

India's Ammonia Industry: Balancing Growth with Sustainability

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Supplementary Information 1

Ammonia Production Process via Steam Methane Reforming (SMR)

Stage 1: Hydrogen production via SMR

It is the most commercialised process, the methane-fed processes represent the best available technique given its higher energy efficiency and lower carbon emissions and thus it will be the benchmark used to compare alternative technologies in this study. Hydrogen is produced by primary and secondary steam methane reforming reactors (SMR), followed by a two-stage water-gas shift reactor, CO₂ removal and methanation. The first SMR reactor operates in allothermal conditions at around 850-900 °C and 25-35 bar and the energy required for the endothermic reaction is provided by external combustion of methane fuel through furnace tubes that run through the catalyst bed (Smith et al., 2020; US DOE, 2022). The second SMR reactor is autothermal, air is compressed and fed to the reactor to provide heat of reaction by partial oxidation of the reagents at 900-1000 °C (Smith et al., 2020). The addition of air also provides the stoichiometric nitrogen required for the downstream Haber-Bosch reaction. The SMR process exports steam to be used elsewhere, mostly for compression energy (Ghavam et al., 2021). The SMR outlet mixture of carbon monoxide, hydrogen, and unreacted steam and methane are introduced into the two-stage water-gas shift (WGS) reactor to maximise CO conversion to hydrogen. The WGS reaction is exothermic and heat must be removed to minimise CO concentration at equilibrium. Although the SMR reactions are endothermic, the high reaction temperature and the need to cool substantially for the water gas shift reaction means that there is substantial waste heat available. This heat is used for raising of high-pressure steam which is expanded in steam turbines for compression, mainly used for compression of the feed in the Haber Bosch loop and the reformer combustion air compressor which are the largest two energy users (Bhat and Sadhukhan, 2009). The use of methane as feedstock inevitably leads to significant CO₂ emissions from the process and this is further compounded by the use of methane as fuel for the primary reformer furnace.

Stage 2: Haber- Bosch

The currently adopted ammonia production process employs the system invented by Fritz Haber and Carl Bosch about 100 years ago. Therefore, this system is well known as Haber-Bosch process. About 85% of total production of ammonia worldwide is produced by this process. The ammonia synthesis occurs according to reaction (S1)



Ammonia synthesis is an exothermic reaction (negative enthalpy change), and it occurs spontaneously at low temperatures (negative entropy change). Although it is favoured at room temperature, the reaction rate at which the reaction occurs at room temperature is too slow to be applicable for at an industrial scale. In order to increase the kinetics of the reaction to achieve the targeted conversion rate, high pressure and temperature are required. To effectively synthesize ammonia from its main components (hydrogen and nitrogen), the reaction should be performed at a relatively high temperature and pressure of 400-500 °C and 10-30 MPa, respectively, with the assistance of an iron-based catalyst (Tian et al., 2024). This condition is demanded due to the high dissociation energy (941 kJ/mol) of triple-bonded nitrogen. However, to bring the reaction under this high temperature and pressure, about 30 MJ/kg-NH₃ of energy is required (Siira, 2024).

Stage 3: Liquid ammonia production

Following ammonia synthesis in the Haber-Bosch reactor, the outlet gas stream consists of ammonia together with unreacted hydrogen and nitrogen (Spatolisano et al., 2023). The gaseous mixture is cooled under elevated pressure to condense ammonia, while the unreacted gases remain in the vapor phase and are recycled back to the synthesis loop. The condensation of ammonia occurs according to the phase equilibrium relationship:



Ammonia liquefaction is achieved through multi-stage refrigeration and compression systems that reduce the temperature sufficiently to reach the saturation conditions of ammonia at the operating pressure. The condensation temperature of ammonia decreases with pressure according to its vapor-liquid equilibrium behaviour, enabling efficient separation in the synthesis loop (Bian et al., 2024). After condensation, the liquid ammonia is separated in a flash separator, while the remaining hydrogen and nitrogen are recompressed and recycled to maximize overall conversion efficiency. Although part of the heat released during ammonia synthesis is recovered through heat integration, the refrigeration and compression requirements make the liquefaction step relatively energy-intensive.

Nitrogen Production (only for the case of SMR/Air)

In some ammonia production configurations, high-purity nitrogen is generated using cryogenic air separation units (ASU). In this process, atmospheric air is first compressed, purified to remove moisture and carbon dioxide, and then cooled to very low temperatures (approximately -170 to -196 °C) where the components of air are separated through fractional distillation based on their different boiling points (Amhamed et al., 2022)



Nitrogen (boiling point -196 °C) is separated from oxygen (boiling point -183 °C) and argon through staged distillation columns. The purified nitrogen stream is then compressed and supplied to the Haber-Bosch reactor to maintain the stoichiometric ratio with hydrogen (Cameli et al., 2024). This cryogenic separation process is widely adopted in large-scale ammonia plants due to its ability to produce nitrogen with high purity required for efficient ammonia synthesis.

Nitrogen Production (SMR)

Nitrogen required for ammonia synthesis is derived from atmospheric air through air separation processes. In conventional SMR-based ammonia plants, nitrogen is partially supplied through the secondary reformer, where compressed air is introduced to provide oxygen for partial oxidation reactions and nitrogen for the downstream Haber-Bosch synthesis loop (Musa et al., 2025). The nitrogen present in the injected air passes through the reformer largely unreacted and becomes part of the synthesis gas mixture required for ammonia formation.

Alkaline Water Electrolysis (AWE):

Alkaline water electrolysis (AWE) is a mature electrochemical technology for hydrogen production that generates hydrogen by splitting water molecules using electricity in the presence of an alkaline electrolyte (Sebbahi et al., 2022; Tuysuz, 2024). In contrast to fossil-based hydrogen production routes such as steam methane reforming (SMR), AWE produces hydrogen without direct carbon emissions when powered by renewable electricity, making it a key technology for green hydrogen production. The electrolyte typically consists of an aqueous solution of potassium hydroxide (KOH) or sodium hydroxide (NaOH), which facilitates ionic conductivity between the electrodes while preventing mixing of the product gases (Tsanaktsis, 2024).

In an alkaline electrolyzer, two electrodes are separated by a porous diaphragm or membrane that allows the transport of hydroxide ions (OH^-) while preventing gas crossover (Henkensmeier et al., 2024). When an external electrical potential is applied across the electrodes, water molecules are reduced at the cathode to produce hydrogen gas, while hydroxide ions are oxidized at the anode to generate oxygen gas (Zuo et al., 2023). The electrochemical reactions occurring in the alkaline electrolyzer can be expressed as follows:

Cathode (Hydrogen Evolution Reaction, HER):**Anode (Oxygen Evolution Reaction, OER):****Overall reaction:**

During the electrolysis process, hydroxide ions produced at the cathode migrate through the electrolyte toward the anode, where they participate in the oxygen evolution reaction. The generated hydrogen and oxygen gases are collected separately and can be utilized for various industrial applications. In ammonia production systems, the hydrogen produced through electrolysis is subsequently combined with nitrogen in the Haber-Bosch synthesis loop.

Industrial alkaline water electrolyzers (AWE) generally operate at temperatures of 60-90 °C and pressures up to 30 bar to maximize efficiency, with cell voltages typically in the 1.8-2.2 V range. Utilizing a 20-40% potassium hydroxide (KOH) electrolyte, these systems achieve current densities of 0.2-0.8 A/cm. Nickel-based catalysts are commonly used for both electrodes due to their stability in alkaline environments. Although AWE technology is commercially mature and widely deployed, its large-scale integration with ammonia production depends on the availability of low-carbon electricity sources and improvements in system efficiency and capital cost reduction.

Justification of the 1:1 displacement assumption:

Methane pyrolysis at temperatures above 800°C without catalysts produces predominantly amorphous or turbostratic solid carbon. The key physical properties of this carbon: surface area (typically 50-100 m²/g, compared with 20-60 m²/g for standard thermal-grade furnace carbon black), bulk density (~0.10-0.15 g/cm³), spheroidal aggregate particle morphology, and electrical conductivity fall within the performance envelope of commercial thermal-grade carbon black used in rubber compounding, conductive coatings, and pigment applications. At the market level, thermal-grade carbon black is priced at approximately USD 500-900 per tonne, broadly consistent with pilot-scale pyrolysis carbon pricing, supporting the economic plausibility of displacement in this market segment. On this basis, 1:1 mass displacement of thermal-grade carbon black is considered a technically defensible base-case assumption. However, for premium reinforcing-grade carbon black (e.g., N110, N220 tyre-grade), which requires tighter specification of surface activity, aggregate structure, and particle size distribution, non-catalytic pyrolysis carbon does not achieve equivalent performance. In such high-value market segments, the 1:1 mass equivalence constitutes an upper-bound assumption. To test the

robustness of the net-negative emission claim, the displacement ratio was varied systematically from 0% (solid carbon assigned no credit, treated as inert waste) to 100% (full 1:1 thermal-grade displacement), and an economic allocation alternative was evaluated. Displacement ratio sensitivity for methane pyrolysis emission intensity (kg CO₂ eq./ton H₂): at 0% displacement (no credit), +0.52 (net positive; not net-negative); at 25% displacement, -0.43; at 50% displacement, -1.38; at 75% displacement, -2.33; at 100% displacement (base case), -3.28; and under economic allocation by mass (H₂ is the lower-mass co-product so receives lower credit share), +0.18 (net positive). The net-negative emission claim is therefore conditional on substantial carbon black displacement (greater than approximately 15%). Critically however, even at 0% displacement, MP emission intensity (+0.52 kg CO₂ eq./ton H₂) remains far below that of conventional SMR (7.02 t CO₂ eq./ton NH₃), confirming that MP delivers meaningful decarbonisation under all tested assumptions. The broad distribution in Fig. 8d is consistent with this sensitivity range and reflects the dominant role of the carbon black displacement ratio as the primary source of variance in the MP life cycle results.

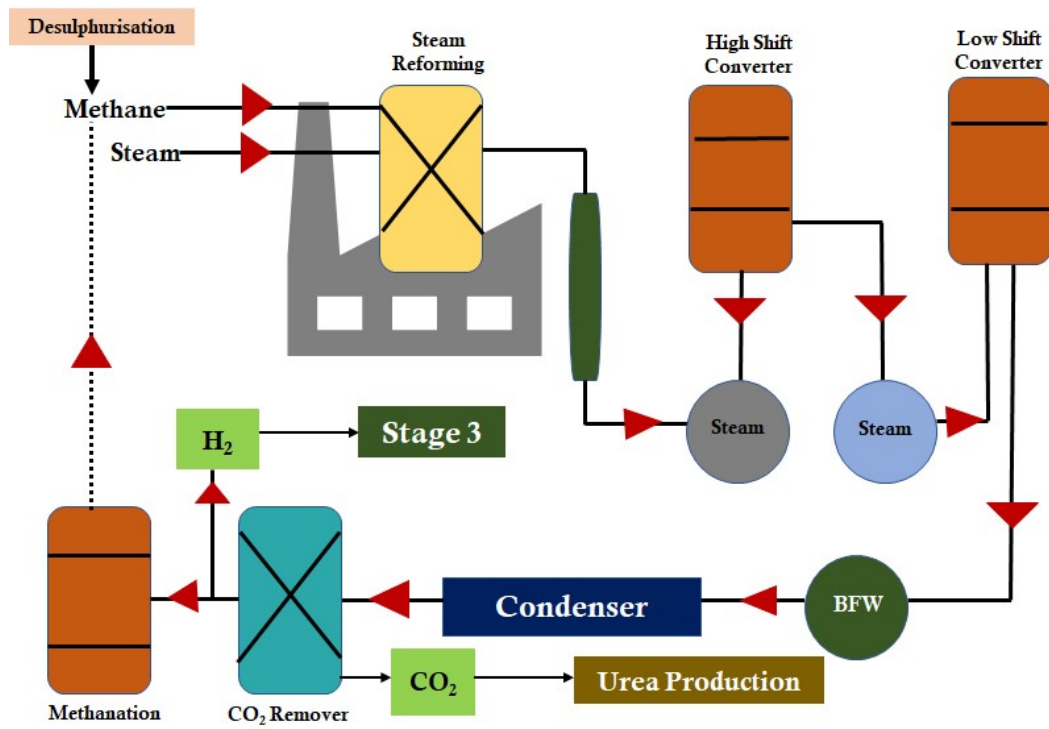


Fig. S1: Process Flow Diagram (PFD) depicting the stages involved in the production of hydrogen

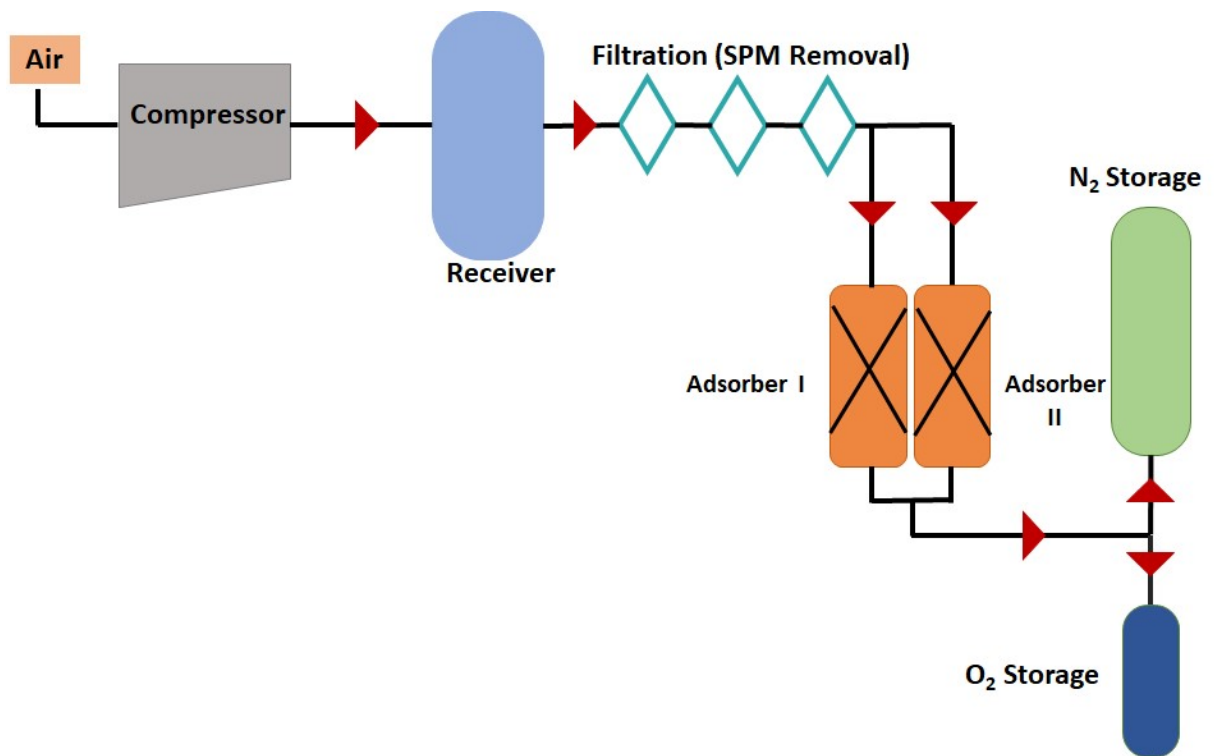


Fig. S2: Process Flow Diagram (PFD) depicting the stages involved in the production of nitrogen

