AMMONIA DECARBONISATION PATHWAYS AND THEIR EFFECTS ON LIFE CYCLE ASSESSMENTS

Integrating future ammonia scenarios into background data for prospective LCAs

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Master of Science in Industrial Ecology

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Abstract

Using the IEA Ammonia Roadmap aligned with the IMAGE electricity scenarios, an extensive database was produced allowing for prospective LCAs across three storylines from 2020 to 2050 (SSP2-Base, SSP2-RCP26, SSP2-RCP19). The scenarios correspond respectively to 3.9, 2.0, and 1.5°C of global warming in 2100 (vs. pre-industrial levels). Regionally, China produces the largest volume of ammonia as well as the ammonia with the largest climate change impact, due to the dominance of coal gasification technology. To meet 1.5°C of warming (the most sustainable scenario) a global decrease of fossil-based ammonia is needed. For many regions, electrolysis (yellow) ammonia becomes the technology with the lowest global warming potential by around 2045 in the RCP26 storyline and 2035 in RCP19. Until the regional electricity mixes are cleaner, steam reforming, steam reforming with carbon capture and storage, or methane pyrolysis offer lower emission options. However, electrolysis using on-site or designated renewable energy can create emission-free green ammonia, without waiting years for a cleaner regional grid. This means that electrolysis is the best choice for new plants if a producer is not making urea on-site (or has an alternative source of carbon dioxide if they are). Reduction in urea demand will be important for reducing reliance on steam reforming and coal gasification, and a swift uptake of electrolysis with designated renewables must be the focus. However, burden shifting associated with the dominance of renewable electricity systems and bioenergy carbon capture and storage in the RCP19 scenario must be taken into account.

List of Key Abbreviations

ADP – Abiotic Depletion Potential
AE – alkaline water electrolysis
ATR – autothermal reforming
BECCS – bioenergy with carbon capture and storage
CCS – carbon capture and storage
CCU – carbon capture and utilisation
CO – carbon monoxide
CO_2 – carbon dioxide
CRM – critical raw material
EF – Environmental Footprint *(impact method)*
GHG – greenhouse gas
GWP – global warming potential
H_2 – hydrogen
H_2O – water
IAM – integrated assessment model
IEA – International Energy Agency
IMAGE – Integrated Model to Assess the Global Environment
IPCC – Intergovernmental Panel on Climate Change
kWh – kilowatt hour
LCA – life cycle assessment
LCI – life cycle inventory
Mt – Megatonnes
N_2 – nitrogen
NH_3 – ammonia
O_2 – oxygen
PEM – polymer electrolyte membrane *or* proton exchange membrane
POX – partial oxidation
SDS – Sustainable Development Scenario *(IEA)*
SMR – steam methane reforming
SOE – solid oxide electrolysis
SSP – Shared Socioeconomic Pathway
STEPS – Stated Policies Scenario *(IEA)*

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1 Introduction

The urgency surrounding climate change action has been growing steadily in scientific and environmental communities for years. This urgency splashed across headlines at the end of summer 2021, when the Intergovernmental Panel on Climate Change (IPCC) released a report of its key findings and emphasized that human influence had “unequivocally” warmed the atmosphere, ocean, and land (IPCC, 2021). Coordinated global action is necessary to slow the damage and mitigate major climate disasters. Many regions, such as the European Union (EU), have pledged to reach net-zero greenhouse gas (GHG) emissions, in alignment with the Paris Agreement (European Commission, 2020). Decarbonisation of heavy industry will be a major challenge, and an understanding of the potential pathways towards this goal will be critical.

The chemical industry uses the most oil and gas (and total energy) of all industrial sectors, and ranks third in direct carbon dioxide (CO_2) emissions (below cement and the iron and steel sector) (IEA, 2021a). Chemicals are ubiquitous in today’s society. While they conjure up an image of dangerous corrosives that would only be found in a lab, they are actually hidden everywhere in plain sight. Chemicals play key roles in plastics, cosmetics, lubricants, cleaning supplies, pharmaceuticals, mining, and agriculture. The reliance on these items, as well as the complexity, profitability, and interconnected nature of the industry, make it no small challenge to decarbonise (Lim, 2021). Beyond emissions, chemicals can also cause serious health effects and other environmental impacts such as aquatic toxicity or other wildlife and habitat threats (Trier, 2017). Many chemical companies have set goals for CO_2 emission reductions, but are not currently on track (Bloomberg Intelligence, 2021).

Identification and quantification of these environmental impacts is an important step towards reducing them, and it is primary focus in the field of Industrial Ecology. The understanding of a chemical’s impact is essential. Not just at the time of use, but covering all stages from the production of the electricity required for manufacturing to the final treatment. Life cycle assessment (LCA) is a method used to evaluate all environmental impacts related to a product’s entire life cycle, including extraction, production of all inputs, use, and disposal (Guinée, 2002). A main application of LCA is to support decision-making between similar products. It can also highlight the most impactful or polluting life cycle stages (hotspots) of a product. LCA is a strong tool, but there are also drawbacks and challenges. Data availability and quality is identified as a significant issue in all phases of an LCA (Reap et al., 2008b).

Prospective (or anticipatory or ex-ante) LCA is used to understand the environmental impacts of emerging technologies at an early stage while modelling them in a more developed future state (Thonemann et al., 2020). It is therefore expected that data quality and availability issues will be exacerbated when making assumptions about the future. Ex-ante LCA can facilitate the assessment of future environmental impacts, the comparison of different policy interventions, and the selection of investment or design pathways (Cucurachi et al., 2018).

1.1 Future Background Data

Prospective LCAs play an important role in evaluating new technologies. They can help avoid sunk costs or unexpected ecological and human health effects, contributing to society and to the environment. While the majority of (standard) LCAs are done on familiar systems with well-defined background process and foreground (system-specific) process data, ex-ante LCAs must explore a technology’s possible future scenarios, which requires projections of process data and system boundaries (Cucurachi et al., 2018). Many LCAs make use of ecoinvent, which is the largest unit process life cycle inventory (LCI) database and allows for the incorporation of important background data into the study (Wernet et al., 2016). For future scenarios, however, this background data is often lacking and these gaps need to be filled. In LCA, inventories consist of the inputs and outputs (including emissions) of a particular process.

Mendoza Beltran et al. (2020) developed a method to improve the robustness of prospective LCAs by systematically changing background processes based on scenarios of the integrated assessment model IMAGE. They demonstrated their approach by adjusting the background electricity sector in a prospective LCA of an internal combustion engine vehicle against an electric vehicle using different scenarios from the baseline Shared Socioeconomic Pathways (SSPs). The five SSP baseline scenarios offer potential ways the world might evolve without climate policy (Riahi et al., 2017). Within the SSP storylines, different levels are climate policy are introduced, corresponding to a level of radiative forcing which is in turn tied to particular global-mean temperature increase in 2100 relative to pre-industrial levels (Fricko et al., 2017).

Building upon the work of Mendoza Beltran et al. (2020), other sectors have been covered, such as copper, nickel, zinc, and lead (Harpprecht et al., 2021) and the critical raw material cobalt (van der Meide et al., 2022). The superstructure approach of Steubing and de Koning (2021) describes the integration of these and other scenarios into a single background LCI database. The superstructure is implemented into the Activity Browser, which is open source LCA software (Steubing et al., 2020). This integration is managed through the Python package *premise,* which streamlines the process of producing these prospective inventory databases (Sacchi et al., 2022). It is then a simple process to run life cycle assessments across multiple scenarios and points in time.

The work of Mendoza Beltran et al. (2020), Harpprecht et al. (2021), van der Meide et al. (2022), Steubing and de Koning (2021), and Sacchi et al. (2022) act as guiding frameworks for this thesis.

Sectors such as chemicals, plastics, agriculture, and the bioeconomy have not yet been covered. Chemical background processes are present in almost all LCAs, and currently prospective LCAs must rely on either historical inventory data or very simplified projections.

