainable option that can be relied upon on industrial scale both from a technological and economic outlook (Mayer et al., 2023).

With respect to blue ammonia, recent advancement challenged the traditional scope limited to CCS only, expanding it to utilization in downstream applications. Saudi Aramco successfully completed the world's first carbon capture and utilization (CCU)-based blue ammonia shipment to Japan in 2020, in which the CO_2 generated during the overall ammonia production was captured and transported subsequently for storage and utilization in an enhanced oil recovery pilot plant in Uthmaniyah, Saudi Arabia, and a methanol production plant in Jubail, Saudi Arabia, respectively (Aramco, 2020). In Southeast Asia, a collaborative initiative between Pupuk Indonesia, the state-owned fertilizer manufacturer, Pertamina, the state-owned oil and gas company, and Mitsubishi Corporation was set to evaluate the viability of establishing a supply chain for hydrogen and ammonia through carbon capture utilization and storage (CCUS) (Pertamina, 2022). Within the Indonesian domain, Pupuk Indonesia boasts an annual ammonia production capacity exceeding five million tons, constituting approximately 3 % of the global production (Atchison, 2022). An extended technical investigation conducted in Mexico delved into the environmental efficacy of carbon capture utilization and storage (CCUS) within an ammonia plant, specifically for its application in an enhanced oil recovery system, carbonated beverages and urea synthesis (Mora et al., 2016).

As more blue ammonia suppliers are opting to utilize the captured CO_2 in downstream applications, the question of assessing the climate change impact of CCU-based blue ammonia emerges. LCA as a method plays a pivotal role in this domain. Though, research suggests that there is no set agreement on the harmonization of LCA to calculate the climate impact of the multi-functional CCU-incorporated processes (Sick et al., 2020).

CCU-based systems are categorically multi-functional in nature, since most CCU-incorporated systems often provide a main product and CO_2 (von der Assen et al., 2014). The initial ISO standards on LCA (ISO14040, 2006, ISO14044, 2006) explored the resolution of multi-functionality through collecting individual process data and employing sub-division. If sub-division proved insufficient, system expansion would then be utilized, acknowledging that outcomes reflected joint impacts from the production of multiple products, not specific to a single product in CCU technology. For product-specific assessments, system expansion via substitution should be prioritized; if unfeasible, allocation (physical or economic) would be applied.

In this context, further guidelines from different industries and entities have been pushed forward to bridge the ISO-generic standards and program-specific guidance, providing for specialized CCU cases. LCA guidance documents by the Global CO_2 Initiative (Langhorst et al., 2022) and National Energy Technology Laboratory – NETL (Skone et al., 2022) offer rudimentary principles that follow the ISO standards with additional guidance specific to CCU projects. Both guidelines favor system expansion as a co-product management method, which means assigning a multiproduct functional unit. These guidelines request that the source of the CO_2 be included in the system boundary and, furthermore, set the tone for a possible comparison of a CCU-based system and a reference system using similar Technology Readiness Levels (TRLs). The system expansion approach entails broadening the system to incorporate the CO_2-emitting main processes (such as ammonia production or electricity generation) without integrating carbon capture. Consequently, all emission reductions are ascribed to the CO_2 co-product and what it entails in downstream applications, while the primary product (e.g., ammonia or electricity) retains the identical climate change impact as that of the primary product in a non-CCU-based system (Langhorst et al., 2022; Skone et al., 2022). This situation is commonly referred to as "fossil-lock in" (TfS, 2024).

The LCA4CCU Guidelines (Ramirez et al., 2022), crafted by a team of experts and commissioned by the European Commission, offer valuable insights into the execution of LCA for CCU. This guideline similarly advocates for the adoption of the ISO hierarchy in addressing multi-functionality issues associated with CCU. While the ISO hierarchy primarily emphasizes avoiding allocation whenever possible, favoring a system expansion approach, certain circumstances necessitate determining the environmental performance of individual products. In such instances, allocation may be deemed appropriate, provided it is justified. The guideline proposes a framework to comprehend and implement allocation procedures within the boundaries of the CO_2 emitter and utilizer. Three reference systems have been devised to highlight the allocation of CO_2 emissions between the proposed boundaries.

1. For CCU plants that are added to existing CO_2 emitting plants without further interaction, 100 % of CO_2 burden should be allocated to the primary emitter. This is because the CCU plant does not change the operation of the primary emitter, and therefore, the primary emitter is still responsible for the emissions.
2. For CCU plants that are added to existing CO_2 emitting plants, changing the operation of the said plant in the process, the reduction in CO_2 burden should be allocated to the CCU plant. However, the change in product output of the primary CO_2 emitter requires compensation by corresponding system expansion and including additional emissions. This additional emission burden should be allocated completely to the CCU plant.
3. For CCU plants that are built together with CO_2 emitting plants, it is more difficult to determine how to allocate CO_2 emissions. Industry-specific technology scenarios should be developed, and Best Available Technology (BAT) should be used to represent the primary CO_2 emitting plant. This will ensure that the allocation is fair and reflects the actual emissions of the system.

The LCA4CCU guidelines underscores the significance of establishing clear and unequivocal rules for CO_2 emissions allocation to mitigate uncertainty or misuse (Ramirez et al., 2022).

A recent publication, which partially focuses on multi-functional output modeling in LCA, highlighted the 'Product Carbon Footprint Guideline for the Chemical Industry' as a meaningful framework. This guideline was developed as part of the Together for Sustainability (TfS) Initiative, which was initiated by the global chemical industry. It set the focus on reporting of indirect GHGs emission that are generated by an organization's activities, but which occur outside of the company's direct control, with the aim of promoting transparency, comparability, and sustainability across the chemical sector and beyond (TfS, 2024). In the report, insights are provided into the modelling of production processes that capture CO_2 for further utilization, with particular interest in the Product Carbon Footprint (PCF) of chemical products. Like other reports discussed, the TfS guidelines offer a similar insight into the hierarchy of solving the multi-functional output of a CCU-based system. Though, it emphasizes a new angle in conducting the system expansion approach.

The TfS guidelines are in favor of system expansion by substitution with avoided DAC as an approach for solving multi-functional output products associated with CCU processes. This approach leverages the environmental benefits of capturing CO_2 within the CCU system itself, thus avoiding the need for additional direct air capture (DAC) infrastructure and its associated emissions. By meeting CO_2 demands internally rather than relying on an independent DACprocess, this method supports the goal of avoiding fossil-lock in and claims incentivization between CO_2-producing and CO_2-utilizing products. Furthermore, the report presents specific examples and scenarios to illustrate how the application of system expansion with avoided DAC can impact the PCFs of chemical products, such as lowering the climate change impact of ammonia (CO_2 source) and achieving similar results for methanol produced through CCU-based processes (CO_2 user) (TfS, 2024).

The proposed LCA modelling approach for CCU processes outlined by the TfS guidelines holds promise for fostering climate change impact reduction amongst all parties involved in the process. That includes producers of CO_2 as co-products (e.g. ammonia producers) and the CO_2 co-product stream utilizers as well. However, there is an observed lack in research exploring the intricacies and implications of implementing this novel methodology. The main aspect of this research is to assess how blue ammonia producers that capture and utilize CO_2 in downstream applications can benefit from climate change impact reduction on their primary product (ammonia) using the proposed method by the TfS guideline.

2. Methods

The framework for LCA modelling adopted in this study was defined based on the ISO 14040 and ISO 14044 standards as well as the newest publication by TfS v.2.1 (TfS, 2024). This chapter defines the system boundaries of grey and blue ammonia production in alignment with the research question, collects the necessary input and output data of ammonia production as well as the reference system to be used in the proposed system expansion approach, including the DAC system. One pivotal Life Cycle Impact Assessment (LCIA) category, climate change, is selected, and different scenarios are proposed, considering a varying aspect of production regionality as well as energy mix and demand of the future.

2.1. System boundary, product systems and solving multi-functionality

To meet the primary goal of this study, it is sufficient to consider the production of ammonia along with the captured CO_2 as a valuable output, with a cradle-to-gate system boundary. Although it would be beneficial to conduct further assessments on products that utilize the captured CO_2, it is not the main purpose of this work. The selected system boundary remains consistent with the research question: What is the climate change impact of blue ammonia production considering CCU through the newly proposed LCA modelling approach by the chemical industry?

In this study, the term 'in-process carbon capture' refers to the thermal CO_2 capture process embedded within in the defined system. This technology captures CO_2 directly as part of the hydrogen production through conventional means in the overall ammonia production process, differentiating it from external capture technologies such as DAC. It should be noted that capital goods are not considered in detail for this analysis, as the primary focus is on the operational processes rather than the supporting infrastructure.

The product systems investigated in this research are divided into two parts as shown in Figs. 1 and 2.