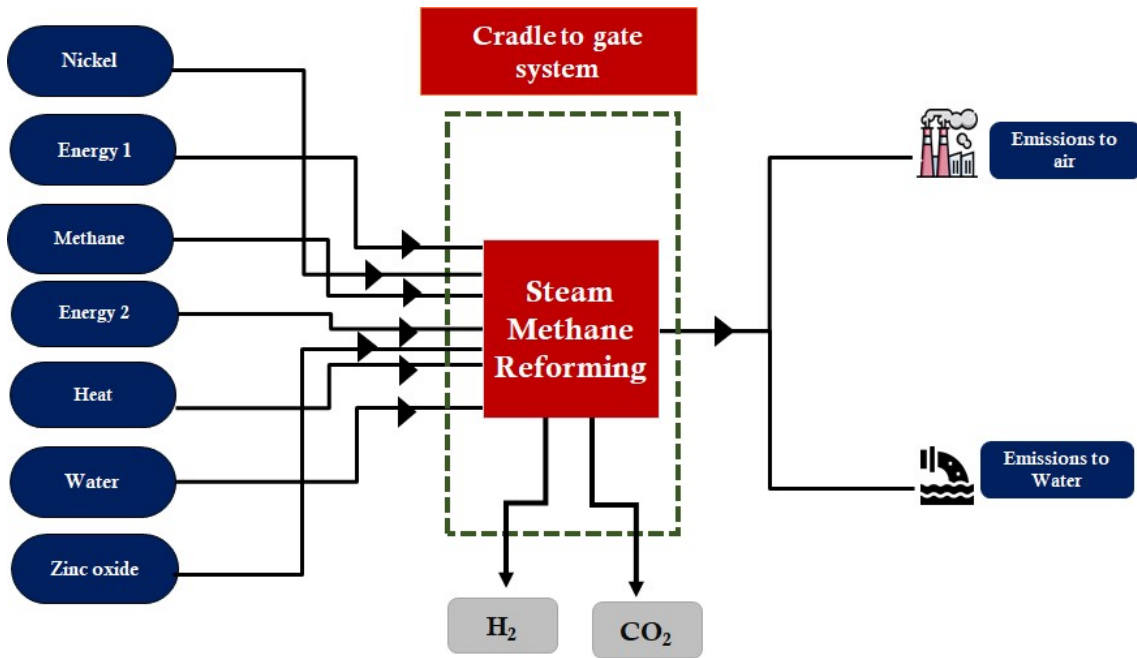


Fig. S3: System boundaries for hydrogen production

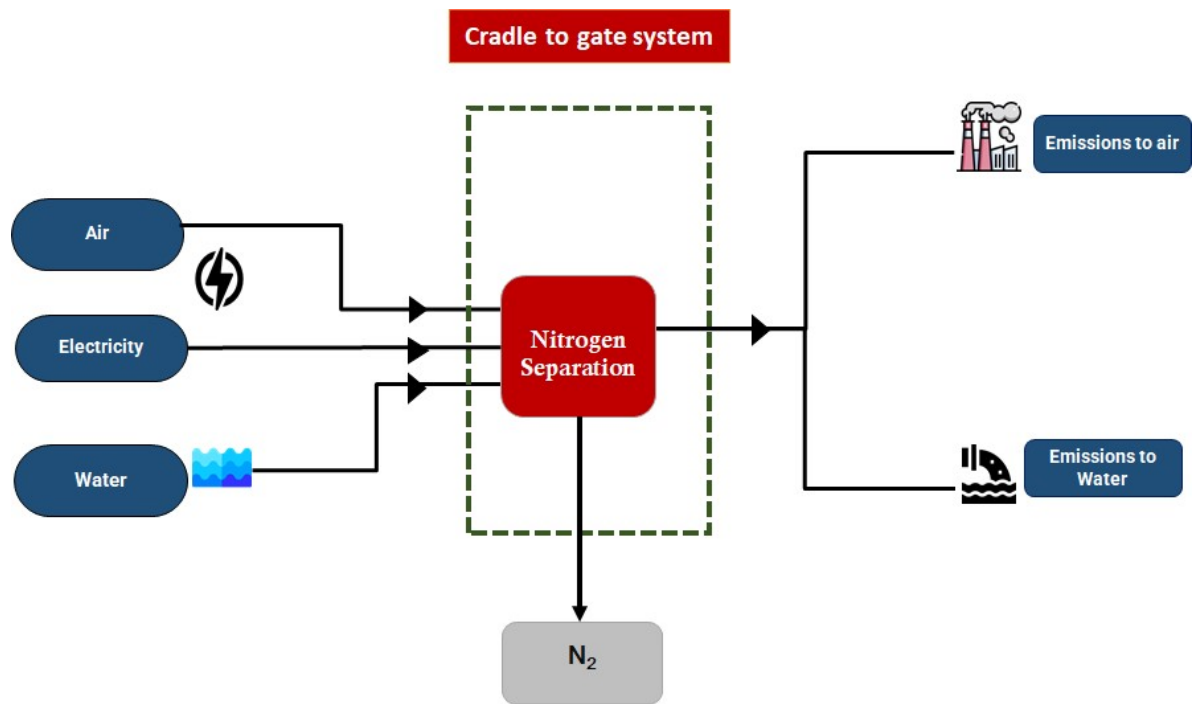


Fig. S4: System boundaries for nitrogen production

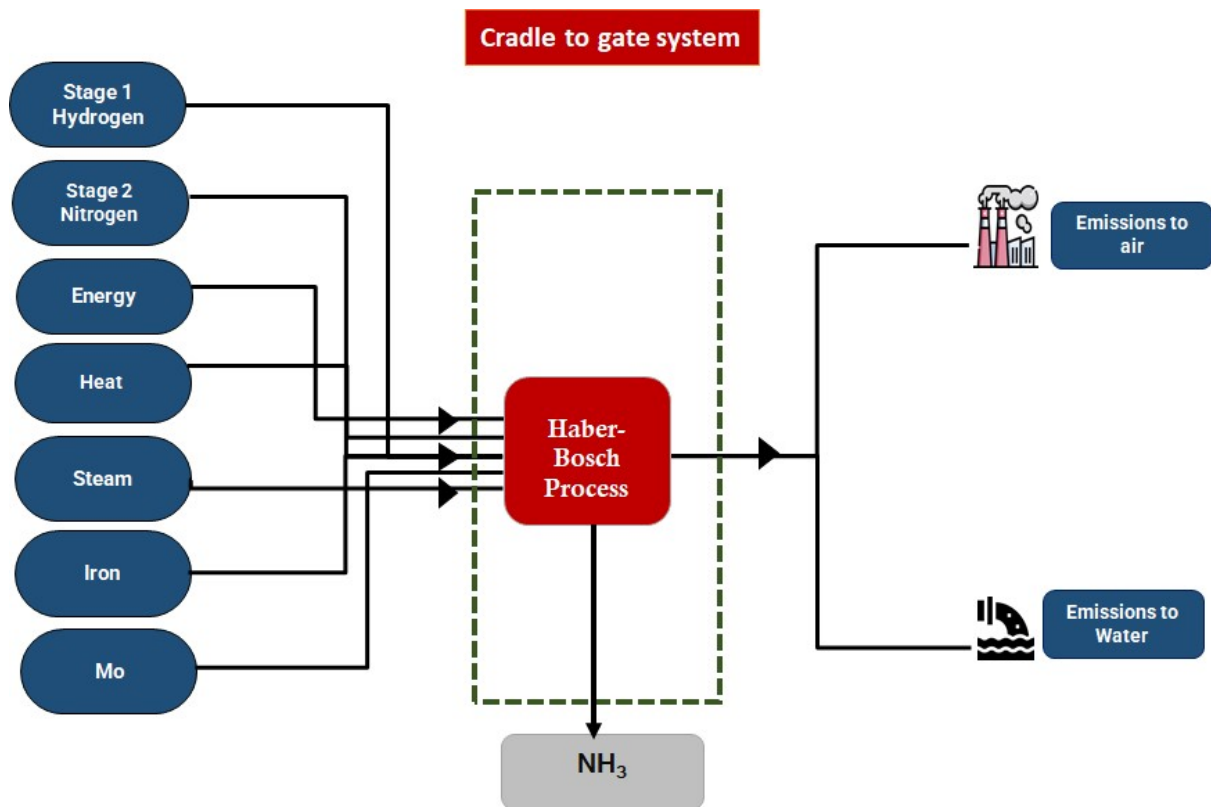


Fig. S5: System boundaries for ammonia production

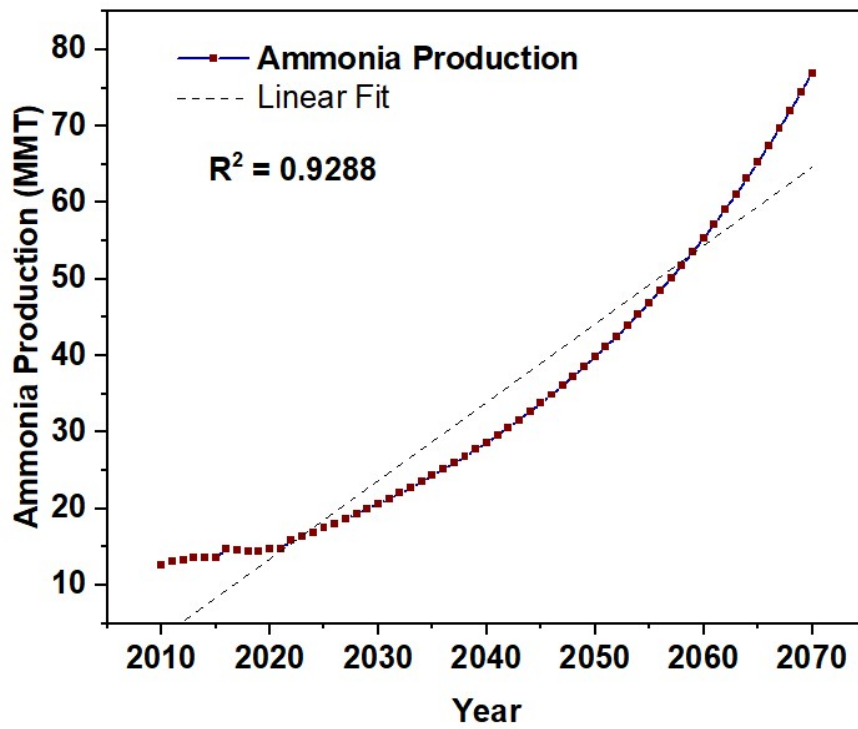


Fig. S6: Co-relation of ammonia production with respect to the GDP for 2010 to 2010: To gain insights into the historical trends and potential future manufacturing capacity for primary aluminium, a correlation was established between country's GDP and production capacity for the year 2010 -2021

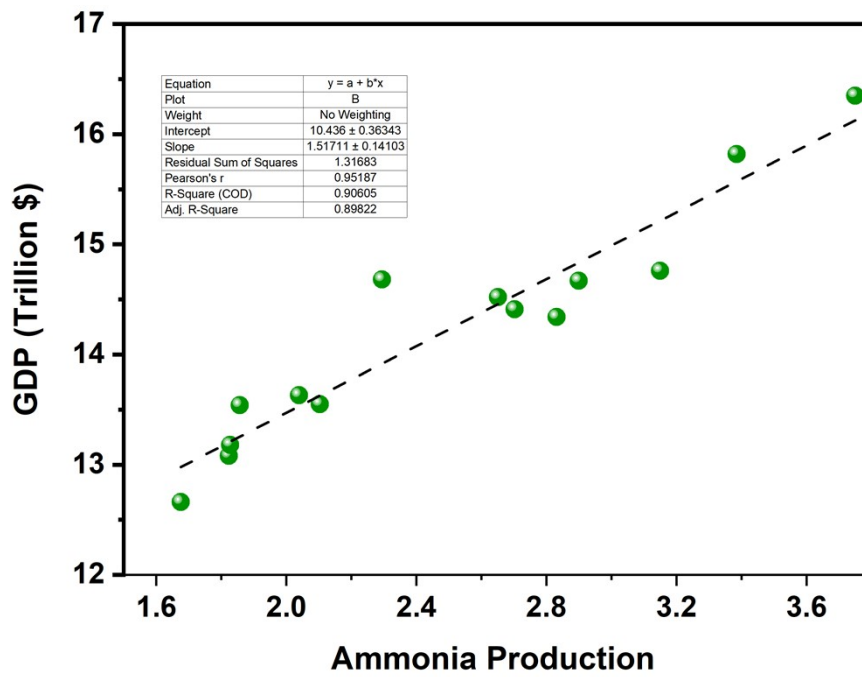


Fig. S7: Co-relation of ammonia production with respect to the GDP

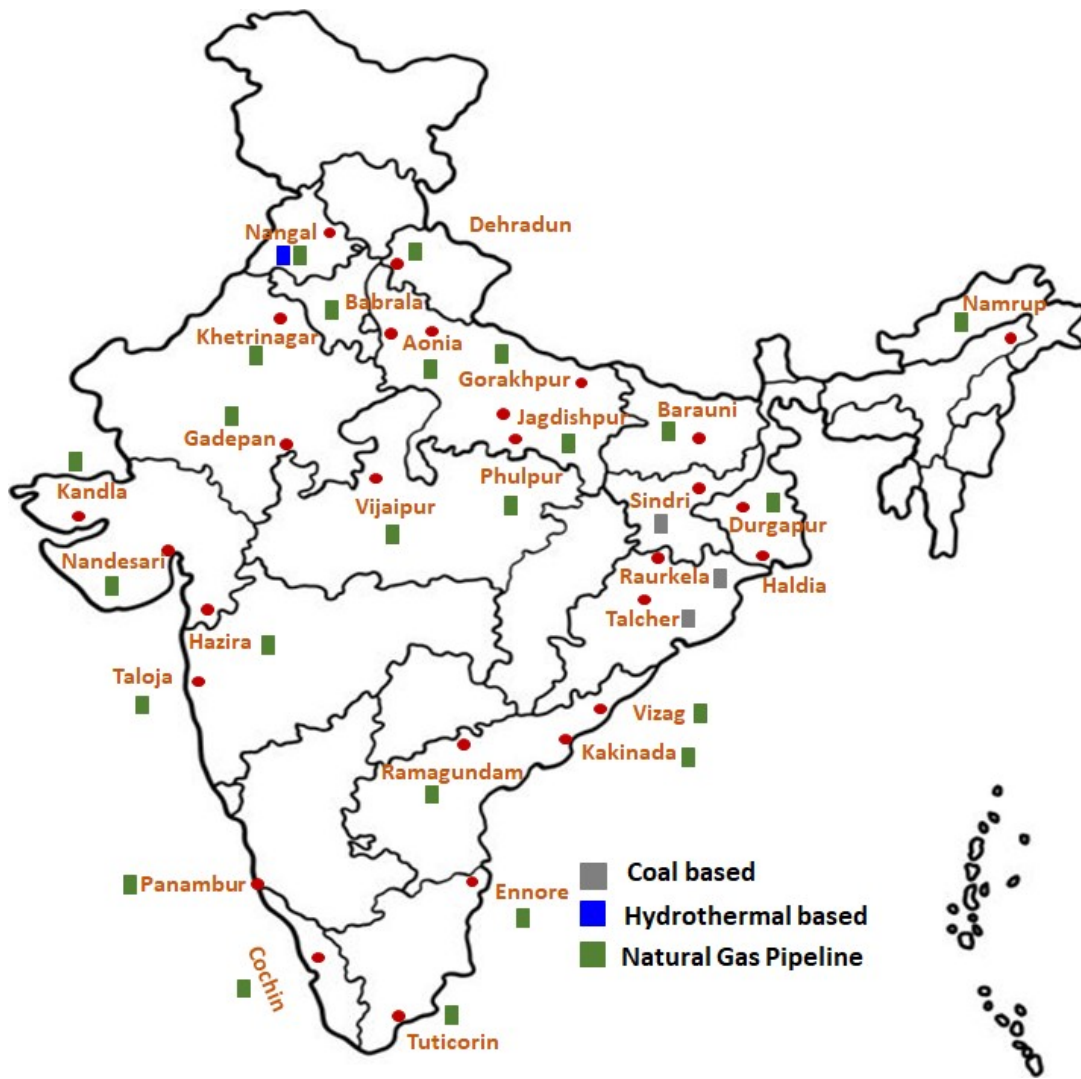


Fig.S8: Indian Map representing the ammonia plants working with natural gas and coal-based feedstock