While thousands of chemicals exist, there are some major groups when it comes to their share of the chemical industry and its environmental effects. In 2020, ammonia was responsible for almost half (49%) of the chemical industry's direct CO_2 emissions, followed by high-value chemicals and methanol (IEA, 2021c). Direct emissions are those produced (directly) during the reaction or conversion process, while indirect emissions can occur due to the *energy* used in their production. A key example of this is chlorine, whose direct emissions are not noteworthy but whose production route (chlor-alkali electrolysis) accounts for 40% of the industry's electricity demand (Fischedick et al., 2014). The environmental impact of chlorine production is therefore based heavily on the electricity systems in the background. This thesis aims to close this research gap for ammonia, while paving the way for similar upgrades to other major chemicals. Urea is often manufactured at the same site as ammonia, using the conveniently located ammonia and CO_2 feedstocks. It is therefore also discussed in this report.

1.2 Integrated Assessment Models

Integrated assessment models (IAMs) have been developed to assist in policy decision-making by describing key global processes and the interactions between human and earth systems (United Nations Framework Convention on Climate Change (UNFCCC), 2022). IMAGE (Integrated Model to Assess the Global Environment), from the Netherlands Environmental Assessment Agency, models up to 2100 and is primarily used to understand the social and economic impacts of policies aimed at reducing land-use change emissions and addressing climate change (UNFCCC, 2022). Using population, economy, policies, technology, lifestyle, and resource drivers, IMAGE can be used to compare a baseline (or business-as-usual) scenario to the implementation of different measures to prevent negative environmental or human impacts (Stehfest et al., 2014). Another useful IAM is the REMIND model, meant to illustrate the outcomes and trade-offs related to population, resources, technologies, policies, and the environment (Stehfest et al., 2014).

As IAMs are influential in climate policy decisions, there are also concerns over their use. There are critiques about transparency (Robertson, 2021) and the appropriateness of scenarios in IAMs since they are very context-dependent, assumption based, and have difficulty modelling human agents (Asefi-Najafabady et al., 2020). Van den Berg et al. (2019) also explain that IAMs typically do not properly include qualitative factors such as lifestyle changes (which can be an essential puzzle piece to meeting climate targets) and could benefit from broader coverage of the system.

However, while models are never perfect and should always be used with caution, they can be a powerful tool when no “real” data is available (which is of course the case for the future). Ellenbeck and Lilliestam (2019) argue that modelling assumptions for IAMs are not arbitrary but shaped by specific social contexts and theories and that IAMs should be used as long as what the model is meant to represent is taken into account. Keppo et al. (2021) emphasise that despite their limitations, IAMs are the best available option to guide climate change policy and mitigation as they simultaneously incorporate complex social, economic, technical, and physical aspects.

1.3 Ammonia: Production and Use

In order to develop the best possible model for current and future ammonia life cycle inventories, an understanding of the methods of producing ammonia is needed.

Ammonia (chemical formula NH_3) is a major player in the chemical industry. Ammonia and its derivatives are widely used as agricultural fertilisers, responsible for feeding a significant portion of the global population, but with unfortunate detrimental environmental side effects such as eutrophication, soil acidification, and others (Sutton et al., 2008). Eutrophication is caused when water bodies are contaminated with excessive nutrients (such as nitrogen), leading to too much plant growth and dangerous repercussions in the surrounding ecosystem (Smith & Schindler, 2009). These downstream consequences of liberal fertilisation are in addition to the environmental effects (particularly greenhouse gas emissions) stemming from the chemical production processes themselves.

For the past century, ammonia has been primarily manufactured through the Haber-Bosch process. Created by Fritz Haber and industrialised by Carl Bosch, who both won Nobel Prizes for their work, the process uses nitrogen (N_2) and hydrogen (H_2) with an iron catalyst and high temperatures and pressures to create NH_3 (Erisman et al., 2008). The future consumption of nitrogen fertilisers will depend on many factors, including population growth, more efficient fertiliser use, crop demand for biofuels, and diet changes (Erisman et al., 2008). Ammonia demand will continue to be closely intertwined with these changing elements.

Ammonia currently accounts for 65% of the hydrogen demand in industry, followed by 25% for methanol, 10% for steel making, and less than 1% for other industrial uses (IEA, 2021e). Traditionally, the hydrogen required for ammonia synthesis has come from fossil fuel sources, particularly natural gas, while the nitrogen is taken directly from the air. The most common process used today is natural gas steam reforming (or steam methane reforming – SMR).

Methane (which is the main component of natural gas) and steam undergo a series of chemical reactions to produce primarily hydrogen, carbon dioxide, and carbon monoxide (CO) (García, 2015).

SMR is an endothermic process which requires heat input, so alternative processes such as partial oxidation (POX) and autothermal reforming (ATR) are now also used to produce hydrogen. Partial oxidation does not need external heat since it is an exothermic reaction. Autothermal reforming combines both SMR and POX, so that the heat created by POX is used in the SMR reaction (García, 2015).

Using a process very similar to POX of heavy oil, coal gasification is the main production route for coal-based hydrogen (Simons & Bauer, 2011). Coal gasification represents a significant 85% of Chinese ammonia production, as well as smaller fractions in other regions such as the United States, South Africa, and Indonesia (IEA, 2021a). Multiple gasification technologies exist including fixed bed, fluidized bed, entrained bed, and plasma gasifiers (Midilli et al., 2021). They will not be differentiated from each other in the scenarios or explored more deeply in this thesis. Globally, slightly more than 70% of ammonia is made from hydrogen produced by natural gas steam reforming, while most of the difference is from coal gasification (IEA, 2021a).

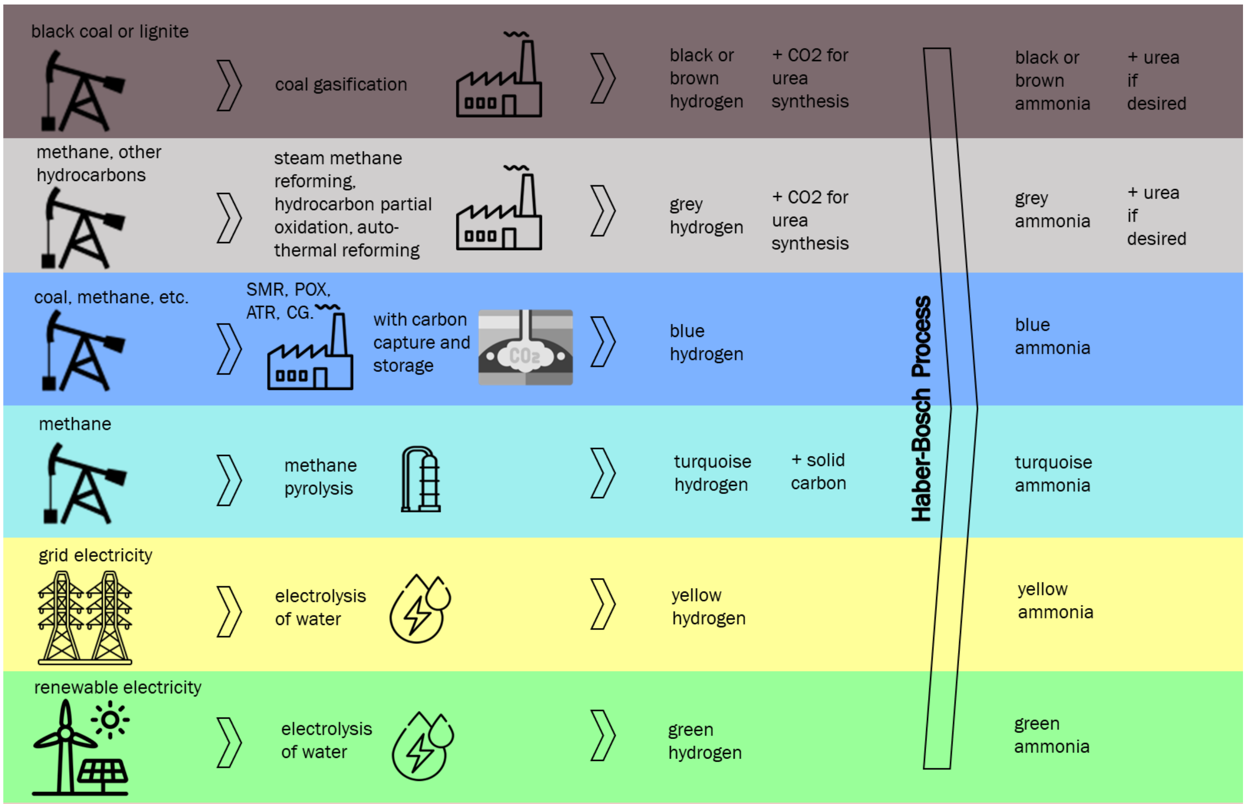
In each of these processes, CO_2 removal is needed to purify the stream of hydrogen. This can be done through processes such as amine-based scrubbing or hot potassium carbonate scrubbing (IEA, 2021a). In many cases, the CO_2 can be used within the same plant for urea synthesis, which is produced by a reaction of ammonia and gaseous CO_2 (Ausfelder et al., 2022). Otherwise, the CO_2 can also be used for other industrial processes or in the food and beverage sector (IEA, 2021a). Urea and other fertiliser products derived from ammonia make up 70% of the global ammonia demand (IEA, 2021a).