- The first product system represents grey ammonia production, which includes all upstream processes such as utilities and feedstock required to produce a specific amount of grey ammonia based on an established production route discussed in section 2.3. The CO_2 stream in this product system is assumed to be directly emitted into the atmosphere.
- The second product system is for blue ammonia production, similarly, following the set up for grey ammonia production route, but in this case the product system considers additionally a capture unit that consists of separation, compression of the CO_2 co product towards the utilization destination. The term "CO_2 capture losses" refers to the quantity of direct CO_2 emissions that remain uncaptured due to inherent limitations in the efficiency of the process.

Another system that is analyzed and utilized for the system expansion method proposed is DAC. As shown in Fig. 3, the modelled system considers the upstream processes necessary to produce a CO_2 stream equivalent to the captured CO_2 in the previous product systems discussed in Fig. 2, ready to be utilized at prospective destination in a similar proposed scope (Cradle-to-Gate). Similarly, the CO_2 capture losses in this figure pertain to the atmospheric CO_2 that remains uncaptured due to limitations in efficiency. In contrast, emissions classified as "Overall System Emission" encompass all emissions associated with the upstream and ancillary processes integral to the overall system operation, excluding the direct CO_2 emissions generated during the primary production process. This category aggregates emissions from energy production, material processing, and other supporting activities that are attributable to the process but are not the direct CO_2 output.

The schematic representations of the system boundaries in Figs. 1–3 are intentionally designed to provide a high-level overview of the

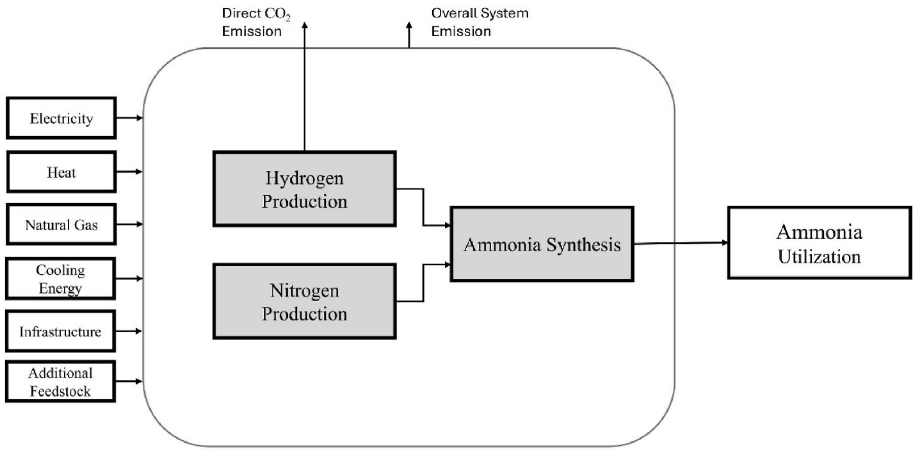

Fig. 1. Schematic representation of system boundaries for grey ammonia production.

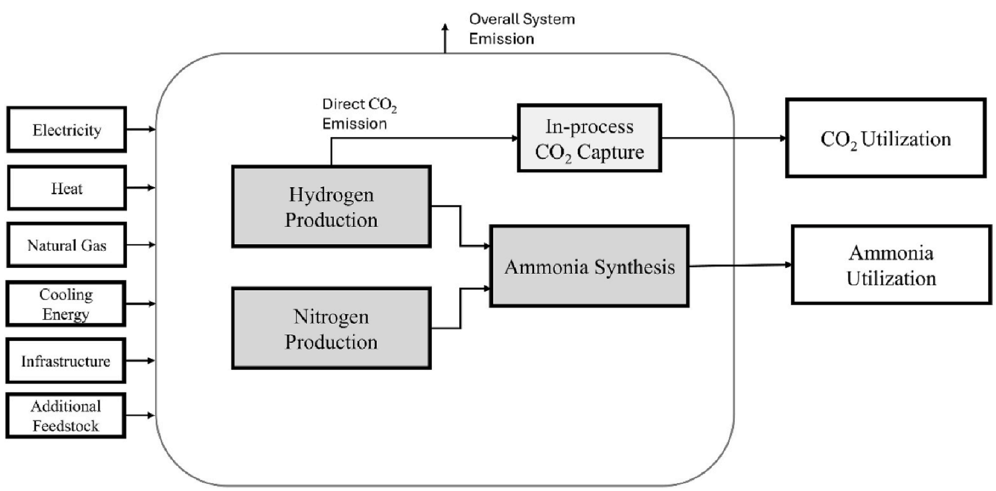

Fig. 2. Schematic representation of system boundaries for blue ammonia production.

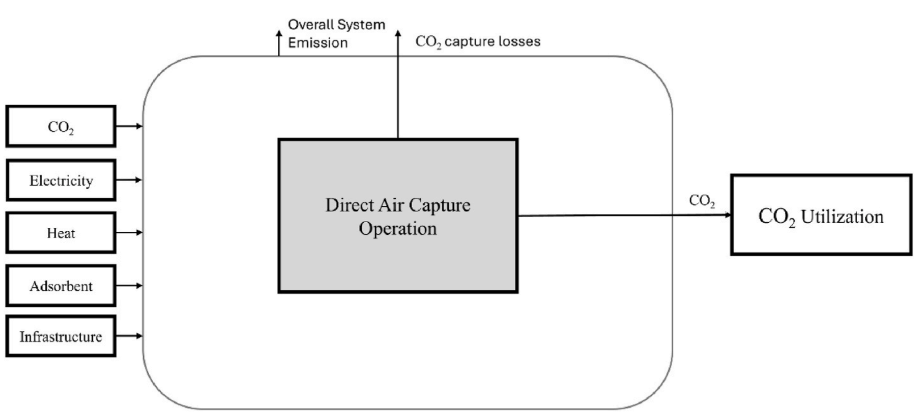

Fig. 3. Schematic representation of system boundaries for CO_2 production from DAC.

process flows to the evaluated systems. These visualizations are not intended to display the exhaustive details of all inputs and emissions; rather, they serve to highlight the methodological consistency across the compared systems and the application of the system expansion approach. For comprehensive breakdown of all inputs and corresponding system emissions, a complete data inventory is presented in the supplementary sheet.This study employs **system expansion by substitution** as recommended in the latest TfS guidelines (TfS, 2024), expanding the system boundary to incorporate a DAC system rather than using grey ammonia as a comparative baseline, as implied in previous work (Langhorst et al., 2022; Skone et al., 2022) and shown in Fig. 4. In this setup, the DAC system operates exclusively to produce CO_2, but its operation is effectively "avoided" by substituting the DAC-derived CO_2 with CO_2 captured in-process within the blue ammonia production system. Through this approach, the climate change impact of blue ammonia is assessed, as illustrated in Fig. 5.

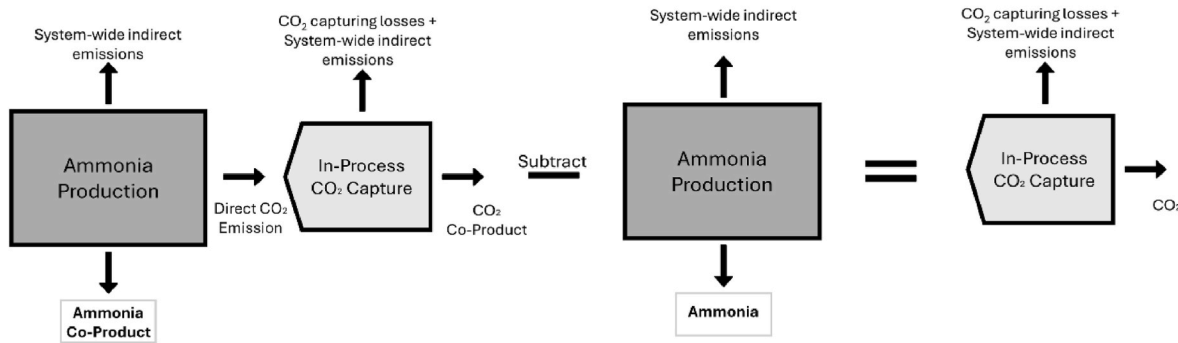

Fig. 4. The system expansion approach proposed in previous work.

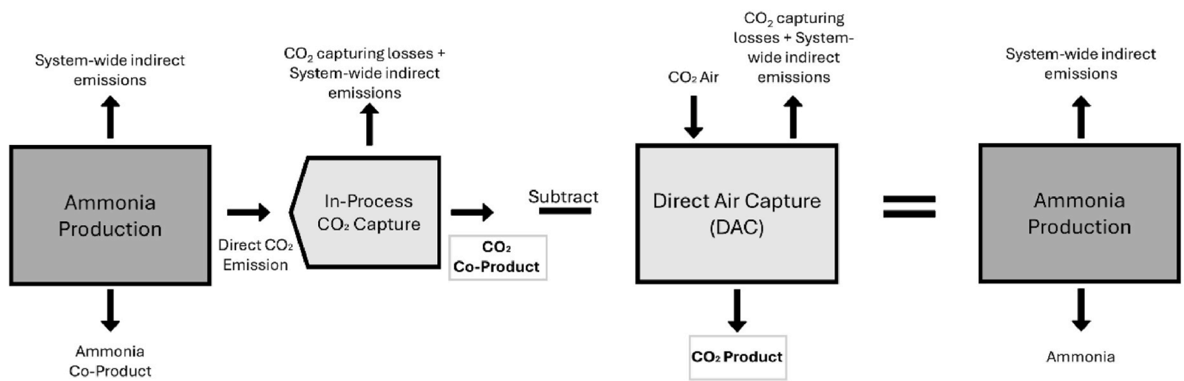

Fig. 5. The proposed system expansion approach by TfS – avoided DAC.