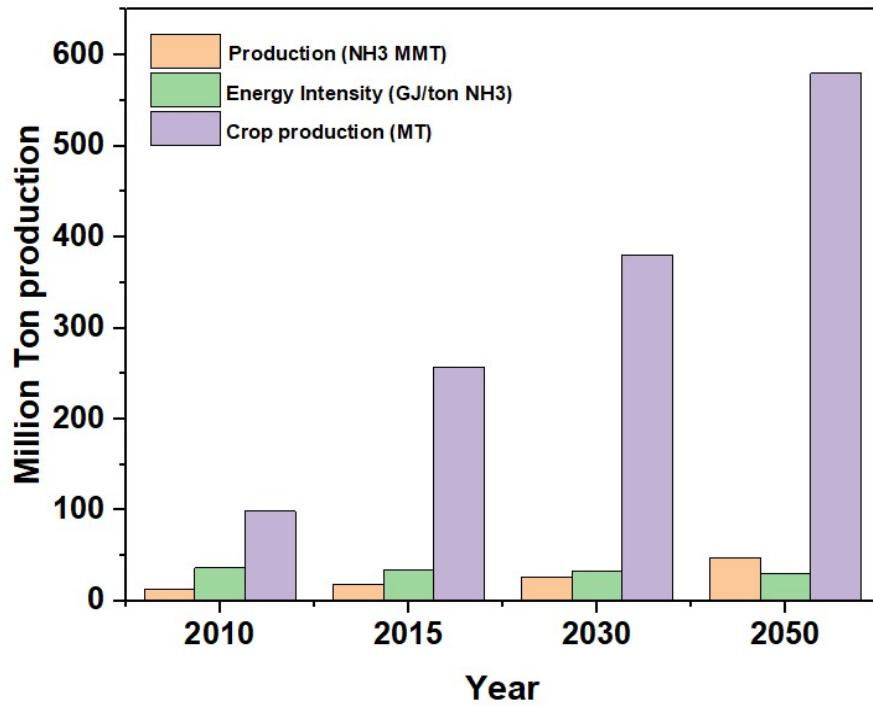


Fig S9: Co-relation of productivity, energy and crop production

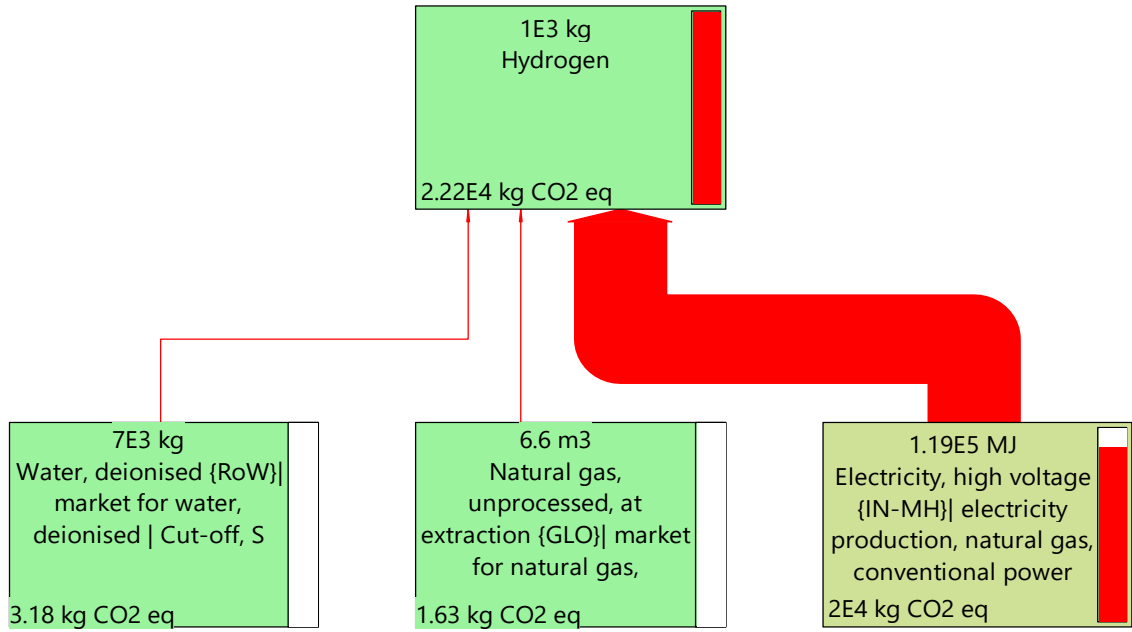


Fig S10: Sankey diagram for 1 ton Hydrogen production with SMR in BAU

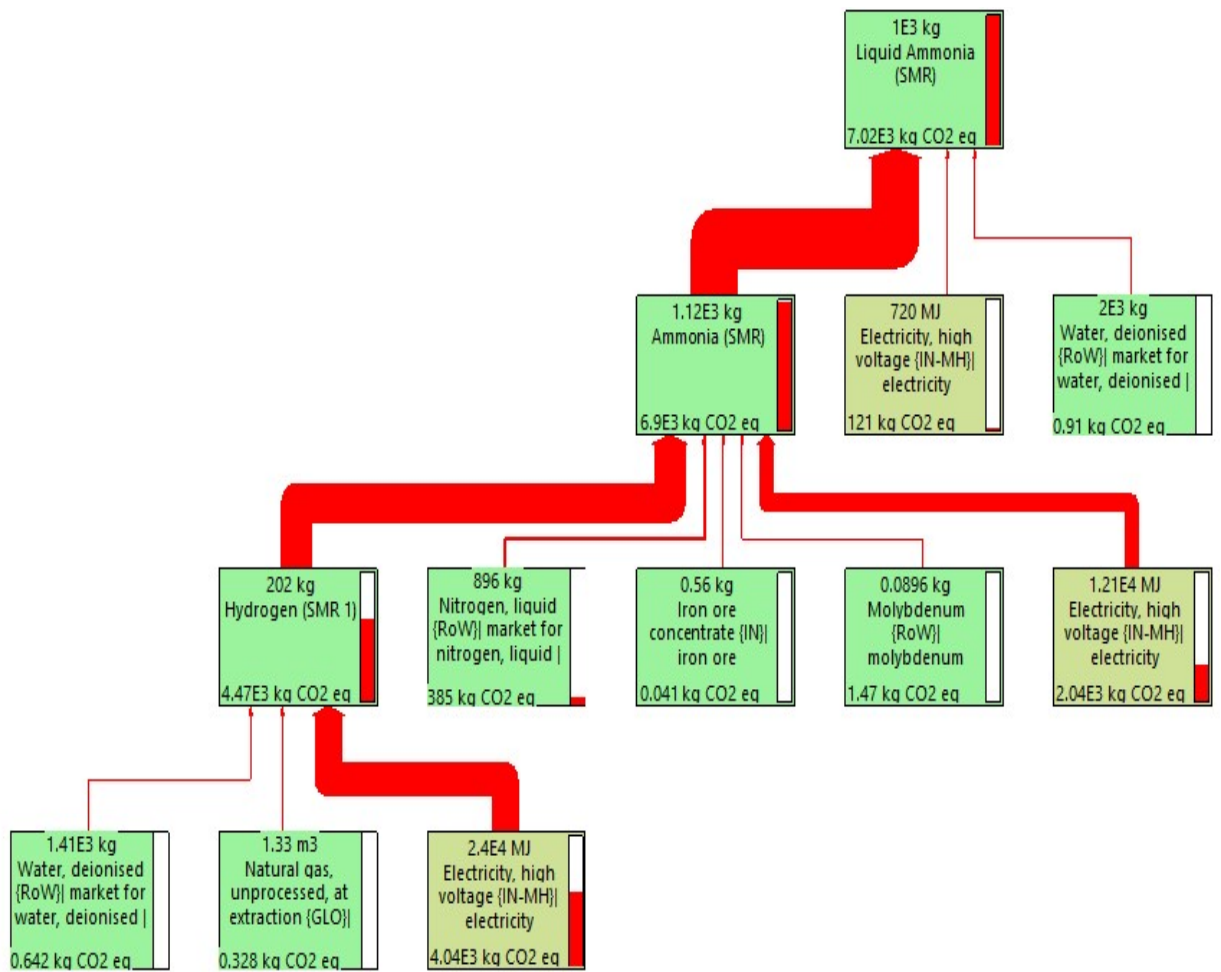


Fig. S11: Sankey diagram for 1 ton liquid ammonia production with SMR in BAU

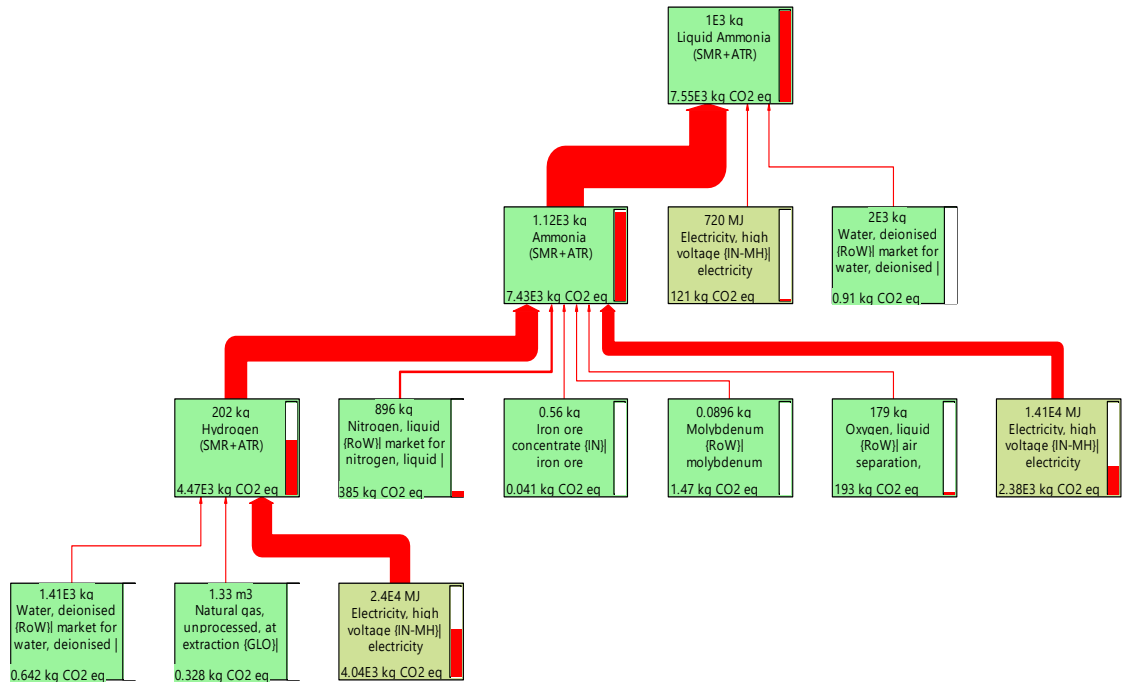


Fig. S12: Sankey diagram for 1 ton liquid ammonia production with SMR+ATR in BAU

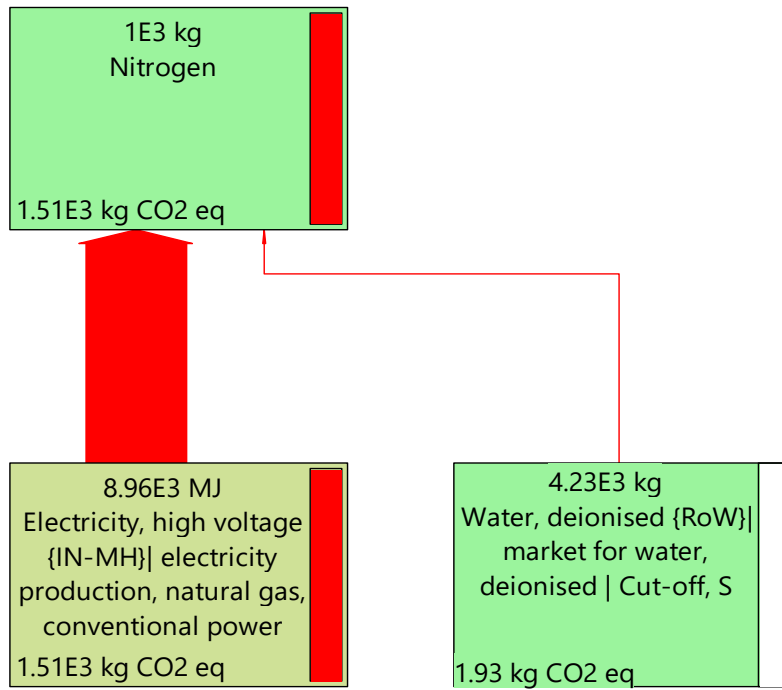


Fig. S13: Sankey diagram for 1 ton Nitrogen production for SMR/Air process

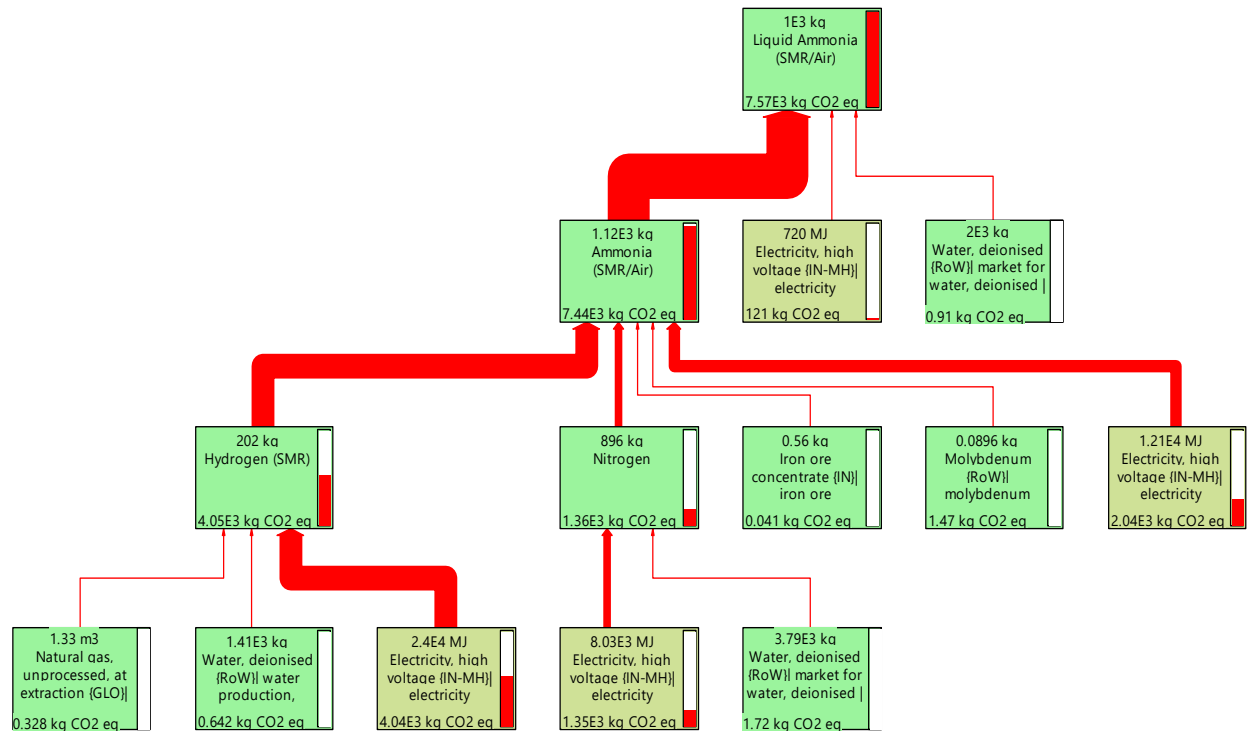


Fig. S14: Sankey diagram for 1 ton liquid ammonia production with SMR/Air in BAU

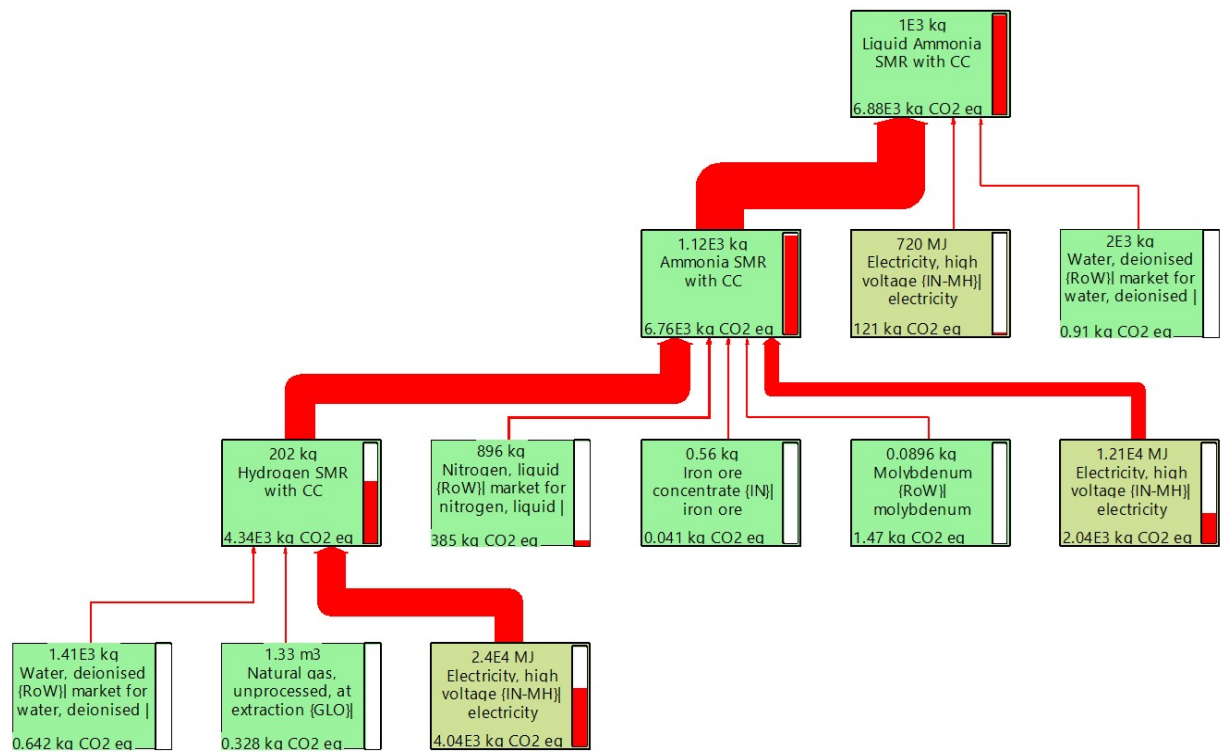


Fig. S15: Sankey diagram for 1 ton of liquid ammonia production with in situ CC in SMR (BAU)