1.3.1 Colours of Ammonia

In order to reduce the emissions associated with ammonia synthesis, the hydrogen feedstock, electricity, and heat sources must be made more sustainable. Decarbonisation of the chemical industry will therefore rely heavily on the decarbonisation of hydrogen production.

Research into cleaner hydrogen production methods is ongoing. This has led to the colour coding of hydrogen production routes. Throughout this thesis, when a colour is used to describe ammonia, it is aligned with the colour of the hydrogen that is used in the Haber-Bosch process.

The methods discussed in the previous section all use fossil fuel feedstocks. Hydrogen made from natural gas is classified as grey hydrogen (Oni et al., 2022). Grey hydrogen is subsequently used to make grey ammonia. Coal gasification produces black (from black coal) or brown (from lignite (brown coal)) hydrogen (Gür, 2021). Natural gas, coal, and other fossil feedstocks are often grouped together as grey hydrogen (Newborough & Cooley, 2020). The colour classifications are illustrated in Figure 1-1, which summarises the inputs, industrial processes, and outputs of the different colours of ammonia.



The colour for hydrogen from biomass gasification hasn't been agreed upon, but is treated separately from grey and green in this report. Others (such as pink hydrogen from nuclear) are not addressed within the scope of this project.

Designed using icons from Flaticon.com

Figure 1-1 Colour classification of hydrogen (and ammonia) production routes

If grey, black, or brown hydrogen uses carbon capture and storage (CCS) to prevent the process emissions from entering the atmosphere, it is classified as blue hydrogen (Giovannini, 2020). However, CCS is not a magic wand. Low CO_2 concentrations make it difficult to separate, and CCS relies on transportation and accessible sites for storage (Ausfelder et al., 2022). It is easier and cheaper to capture CO_2 from the syngas than the flue gas, and neither will prevent 100% of the emissions.

Hydrogen produced from methane pyrolysis is classified as turquoise hydrogen (Newborough & Cooley, 2020). Despite the fossil fuel feedstock, turquoise hydrogen is seen as a technological tool towards a more sustainable hydrogen economy due to the fact that solid carbon (rather than CO_2 gas) is the by-product (Sánchez-Bastardo et al., 2021). Methane pyrolysis is not yet ready to be used at an industrial scale, and before full commercialisation it will require more development and adaptation to challenges such as a natural gas (rather than pure methane) feed (Schneider et al., 2020).

Another key technology for the development of sustainable hydrogen (and ammonia) is water electrolysis. This technology uses an electric current to split water (H_2O) into hydrogen and oxygen ($H_2O \rightarrow H_2 + \frac{1}{2} O_2$) (Chi & Yu, 2018). The three main electrolysis methods are alkaline water electrolysis (AE), polymer electrolyte membrane or proton exchange membrane (PEM) electrolysis, and solid oxide electrolysis (SOE) (Grigoriev et al., 2020). Alkaline electrolysis is a mature technology which is the commonly used, followed by PEM which is commercially available and becoming more widespread, while solid oxide electrolysis is still in the development phase (Grigoriev et al., 2020).

Hydrogen produced from the electrolysis of water is classified yellow if it comes from the electricity grid mix that is available, and green if the electricity comes from renewable energy sources (Giovannini, 2020). This distinction is important because the upstream process can contribute a lot of environmental impacts, despite electrolysis itself being emission-free. This will have a big impact, as two thirds of modern global electricity production is made using fossil fuels (Ritchie et al., 2020). While green hydrogen has the lowest *direct* greenhouse gas emissions, renewable energy will not be available at the scale needed for global hydrogen supply in the short term, making the alternatives such as turquoise hydrogen interesting as transition technologies (Sánchez-Bastardo et al., 2021).

Electrolysis is currently responsible for only about 0.03% of global hydrogen production, due to the high cost and to the fact that the electricity mix produces (yellow) hydrogen that has almost triple the emission intensity of grey hydrogen (IEA, 2021e).

In place of coal, the gasification process can also be used on biomass. A colour classification for biomass gasification has not yet been agreed upon, but it should be considered separately from the others. The life cycle environmental impacts are more complex to quantify than for grey and green hydrogen, due to accounting for negative emissions (CO_2 uptake), socio-economic trade-offs, and the risk of burden shifting (Sevigné-Itoiz et al., 2021).

There are also other categories, such as pink hydrogen which uses nuclear electricity for water electrolysis (Giovannini, 2020). Pink hydrogen is not specifically discussed in this report.

The question then remains: what will the ammonia rainbow look like in the future? Presently predominantly made from natural gas and coal, with almost no carbon capture, the state of ammonia production must change drastically if climate targets are to be met.

1.4 Research Objectives

This thesis aims to understand how the ammonia industry and its environmental impacts will develop in the future. The goal is to extend the coupling of ecoinvent and IMAGE or REMIND electricity data with ammonia scenarios to generate LCI databases that represent future technologies and scenarios. The integration of possible future pathways for the ammonia industry will add a more complete background than the ecoinvent database alone, for use in prospective life cycle assessments. These extended future LCIs can be considered “prospective LCI databases”.

It is important to note that this research focuses on ammonia as a chemical (primarily for fertilisers), rather than ammonia as a fuel or energy carrier.

The main research question to be addressed is:

How will the scale and technology mix of ammonia production for existing applications develop in the future, and what will that mean for the climate?

This will be answered by exploring the relative environmental impacts of different ammonia synthesis technologies as well as the overall impact of ammonia production across different future scenarios.

2 *Method*

2.1 Scenario Selection

As discussed, there is extensive work being done to model the policies and technological trends which will correspond to particular global temperature increases. The aim of this research was not to create new scenarios, but to integrate existing scenarios to create the prospective LCI databases introduced in Section 1.4. Integrated assessment models such as IMAGE and REMIND provide several scenarios that are aligned with different radiative forcing levels (and associated degrees of warming) for the year 2100. IAM data for ammonia would ideally have been used for consistency, but they do not have the resolution to model changes in ammonia production.

Based on a review of the literature and available scenarios, the IEA Ammonia Technology Roadmap (also referred to as the "IEA Roadmap" later in this thesis) was identified to be a robust and thorough illustration of potential future ammonia scenarios (IEA, 2021a). It includes regional and global production volumes and technology shares. It was therefore selected as the data source for the ammonia scenarios in this research, despite requiring some adjustments to align it with the IAMs.