2.2. Functional unit

The functional unit in the assessment is contingent on the specific product system under evaluation. In this study, three distinct product systems are analyzed.

- **System A** - Grey ammonia production: This system represents conventional SMR-based ammonia production without CO_2 capture. The functional unit for this system is 1 kg of grey ammonia produced.
- **System B** – Blue ammonia production with in-process CO_2 capture: This system incorporates CO_2 capture directly within the production process, without system expansion, or any allocation procedure, to solve the multi-output product. The functional unit for this system is 1 kg of produced blue ammonia plus the associated CO_2 captured during the production.
- **System C** – Blue ammonia production with in-process CO_2 capture and system expansion with DAC: Similar to system B, this product system includes in-process CO_2 and additionally uses a system expansion approach where DAC-derived CO_2 substitutes CO_2 co-product captured in the system. Here, the functional unit is also 1 kg of produced blue ammonia plus the associated CO_2 captured, with the system boundary expanded to incorporate DAC to address the multi-functional output. The results for blue ammonia and the captured CO_2 are calculated and presented independently to ensure a clear evaluation of each co-product's impact.

2.3. Life cycle inventory

In the exploration of the Life Cycle Inventory (LCI) within the context of the proposed LCA, a systematic tracking of inputs and outputs throughout the studied processes is conducted. Given the theoretical nature of this study, no primary data collection was required; instead the research compiled comprehensive secondary data from literature and the Ecoinvent database - version 3.9.1, cut-off system model (ECOINVENT, 2023). The analysis was conducted using the LCA software 'LCA for Experts'. An overview of secondary data is presented in the supplementary material (Tables S1–S9). The initial LCA model considers ammonia production location in Germany modelled for the year 2023 with focus on the German electricity mix as illustrated in Table 1.

2.3.1. Ammonia production

The proposed ammonia plant is composed of three distinct and separately modelled sections: hydrogen production, nitrogen production, and ammonia synthesis. H-B process. Since the modelled production site is hypothetical, a capacity of 1000 t/day is assumed over 30-year lifespan. The facility is assumed to operate continuously at full capacity, corresponding to 8760 full-load hours per year.

Data for hydrogen production needed for the H-B process is taken from the Ecoinvent database 3.9.1. The dataset includes the production of 1 kg of gaseous hydrogen through steam methane reforming (SMR) with natural gas, pressurized to 200 bar. However, it is important to note

Table 1
Electricity mix in Germany for the year 2023 (Ag Energiebilanzen e. V., 2023).

Sources of Energy	Percentages
Wind	27.40 %
Lignite	17.39 %
Natural Gas	15.90 %
Photovoltaics	12.14 %
Hard coal	8.76 %
Biomass	8.70 %
Hydropower	5.03 %
Municipal Solid Waste	2.18 %
Nuclear Energy	1.43 %
Others (Mineral oils, Geothermal)	1.01 %

that the recent shift in the origin of natural gas for Germany was not included in this analysis. SMR involves the reforming of natural gas with steam, resulting in the formation of carbon monoxide and hydrogen (synthesis gas). The hydrogen yield is enhanced by a water gas shift reaction, in which the generated carbon monoxide reacts with water, producing CO_2 and additional hydrogen. Notably, this process excludes any considerations for CO_2 capture after shifting with respect to grey ammonia production. Carbon capture consideration in blue ammonia production is discussed in section 2.3.2. The endothermic reforming reaction necessitates heat in the form of high-pressure steam, which is supplied by an external natural gas industrial furnace. Consequently, natural gas serves dual roles as both feedstock for the reaction and fuel for the furnace (Antonini et al., 2020). Additionally, nitrogen production is facilitated through the utilization of a pressure swing absorption (PSA) unit reported in a previous study for ammonia synthesis (Osorio-Tejada et al., 2022).

Data for the H-B process is acquired from the same study based on an Aspen Plus model (Osorio-Tejada et al., 2022). In terms of energy requirements for cooling and synthesis, 3.89 MJ and 0.39 kWh are utilized, respectively, to produce 1 kg of ammonia, while approximately 0.91 kg and 0.23 kg of nitrogen and hydrogen are required. Additionally, the generated steam can be utilized in downstream applications or recycled back into the production system. In this assessment, the steam, as a co-product, is credited to a conventional steam generation process from natural gas and reflected in the results. A summary of the technical requirements for ammonia synthesis is given in Table 2. The environmental impacts associated with the infrastructure necessary for ammonia synthesis are relatively insignificant when compared to the impacts of the actual production processes (Althaus et al., 2007). As a result, a less detailed inventory of the infrastructure is acceptable, relying on the available models provided by Ecoinvent.

In both grey and blue ammonia production, the fundamental synthesis route is the conventional H–B process. That is, the ammonia plant is divided into three sections—hydrogen production, nitrogen production, and ammonia synthesis via the H–B process. In the case of grey ammonia, no carbon capture is applied after the water gas shift reaction; whereas for blue ammonia, the process integrates a carbon capture step (detailed in Section 2.3.2). Thus, aside from the additional capture process in blue ammonia production, the underlying production pathway remains identical.

2.3.2. Carbon capture

In research discourse and industrial applications, the prevailing method for carbon capture is anchored in amine-based technologies, notably the monoethanolamine (MEA) absorption process (Metz et al., 2005; Markewitz et al., 2012). Such amine-driven process routinely achieves CO_2 capture rates ranging from 85 % to 90 % within a gaseous medium (Duval-Dachary et al., 2023). Subsequently, the CO_2-enriched amine undergoes a thermal treatment to release CO_2, facilitating the recycling of CO_2-lean amine. The resultant captured CO_2 undergoes compression and is transported via pipelines for storage or utilization, while the amine is recycled.

Table 2
Brief technical description of major inputs and outputs of ammonia synthesis (Osorio-Tejada et al., 2022).

Input	Amount	Unit
Cooling Energy	3.89	MJ
Electricity	0.39	kWh
Heat	0.05	MJ
Hydrogen	0.23	kg
Nitrogen	0.91	kg
Process Water	0.93	kg
Output		
Ammonia	1	kg
Steam	0.93	MJ

Duval-Dachary et al. (2023) recently compiled an in-detail life cycle inventory of CO_2 capture, including the transportation and storage phases. In this study, and based on the scope defined, the data is used up to CO_2 compression. It is further assumed that the capturing efficiency of the modelled system is 90 % at a CO_2 purity of 99 %, while the lifetime of the capture and compressor units are 30 and 18 years, respectively.

2.3.3. Direct air capture

Deutz and Bardow (2021) explored the potential of DAC as a negative emission technology. They provided thorough analysis, showing a potential trade-off between the benefits of DAC and other environmental impacts. The study has its focus on a commercial DAC plant in Hinwil, Switzerland, operated by Climeworks, achieving a carbon capturing efficiency of 85.4 % at a capacity of 4 kt/year over 20 years of approximated lifetime. Due to the thoroughness of this study, DAC is modelled based on Deutz and Bardow (2021) data collection (Table S6), with supplementary data for DAC construction approximated by Terlouw et al. (2021) (Table S7).

2.4. Impact assessment

In this study, the evaluation of impacts on climate change at midpoint level is evaluated, as the objective is to assess GHG emission reduction on CCU-based blue ammonia. The IPCC's Global Warming Potential over 100 years (GWP 100) is a method developed by the Intergovernmental Panel on Climate Change and is widely applied in LCA to assess climate change impact. The modelled impact factors are derived from the most comprehensive and scientifically rigorous consensus model available (INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE, 2023). The latest impact factors published in the IPCC's Sixth Assessment Report (AR6) are currently employed at midpoint level.

2.5. Scenario analysis

To further evaluate the proposed method advocated by the TfS guideline, scenario analyses are systematically undertaken. Different production regions are considered, namely in Poland and Austria, directly incorporating diverse electricity mixes associated as shown in Table 3 (ECOINVENT, 2023). Specifically, the scenarios were developed each representing distinct electricity mixes. Germany's mix reflects a transitional state with moderate fossil fuel reliance, Poland's is predominantly fossil-based, and Austria's is largely renewable. This selection allows to assess the sensitivity of the LCA outcomes to the electricity mix, which is a critical driver of emissions in energy-intensive processes such as DAC used in the proposed system expansion approach under study. Additionally, the initial system is subject to a forward-looking examination, where the maturing of DAC as a technology is included (Deutz and Bardow, 2021) as highlighted in the supplementary sheet. The overall German electricity mix' future defossilized projection (Prognos et al., 2021) is shown in Table 4. With this, the robustness and adaptability of the proposed approach shall be clarified in the context of evolving production landscapes and long-term sustainability considerations.