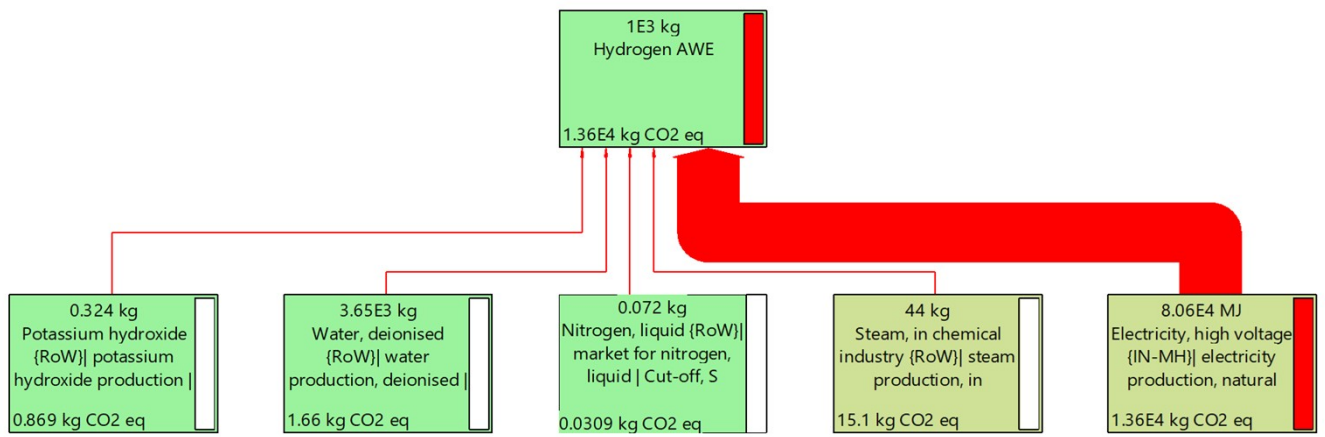


Fig. S16: Sankey diagram for 1 ton of hydrogen production with AWE

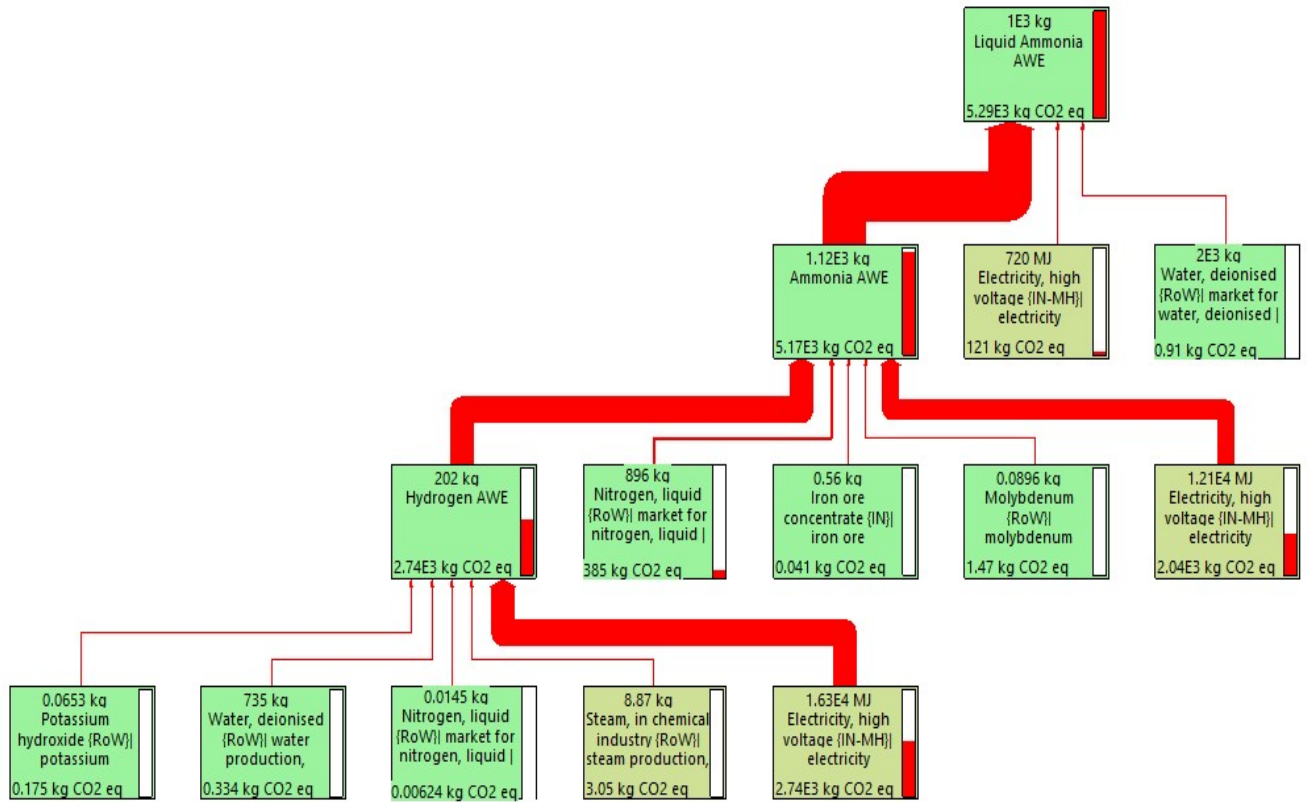


Fig. S17: Sankey diagram for 1 ton of liquid ammonia production with AWE

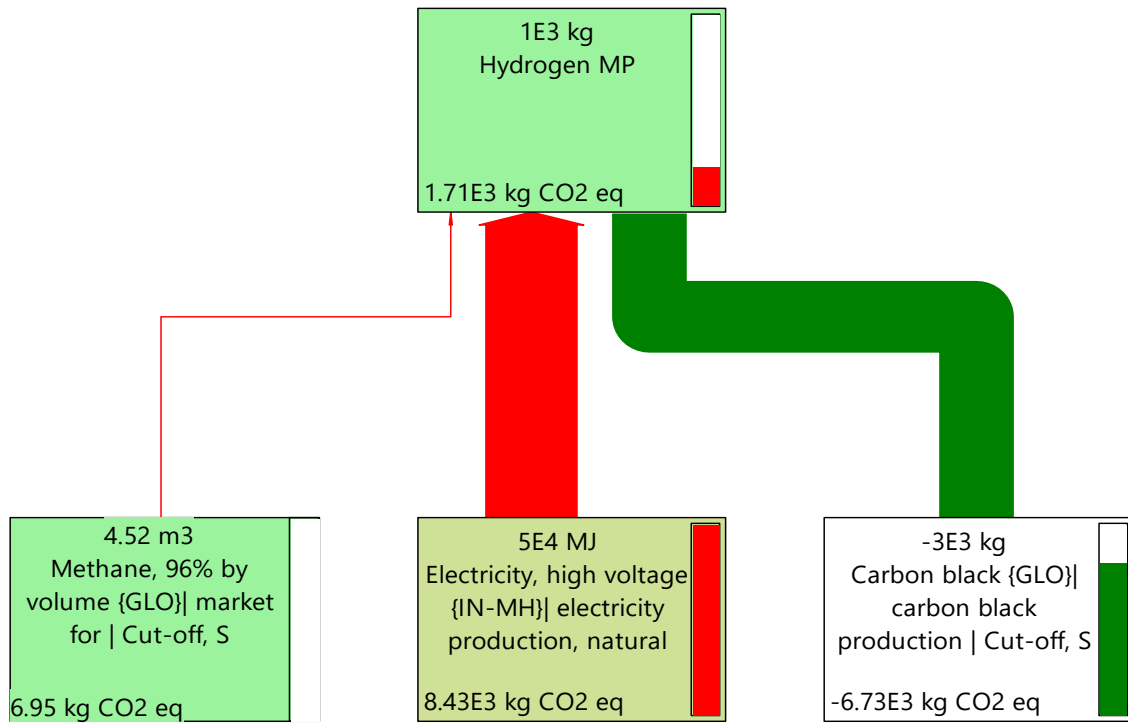


Fig. S18: Sankey diagram for Methane Pyrolysis for 1 ton Hydrogen production

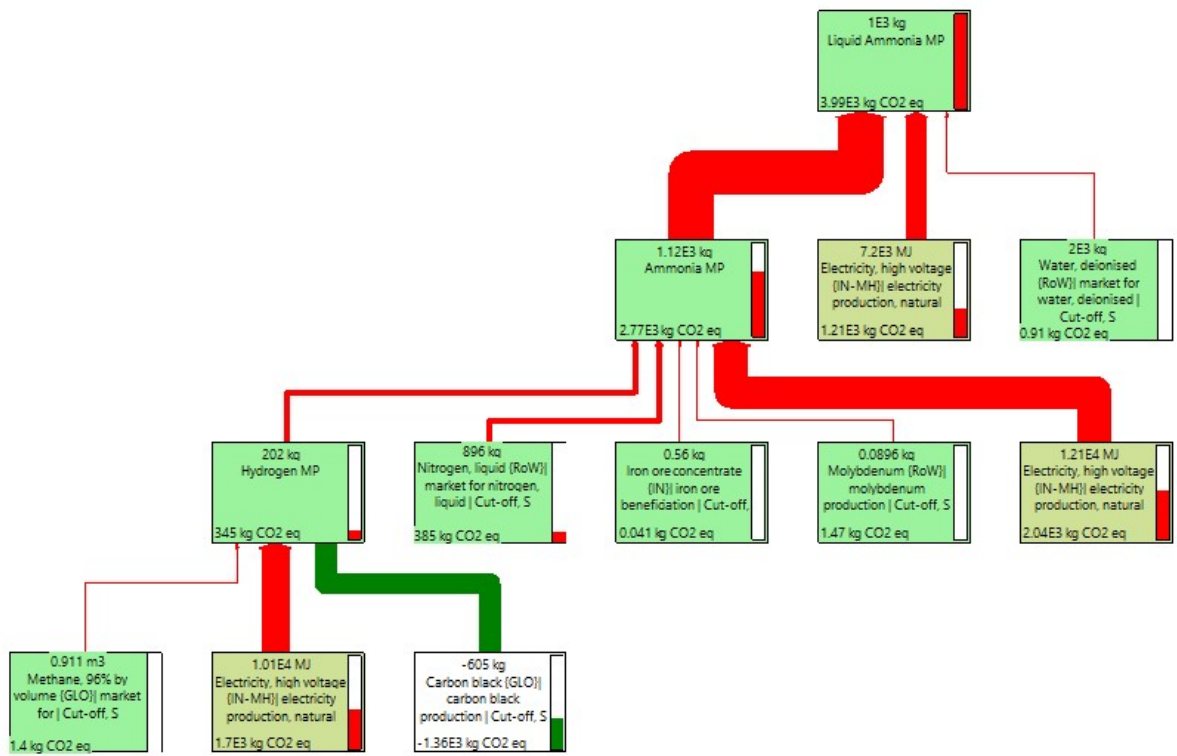


Fig. S19: Sankey for Methane Pyrolysis for 1 ton Liq. Ammonia production (BAU)