Other scenarios exist, such as the DECHEMA Perspective Europe 2030 which highlights the challenge of increasing renewable electricity supply to support green hydrogen, recognises the future potential of turquoise hydrogen and includes blue hydrogen as a necessary transition technology (Ausfelder et al., 2022). However, it lacks the IEA's global coverage. There are also several projections for the hydrogen industry in general, but these were not followed as ammonia will likely follow a different pattern than "average" hydrogen due to the prevalence of urea plants which require the convenient ammonia and CO_2 feedstocks. The International Renewable Energy Agency and Ammonia Energy Association also reported on the future of renewable ammonia, but with the inclusion of ammonia as a fuel and as an energy carrier (IRENA & AEA, 2022), while the IEA Roadmap (and this thesis) look specifically at the existing uses for ammonia (as a chemical product for the agricultural (fertiliser) and industrial sectors).

To match the ammonia prospective LCI with IMAGE background electricity data, the IEA scenarios were aligned with the integrated assessment model SSP2 (middle of the road) storylines. The main analysis followed the IMAGE electricity scenario at SSP2-Base, SSP2-RCP26, and SSP2-RCP19. To develop prospective LCI databases that are compatible with both existing IMAGE and REMIND models, and to test the robustness of the method, the ammonia scenario was also later overlayed with the REMIND SSP2 storylines.

The IEA Roadmap aligns with the IEA's World Energy Model. It contains four scenarios (Net Zero Emissions by 2050 Scenario (NZE), Announced Pledges Scenario (APS), Stated Policies Scenario (STEPS), Sustainable Development Scenario (SDS)) and has newly improved modelling of low carbon hydrogen and ammonia (IEA, 2021b). While they are not a perfect match with the IMAGE SSP2 storylines, Table 2-1 shows how the IEA scenarios were paired with the IMAGE and REMIND electricity scenarios in this thesis.

Table 2-1 Alignment between IMAGE and REMIND storylines and the IEA scenarios

Integrated Assessment Model				IEA	
IMAGE	REMIND	radiative forcing (W/m2)	°C of warming (in 2100 vs. pre-industrial levels)	scenario	°C of warming (in 2100 vs. pre-industrial levels)
SSP2-Base	SSP2-Base	6.7	3.9	-	-
SSP2-RCP26	SSP2-PkBudg1100	2.6	2.0	STEPS	2.6
SSP2-RCP19	SSP2-PkBudg900	1.9	1.5	SDS	1.65

The IEA Roadmap did not provide an equivalent to the SSP2-Base scenario, but as the Base scenario represents an absence of climate policy, the 2020 regional technology shares were simply assumed to remain constant in the Base scenario. While the IEA scenarios provide the ammonia data, the IMAGE (or REMIND) scenario names will be most often used in the discussion of the results in this report.

2.2 Life Cycle Inventory Model Development

Life cycle inventories then needed to be developed to match the IEA scenarios. The IEA Roadmap, which provides the 2020 technology mix and two potential 2050 mixes, differentiates the technologies (across eight regions) as follows: Electrolysis, Pyrolysis, Coal, Coal with CCS, Gas, Gas with CCS, Oil, Fossil with CCU (carbon capture and utilisation) (IEA, 2021a). This means that different electrolysis technologies need to be grouped together, as well as the different natural gas technologies. Here Fossil with CCU refers to CO_2 capture for use in the industry (typically for urea production) and CCS denotes that the emissions are compressed, transported, and stored underground (IEA, 2021a). Biomass gasification is not included in the SDS or STEPS scenarios of the IEA Roadmap so it is not included in this thesis, but it does play a small role in the Net Zero Emissions by 2050 scenario.

In order to project ammonia production into the future, the first step was to expand the current technology coverage in ecoinvent 3.8. New inventories needed to be introduced for water electrolysis, methane pyrolysis, and coal/natural gas technologies with carbon capture. Existing inventories were upgraded where newer or more complete data was found. The inventories for several of the ammonia production alternatives were taken from Carlo D'Angelo et al. (2021).

Figure 2-1 provides an overview of the modelled system. This is a simplified diagram of the main processes and key flows. Some flows (such as electricity input) are not shown as they are required for all of the processes in the figure. The full list of inputs and outputs can be found in the inventory file in the supplementary information (new_activities.xlsx). Also note that while the IEA treats CCU separately, there is no difference to the SMR unit process if the CO_2 is vented or later used, so this model groups gas and gas w/ CCU together. As the CO_2 emissions "stored" in urea are eventually released in the fertiliser use phase, it's appropriate to consider these both "grey" ammonia. The same applies to coal with CCU (which is specific to China). This means that seven main ammonia production processes exist in the new model. The dominance of each of the seven varies over time and by region.

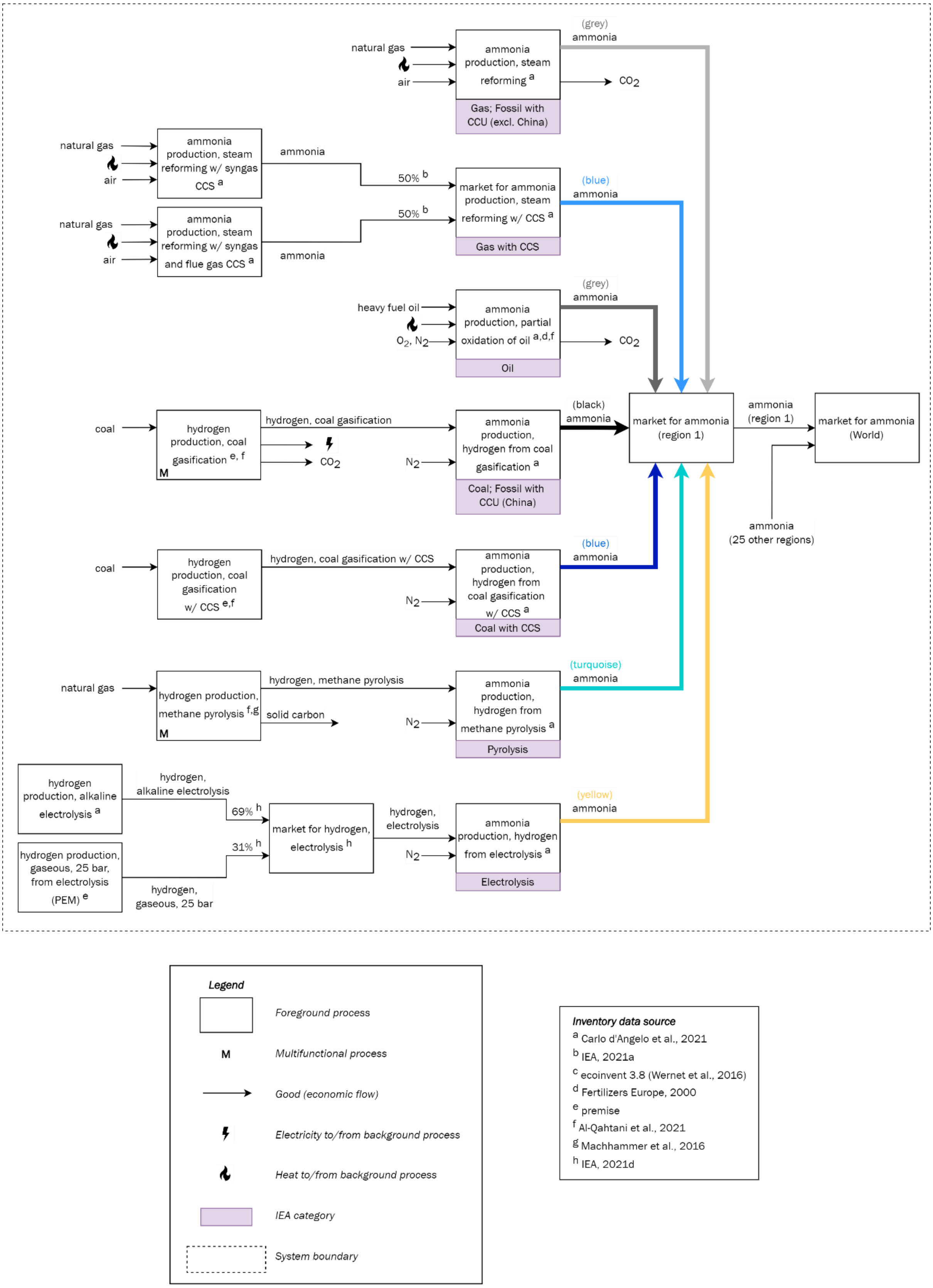


Figure 2-1 Key inventories in the new ammonia model and the corresponding IEA categories

The data sources used for each process are indicated by letters in superscript. The purple boxes represent the IEA category name associated with the process in the LCA model.