Table 3
Current day electricity mix in Austria and Poland (ECOINVENT, 2023).

Sources of Energy	Austria	Poland
Wind	11.78 %	11.04 %
Lignite	–	28.44 %
Natural Gas	15.16 %	4.82 %
Hard coal	2.64 %	49.83 %
Biomass	2.33 %	3.12 %
Biogas	0.82 %	0.42 %
Hydropower	68.00 %	1.94 %
Others (Mineral oils, Geothermal)	0.002 %	0.33 %

Table 4
Future electricity mix in Germany for 2045 (Prognos et al., 2021).

Sources of Energy	Percentages
Wind	59.24 %
Photovoltaics	37.48 %
Hydropower	2.22 %
Biogas	1.05 %

3. Results

This chapter is divided into three subsections. The first subsection explores the present-day German context with grey and blue ammonia. The subsequent subsection delves into additional scenarios based on geographical distinctions, showcasing the proposed method's versatility across varying production regions and their corresponding electricity mixes. The final subsection explores how the system employed will evolve as the DAC technology matures and the demand for energy and heat decreases, and the German electricity mix moves toward decarbonization.

3.1. Base case: ammonia production in Germany

Findings based on the inventory described in the previous chapter showcase a climate change impact associated with the production of 1 kg grey ammonia in present-day Germany to be 3.12 $kgCO_{2eq}$. As shown in Fig. 5, System A dominant contributor is the GHG emission-intensive SMR process, contributing approximately 2.65 $kgCO_{2eq}$, of which 2.06 $kgCO_{2eq}$ are direct CO_2 emissions. Notably, electricity demand during both synthesis and cooling stages in the H-B process is significant, accounting for about 0.43 $kgCO_{2eq}$. The role of ammonia plant construction plays a marginal part in the overall results.

From Fig. 6, System B can be clarified as 1 kg of blue ammonia plus 1.85 kg of captured CO_2, factoring in the system's capturing efficiency. The results from the initial scenario reveal a climate change impact of 1.79 $kgCO_{2eq}$ for the extended functional unit.

In preparation of assessing the system expansion approach, a comparison between the MEA-based in-process carbon capture system and DAC is illustrated in Fig. 7. Evaluating for 1 kg of captured CO_2, the in-process MEA-based carbon capture system shows a negative net climate change impact of −0.65 $kgCO_{2eq}$. Similarly, DAC exhibits a negative impact, albeit less competitive, at −0.39 $kgCO_{2eq}$. It is important to acknowledge that the MEA-based system heavily relies on heat traditionally derived from natural gas, contributing to approximately 60 % of the recorded impact. In contrast, the DAC system's operation is significantly influenced by electricity, constituting approximately 44 % of the system's impact. Additionally, the electrified heat pump in the DAC system, used for heating up the adsorbent and metals as well as to initiate the desorption of CO_2, contributes approximately for around 18 % of the total emissions.

Taking this into consideration, the proposed system expansion approach is applied, with the DAC system scaled to align with the specified quantity of captured CO_2 in the blue ammonia production process. The climate change results of System C are determined and presented in Fig. 8. Under the expanded system, the climate change impact of 1 kg of blue ammonia demonstrates a notable reduction, approximately 20 % compared to that of the grey ammonia counterpart presented in Fig. 5, resulting in an impact of 2.64 $kgCO_{2eq.}$ The climate change result of the 1.85 kg of captured CO_2, treated as a co-product, exhibits a negative net climate change impact of −0.85 $kgCO_{2eq.}$

In our analysis, the DAC system's performance is characterized by an effective capture of only 0.85 kg CO_2 per 1 kg of CO_2 targeted for capture (i.e., a 15 % loss due to inefficiency). The net emission credit is applied at an emission factor of −0.39 kg CO_{2eq} for every 0.85 kg of CO_2 captured. This relationship can be expressed algebraically as:

$$\text{Net Emission Credit} = (\text{Captured CO2}) \times \left(\frac{-0.39}{0.85}\right)$$

As highlighted in the TfS guidelines, this approach establishes a pathway for a shared incentive between ammonia and CO_2 ready for further utilization in downstream applications. This represents a shift from previous methods that only incentivized downstream CO_2 users, leaving the ammonia product's climate change results unchanged.

3.2. Scenario analysis: different production regions

Different production regions contribute varying climate impact results, primarily due to differences in supply structure, while direct emissions from the SMR process are consistent across countries. The production of 1 kg of grey ammonia in Poland and Austria result in an impact of 3.64 $kgCO_{2eq.}$ and 3.20 $kgCO_{2eq.}$, respectively, as depicted in Fig. 9 for System A (Polish and Austrian Scenarios). Several observations from these results help clarify the differences in comparison to the German base case result.

In the context of Poland, the higher climate change results for grey ammonia production can be attributed to a greater reliance on fossil-based utilities throughout the production process. This is evident in various subprocesses leading to the output of grey ammonia. Notably, the increased climate change impact for hydrogen production, with

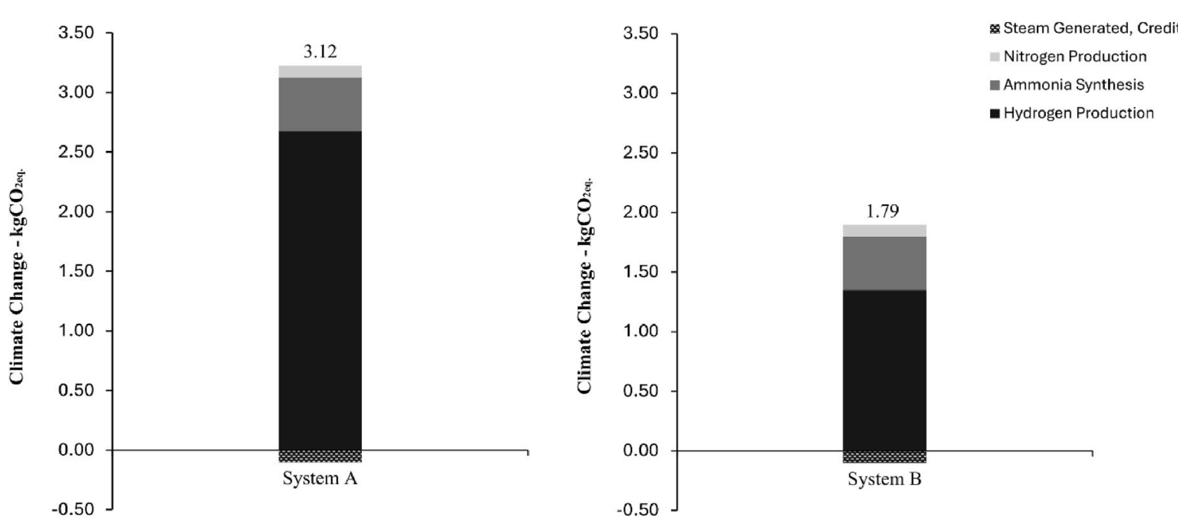

Fig. 6. Climate change impact of System A (grey ammonia) and System B (blue ammonia - extend functional unit) in present-day Germany.

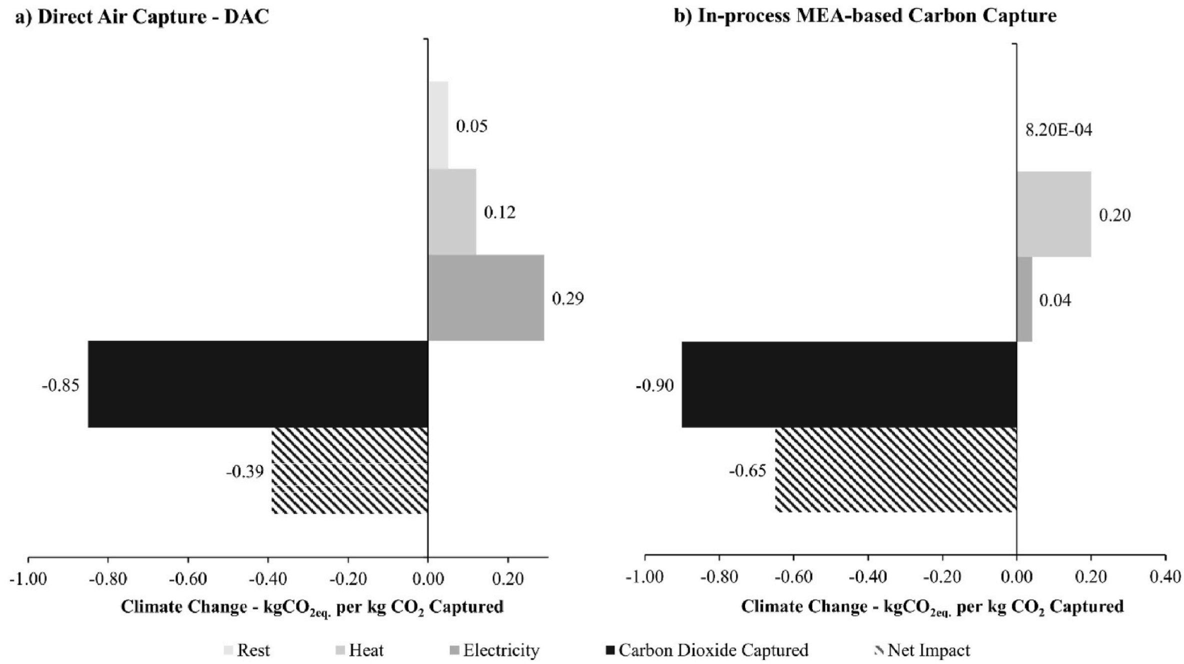

Fig. 7. Comparative climate change results per capturing process of 1 kg of CO_2 (a) DAC and (b) In-process MEA-based carbon capture system, in present-day Germany.