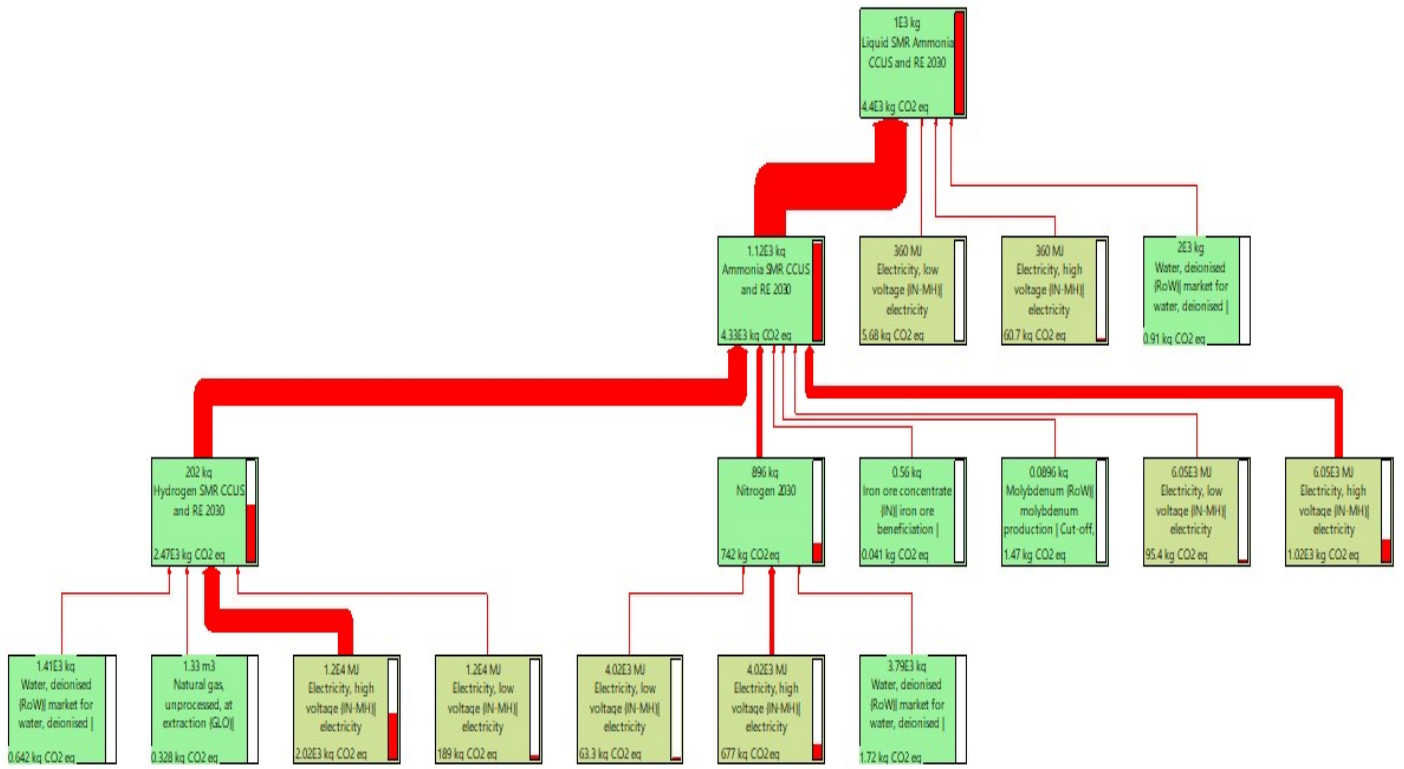


Fig. S20: Sankey for 1 ton Liq. Ammonia production with SMR (CC+RE) 2030

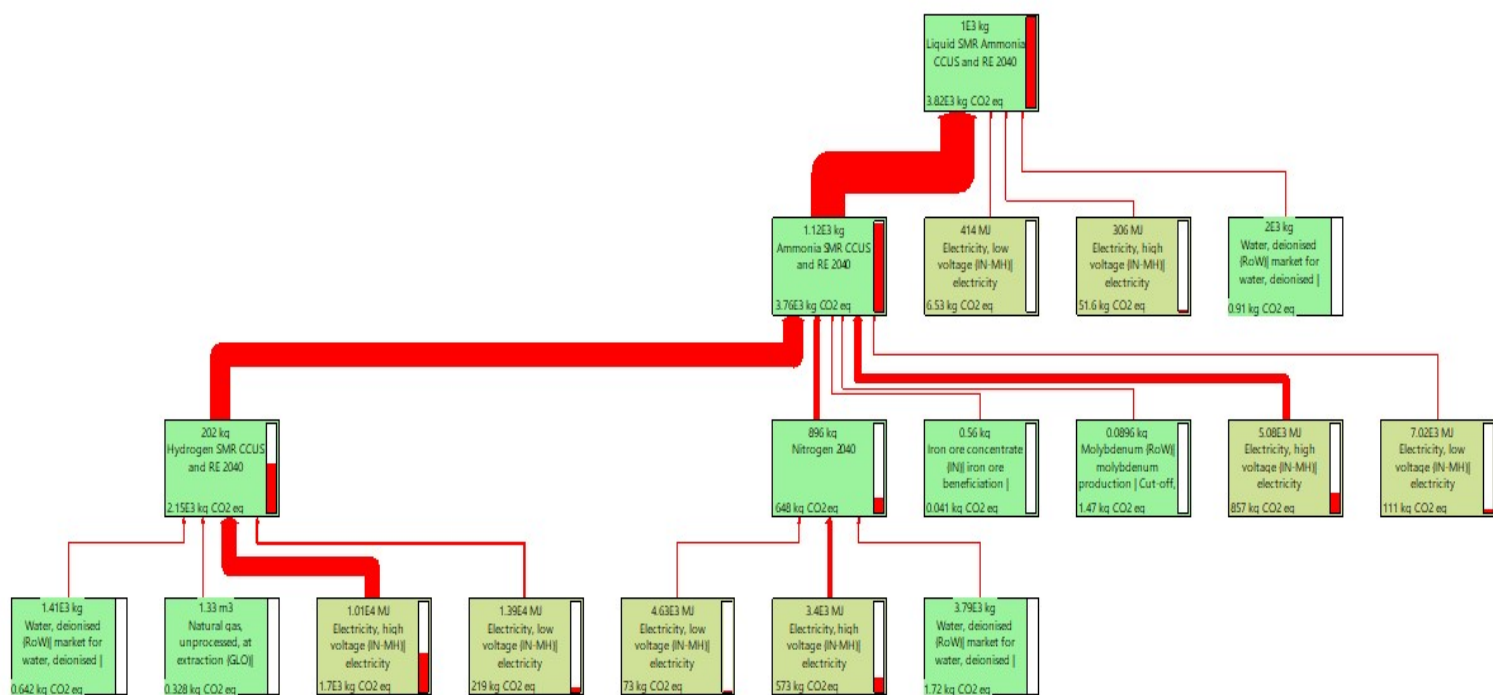


Fig. S21: Sankey for 1 ton Liq. Ammonia production with SMR (CC+RE) 2040

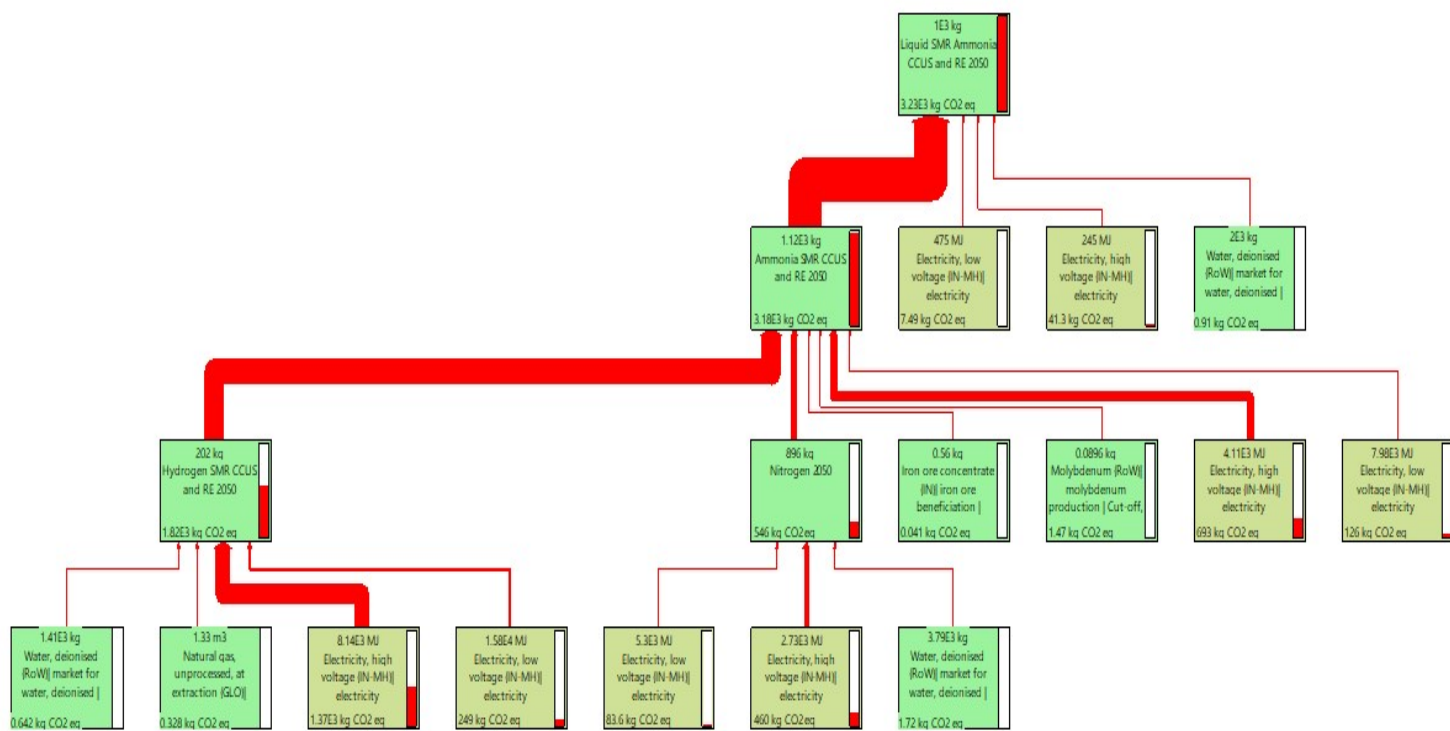


Fig. S22: Sankey for 1 ton Liq. Ammonia production with SMR (CC+RE) 2050

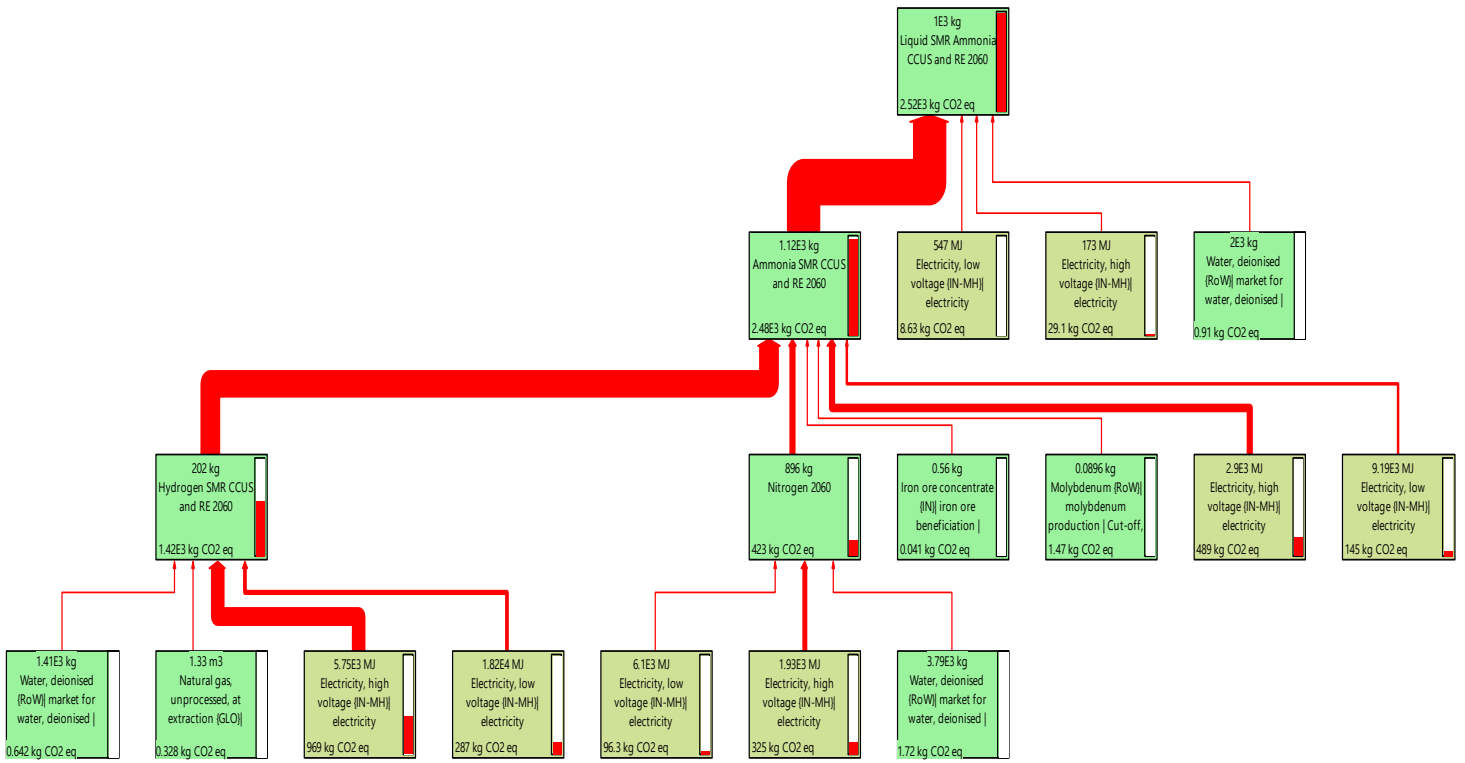


Fig. S23: Sankey for 1 ton Liq. Ammonia production with SMR (CC+RE) 2060

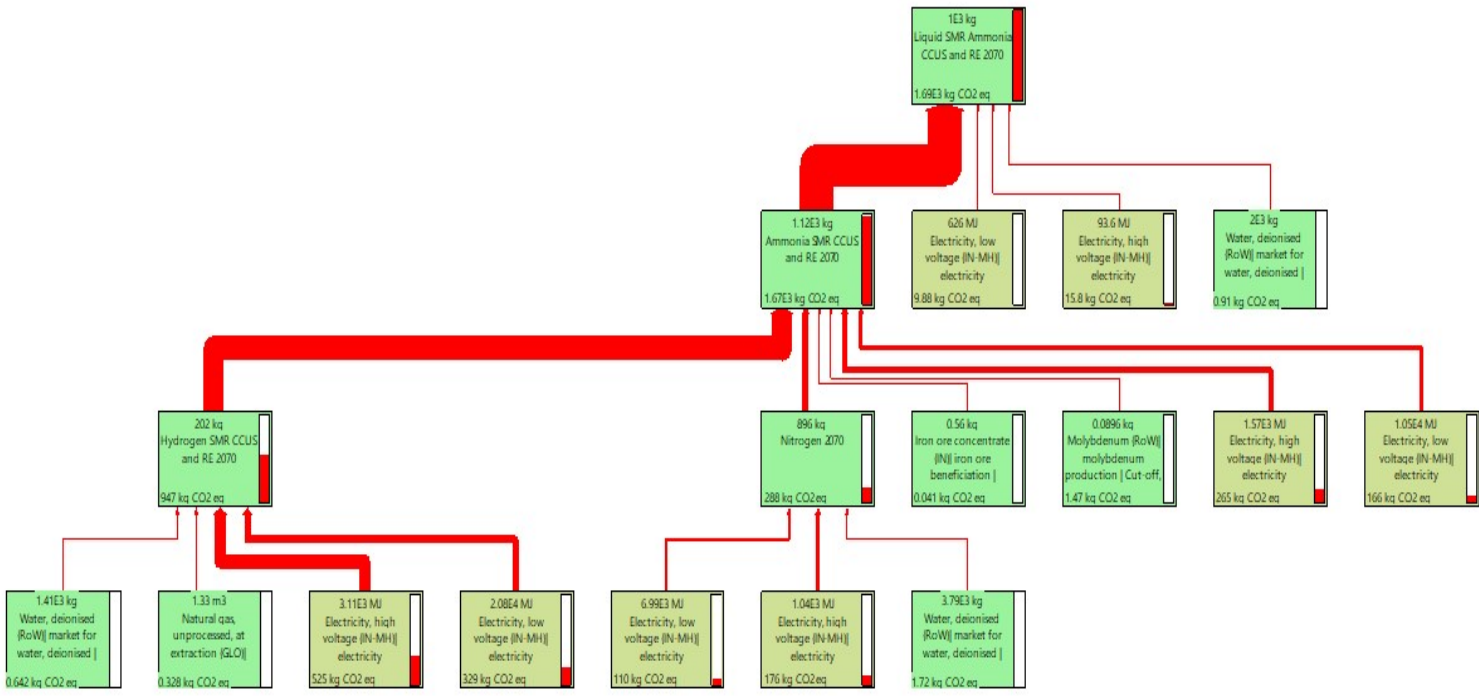


Fig. S24: Sankey for 1 ton Liq. Ammonia production with SMR (CC+RE) 2070

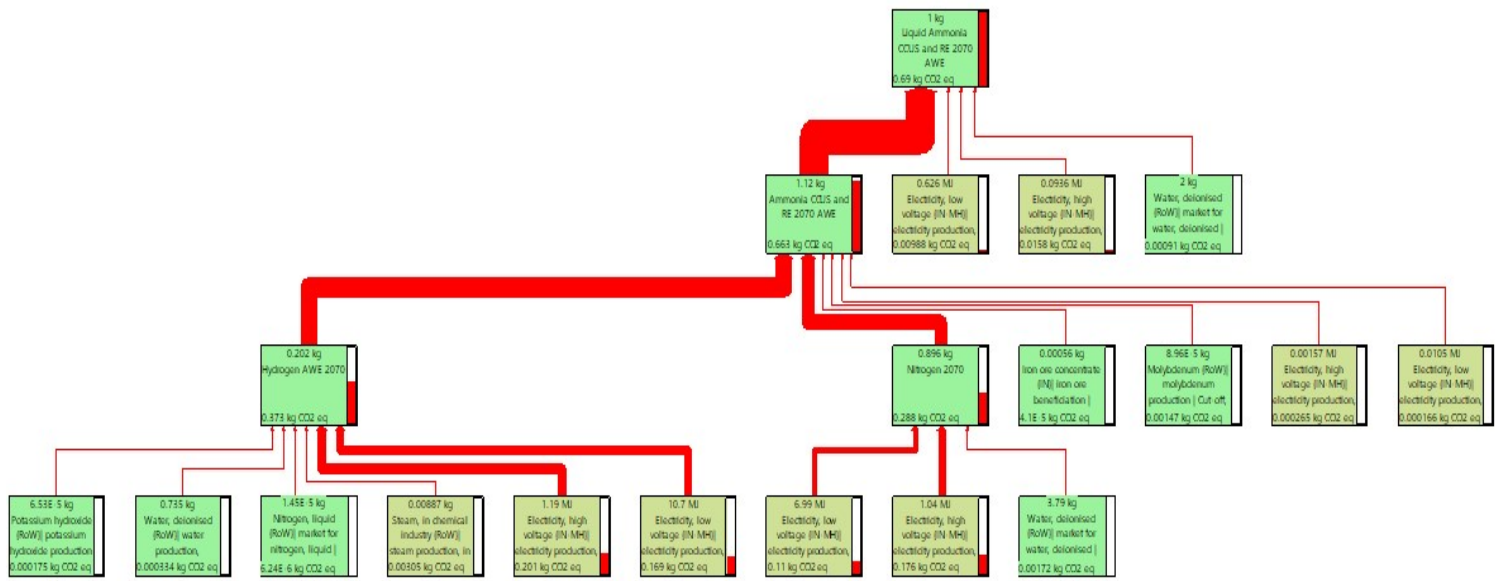


Fig. S25: Sankey for 1 ton Liq. Ammonia production with AWE, CC+RE 2070

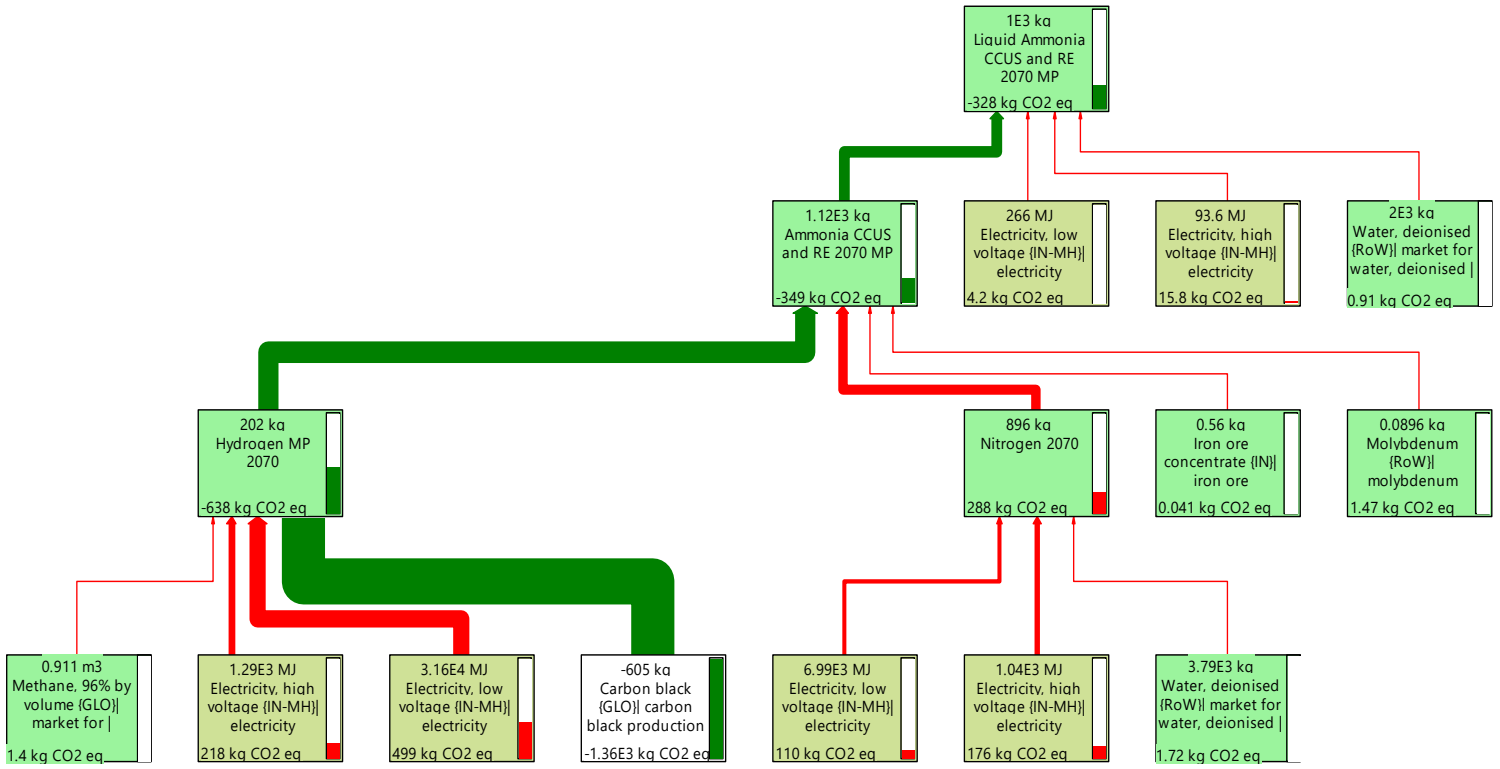


Fig. S26: Sankey for 1 ton Liq. Ammonia production with MP CC+RE 2070

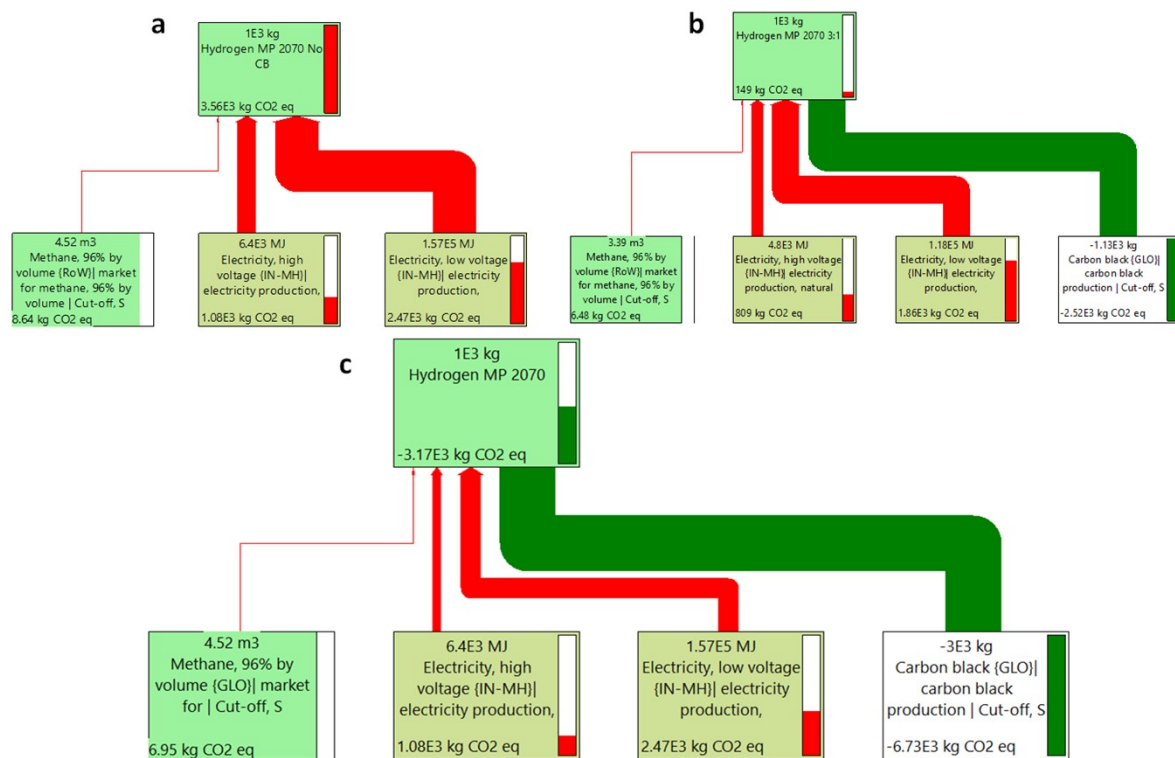


Fig. S27: Sankey for 1 ton Hydrogen production with MP 2070: a) with 0% carbon utilization; b) with 50% carbon utilization and c) 100 % carbon utilization.