A “market” in ecoinvent represents a consumption mix (or in this case a production technology mix) for a particular region (Wernet et al., 2016). Markets play an important role in ecoinvent, as most downstream users of ammonia will pull from an ammonia market. The environmental impacts of e.g. a food product, will have background impacts related to the fertiliser used in crop cultivation. Figure 2-1 gives an example of a region (region 1) whose seven ammonia processes are combined (at a particular ratio, defined by the scenarios) to create the regional market. The IEA Roadmap provides the production mixes for eight IEA regions. After being converted to the 26 IMAGE regions, these regional markets form the basis of the World market.

Some key assumptions will be discussed below. Further details and other modelling choices can be found in Appendix 1: Model Assumptions (Table A1- 1).

The new SMR (IEA: Gas) process replaces the existing ecoinvent 3.8 steam reforming inventory. The upgraded process uses steam produced during operation as an offset to its electricity needs, so the co-product of steam (which was present in the ecoinvent 3.8 inventory) is no longer included (Carlo D’Angelo et al., 2021).

Gas with CCS is a new inventory which consists of equal shares "steam reforming w/ syngas CCS" and "steam reforming w/ syngas and flue gas CCS" to result in a 90% capture rate (IEA, 2021a).

All ammonia production processes described here use the Haber-Bosch process to convert hydrogen and nitrogen into ammonia. In SMR the nitrogen is taken directly from the air, but all others require a designated nitrogen input (in this model, from cryogenic air separation). In SMR, SMR with CCS, and POX of oil, the hydrogen production and Haber-Bosch process were grouped within the same unit process (or inventory). The remaining four were modelled with the hydrogen production and ammonia production (via Haber-Bosch) separately.

The coal gasification process is multifunctional (labelled M), meaning that it has two economic products (hydrogen and electricity). The environmental burden was economically allocated based on \$1.11/kg H_2 and \$0.04/kWh electricity (von Wald et al., 2020). Coal w/ CCS requires a net input of electricity, so it is not considered multifunctional.

Methane pyrolysis, which produces hydrogen and solid carbon, was economically allocated based on \$1.11/kg H_2 and \$0.15/kg C (von Wald et al., 2020)).

For ammonia from electrolysis, the hydrogen input is a mixture of 69% alkaline electrolysis (new inventory) and 31% PEM (from *premise*). This assumption was based on the 2020 installed capacity of 61% AE, 31% PEM, 8% unspecified or SOE (IEA, 2021d) with SOE excluded and the dominant technology (AE) assumed to cover the difference. Ammonia from electrolysis hydrogen was modelled as being connected to the region-specific electricity grid, meaning that this is yellow ammonia (not green). This assumption may not reflect reality in the future, as there may be a shift to designated on-site renewables for hydrogen production.

2.3 Prospective LCI Database Creation

A scenario data file was built based on the IEA Roadmap’s global production quantities in megatonnes (Mt or million tonnes) for 2020 (actual) and 2030, 2040, 2050 under STEPS and SDS scenarios as well as the technology shares in eight regions for 2020 (actual) and 2050 (under the STEPS and SDS scenarios). Linear interpolation was used for the intervening years. The development of the scenario file is described in the following sections.

2.3.1 Regional Market (Technology) Mixes

In order to generate an output compatible with the IMAGE electricity scenarios, the IEA regions were matched with their corresponding IMAGE regions, shown in Table 2-2. Where there were multiple IMAGE regions corresponding to a single IEA region, the technology mixes were assumed to be the same for all the linked IMAGE regions. This means that same fractions of the seven technology types (Gas, Coal, Electrolysis, etc.) provided for Europe (IEA) were applied to the regions Central Europe, Turkey, Ukraine, and Western Europe (IMAGE).

Table 2-2 IEA and IMAGE regional divisions

IEA region	IMAGE region
India	India (INDIA)
China	China region (CHN)
Eurasia	Russia region (RUS) Central Asia (STAN)
Europe	Central Europe (CEU) Turkey (TUR) Ukraine region (UKR) Western Europe (WEU)
Africa	Eastern Africa (EAF) Northern Africa (NAF) Rest of Southern Africa (RSAF) South Africa (SAF) Western Africa (WAF)
Asia Pacific (minus India, China) *	Indonesia region (INDO) Japan (JAP) Korea region (KOR) Oceania (OCE) Rest of South Asia (RSAS) Southeastern Asia (SEAS)
Central & South America	Brazil (BRA) Central America (RCAM) Rest of South America (RSAM)
North America	Canada (CAN) United States of America (USA) Mexico (MEX)
Middle East	Middle East (ME)

* Note that technology share projections for Asia Pacific (minus India, China) are not shown in the IEA Ammonia Technology Roadmap. However, as the corresponding six IMAGE regions do all produce ammonia (WITS, 2021), the decision was made to include them in the scenario data file. Projected in the SDS scenario to have a lot of CCUS deployment and an increasing shift toward electrolysis due to high natural gas prices (IEA, 2021a), the assumption was made to match Asia Pacific to the technology mix trajectory as Africa, which in SDS 2050 contains almost 20% electrolysis and almost 60% SMR with CCU or CCS.

2.3.2 Regional Production Volumes

The initial regional contribution to these total volumes was provided for the top ammonia producers (China, Russia, Europe, USA, Middle East, India). More detail was provided for SDS (such as the significant growth in India and the plateaus in Europe and North America), so this was incorporated into the calculated regional volumes (IEA, 2021a). Otherwise, growth was assumed to be linear. For the Base scenario, the 1.5% annual (global) production growth rate of the last three decades (IEA, 2021a) is simply assumed to continue. For Base and RCP26 the regional producer fractions remain static (e.g. China is responsible for 29% of the total ammonia production each year). These volumes are visualised in Figure 2-2.

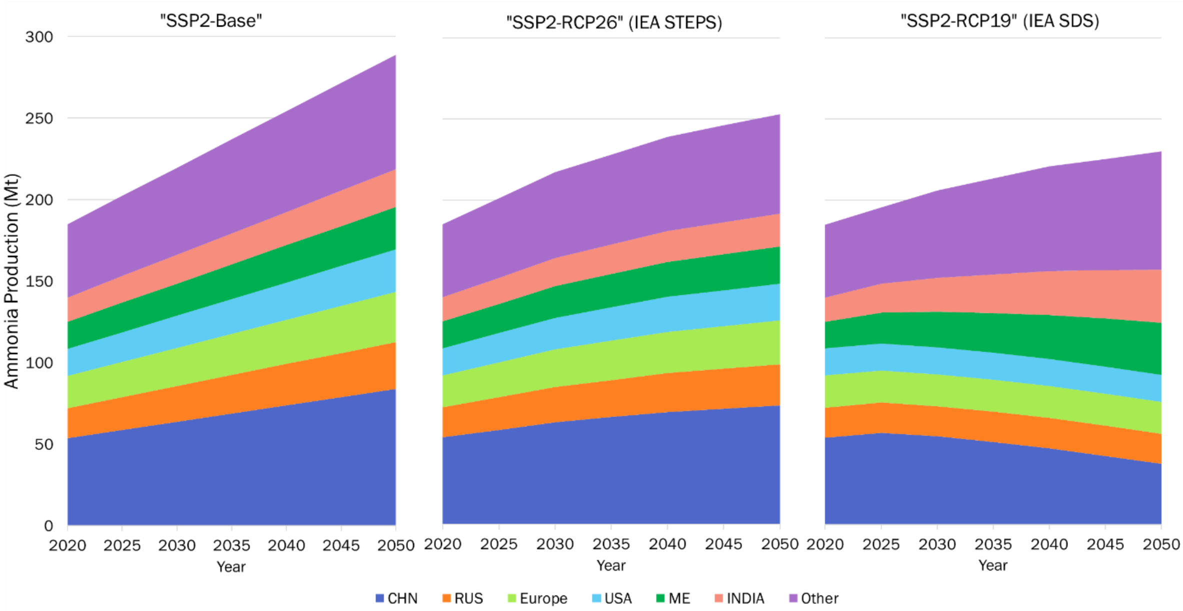


Figure 2-2 Regional ammonia production quantities used in the model scenarios

The assumptions and calculations used to determine the regional production volumes can be found in the supplementary information file regional_production.xlsx.