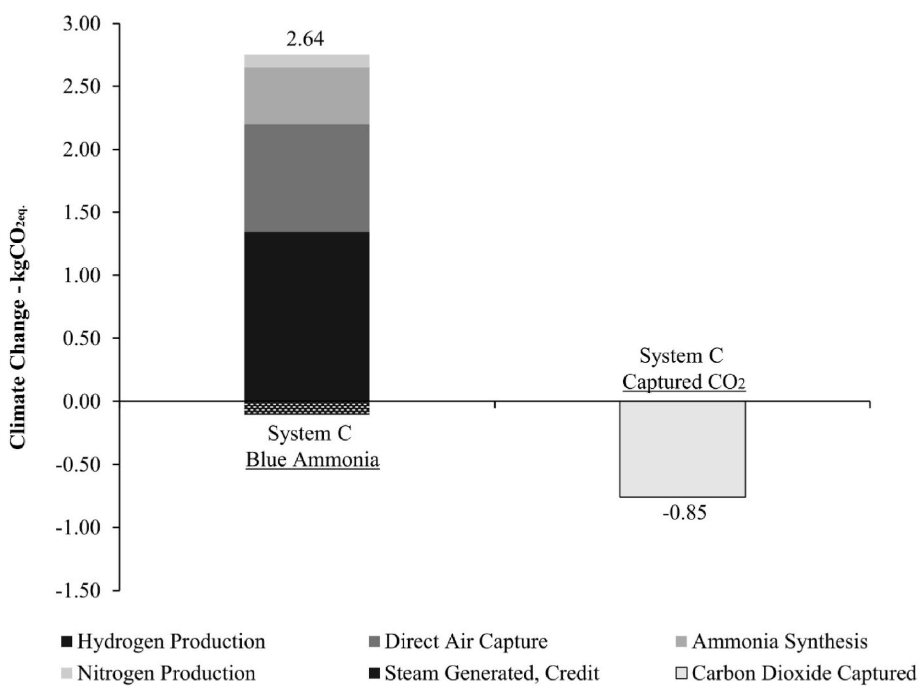

Fig. 8. Climate change results of blue ammonia and captured CO2 co-products after system expansion via DAC.

emissions of 2.90 kg $CO_{2eq.}$, can be attributed to the assumptions about the Polish natural gas market modelling. While Ecoinvent approximates the Polish natural gas market process to its German counterpart, the Polish market shows more diverse imports and transportation modeling, likely contributing to the higher climate change results observed. Whereas direct emissions from SMR process remain consistent with the initial scenario at 2.06 $kgCO_{2eq.}$ Additionally, the fossil-intensive electricity mix employed in the H-B process contributes to the overall high impact of 0.67 $kgCO_{2eq.}$, as can be seen in Fig. 9 (Polish Scenario)

Similar observations can be made for Austria concerning natural gas procurement, processing, and transportation, akin to the trends noted in the Polish scenario, where the hydrogen production contributes to approximately 2.90 $kgCO_{2eq.}$, of which 2.06 $kgCO_{2eq.}$ are direct emissions. However, a notable distinction lies in the electricity mix, where Austria shows a predominant presence of renewable energies. This energy mix is visibly evident in the assessment of ammonia synthesis, where the impact is at 0.34 $kgCO_{2eq.}$, as illustrated in Fig. 9 for System A (Austrian Scenario).

Furthermore, the visual contrast between the Austrian and Polish scenarios is apparent in Fig. 9, particularly in the context of carbon

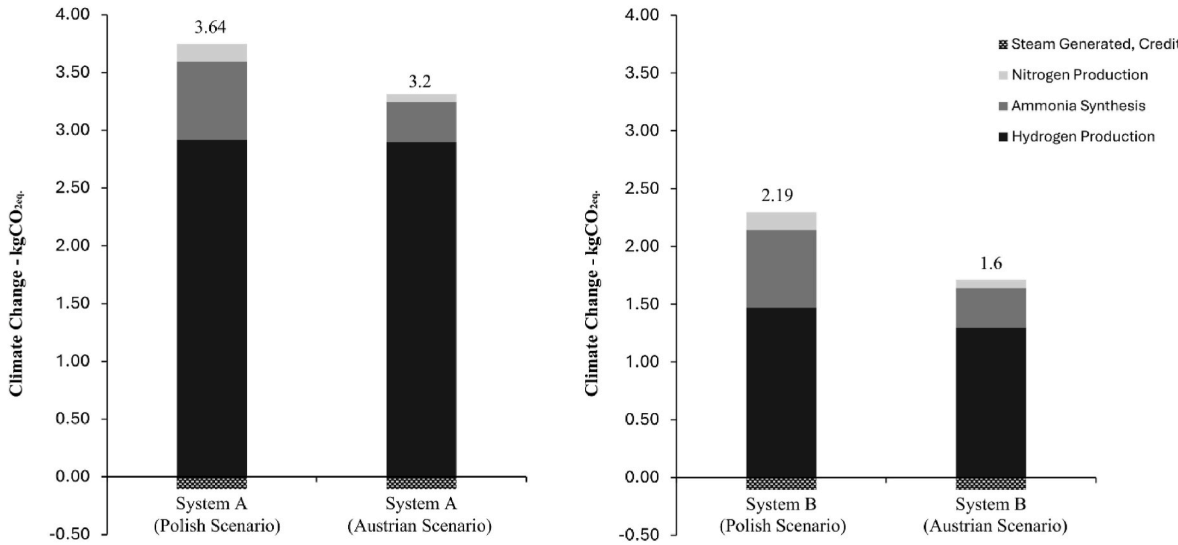

Fig. 9. Climate change results of the assessed System A and B in Poland and Austria.

capture-based hydrogen production of System B. In the Austrian case, the climate change impact of blue ammonia in its extended functional unit form is significantly lower, registering a joint impact of 1.60 $kgCO_{2eq.}$, as opposed to the Polish case at 2.19 $kgCO_{2eq.}$

The application of the proposed system expansion approach highlights the significance of production regionality in shaping the final outcomes. It is important to note that, in the scenario analysis, the DAC is modelled in the same country as the ammonia production, ensuring the use of a consistent electricity mix for system expansion. In the case of the Polish scenario in Fig. 10 (a), a relatively low climate change impact of 1.80 $kgCO_{2eq.}$ for 1 kg of blue ammonia was attainable, albeit at a substantial disadvantage. The net climate change results of the captured CO_2 co-product are no longer a negative emission, reaching at 0.39 $kgCO_{2eq.}$ for 1.85 kg of captured CO_2. Under the proposed system expansion, this positive climate impact from DAC is then reflected in the results for ammonia production negatively. This is a direct result of the mathematical relation where the overall climate impact (2.19 $kgCO_{2eq}$) shown in Fig. 10 is the sum of the process emissions for ammonia (1.8 $kgCO_{2eq}$) and the additional burden from DAC (0.39 $kgCO_{2eq}$). The incentive generated for blue ammonia in this case becomes obsolete when the captured CO_2 would be employed in further downstream applications.

In contrast, the Austrian-based scenario, shown in Fig. 10 (b), demonstrates more favorable outcomes for both blue ammonia and the captured CO_2 co-products, with a particularly significant benefit for the latter. Compared to the grey ammonia production scenario (System A: Austria Scenario) shown in Fig. 9, the results indicate an approximate 8 % reduction in climate change impacts. However, this reduction is relatively modest compared to the reductions observed in the German and Polish scenarios. Notably, the 1.85 kg of captured CO_2 in the Austrian scenario achieves a negative climate change impact of −1.34 $kgCO_{2eq.}$, marking a significant improvement over the other scenarios discussed.