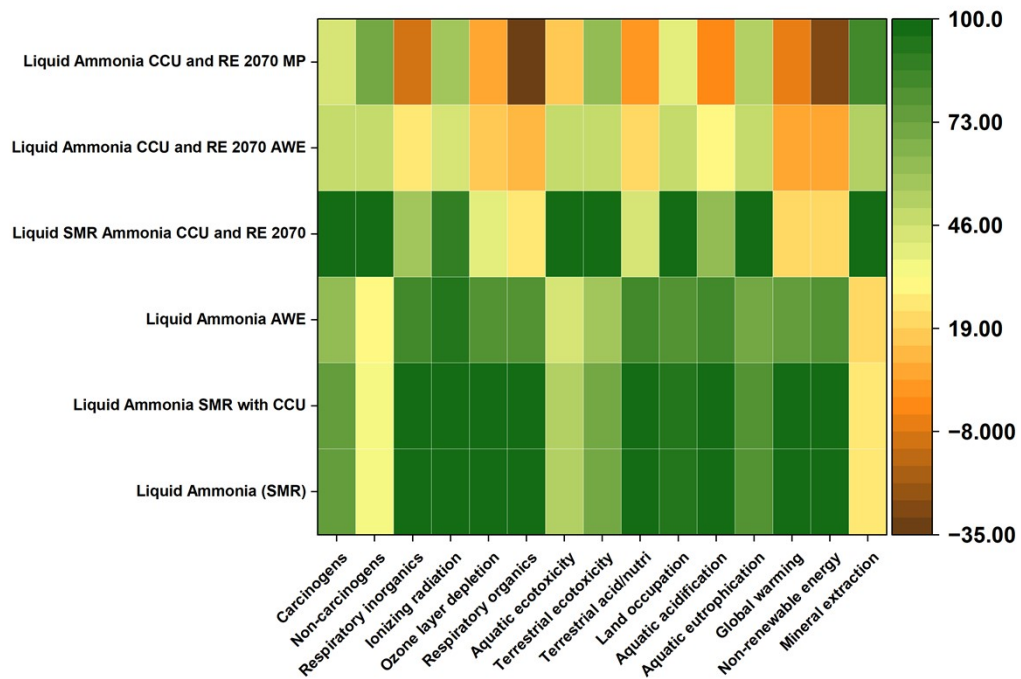


Fig. S28: Comparative midpoint impact assessment for 1 ton of liquid ammonia production under different technology scenarios, including conventional SMR, SMR with CCU, alkaline water electrolysis (AWE), and future decarbonization pathways integrating CCU and renewable energy (RE) by 2070. The heatmap illustrates the relative change in environmental impacts across midpoint categories using the IMPACT 2002+ method, where color intensity represents the percentage variation compared to the baseline SMR process. Positive values indicate higher impacts relative to the baseline, while negative values indicate impact reductions, highlighting the environmental benefits of integrating renewable hydrogen and CCU technologies.

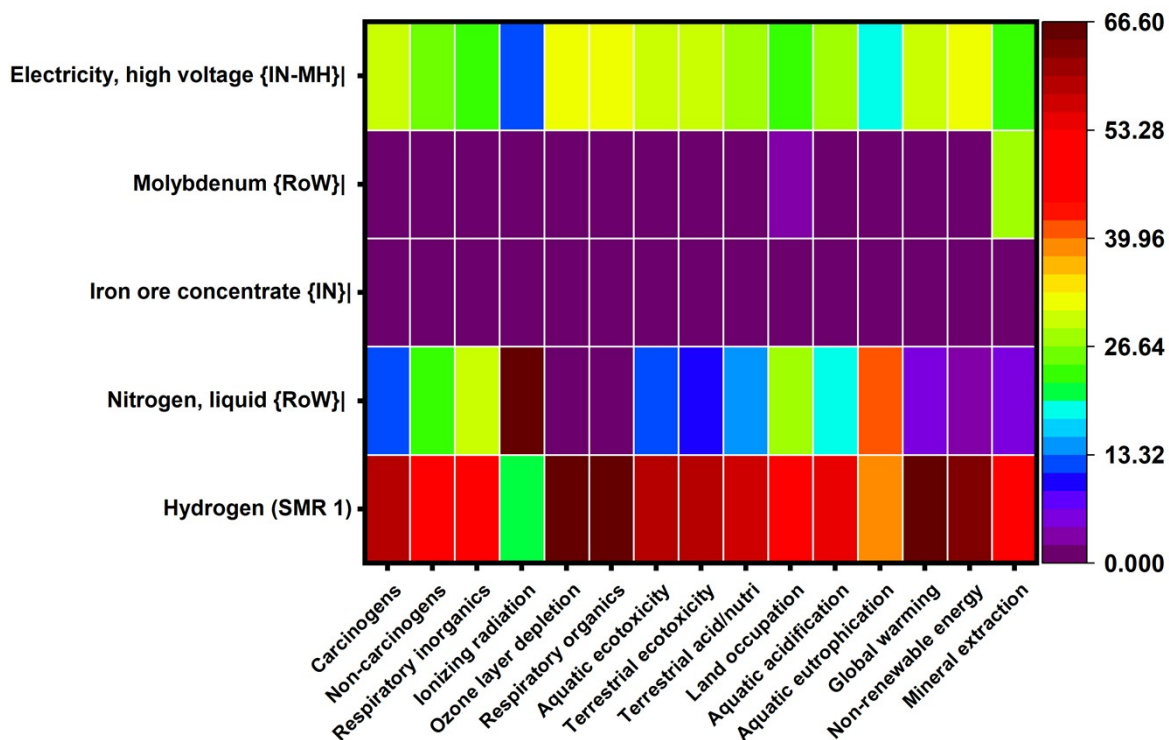


Fig. S29: Midpoint impact assessment for the production of 1 ton of liquid ammonia via SMR using the IMPACT 2002+ method. The heatmap shows the contribution of key inventory inputs (hydrogen from SMR, liquid nitrogen, electricity, iron ore concentrate, and molybdenum) across different environmental impact categories. The color scale represents the relative contribution of each input to the respective midpoint impact category, highlighting the dominant influence of SMR-derived hydrogen and electricity consumption on several environmental indicators.

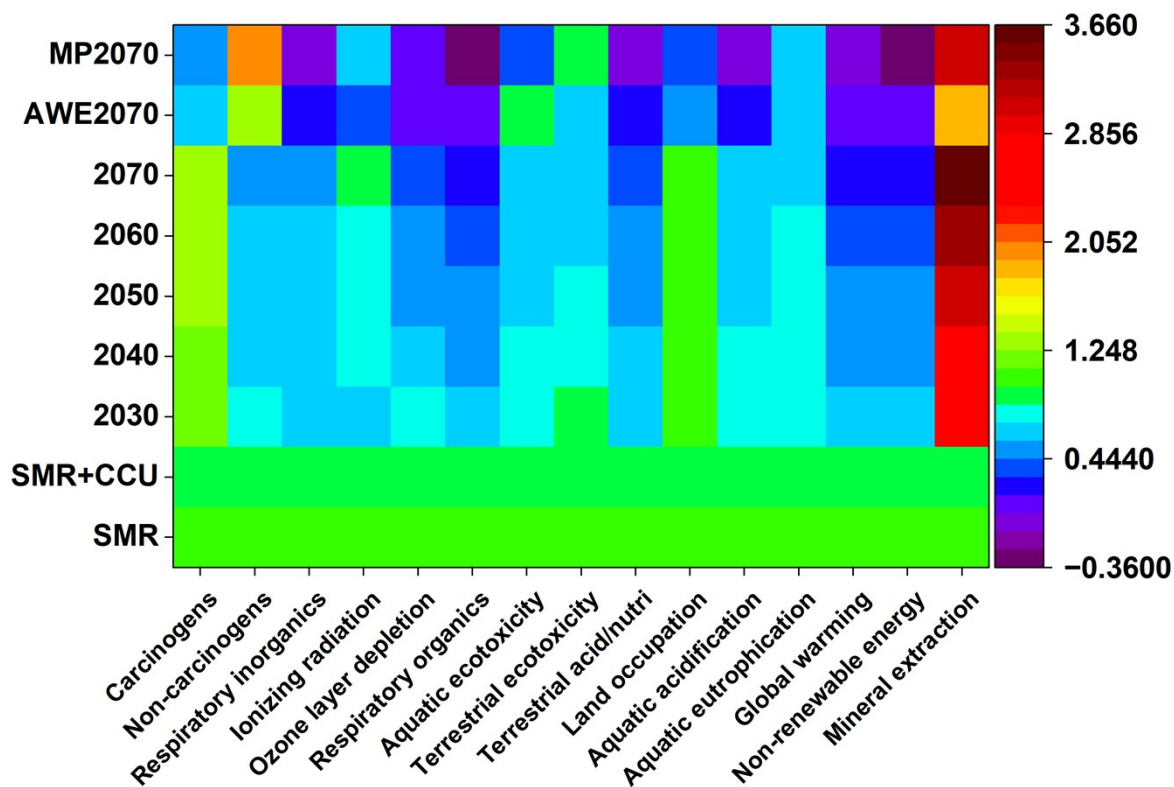


Fig. S30: Normalized midpoint impact assessment for 1 ton of liquid ammonia production across different technology scenarios, including conventional SMR (BAU), SMR with CCU, and future decarbonization pathways incorporating CCU and renewable energy integration for the years 2030-2070, as well as alkaline water electrolysis (AWE 2070) and methane pyrolysis (MP 2070). Environmental impacts were calculated using the IMPACT 2002+ method and normalized relative to the SMR baseline (SMR = 1). The heatmap illustrates the relative change in impact categories across scenarios, highlighting the progressive environmental benefits of integrating renewable electricity, CCU technologies, and alternative hydrogen production pathways.

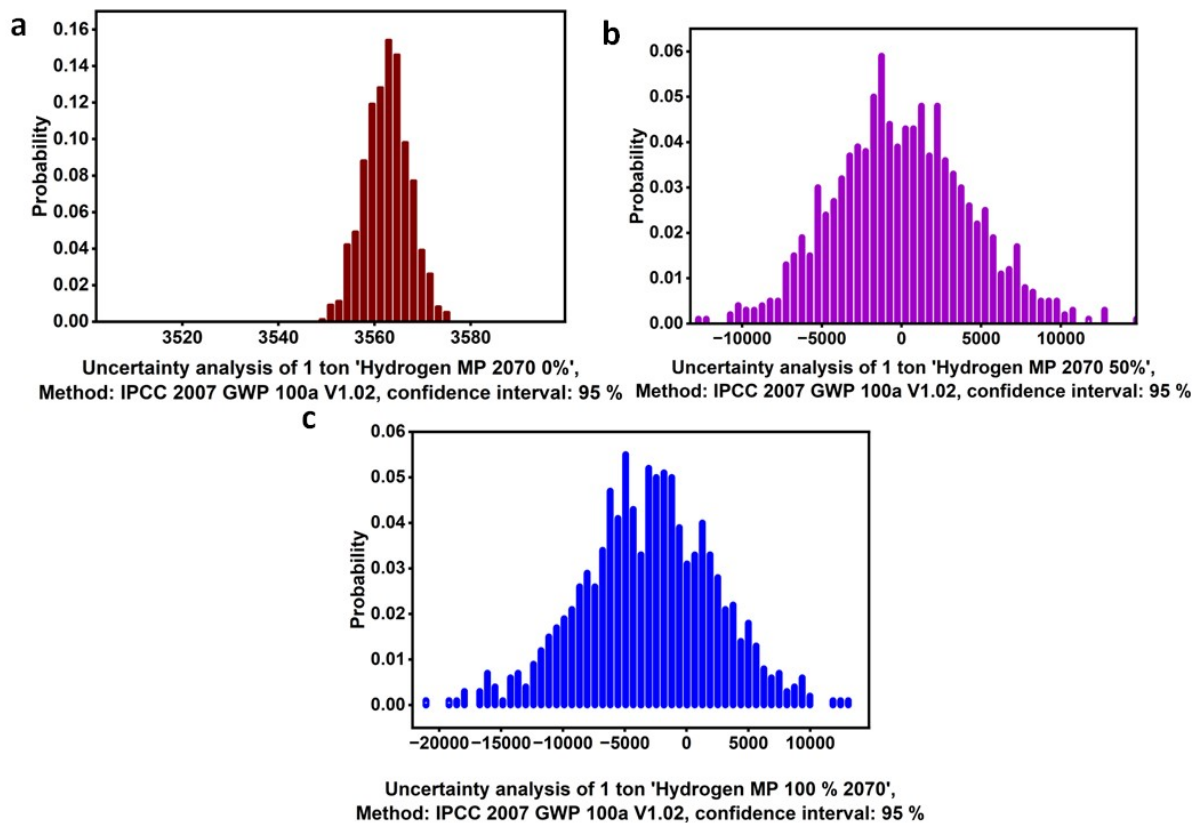


Fig. S31: The Monte Carlo uncertainty analysis (IPCC GWP 100a V1.02, 95% confidence interval, 1,000 iterations) was applied to all three methane pyrolysis co-product scenarios to evaluate the robustness of emission estimates under parameter variability: a), representing the 0% carbon utilization scenario, shows a narrow, symmetric distribution entirely within positive emission values (approximately 3,500-3,600 CO₂ eq. kg/ton H₂), indicating low sensitivity to input uncertainty when no co-product credit is applied. This narrow spread confirms that the process emissions of MP without any carbon credit are reliably positive and well-constrained; b), representing the 50% carbon utilization scenario, exhibits a markedly wider distribution spanning both negative and positive emission values (approximately -12,750 to +14,500 CO₂ eq. kg/ton H₂), reflecting the higher uncertainty introduced when a relatively small carbon credit is applied; c), representing the 100 % carbon utilization base case scenario, shows a distribution centred in negative territory (approximately -3,000 to -3,500 CO₂ eq. kg/ton H₂) with a spread of roughly -20,000 to +13,000 kg CO₂ eq/ton H₂. While the distribution is wide consistent with the broader uncertainty reported for emerging technology pathways the majority of the probability mass lies below zero, supporting the net-negative characterisation of this pathway.

Table S1: Inventory data for 1 ton of liq. ammonia production (SMR- BAU Scenario)

Stage 1: Hydrogen production

| Inputs | | Amount | Unit |
|---------------|-----------------|---------------|-------------|
| 1 | Water | 7 | Ton |
| 2. | Electricity | 33 | MWh |
| 3. | Natural gas | 3 (6.6 m3) | Ton |
| Output | | | |
| 1. | Hydrogen | 1 | Ton |
| 2. | Wastewater | 1 | Ton |
| 4. | CO ₂ | 1.7 | Ton |
| 5. | NO | 0.0058 | Ton |
| 6 | CO | 0.0048 | Ton |
| 7 | CH ₄ | 0.0183 | Ton |

Stage 2: Ammonia production (Haber-Bosch Process)

| Inputs | | Amount | Unit |
|---------------|----------------------|---------------|-------------|
| 1 | Stage 1 (Hydrogen) | 0.18 | Ton |
| 2 | Nitrogen | 0.8 | Ton |
| 3 | Iron | 0.5 | Kg |
| 4 | Molybdenum | 0.08 | Kg |
| 5 | Energy | 3 | MWh |
| Output | | | |
| 1. | Ammonia (gas) | 1 | Ton |
| 2. | waste stream | 40 | Kg |

Stage 3: Liquid ammonia production

| Inputs | | Amount | Unit |
|---------------|-----------------------|---------------|-------------|
| 1 | Water | 2 | Ton |
| 2. | Energy | 0.2 | MWh |
| Output | | | |
| 1. | NH₃ | 1 | Ton |

Table S2: Inventory data for 1 ton of liq. ammonia production (SMR+ATR- BAU Scenario)

Stage 1: Hydrogen production

| Inputs | | Amount | Unit |
|---------------|-----------------|------------|------------|
| 1 | Water | 7 | Ton |
| 2. | Electricity | 33 | MWh |
| 3. | Natural gas | 3 (6.6 m3) | Ton |
| Output | | | |
| 1. | Hydrogen | 1 | Ton |
| 2. | Wastewater | 1 | Ton |
| 4. | CO ₂ | 1.7 | Ton |
| 5. | NO | 0.0058 | Ton |
| 6 | CO | 0.0048 | Ton |
| 7 | CH ₄ | 0.0183 | Ton |

Stage 2: Ammonia production (Haber-Bosch Process)

| Inputs | | Amount | Unit |
|---------------|----------------------|----------|------------|
| 1 | Stage 1 (Hydrogen) | 0.18 | Ton |
| 2 | Nitrogen | 0.8 | Ton |
| 3 | Iron | 0.5 | Kg |
| 4 | Molybdenum | 0.08 | Kg |
| 5 | Energy | 3 | MWh |
| Output | | | |
| 1. | Ammonia (gas) | 1 | Ton |
| 2. | waste stream | 40 | Kg |

Stage 3: Liquid ammonia production

| Inputs | | Amount | Unit |
|---------------|-----------------------|----------|------------|
| 1 | Water | 2 | Ton |
| 2. | Energy | 0.2 | MWh |
| Output | | | |
| 1. | NH₃ | 1 | Ton |

Table S3: Inventory data for 1 ton of liq. ammonia production (SMR+ATR- BAU Scenario)

Stage 1: Hydrogen Production

| Inputs | | Amount | Unit |
|---------------|-----------------|------------|------------|
| 1 | Water | 7 | Ton |
| 2. | Electricity | 33 | MWh |
| 3. | Natural gas | 3 (6.6 m3) | Ton |
| Output | | | |
| 1. | Hydrogen | 1 | Ton |
| 2. | Wastewater | 1 | Ton |
| 4. | CO ₂ | 1.7 | Ton |
| 5. | NO | 0.0058 | Ton |
| 6 | CO | 0.0048 | Ton |
| 7 | CH ₄ | 0.0183 | Ton |