With regional production volumes and regional market shares (technology mixes), the amount of ammonia produced via each technology type could be calculated.

2.3.3 Integration of the Scenario Files

The scenario data file ended up with 26 regions, each with a particular quantity of the seven technologies, across the three scenarios, evolving over time from 2020-2050.

In addition to these volume changes, electrolysis efficiency improvements from 66% to 76% (Ausfelder et al., 2022) were also included in the scenario data file for all three scenarios. Since SMR and coal gasification are already quite mature and efficient technologies, it’s unlikely that they will change much and no efficiency improvement was allocated to them.

The next step was to integrate the IEA scenarios into ecoinvent, using the python package *premise*, as explained in the approach of Steubing and de Koning (2021) and (Sacchi et al., 2022). *Premise* incorporates the background IAM scenarios and generates prospective LCI databases (or an amalgamated “superstructure” database) which are the extended future versions of the ecoinvent database.

An external tool was made by the *premise* developer for the manual addition of sector-specific custom scenarios. This Custom Scenario Tool is described in more detail in the supplementary information (Custom_Scenario_Tool_Guide.docx). Based on the production volumes in the scenario data file (scenario_ammonia.xlsx), the Custom Scenario Tool created markets for the 26 IMAGE regions plus a World market, which superseded the old (ecoinvent) ammonia markets. In addition to the custom ammonia scenarios, the IMAGE background electricity scenarios were updated in the new database.

2.4 Life Cycle Impact Assessment

To assess the outcomes of the new inventories and scenarios, several LCAs were performed to explore the impact of (1 kg) ammonia produced by different technologies, regions, and scenarios. The total impact of ammonia production regionally and globally was also calculated.

Several methods to measure and characterise the life cycle impacts of a process or product. The European Commission (2021) recommends the use of the Environmental Footprint (EF) methods for reliable and consistent measurement and communication of environmental performance. To investigate the impact category “climate change” the Joint Research Centre (JRC) of the European Commission recommends using the midpoint indicator “radiative forcing as Global Warming Potential (GWP100)” measured in kilograms of CO_2-equivalent (kg CO2-eq) (Fazio et al., 2018). Different EF versions treat biogenic carbon (emissions resulting from the combustion or breakdown of *organic* material) differently. In EF v3.0, biogenic CO and CO_2 have a zero characterisation factor, but in the EN 15804 standard biogenic emissions cause the same amount of climate change as fossil emissions (characterisation factor of 1.57 and 1 for CO and CO_2 respectively) but CO_2 can also be removed from the atmosphere with a factor of -1 (PRé, 2020).

Because negative emissions are used in the IMAGE storylines in order to reach climate targets, the impact assessments performed in this research all use the EF v3.0 EN15804 standard available on the Activity Browser.

Both IMAGE and REMIND focus primarily on climate change (global warming potential (GWP) due to GHG emissions) and do not dive deep into other life cycle impact categories. For this reason, climate change will be the main impact category of focus throughout this report.

For clarity, a summary of the steps in this Method section is shown in Figure 2-3.

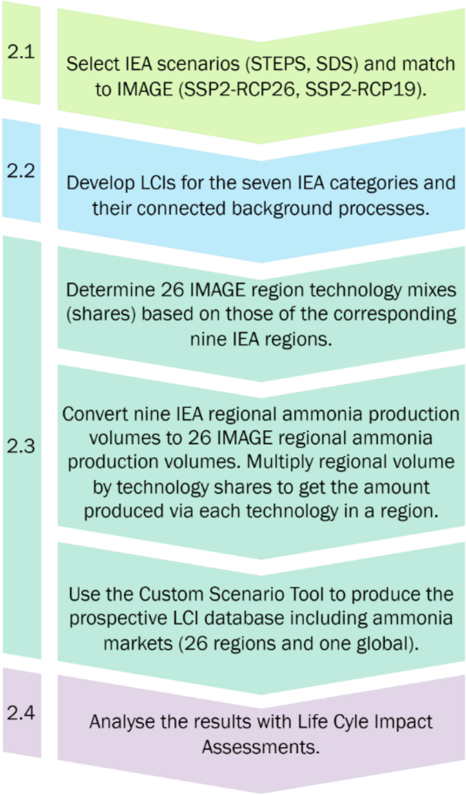


Figure 2-3 Method Overview

3 Results and Discussion

3.1 Relative Impacts

To understand the individual impacts of different technologies within a region, the production of 1 kg of ammonia via the different production routes can be compared through an LCA. Regions can also be compared to each other, by looking at the production of 1 kg of ammonia from different regional markets. These markets, as discussed earlier, contain specific ratios of each technology type used in a region. These LCAs would be considered “cradle to gate” since they include impacts from the origin of the resources up to and including transportation of the produced ammonia. They do not cover the downstream processing into different products or fertilisers, the use phase, or any final disposal.

3.1.1 Relative Technology Impacts - China

In Figure 3-1 below, climate change impacts (shown as the global warming potential in kg CO2-eq) are compared for the different production technologies used in China (CHN). Note that these technologies are used at some point in time in at least one of the three scenarios; all five are not necessarily in the mix for all situations. Electrolysis and CCS only play a role in the sustainable scenario (the changing technology market shares used in the model for China can be seen in Appendix 2, Figure A2- 1).

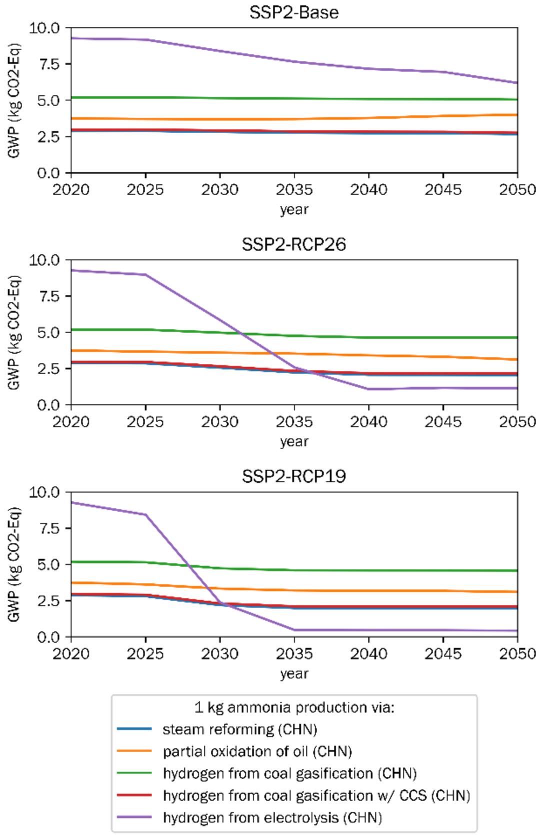


Figure 3-1 GWP per ammonia production technology (China)

Initially, the technology with the lowest emissions is ammonia from steam reforming, but SMR is not heavily used in China. Currently, most of their ammonia is produced via coal gasification. The clearest observation is that the choice of scenario makes a significant impact on ammonia using hydrogen from electrolysis. As discussed, this is considered yellow ammonia, since it is linked to the Chinese electricity mix, rather than designated renewable energy sources. For green ammonia, the results would be different (in a very basic model linking electrolysis to onshore wind power (without considering storage, intermittency, or other limitations), green ammonia has about 0.3 kg emissions per kg ammonia in 2020 already, the lowest of all technologies).