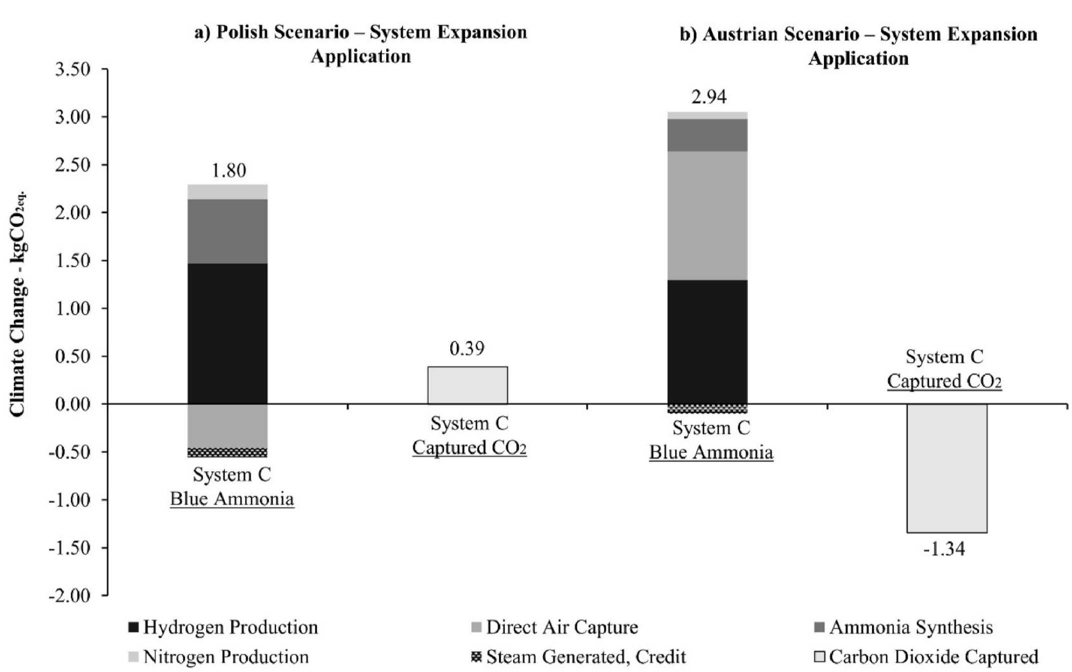

Fig. 10. Climate change results of blue ammonia and captured CO_2 co-products after system expansion via DAC in (a) Poland and (b) Austria.

3.3. Scenario analysis: future direct air capture system and electricity mix

In the foreseeable future, significant changes are anticipated in the energy demand for DAC and the composition of the electricity mix and heat source. While the hydrogen production process through SMR is well-established and highly optimized, little to no change is assumed. However, the global electricity mix, including that of Germany, is poised to undergo a transformation, thereby influencing the environmental outputs of both ammonia synthesis and carbon capture processes. As depicted in Fig. 11, the German production is projected along a futuristic trajectory. This projection models the anticipated electricity mix of Germany in the year 2045 to be fully renewable-based and defossilized (Prognos et al., 2021).

In the projected future scenario for the year 2045, the climate change results for 1 kg grey ammonia experience a slight reduction, decreasing from 3.12 $kgCO_{2eq.}$ in 2023 to 2.94 $kgCO_{2eq.}$ in 2045. This reduction is attributed to the substantial defossilization of the electricity mix, leading to a consequent decrease in the climate change impact associated with nitrogen production and ammonia synthesis.

Furthermore, the climate change impact of the in-process carbon capture significantly reduced due to prospective sustainable heat source required for sorbent regeneration and CO_2 separation, which was assumed to come from sustainable biomethane. As a result, blue ammonia impact is notably reduced to 1.36 $kgCO_{2eq.}$ for the extended functional unit.

Additionally, it has been assumed that the electricity and heat demand for DAC are expected to decrease significantly as the technology matures in the market, with anticipated reductions of 30 % in electricity demand and 53 % in heat demand, as projected in Deutz and Bardow (2021). Coupled with a defossilized German electricity mix, this presents a highly favorable environmental outcome for DAC.

In the application of the system expansion approach, as illustrated in Fig. 12, it becomes evident that the substitution of DAC is particularly advantageous for the captured CO_2 co-product. This is exemplified by a negative result recorded at −1.64 $kgCO_{2eq.}$ for every 1.85 $kgCO_2$ captured. However, despite the positive attributes associated with DAC as a negative emission system, it undoubtedly outperforms in-process carbon capture at ammonia plants energetically and environmentally. Consequently, the climate change impact of blue ammonia in this system expansion approach stands at 3.00 $kgCO_{2eq.}$, representing a minor increase compared to its grey ammonia counterpart. Importantly, there is no shared incentivization observed between the two co-products; rather, there is a counter-incentivization for producing blue ammonia in this specific case.

4. Discussion

After assessing the proposed methodology against the backdrop of blue ammonia incentivization, several main points can be drawn up and elaborated to provide further clarity regarding the decision to adopt such approach to achieve a reduced climate change impact in the chemical industry and beyond. It is noteworthy that previous studies, such as those underpinning the Global CO_2 Initiative (Langhorst et al., 2022), NETL guidelines (Skone et al., 2022), and LCA4CCU recommendations (Ramirez et al., 2022), have primarily addressed multi-functional handling in carbon capture and utilization. However, these frameworks do not facilitate the mutual co-product climate impact incentivization that is central to the TfS guidelines. Consequently, our discussion concentrates on critically evaluating the novel and as yet untested system expansion approach via DAC substitution, which represents a significant departure from existing methodologies.

4.1. Grey ammonia, carbon capture systems and blue ammonia incentivization

At an initial stage, the examination of grey ammonia production with hydrogen from SMR falls within the range of previously reported research (Zhang et al., 2013; Liu et al., 2020). It underscores that SMR contributes the largest share of the total impact of overall grey ammonia production regardless of regionality.

Furthermore, the comparative analysis of the in-process MEA carbon capture and DAC systems highlights major disparities. The dependence of the former on natural gas and the latter on electricity in direct operations underlines the importance of carefully understanding the systems, prior to the application of system expansion to solve the multi-functionality output of CCU-based blue ammonia production. Additionally, it is important to consider that due to the variance in technological maturity, the application of the proposed system expansion may not achieve the same level of representativeness and reliability for the end results.

The proposed system expansion approach, as evidenced by the extended functional unit for blue ammonia production, presents an innovative strategy for simultaneous incentivization of both blue ammonia and captured CO_2 as output products. Previous modelling approaches fell short of offering a mutually beneficial solution for product suppliers who have excess CO_2 and want to collaborate in decreasing the environmental impact of their products. Hence, the TfS approach stands as a pivotal point worth investigating.

In today's Germany, the modelling of CCU-based blue ammonia has shown a 20 % decrease in the climate change impact compared to grey

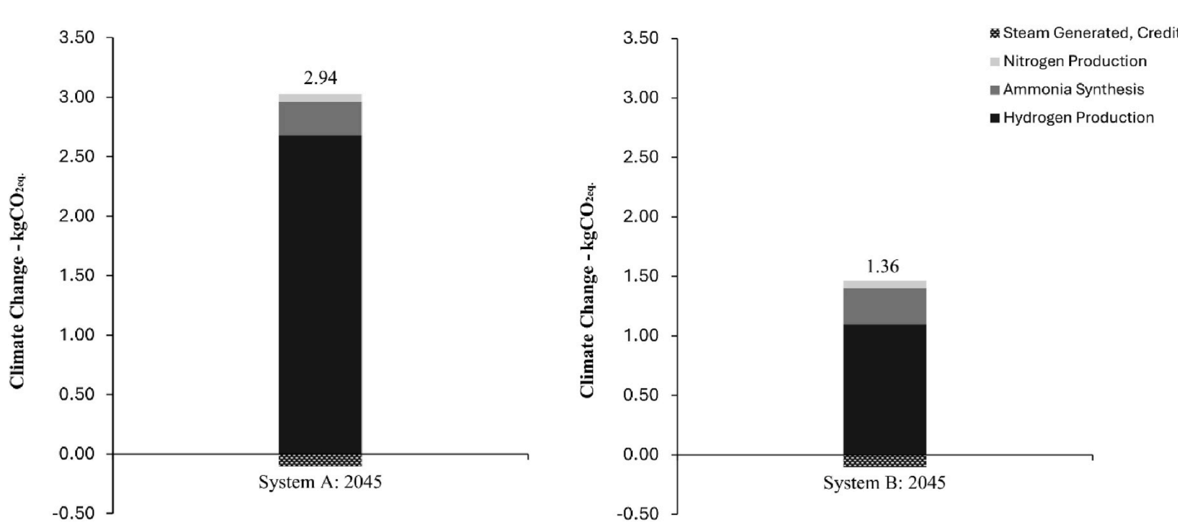

Fig. 11. Climate change results of grey ammonia and blue ammonia (extend functional unit) in Germany – future scenario 2045.