Stage 2: Nitrogen Production

| Inputs | | Amount | Unit |
|---------------|-----------------|----------|------------|
| 1 | Water | 5.1 | Ton |
| 2. | Energy | 3 | MWh |
| 3. | Air | 3.5 | Ton |
| Output | | | |
| 1. | Nitrogen | 1 | Ton |
| 3. | O ₂ | 0.4 | Ton |

Stage 3: Ammonia production (Haber-Bosch Process)

| Inputs | | Amount | Unit |
|---------------|----------------------|----------|------------|
| 1 | Stage 1 (Hydrogen) | 0.18 | Ton |
| 2 | Stage 2 (Nitrogen) | 0.8 | Ton |
| 3 | Iron | 0.5 | Kg |
| 4 | Molybdenum | 0.08 | Kg |
| 5 | Energy | 3 | MWh |
| Output | | | |
| 1. | Ammonia (gas) | 1 | Ton |
| 2. | waste stream | 40 | Kg |

Stage 4: Liquid ammonia production

| Inputs | | Amount | Unit |
|---------------|--------|--------|------|
| 1 | Water | 2 | Ton |
| 2. | Energy | 0.2 | MWh |
| Output | | | |

| | | | |
|-----------|-----------------------|----------|------------|
| 1. | NH₃ | 1 | Ton |
|-----------|-----------------------|----------|------------|

Table S4: Inventory data for Alkaline Water Electrolysis

| Inputs | | Amount | Unit |
|---------------|-----------------|---------------|-------------|
| 1 | Electricity | 56 | KWh |
| 2. | KOH | 0.81 | g |
| 3. | Distilled water | 9.12 | Kg |
| 4. | Nitrogen | 0.18 | g |
| 5. | Steam | 0.11 | Kg |
| Output | | | |
| 1. | Hydrogen | 1 | Kg |
| 2. | Oxygen | 8.12 | Kg |

Table S5: Methane Pyrolysis Inventory Data

| Inputs | | Amount | Unit |
|---------------|-----------------|---------------|-------------|
| 1 | Methane | 4 | Ton |
| 2. | Energy | 50000 | MJ |
| Output | | | |
| 1. | Hydrogen | 1 | Ton |
| 2. | Carbon | 3 | Ton |

Table S6: List of ammonia plants with location and production capacity

| Sl. No. | Plants | Capacity | Plant Location |
|---------|---|--|-----------------------------|
| 1 | Nagarjuna Fertilisers & Chemicals Ltd., Kakinada | 2000 MTPD | Kakinada, Andhra Pradesh |
| 2 | MATIX Fertilisers & Chemicals Ltd., Kolkata | 2200 MTPD Ammonia Plant | Panagarh, West Bengal |
| 3 | MATIX Fertilisers & Chemicals Ltd., Kolkata | Ammonia-Urea plant | Panagarh, West Bengal |
| 4 | Nagarjuna Fertilisers & Chemicals Ltd., Kakinada | 900 MTPD Ammonia and 1500 MTPD Urea Plant | Kakinada, Andhra Pradesh |
| 5 | National Fertilisers Ltd., Vijaipur | Ammonia Plant, 2 x 1100 MTPD Urea Plant | Vijaipur, Madhya Pradesh |
| 6 | Indian Farmers Fertilisers Cooperatives Ltd., Phulpur | 1350 MTPD Ammonia Plant, 2 x 1100 MTPD Urea Plant | Phulpur, Uttar Pradesh |
| 7 | Indian Farmers Fertilisers Cooperatives Ltd., Aonla | 1350 MTPD Ammonia Plant and 2 x 1100 MTPD Urea Plant | Aonla, Uttar Pradesh |
| 8 | Oswal Chemicals & Fertilisers Ltd., Shahjahanpur | 1350 MTPD Ammonia Plant and 2 x 1120 MTPD Urea Plant | Shahjahanpur, Uttar Pradesh |
| 9 | Chambal Fertilisers & Chemicals Ltd., Gadepan | 1350 MTPD Ammonia Plant and 2 x 1125 MTPD Urea Plant | Gadepan, Rajasthan |
| 10 | Tata Chemicals Ltd., Babrala | 1350 MTPD Ammonia Plant and 2 x 1125 MTPD Urea Plant | Babrala, Uttar Pradesh |
| 11 | Hindustan Fertiliser Corporation Ltd., Durgapur | 600 MTPD Ammonia Plant, 1000 MTPD Urea Plant | Durgapur, West Bengal |
| 12 | Fertilisers and Chemicals Travancore Ltd., Kerala | 600 MTPD Ammonia Plant, 1000 MTPD Urea | Cochin, Kerala |
| 13 | National Fertilisers Ltd., Nangal | 900 MTPD Ammonia Plant, 1000 MTPD Urea Plant | Nangal, Punjab |
| 14 | Hindustan Fertilisers Corporation Ltd., Namrup | 600 MTPD Ammonia Plant, 1000 MTPD Urea Plant | Namrup, Assam |
| 15 | Hindustan Fertilisers Corporation Ltd., Barauni | 600 MTPD Ammonia Plant, 1000 MTPD Urea Plant | Barauni, Bihar |
| 16 | Fertilizer Corporation of India, Gorakhpur | Ammonia Plant from 340 MTPD to 570 MTPD and Urea Plant from 570 MTPD to 950 MTPD | Gorakhpur, Uttar Pradesh |
| 17 | Krishak Bharti Cooperatives Ltd., Hazira | 768 MTPD Ammonia Synthesis Unit | Hazira, Gujarat |

| | | | |
|----|---|---|----------------------------|
| 18 | Nagarjuna Fertilisers & Chemicals Ltd., Kakinada | 900 MTPD Ammonia Plant and 1500 MTPD Urea Plant | Kakinada, Andhra Pradesh |
| 19 | Rashtriya Chemicals & Fertilisers Ltd., Mumbai | 350 MTPD | Trombay, Maharashtra |
| 20 | National Fertilisers Ltd., Vijaipur | 1350 MTPD Ammonia Plant, 2 x 1100 MTPD Urea Plant | Vijaipur, Madhya Pradesh |
| 21 | Indian Farmers Fertilisers Cooperatives Ltd., Aonla | 1350 MTPD Ammonia Plant and 2 x 1100 MTPD Urea Plant | Aonla, Uttar Pradesh |
| 22 | Hindustan Fertilizer Corporation Ltd., Namrup | 600 MTPD Ammonia Plant, 1167 MTPD Urea Plant | Namrup, Assam |
| 23 | Indo Gulf Corporation Ltd., Jagdishpur | 1350 MTPD Ammonia Plant, 2 x 1100 MTPD Urea Plant | Jagdishpur, Uttar Pradesh |
| 24 | Rashtriya Chemicals & Fertilisers Ltd., Mumbai | 768 MTPD Ammonia Synthesis Unit | Thal Vaishet, Maharashtra |
| 25 | Rashtriya Chemicals & Fertilisers Ltd., Mumbai | 2 x 1350 MTPD Ammonia Plants, 3 x 1500 MTPD Urea Plants | Thal Vaishet, Maharashtra |
| 26 | Krishak Bharti Cooperatives Ltd., Hazira | 4 x 1100 MTPD Urea Plants | Hazira, Gujarat |
| 27 | Hindustan Fertilizer Corporation Ltd., Haldia | 600 MTPD Ammonia Plant, 500 MTPD Urea Plant, 400 MTPD Ammonium Sulphate Plant, 1600 MTPD NPK Plant, 100 MTPD Phosphoric Acid Plant, 475 MTPD Nitric Acid Plant, 200 MTPD Soda Ash Plant, 125 MTPD Methanol Plant, 240 MTPD Sulphuric Acid Plant | Haldia, West Bengal |
| 28 | Rashtriya Chemicals & Fertilisers Ltd., Mumbai | 900 MTPD Ammonia Plant, 1000 MTPD Urea Plant | Trombay, Maharashtra |
| 29 | Fertilizer Corporation of India, Talcher | 900 MTPD Ammonia Plant, 1500 MTPD Urea Plant | Talcher, Orissa |
| 30 | Fertilizer Corporation of India, Ramagundam | 900 MTPD Ammonia Plant, 1500 MTPD Urea Plant | Ramagundam, Andhra Pradesh |
| 31 | Fertilizer Corporation of India, Sindri | 900 MTPD Ammonia Plant, 1000 MTPD Urea Plant | Sindri, Bihar |

Table S7: Annual and Decadal CO₂ Emissions (2020-2070)

| Year | Ammonia Production (MMT NH₃/yr) | BAU-SMR Annual (MMT CO₂/yr) | BAU-SMR Running Cumulative (MMT CO₂) | BAU-SMR+ATR Annual (MMT CO₂/yr) | BAU-SMR+ATR Running Cumulative (MMT CO₂) | SMR/Air Annual (MMT CO₂/yr) | SMR/Air Running Cumulative (MMT CO₂) | Decade |
|-------------|---|---|--|---|--|---|--|---------------|
| 2020 | 14.7 | 103.0 | 103.0 | 110.8 | 110.8 | 111.1 | 111.1 | 2020–2029 |
| 2021 | 14.8 | 103.6 | 206.6 | 111.4 | 222.2 | 111.7 | 222.8 | 2020–2029 |
| 2022 | 15.8 | 111.1 | 317.7 | 119.4 | 341.6 | 119.8 | 342.5 | 2020–2029 |
| 2023 | 16.4 | 114.8 | 432.4 | 123.4 | 465.1 | 123.8 | 466.3 | 2020–2029 |
| 2024 | 16.9 | 118.6 | 551.1 | 127.6 | 592.7 | 127.9 | 594.3 | 2020–2029 |
| 2025 | 17.5 | 122.6 | 673.7 | 131.9 | 724.6 | 132.2 | 726.5 | 2020–2029 |
| 2026 | 18.1 | 126.7 | 800.4 | 136.3 | 860.9 | 136.6 | 863.1 | 2020–2029 |
| 2027 | 18.7 | 131.0 | 931.4 | 140.9 | 1,001.7 | 141.3 | 1,004.4 | 2020–2029 |
| 2028 | 19.3 | 135.3 | 1,066.8 | 145.6 | 1,147.3 | 145.9 | 1,150.3 | 2020–2029 |
| 2029 | 19.9 | 139.9 | 1,206.7 | 150.5 | 1,297.8 | 150.9 | 1,301.2 | 2020–2029 |
| 2030 | 20.6 | 144.5 | 1,351.2 | 155.5 | 1,453.2 | 155.9 | 1,457.1 | 2030–2039 |
| 2031 | 21.3 | 149.4 | 1,500.6 | 160.7 | 1,613.9 | 161.1 | 1,618.2 | 2030–2039 |
| 2032 | 22.0 | 154.4 | 1,655.0 | 166.1 | 1,780.0 | 166.5 | 1,784.7 | 2030–2039 |
| 2033 | 22.7 | 159.6 | 1,814.6 | 171.6 | 1,951.6 | 172.1 | 1,956.8 | 2030–2039 |
| 2034 | 23.5 | 165.0 | 1,979.6 | 177.4 | 2,129.0 | 177.9 | 2,134.7 | 2030–2039 |
| 2035 | 24.3 | 170.4 | 2,150.0 | 183.3 | 2,312.3 | 183.8 | 2,318.5 | 2030–2039 |
| 2036 | 25.1 | 176.2 | 2,326.2 | 189.5 | 2,501.8 | 190.0 | 2,508.5 | 2030–2039 |
| 2037 | 25.9 | 182.1 | 2,508.3 | 195.8 | 2,697.7 | 196.4 | 2,704.8 | 2030–2039 |
| 2038 | 26.8 | 188.2 | 2,696.5 | 202.4 | 2,900.1 | 203.0 | 2,907.8 | 2030–2039 |
| 2039 | 27.7 | 194.5 | 2,891.1 | 209.2 | 3,109.3 | 209.8 | 3,117.6 | 2030–2039 |
| 2040 | 28.6 | 201.0 | 3,092.0 | 216.2 | 3,325.5 | 216.7 | 3,334.3 | 2040–2049 |
| 2041 | 29.6 | 207.7 | 3,299.8 | 223.4 | 3,548.9 | 224.0 | 3,558.3 | 2040–2049 |
| 2042 | 30.6 | 214.7 | 3,514.4 | 230.9 | 3,779.8 | 231.5 | 3,789.8 | 2040–2049 |
| 2043 | 31.6 | 221.9 | 3,736.3 | 238.7 | 4,018.4 | 239.3 | 4,029.1 | 2040–2049 |

| | | | | | | | | |
|------|------|-------|----------|-------|----------|-------|----------|-----------|
| 2044 | 32.7 | 229.3 | 3,965.7 | 246.7 | 4,265.1 | 247.3 | 4,276.4 | 2040–2049 |
| 2045 | 33.8 | 237.0 | 4,202.7 | 254.9 | 4,520.0 | 255.6 | 4,531.9 | 2040–2049 |
| 2046 | 34.9 | 244.9 | 4,447.6 | 263.4 | 4,783.4 | 264.1 | 4,796.1 | 2040–2049 |
| 2047 | 36.1 | 253.1 | 4,700.7 | 272.3 | 5,055.6 | 273.0 | 5,069.0 | 2040–2049 |
| 2048 | 37.3 | 261.6 | 4,962.4 | 281.4 | 5,337.0 | 282.1 | 5,351.2 | 2040–2049 |
| 2049 | 38.5 | 270.4 | 5,232.8 | 290.8 | 5,627.9 | 291.6 | 5,642.8 | 2040–2049 |
| 2050 | 39.8 | 279.5 | 5,512.2 | 300.6 | 5,928.4 | 301.4 | 5,944.1 | 2050–2059 |
| 2051 | 41.1 | 288.8 | 5,801.1 | 310.6 | 6,239.0 | 311.4 | 6,255.6 | 2050–2059 |
| 2052 | 42.5 | 298.5 | 6,099.5 | 321.0 | 6,560.0 | 321.9 | 6,577.4 | 2050–2059 |
| 2053 | 44.0 | 308.5 | 6,408.1 | 331.8 | 6,891.9 | 332.7 | 6,910.1 | 2050–2059 |
| 2054 | 45.4 | 318.8 | 6,726.9 | 342.9 | 7,234.8 | 343.8 | 7,254.0 | 2050–2059 |
| 2055 | 46.9 | 329.5 | 7,056.4 | 354.4 | 7,589.2 | 355.3 | 7,609.3 | 2050–2059 |
| 2056 | 48.5 | 340.5 | 7,397.0 | 366.3 | 7,955.4 | 367.2 | 7,976.5 | 2050–2059 |
| 2057 | 50.1 | 352.0 | 7,749.0 | 378.6 | 8,334.0 | 379.6 | 8,356.1 | 2050–2059 |
| 2058 | 51.8 | 363.8 | 8,112.7 | 391.2 | 8,725.2 | 392.3 | 8,748.4 | 2050–2059 |
| 2059 | 53.6 | 376.0 | 8,488.7 | 404.4 | 9,129.6 | 405.4 | 9,153.8 | 2050–2059 |
| 2060 | 55.4 | 388.6 | 8,877.3 | 417.9 | 9,547.5 | 419.0 | 9,572.8 | 2060–2070 |
| 2061 | 57.2 | 401.5 | 9,278.8 | 431.9 | 9,979.4 | 433.0 | 10,005.8 | 2060–2070 |
| 2062 | 59.1 | 415.0 | 9,693.9 | 446.4 | 10,425.7 | 447.5 | 10,453.3 | 2060–2070 |
| 2063 | 61.1 | 428.9 | 10,122.8 | 461.3 | 10,887.0 | 462.5 | 10,915.9 | 2060–2070 |
| 2064 | 63.2 | 443.3 | 10,566.1 | 476.8 | 11,363.8 | 478.0 | 11,393.9 | 2060–2070 |
| 2065 | 65.3 | 458.2 | 11,024.3 | 492.8 | 11,856.6 | 494.1 | 11,888.0 | 2060–2070 |
| 2066 | 67.5 | 473.5 | 11,497.8 | 509.2 | 12,365.8 | 510.6 | 12,398.6 | 2060–2070 |
| 2067 | 69.7 | 489.4 | 11,987.1 | 526.3 | 12,892.2 | 527.7 | 12,926.3 | 2060–2070 |
| 2068 | 72.1 | 505.8 | 12,492.9 | 544.0 | 13,436.1 | 545.4 | 13,471.7 | 2060–2070 |
| 2069 | 74.5 | 522.7 | 13,015.6 | 562.2 | 13,998.3 | 563.7 | 14,035.4 | 2060–2070 |
| 2070 | 77.0 | 540.3 | 13,555.9 | 581.0 | 14,579.4 | 582.6 | 14,618.0 | 2060–2070 |

| Decade | Start Year | End Year | N Years | BAU-SMR Decadal Sum (MMT CO ₂) | BAU-SMR+ATR Decadal Sum (MMT CO ₂) | SMR/Air Decadal Sum (MMT CO ₂) |
|------------------------|-------------|-------------|-----------|--|--|--|
| 2020-2029 | 2020 | 2029 | 10 | 1,206.7 | 1,297.8 | 1,301.2 |
| 2030-2039 | 2030 | 2039 | 10 | 1,684.4 | 1,811.6 | 1,816.4 |
| 2040-2049 | 2040 | 2049 | 10 | 2,341.7 | 2,518.5 | 2,525.2 |
| 2050-2059 | 2050 | 2059 | 10 | 3,256.0 | 3,501.8 | 3,511.0 |
| 2060-2070 | 2060 | 2070 | 11 | 5,067.2 | 5,449.7 | 5,464.2 |
| 2020-2070 Total | 2020 | 2070 | 51 | 13,555.9 | 14,579.4 | 14,618.0 |

| To Year (inclusive) | BAU-SMR Cumulative (MMT CO ₂) | BAU-SMR+ATR Cumulative (MMT CO ₂) | SMR/Air Cumulative (MMT CO ₂) |
|---------------------------------|--|--|--|
| End of 2020s (2020-2029) | 1,206.7 | 1,297.8 | 1,301.2 |
| End of 2030s (2020-2039) | 2,891.1 | 3,109.3 | 3,117.6 |
| End of 2040s (2020-2049) | 5,232.8 | 5,627.9 | 5,642.8 |
| End of 2050s (2020-2059) | 8,488.7 | 9,129.6 | 9,153.8 |
| End of 2060s (2020-2070) | 13,555.9 | 14,579.4 | 14,618.0 |

Table S8: Scope-wise emission intensity under progressive Carbon capture utilization deployment

| Year | Nominal capture (Scope 1) | Scope 1 (t CO₂/t NH₃) | Scope 2 (t CO₂/t NH₃) | Total intensity |
|-------------------|----------------------------------|--|--|------------------------|
| Baseline (no CCU) | 0% | 4.47 | 2.55 | 7.02 |
| 2024 | 40% | 4.34 | 2.54 | 6.88 |
| 2030 | 50% | 3.95 | 2.55 | 6.50 |
| 2040 | 60% | 3.73 | 2.55 | 6.28 |
| 2050 | 70% | 3.51 | 2.55 | 6.06 |
| 2060 | 80% | 3.29 | 2.55 | 5.84 |
| 2070 | 100% | 3.07 | 2.55 | 5.62 |

*The 2024 Carbon capture utilization scenario assumes a baseline nominal capture level of 40% applied to high-purity process CO₂ streams from SMR and water-gas shift units. Capture percentages reported for future years represent nominal capture of these process streams rather than total plant emissions. As a result, Scope 1 emissions decrease progressively while Scope 2 emissions remain largely unchanged due to the additional energy demand of capture and compression. Residual Scope 1 emissions persist because combustion-related flue gas streams remain outside the capture boundary.