In the Base scenario (which is the least ambitious in terms of sustainability as it doesn't deviate from historical trends), electrolysis remains the most impactful technology across the whole time period. In RCP26 however, electrolysis has a lower GWP than coal gasification (the dominant Chinese technology) by 2035. In RCP19, the most ambitious scenario, electrolysis has the lowest emissions by 2035.

To get a rough idea of the impact of green ammonia, the results of RCP19 in later years should be considered. Exact results would depend on type, location, and quantities of green energy used. While modelling green ammonia separately did not fit in the scope of this thesis, it's safe to say that electrolysis ammonia should only be introduced with designated renewable energy sources until the electricity mixes are cleaner. Otherwise, electrolysis will be worse for the climate than just using the coal or natural gas directly.

Since the ammonia production technologies themselves are not modified over time, except for electrolyser efficiency, any changes in GWP are due to the background processes such as the electricity mix.

3.1.2 Background Electricity Changes

The electrolysis trends are driven primarily by the background electricity mix. Since electricity is still predominantly coal-based in China, the GWP of yellow ammonia only decreases as the GWP of the electricity mix goes down. A comparison of the two can be seen in Appendix 2, Figure A2-2, and the electricity mixes for the top ammonia producers are in Figure A2- 3. In some regions, the GWP of electricity goes below zero. These come from electricity mixes which rely on combinations of low-emission (or negative emission) technologies such as fossil fuels with CCS, renewable energy, nuclear power, and bioenergy with carbon capture and storage (BECCS). Because growing biomass acts as a carbon sink, the full process can be net negative if the downstream emissions are captured (at the cost of major land requirements) (PBL, 2020). The negative characterisation factor used in the EN15804 model then produces a negative GWP.

Almost all scenarios used to meet net-zero carbon goals rely on negative emissions (typically via BECCS or afforestation) along with deep decarbonisation of hard-to-abate sectors (García-Freites et al., 2021). Reliance on BECCS and afforestation has raised concerns over land-use competition with food crops (leading to higher food prices) as well as other environmental impacts, and it's critical that they are not seen as a magic solution but as a tool to be used in combination with sharp global decreases in emissions (Fajardy et al., 2021).

BECCS can be done with sources that do not require designated energy crops (such as pulp and paper, wastewater treatment, crop residues, organic waste), but this has challenges related to source-sink distribution, the availability of CO_2 storage sites, and transportation of the CO_2 itself (Rosa et al., 2021). The IMAGE scenarios with climate policy include a carbon price which results in higher shares of renewables and alternative technologies like CCS/BECCS (by making them more affordable) (Stehfest et al., 2014).

The question of to what extent BECCS can or should be relied on falls outside the scope of this thesis. The main takeaway should be: under the conditions of the IMAGE RCP19 and RCP26 scenario, BECCS does assist in decarbonising ammonia from electrolysis hydrogen. For even faster decarbonisation, ammonia producers can use designated renewable energy to produce green electrolysis, without waiting years for the regional electricity mix to become cleaner.

3.1.3 Relative Technology Impacts - Western Europe

In contrast to the Chinese ammonia production mix, the sustainable scenario for a region which currently relies more heavily on steam methane reforming (Western Europe) is shown below in Figure 3-2.

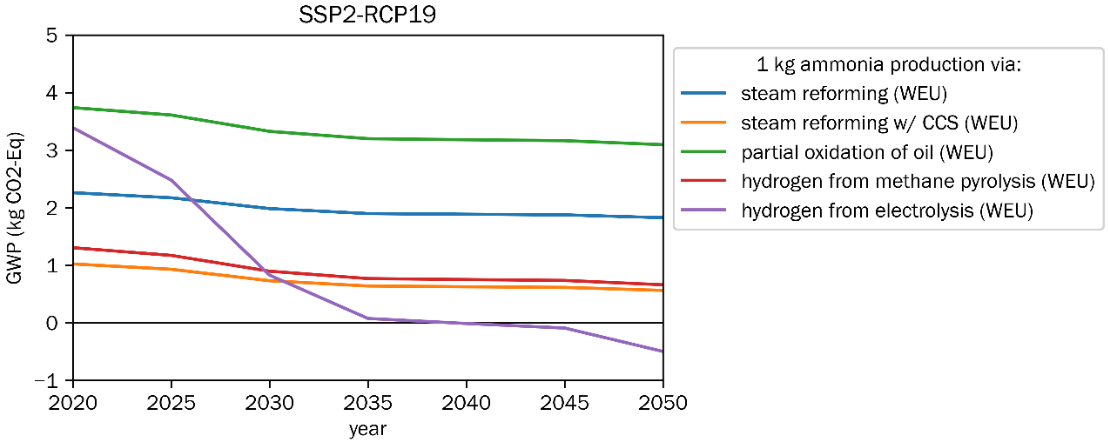


Figure 3-2 GWP per ammonia production technology (Western Europe, SSP2-RCP19)

In this case, ammonia from electrolysis actually becomes emission-free around 2040 in RCP19 (and closer to 2050 in RCP26). This is due to the use of BECCS in the chosen IMAGE storylines.

"Burden shifting" from one impact category to another is another reason LCAs are a useful tool. Climate change is the focus of this thesis, but it's always valuable to check if there are unexpected consequences in the other categories. A look at land use in Western Europe shows the increase in electrolysis' land use impact in the later years of the RCP26/19 scenarios where BECCS are being used to achieve negative emissions (Appendix 2, Figure A2- 4). It's also interesting to check water use, since freshwater scarcity is often listed as a concern in discussions of electrolysis hydrogen. However, Beswick et al. (2021) found that, assuming renewable electricity is used, the hydrogen economy will have a lower water demand than fossil energy. This LCA agrees with that outcome, as the water use for ammonia from SMR is at least 1.5 times higher than ammonia from electrolysis hydrogen (Appendix 2, Figure A2- 5).

In WEU as with CHN, electrolysis changes the most dramatically, but the remaining ammonia production routes also evolve over time (the impacts decrease slightly). No efficiency changes are applied to these processes, so the ammonia production process itself does not actually change over time; SMR in 2050 is modelled to be the same as SMR in 2020. Therefore, the cause of these fluctuations is again the background changes.

The changing technology market shares used in the model for WEU can be seen in Appendix 2, Figure A2- 6. In the sustainable scenario, a significant portion of the SMR ammonia is replaced by electrolysis ammonia.

3.1.4 Relative Technology Impacts - Other Top Producers

The technology comparison graphs (for climate change (GWP)) of the other top producers can be seen in Appendix 2, Figures A2- 7 through A2-12. A brief summary is given here. For Russia, methane pyrolysis has the lowest emissions in all scenarios, followed closely by SMR. Electrolysis (yellow ammonia) only becomes a better option than SMR by almost 2050 in RCP26 and 2035 in RCP19. Russia's electricity mix does not decarbonise to the extent of the other regions. In Central Europe, SMR with CCS has the lowest emissions the whole time period for Base and RCP26, but electrolysis is the lowest by 2035 in RCP19. SMR with CCS is the best choice in the USA and

India until 2045 and 2035 for RCP26 and RCP19 respectively, where it is beaten by electrolysis. In the Middle East this is the case in about 2045 and 2030.

3.1.5 Regional Ammonia Markets

Instead of looking at each technology individually, the regional markets can also be compared. The GWP of 1 kg ammonia produced by the “market for ammonia” for each top producer is shown in Figure 3-3.