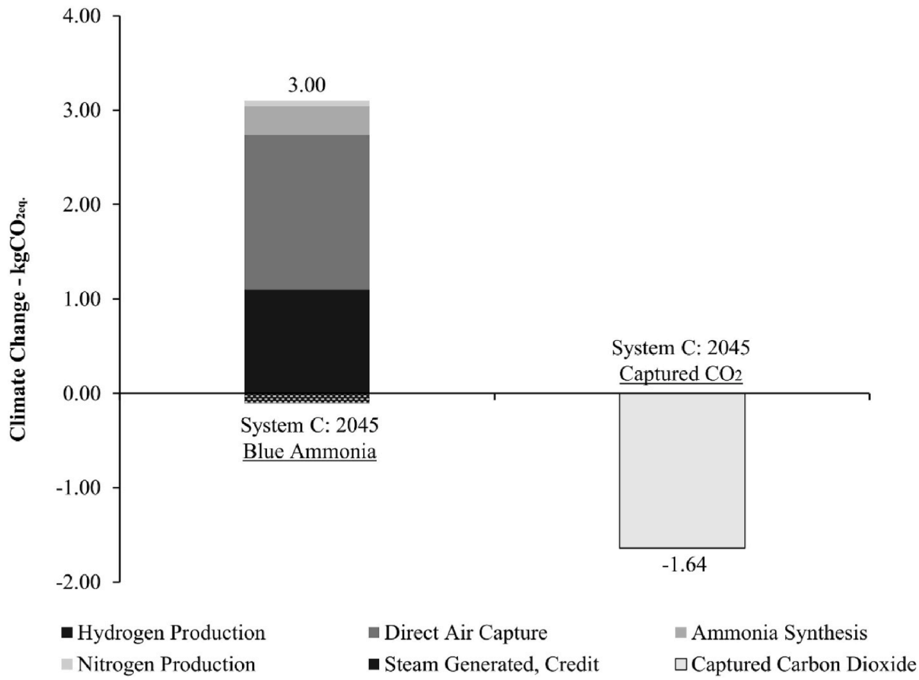

Fig. 12. Climate change results of blue ammonia and captured CO_2 co-products after system expansion via DAC - future scenario 2045.

ammonia. The captured CO_2 co-product retains its negative emission status, which encourages further incentivization of its downstream application to mitigate climate change impact. Previous modelling approaches failed to provide a mutually beneficial solution for product providers to effectively use and benefit from CO_2 while also incentivizing the reduction of their main products' impact on climate change. This results arguably encourages ammonia suppliers in Germany to promote a CCU-based blue ammonia alternative that can potentially benefit everyone in their journey of reducing climate change impact in downstream applications.

4.2. Regionality impact on shared incentivization between blue ammonia and captured CO_2

The scenario analysis of production regionality, especially in Poland and Austria, shows that regional factors influence climate change results incentivization for blue ammonia through the proposed approach. As Poland relies on electricity generated from fossil fuels, whereas Austria obtains its electricity from renewable energy sources, the suggested system expansion approach, which adjusts outcomes based on regional modelling tied to the GHG emissions of provided electricity, highlights the complexity of achieving a universally shared incentivization pattern for climate change. According to positive results seen in Austria, a low-fossil electricity mix can slightly decrease the impact of ammonia on the environment. However, this effect is more apparent as seen in Germany, where the electricity mix is much less 'renewable'. In Poland, there is a negative incentive for the blue ammonia byproduct, which sets the tone for possible conclusions about how 'unsuitable' the proposed approach would work in a fossil-heavy production area.

4.3. Prospective impact on shared incentivization between blue ammonia and captured CO_2

A fully carbon-neutral energy system is expected to exist in Germany by 2045. This is a positive prediction for how DAC will operate and mature as a technology. However, with this advancement, the DAC becomes practically more efficient both energetically and environmentally than in-process carbon capture. Using the suggested system expansion method in this case would lead to counter incentivization of blue ammonia production, while the CO_2 that was captured, eventually utilized in downstream applications, would see an incentivization that goes beyond the capability limits of the system that captured it.

5. Conclusion

This study advances the understanding of industry-focused LCA approaches, specifically addressing the multifunctional modelling challenges proposed by the chemical industry. The latest publication guideline by TfS offers a new insight into solving such multifunctionality through system expansion via DAC substitution. As this method was not assessed on a scientific research level, this work enables further understanding of such a methodology, highlighting its mechanisms and limitations.

The outcome of this work can be summarized and concluded in these points.

- Hydrogen production via SMR, as part of the ammonia production process, holds the majority of the emission burden of the GHG emissions, particularly CO_2, throughout the entire process.
- MEA-based carbon capture processes and DAC exhibit significant differences in operational requirements and climate change impact outcomes, depending on the scenario modelled. These variations can pose challenges for LCA practitioners when attempting to integrate these technologies into the proposed system expansion approach, especially when adapting the model to their specific scenarios.
- The promised shared incentivization, via the proposed system expansion, can be recorded in a production regionality with balanced or transitioning energy mix, between fossil-based and renewable-based sources of energy, as such in Germany and Austria.
- A heavily fossil-based energy mix, like that in Poland, discourages the use of CO_2 as a co-production for downstream utilization, making it less attractive or feasible. It will no longer hold negative climate change results as initially outlined and potentially perpetuating high climate change impact overall.

- A fully renewable energy mix leads to full incentivization towards CO_2 co-product heading towards utilization, leaving blue ammonia as a co-product unincentivized.
- The utilization of the proposed system expansion method using DAC will not lead to shared incentivization in a future decarbonized electricity scenario, therefore, such an approach should be designated as a "short-term outlook" in providing shared incentivization of blue ammonia as well as captured CO_2.
- As highlighted in the TfS guidelines, this method is heavily intertwined with the GHG emissions of electricity that powers DAC. It is important to examine the possibility that both DAC and ammonia production are geographically distinct to maintain consistent incentivization while avoiding the pitfalls of greenwashing practices.
- The guideline's recommendation that 'CO_2 emission factor shall be adjusted to reflect the electricity consumption mix of the country where the CO_2 producer is located' in DAC modelling may lead to inconsistent incentivization between co-products, as demonstrated in this study, compared to the guideline's claim.
- Variations in electricity mixes, which can change significantly across regions and over time, introduce uncertainties that hinder the consistency and comparability of the proposed method in the TfS guideline.

This study highlights important recommendations moving forward.

- The proposed approach should be emphasized as a short-term solution to address the multifunctionality challenge in CCU for co-products incentivization, particularly given its disadvantages in future defossilized electricity mix scenario analysis.
- The system expansion approach is most suitable and recommended for application in regions with a transitioning energy mix, where shared incentivization can be achieved.
- The application of the proposed approach should be avoided in regions dominated by either fossil-based or fully renewable energy systems, if the goal is the highlighted co-product incentivization.

CRediT authorship contribution statement

Mutaz Chahrour: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Conceptualization. **Christina Wulf:** Writing – review & editing, Validation, Supervision. **Petra Zapp:** Writing – review & editing, Validation, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jenvman.2025.125438.

Data availability

All data used in the article are either published in the article itself or in the supplementing material.

References

Ag Energiebilanzen, E.V., 2023. Gross electricity generation in Germany by source [Online]. Münster. Available: https://ag-energiebilanzen.de/en/. (Accessed 20 September 2024).

Althaus, H., Chudacoff, M., Hischier, R., Jungbluth, N., Osses, M., Primas, A., 2007. Life Cycle Inventories of Chemicals. *Ecoinvent Report No. 8.* EMPA Dübendorf. Swiss Centre for Life Cycle Inventories.

Amhamed, A.I., Shuibul Qarnain, S., Hewlett, S., Sodiq, A., Abdellatif, Y., Isaifan, R.J., Alrebei, O.F., 2022. Ammonia production plant - a review. Fuels 3, 408–435. https://doi.org/10.3390/fuels3030026.

Antonini, C., Treyer, K., Streb, A., Van Der Spek, M., Bauer, C., Mazzotti, M., 2020. Hydrogen production from natural gas and biomethane with carbon capture and storage - a techno-environmental analysis. Sustain. Energy Fuels 4, 2967–2986. https://doi.org/10.1039/d0se00222d.

ARAMCO, 2020. How can we deliver one of the fuels of the future? [Online]. Dhahran. Available: https://www.aramco.com/en/about-us/our-brand/powered-by-how/blue-hydrogen. (Accessed 20 September 2024).

Atchison, J., 2022. *Building hydrogen and ammonia value chains in Indonesia* [online]. Ashburn: ammonia energy association. Available: https://ammoniaenergy.org/articles/building-hydrogen-and-ammonia-value-chains-in-indonesia/. (Accessed 20 September 2024).

Bicer, Y., Dincer, I., Vezina, G., Raso, F., 2017. Impact assessment and environmental evaluation of various ammonia production processes. Environ. Manag. 59, 842–855. https://doi.org/10.1007/s00267-017-0831-6.