Table S9: Comparative Midpoint categories for 1 ton Liq. Ammonia production with SMR, SMR/Air, SMR+ATR

| Impact category | Unit | Liquid Ammonia (SMR) | Liquid Ammonia (SMR/Air) | Liquid Ammonia (SMR+ATR) |
|-------------------------|--------------|----------------------|--------------------------|--------------------------|
| Carcinogens | kg C2H3Cl eq | 12.93357 | 13.85112 | 14.33543 |
| Non-carcinogens | kg C2H3Cl eq | 26.93626 | 25.17388 | 31.21383 |
| Respiratory inorganics | kg PM2.5 eq | 2.155291 | 1.857886 | 2.554605 |
| Ionizing radiation | Bq C-14 eq | 2503.31 | 1042.368 | 3383.142 |
| Ozone layer depletion | kg CFC-11 eq | 0.000222 | 0.000269 | 0.000235 |
| Respiratory organics | kg C2H4 eq | 5.148706 | 6.13422 | 5.46976 |
| Aquatic ecotoxicity | kg TEG water | 20980.53 | 22582.66 | 23153.27 |
| Terrestrial ecotoxicity | kg TEG soil | 13858.02 | 15127.33 | 15155.98 |
| Terrestrial acid/nutri | kg SO2 eq | 44.73657 | 47.13953 | 49.84256 |
| Land occupation | m2org.arable | 13.51221 | 11.91604 | 15.76967 |
| Aquatic acidification | kg SO2 eq | 8.621109 | 8.496374 | 9.827014 |
| Aquatic eutrophication | kg PO4 P-lim | 0.142073 | 0.104591 | 0.174974 |
| Global warming | kg CO2 eq | 6600.63 | 7149.816 | 7104.813 |
| Non-renewable energy | MJ primary | 121127.7 | 141487.6 | 129997.7 |
| Mineral extraction | MJ surplus | 43.96158 | 48.78085 | 46.59819 |

Table S10: Midpoint categories for 1 ton Liq. Ammonia production with SMR (CC+RE) 2030

| Impact category | Unit | Total | Liquid SMR Ammonia CCUS and RE 2030 | Ammonia SMR CCUS and RE 2030 | Electricity, low voltage {IN-MH} electricity production, photovoltaic, 3kWp Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|-------------------------------------|------------------------------|--|---|--------------------------------------|
| Carcinogens | kg C2H3Cl eq | 15.76765 | 0 | 15.50274 | 0.141417 | 0.110614 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 53.61027 | 0 | 52.67654 | 0.655342 | 0.198307 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | 1.49742 | 0 | 1.47219 | 0.009015 | 0.014821 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 1742.02 | 0 | 1711.241 | 19.49248 | 8.247537 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 0.000162 | 0 | 0.000159 | 4.34E-07 | 2.15E-06 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | 3.401482 | 0 | 3.346823 | 0.005007 | 0.049249 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 33091.47 | 0 | 32477.3 | 345.9071 | 177.0073 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 18048.16 | 0 | 17737.17 | 166.0094 | 119.0652 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 30.88076 | 0 | 30.36968 | 0.115926 | 0.377081 | 0.018073 |
| Land occupation | m2org.arable | 13.39967 | 0 | 13.17513 | 0.115735 | 0.09189 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 6.659881 | 0 | 6.546486 | 0.038354 | 0.067851 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.145722 | 0 | 0.143274 | 0.001482 | 0.000821 | 0.000144 |
| Global warming | kg CO2 eq | 4112.333 | 0 | 4048.718 | 5.406762 | 57.38554 | 0.822546 |
| Non-renewable energy | MJ primary | 75582.79 | 0 | 74358.16 | 76.86291 | 1136.099 | 11.67333 |
| Mineral extraction | MJ surplus | 112.8231 | 0 | 111.0496 | 1.323124 | 0.293823 | 0.156595 |

Table S11: Midpoint categories for 1 ton Liq. Ammonia production with SMR (CC+RE) 2040

| Impact category | Unit | Total | Liquid SMR Ammonia CCUS and RE 2040 | Ammonia SMR CCUS and RE 2040 | Electricity, low voltage {IN-MH} electricity production, photovoltaic, 3kWp Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|-------------------------------------|------------------------------|--|---|--------------------------------------|
| Carcinogens | kg C2H3Cl eq | 16.07169 | 0 | 15.80217 | 0.162629 | 0.094022 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 58.12153 | 0 | 57.11925 | 0.753644 | 0.168561 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | 1.44011 | 0 | 1.415751 | 0.010368 | 0.012598 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 1853.015 | 0 | 1820.55 | 22.41635 | 7.010407 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 0.000145 | 0 | 0.000143 | 5.00E-07 | 1.83E-06 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | 2.964784 | 0 | 2.916761 | 0.005759 | 0.041862 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 34758.63 | 0 | 34119.12 | 397.7932 | 150.4562 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 18511.53 | 0 | 18193.5 | 190.9108 | 101.2055 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 28.30297 | 0 | 27.83107 | 0.133314 | 0.320519 | 0.018073 |
| Land occupation | m2org.arable | 13.63504 | 0 | 13.40693 | 0.133095 | 0.078106 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 6.368731 | 0 | 6.259761 | 0.044107 | 0.057673 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.152247 | 0 | 0.1497 | 0.001705 | 0.000698 | 0.000144 |
| Global warming | kg CO2 eq | 3564.994 | 0 | 3509.176 | 6.217776 | 48.77771 | 0.822546 |
| Non-renewable energy | MJ primary | 65127.39 | 0 | 64061.64 | 88.39235 | 965.6839 | 11.67333 |
| Mineral extraction | MJ surplus | 122.983 | 0 | 121.0551 | 1.521592 | 0.24975 | 0.156595 |

Table S12: Midpoint categories for 1 ton Liq. Ammonia production with SMR (CC+RE) 2050

| Impact category | Unit | Total | Liquid SMR Ammonia CCUS and RE 2050 | Ammonia SMR CCUS and RE 2050 | Electricity, low voltage {IN-MH} electricity production, photovoltaic, 3kWp Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|-------------------------------------|------------------------------|---|---|------------------------------------|
| Carcinogens | kg C2H3Cl eq | 16.38094 | 0 | 16.10618 | 0.18667 | 0.075217 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 62.70992 | 0 | 61.62994 | 0.865052 | 0.134849 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | 1.381821 | 0 | 1.358449 | 0.0119 | 0.010079 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 1965.908 | 0 | 1931.531 | 25.73008 | 5.608325 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 0.000128 | 0 | 0.000126 | 5.73E-07 | 1.46E-06 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | 2.520621 | 0 | 2.480119 | 0.00661 | 0.033489 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 36454.29 | 0 | 35786.07 | 456.5974 | 120.365 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 18982.82 | 0 | 18656.81 | 219.1324 | 80.96436 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 25.68112 | 0 | 25.25361 | 0.153022 | 0.256415 | 0.018073 |
| Land occupation | m2org.arable | 13.87443 | 0 | 13.64227 | 0.15277 | 0.062485 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 6.072603 | 0 | 5.968648 | 0.050627 | 0.046138 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.158884 | 0 | 0.156225 | 0.001957 | 0.000559 | 0.000144 |
| Global warming | kg CO2 eq | 3008.884 | 0 | 2961.902 | 7.136926 | 39.02217 | 0.822546 |
| Non-renewable energy | MJ primary | 54493.26 | 0 | 53607.58 | 101.4591 | 772.5471 | 11.67333 |
| Mineral extraction | MJ surplus | 133.3166 | 0 | 131.2137 | 1.746523 | 0.1998 | 0.156595 |

Table S13: Midpoint categories for 1 ton Liq. Ammonia production with SMR (CC+RE) 2060

| Impact category | Unit | Total | Liquid SMR Ammonia CCUS and RE 2060 | Ammonia SMR CCUS and RE 2060 | Electricity, low voltage {IN-MH} electricity production, photovoltaic Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|-------------------------------------|------------------------------|---|---|------------------------------------|
| Carcinogens | kg C2H3Cl eq | 16.76424 | 0 | 16.48332 | 0.214953 | 0.053095 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 68.39719 | 0 | 67.22581 | 0.996121 | 0.095187 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | 1.309571 | 0 | 1.28736 | 0.013703 | 0.007114 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 2105.838 | 0 | 2069.212 | 29.62857 | 3.958818 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 0.000107 | 0 | 0.000105 | 6.60E-07 | 1.03E-06 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | 1.970083 | 0 | 1.938429 | 0.007611 | 0.02364 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 38556.06 | 0 | 37854.05 | 525.7788 | 84.9635 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 19566.99 | 0 | 19231.59 | 252.3343 | 57.15131 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 22.43134 | 0 | 22.05606 | 0.176207 | 0.180999 | 0.018073 |
| Land occupation | m2org.arable | 14.17116 | 0 | 13.93422 | 0.175917 | 0.044107 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 5.705555 | 0 | 5.607499 | 0.058298 | 0.032568 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.16711 | 0 | 0.164319 | 0.002253 | 0.000394 | 0.000144 |
| Global warming | kg CO2 eq | 2327.797 | 0 | 2291.211 | 8.218278 | 27.54506 | 0.822546 |
| Non-renewable energy | MJ primary | 41312.3 | 0 | 40638.46 | 116.8316 | 545.3274 | 11.67333 |
| Mineral extraction | MJ surplus | 146.1251 | 0 | 143.8163 | 2.011148 | 0.141035 | 0.156595 |

Table S14: Midpoint categories for 1 ton Liq. Ammonia production with SMR (CC+RE) 2070

| Impact category | Unit | Total | Liquid SMR Ammonia CCUS and RE 2070 | Ammonia SMR CCUS and RE 2070 | Electricity, low voltage {IN-MH} electricity production, photovoltaic, 3kWp Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|-------------------------------------|------------------------------|---|---|------------------------------------|
| Carcinogens | kg C2H3Cl eq | 17.18588 | 0 | 16.89818 | 0.246065 | 0.02876 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 74.6532 | 0 | 73.38126 | 1.140296 | 0.05156 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | 1.230097 | 0 | 1.209163 | 0.015687 | 0.003854 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 2259.762 | 0 | 2220.662 | 33.91692 | 2.14436 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 8.34E-05 | 0 | 8.17E-05 | 7.56E-07 | 5.59E-07 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | 1.364491 | 0 | 1.34257 | 0.008713 | 0.012805 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 40868 | 0 | 40128.83 | 601.8784 | 46.02189 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 20209.57 | 0 | 19863.84 | 288.8563 | 30.95696 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 18.85658 | 0 | 18.53876 | 0.201711 | 0.098041 | 0.018073 |
| Land occupation | m2org.arable | 14.49755 | 0 | 14.25538 | 0.201379 | 0.023891 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 5.301802 | 0 | 5.210234 | 0.066736 | 0.017641 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.176159 | 0 | 0.173222 | 0.002579 | 0.000214 | 0.000144 |
| Global warming | kg CO2 eq | 1547.755 | 0 | 1522.605 | 9.407766 | 14.92024 | 0.822546 |
| Non-renewable energy | MJ primary | 26813.24 | 0 | 26372.44 | 133.7415 | 295.3857 | 11.67333 |
| Mineral extraction | MJ surplus | 160.2144 | 0 | 157.6792 | 2.302235 | 0.076394 | 0.156595 |

Table S15: Midpoint categories for 1 ton Liq. Ammonia production with AWE, CC+RE 2070

| Impact category | Unit | Total | Liquid Ammonia CCUS and RE 2070 AWE | Ammonia CCUS and RE 2070 AWE | Electricity, low voltage {IN-MH} electricity production, photovoltaic, 3kWp Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|-------------------------------------|------------------------------|---|---|------------------------------------|
| Carcinogens | kg C2H3Cl eq | 8.009009 | 0 | 7.72131 | 0.246065 | 0.02876 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 35.08757 | 0 | 33.81564 | 1.140296 | 0.05156 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | 0.569743 | 0 | 0.54881 | 0.015687 | 0.003854 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 1062.812 | 0 | 1023.712 | 33.91692 | 2.14436 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 3.76E-05 | 0 | 3.58E-05 | 7.56E-07 | 5.59E-07 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | 0.578837 | 0 | 0.556917 | 0.008713 | 0.012805 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 19210.01 | 0 | 18470.85 | 601.8784 | 46.02189 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 9551.254 | 0 | 9205.528 | 288.8563 | 30.95696 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 8.575709 | 0 | 8.257884 | 0.201711 | 0.098041 | 0.018073 |
| Land occupation | m2org.arable | 6.97996 | 0 | 6.737781 | 0.201379 | 0.023891 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 2.452005 | 0 | 2.360438 | 0.066736 | 0.017641 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.083306 | 0 | 0.080369 | 0.002579 | 0.000214 | 0.000144 |
| Global warming | kg CO2 eq | 653.9315 | 0 | 628.7809 | 9.407766 | 14.92024 | 0.822546 |
| Non-renewable energy | MJ primary | 11366.26 | 0 | 10925.45 | 133.7415 | 295.3857 | 11.67333 |
| Mineral extraction | MJ surplus | 81.4743 | 0 | 78.93907 | 2.302235 | 0.076394 | 0.156595 |

Table S16: Midpoint categories for 1 ton Liq. Ammonia production with MP, CC+RE 2070

| Impact category | Unit | Total | Liquid Ammonia CCUS and RE 2070 MP | Ammonia CCUS and RE 2070 MP | Electricity, low voltage {IN-MH} electricity production, photovoltaic, 3kWp Cut-off, S | Electricity, high voltage {IN-MH} electricity production, natural gas, conventional power plant Cut-off, S | Water, deionised {RoW} Cut-off, S |
|-------------------------|--------------|----------|------------------------------------|-----------------------------|--|---|-----------------------------------|
| Carcinogens | kg C2H3Cl eq | 7.142103 | 0 | 6.995821 | 0.104648 | 0.02876 | 0.012874 |
| Non-carcinogens | kg C2H3Cl eq | 53.60709 | 0 | 52.9905 | 0.484953 | 0.05156 | 0.080077 |
| Respiratory inorganics | kg PM2.5 eq | -0.18464 | 0 | -0.19656 | 0.006671 | 0.003854 | 0.001393 |
| Ionizing radiation | Bq C-14 eq | 1452.95 | 0 | 1433.342 | 14.42444 | 2.14436 | 3.038816 |
| Ozone layer depletion | kg CFC-11 eq | 2.04E-05 | 0 | 1.90E-05 | 3.21E-07 | 5.59E-07 | 4.48E-07 |
| Respiratory organics | kg C2H4 eq | -1.79799 | 0 | -1.8149 | 0.003705 | 0.012805 | 0.000403 |
| Aquatic ecotoxicity | kg TEG water | 7333.121 | 0 | 6939.865 | 255.9713 | 46.02189 | 91.26292 |
| Terrestrial ecotoxicity | kg TEG soil | 12364.57 | 0 | 12184.85 | 122.8469 | 30.95696 | 25.91291 |
| Terrestrial acid/nutri | kg SO2 eq | 1.094412 | 0 | 0.892514 | 0.085785 | 0.098041 | 0.018073 |
| Land occupation | m2org.arable | 5.732606 | 0 | 5.606161 | 0.085644 | 0.023891 | 0.016909 |
| Aquatic acidification | kg SO2 eq | 0.003444 | 0 | -0.04977 | 0.028382 | 0.017641 | 0.00719 |
| Aquatic eutrophication | kg PO4 P-lim | 0.094213 | 0 | 0.092758 | 0.001097 | 0.000214 | 0.000144 |
| Global warming | kg CO2 eq | -247.842 | 0 | -267.586 | 4.001004 | 14.92024 | 0.822546 |
| Non-renewable energy | MJ primary | -34036.6 | 0 | -34400.5 | 56.87856 | 295.3857 | 11.67333 |
| Mineral extraction | MJ surplus | 133.9773 | 0 | 132.7652 | 0.979112 | 0.076394 | 0.156595 |

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