Deutz, S., Bardow, A., 2021. Life-cycle assessment of an industrial direct air capture process based on temperature-vacuum swing adsorption. Nat. Energy 6, 203–213. https://doi.org/10.1038/s41560-020-00771-9.

Duval-Dachary, S., Beauchet, S., Lorne, D., Salou, T., Helias, A., Pastor, A., 2023. Life cycle assessment of bioenergy with carbon capture and storage systems: critical review of life cycle inventories. Renew. Sustain. Energy Rev. 183. https://doi.org/10.1016/j.rser.2023.113415.

ECOINVENT, 2023. Ecoinvent Database. Swiss Centre for Life Cycle Inventories, Dübendorf, Version 3.9.1.

El-Shafie, M., Kambara, S., 2023. Recent advances in ammonia synthesis technologies: toward future zero carbon emissions. Int. J. Hydrogen Energy 48, 11237–11273. https://doi.org/10.1016/j.ijhydene.2022.09.061.

IEA, 2021. Ammonia Technology Roadmap: towards More Sustainable Nitrogen Fertiliser Production. International Energy Agency, Paris.

INTERGOVERNMENTAL PANEL ON CLIMATE CHANGE, 2023. Climate Change 2021 – the Physical Science Basis: Working Group I Contribution to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge.

Ishaq, H., Dincer, I., Crawford, C., 2022. A review on hydrogen production and utilization: challenges and opportunities. Int. J. Hydrogen Energy 47, 26238–26264. https://doi.org/10.1016/j.ijhydene.2021.11.149.

ISO14040, 2006. Environmental Management: Life Cycle Assessment; Principles and Framework. International Organization for Standardization, Geneva, Switzerland.

ISO14044, 2006. Environmental Management: Life Cycle Assessment; Requirements and Guidelines. International Organization for Standardization Geneva, Switzerland.

Langhorst, T., Mccord, S., Zimmermann, A., Müller, L., Cremonese, L., Strunge, T., Wang, Y., Zaragoza, A.V., Wunderlich, J., Marxen, A., Armstrong, K., Buchner, G., Kätelhön, A., Bachmann, M., Sternberg, A., Michailos, S., Naims, H., Winter, B., Roskosch, D., Faber, G., Mangin, C., Olfe-Kräutlein, B., Styring, P., Schomäcker, R., Bardow, A., Sick, V., 2022. Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO2 Utilization (Version 2), pp. 133–186. Ann Arbor.

Liu, X.Y., Elgowainy, A., Wang, M., 2020. Life cycle energy use and greenhouse gas emissions of ammonia production from renewable resources and industrial by-products. Green Chem. 22, 5751–5761. https://doi.org/10.1039/d0gc02301a.

Macfarlane, D.R., Cherepanov, P.V., Choi, J., Suryanto, B.H.R., Hodgetts, R.Y., Bakker, J. M., Vallana, F.M.F., Simonov, A.N., 2020. A roadmap to the ammonia economy. Joule 4, 1186–1205. https://doi.org/10.1016/j.joule.2020.04.004.

Markewitz, P., Kuckshinrichs, W., Leitner, W., Linssen, J., Zapp, P., Bongartz, R., Schreiber, A., Müller, T.E., 2012. Worldwide innovations in the development of carbon capture technologies and the utilization of CO_2. Energy Environ. Sci. 5, 7281–7305. https://doi.org/10.1039/C2EE03403D.

Mayer, P., Ramirez, A., Pezzella, G., Winter, B., Sarathy, S.M., Gascon, J., Bardow, A., 2023. Blue and green ammonia production: a techno-economic and life cycle assessment perspective. iScience 26. https://doi.org/10.1016/j.isci.2023.107389.

Metz, B., Davidson, O., De Coninck, H., Loos, M., Meyer, L., 2005. IPCC Special Report on Carbon Dioxide Capture and Storage. Cambridge University Press, Cambridge.

Mora, M.A.M., Vergara, C.P., Leiva, M.A., Delgadillo, S.A.M., Rosa-Domínguez, E.R., 2016. Life cycle assessment of carbon capture and utilization from ammonia process in Mexico. J. Environ. Manag. 183, 998–1008. https://doi.org/10.1016/j.jenvman.2016.09.048.

Morlane, N., Katikaneni, S.P., Paglieri, S.N., Harale, A., Solami, B., Sarathy, S.M., Gascon, J., 2021. A technological roadmap to the ammonia energy economy: current state and missing technologies. Chem. Eng. J. 408. https://doi.org/10.1016/j.cej.2020.127310.

Osorio-Tejada, J., Tran, N.N., Hessel, V., 2022. Techno-environmental assessment of small-scale Haber-Bosch and plasma-assisted ammonia supply chains. Sci. Total Environ. 826, 154162. https://doi.org/10.1016/j.scitotenv.2022.154162.

PERTAMINA, 2022. Pertamina, PT Pupuk Indonesia, and Mitsubishi corporation agree to develop blue/green hydrogen and ammonia business [Online]. Jakarta. Available: https://www.pertamina.com/en/news-room/news-release/pertamina-pt-pupuk-in donesia-and-mitsubishi-corporation-agree-to-develop-blue-green-hydrogen-and-ammonia-business. (Accessed 20 September 2024).

PROGNOS, ÖKO-INSTITUT & WUPPERTAL-INSTITUT, 2021. Towards a climate-neutral Germany by 2045. How Germany Can Reach its Climate Targets before 2050 - Executive Summary. Berlin: Stiftung Klimaneutralität, Agora Energiewende and Agora Verkehrswende.

Rafiqul, I., Weber, C., Lehmann, B., Voss, A., 2005. Energy efficiency improvements in ammonia production - perspectives and uncertainties. Energy 30, 2487–2504. https://doi.org/10.1016/j.energy.2004.12.004.

Ramirez, A., El Khamlichi, A., Markowz, G., Rettenmaier, N., Baitz, M., Jungmeier, G., Bradley, T., 2022. LCA4CCU – Guidelines for Life Cycle Assessment of Carbon Capture and Utilisation. Publications Office of the European Union, Luxembourg.

Rouwenhorst, K., 2023. *Technology status: ammonia production from electrolysis-based hydrogen* [Online]. Ashburn: Ammonia Energy Association. Available: https://ammoniaenergy.org/articles/technology-status-ammonia-production-from-electrolysis-based-hydrogen/. (Accessed 20 September 2024).

Sick, V., Armstrong, K., Cooney, G., Cremonese, L., Eggleston, A., Faber, G., Hackett, G., Kätelhön, A., Keoleian, G., Marano, J., Marriott, J., Mccord, S., Miller, S.A., Mutchek, M., Olfe-Kräutlein, B., Ravikumar, D., Roper, L.K., Schaidle, J., Skone, T., Smith, L., Strunge, T., Styring, P., Tao, L., Völker, S., Zimmermann, A., 2020. The need for and path to harmonized life cycle assessment and techno-economic assessment for carbon dioxide capture and utilization. Energy Technol. 8. https://doi.org/10.1002/ente.201901034.

Skone, T.J., Mutchek, M., Krynock, M., Moni, S., Rai, S., Chou, J., Carlson, D.R., Jamieson, M., Dale, E., Cooney, G., Kumar, A., 2022. Carbon Dioxide Utilization Life Cycle Analysis Guidance for the U.S. DOE Office of Fossil Energy and Carbon Management. National Energy Technology Laboratory, Pittsburgh, Version 2.0.

Terlouw, T., Treyer, K., Bauer, C., Mazzotti, M., 2021. Life cycle assessment of direct air carbon capture and storage with low-carbon energy sources. Environ. Sci. Technol. 55, 11397–11411. https://doi.org/10.1021/acs.est.1c03263.

TFS, 2024. The Product Carbon Footprint Guideline for the Chemical Industry: Specification for Product Carbon Footprint and Corporate Scope 3.1 Emission Accounting and Reporting (Version 2.1). Together for Sustainability, Brussels.

Von Der Assen, N., Voll, P., Peters, M., Bardow, A., 2014. Life cycle assessment of CO_2 capture and utilization: a tutorial review. Chem. Soc. Rev. 43, 7982–7994. https://doi.org/10.1039/c3cs60373c.

Zhang, W.F., Dou, Z.X., He, P., Ju, X.T., Powlson, D., Chadwick, D., Norse, D., Lu, Y.L., Zhang, Y., Wu, L., Chen, X.P., Cassman, K.G., Zhang, F.S., 2013. New technologies reduce greenhouse gas emissions from nitrogenous fertilizer in China. Proc. Natl. Acad. Sci. U. S. A 110, 8375–8380. https://doi.org/10.1073/pnas.1210447110.

Zhang, Y.L., Liu, H., Li, J.J., Deng, Y.L., Miao, X.P., Xu, D.P., Liu, S.Q., Xie, K.C., Tian, Y. J., 2022. Life cycle assessment of ammonia synthesis in China. Int. J. Life Cycle Assess. 27, 50–61. https://doi.org/10.1007/s11367-021-02010-z.