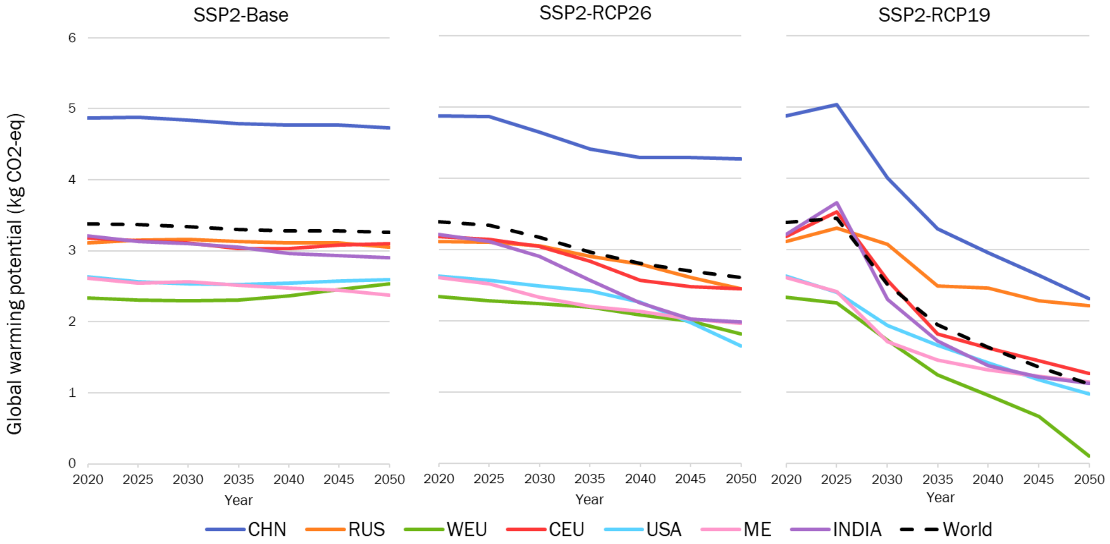


Figure 3-3 GWP of 1 kg ammonia from the top producers’ ammonia markets

Note that in Figure 3-3, Western and Central Europe are shown separately for comparison purposes, while the top producer is technically IEA’s Europe as a whole (which also includes Turkey and Ukraine).

In 2020, the average global impact (black dashed line) is 3.4 kg CO2-eq/kg ammonia. By 2050, this per-kilogram impact decreases by 4%, 23%, and 67% for SSP2-Base, RCP26, and RCP19 respectively. In the most sustainable scenario, the 2050 average global impact is 1.1 kg CO2-eq/kg ammonia.

As expected, the Chinese technology mix initially has the highest global warming potential due to its heavy use of coal gasification. Under the RCP19 scenario, it manages to make substantial improvements, but remains the worst emitter. However, it becomes almost comparable to Russia in 2050, as Russia does not have a steep ammonia decarbonisation. The other regions show a much stronger emissions reductions. Though Western Europe gets very close, none of the regions achieve net-zero GHG emissions with respect to ammonia, under these scenario conditions.

3.1.6 Process Contributions to GWP

Contribution analysis is used in LCA to identify hotspots and important emissions. This allows the identification of issues at a detailed process level. The first contribution analysis in Figure 3-4 compares 1 kg ammonia from the market for ammonia (World) activity at 2020 and the three scenarios at 2050. The processes were aggregated by activity name and the top five contributors for each year/scenario were included (which led to seven total activities and the remaining contributions filling the “rest” category).

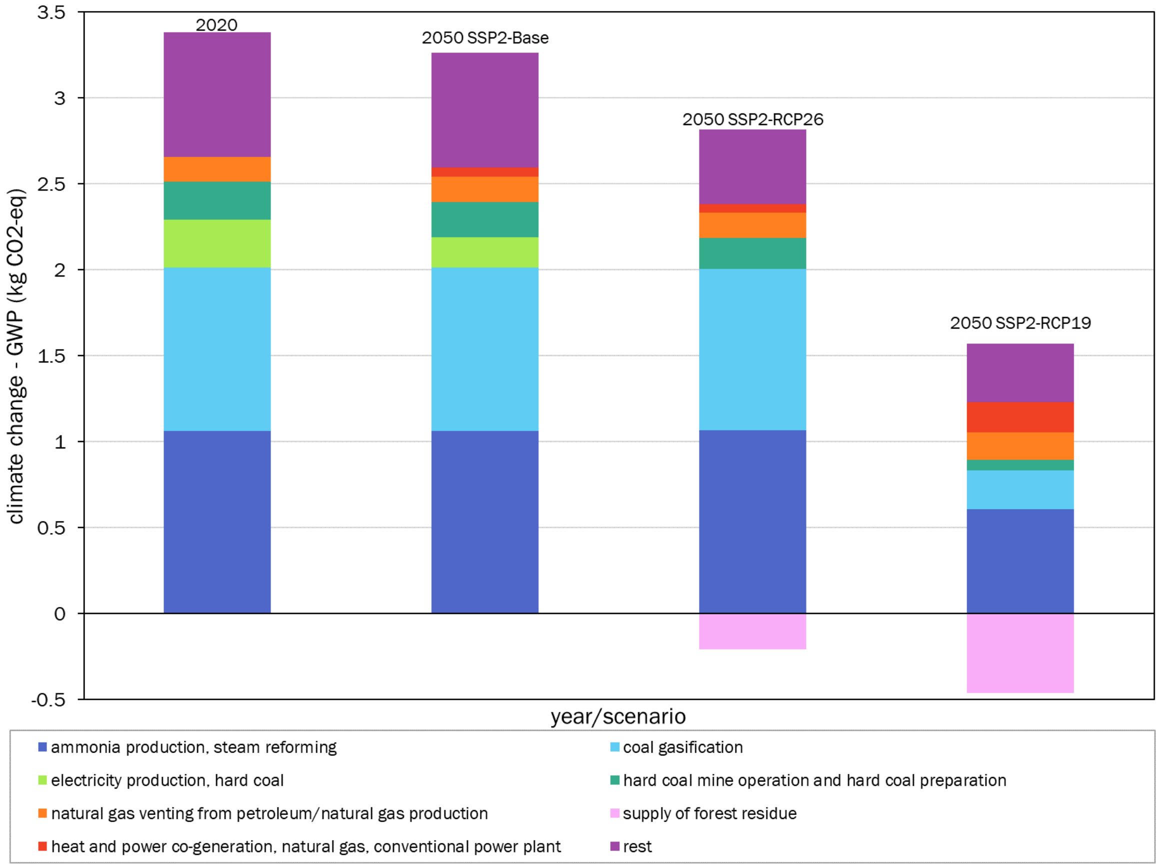


Figure 3-4 GWP contribution analysis of 1 kg ammonia (new market for ammonia (World))

This identifies steam reforming and coal gasification as the main process hotspots, followed by electricity production and coal mining. This is quite logical, as the World market is made of regional markets which are made of varying amounts of SMR, coal gasification, and other ammonia technologies. In 2050 in the RCP26 and RCP19 scenarios, the negative contribution due to carbon uptake is seen. In RCP19 in particular, the contribution of the traditional ammonia production techniques (especially coal gasification) has decreased significantly.

For 2020, 2050 Base and 2050 RCP26, the SMR and coal gasification contributions are quite similar. The main reason for this is that the technology mixes do not change much in the IEA STEPS scenario. If they do, it is often a shift from SMR to SMR with carbon capture and *use* which is the same as standard SMR in ecoinvent. It is only in the RCP19 (IEA SDS) scenario that there is a strong shift to new technologies (electrolysis in particular).

These contributions look different on a regional level, since the global market is quite heavily influenced by China. Using the same method to examine 1 kg ammonia from the new market for ammonia of Western Europe (WEU) results in Figure 3-5. The top four contributors to each year/scenario were included, which led to eight total activities and the remaining contributions filling the “rest” category.

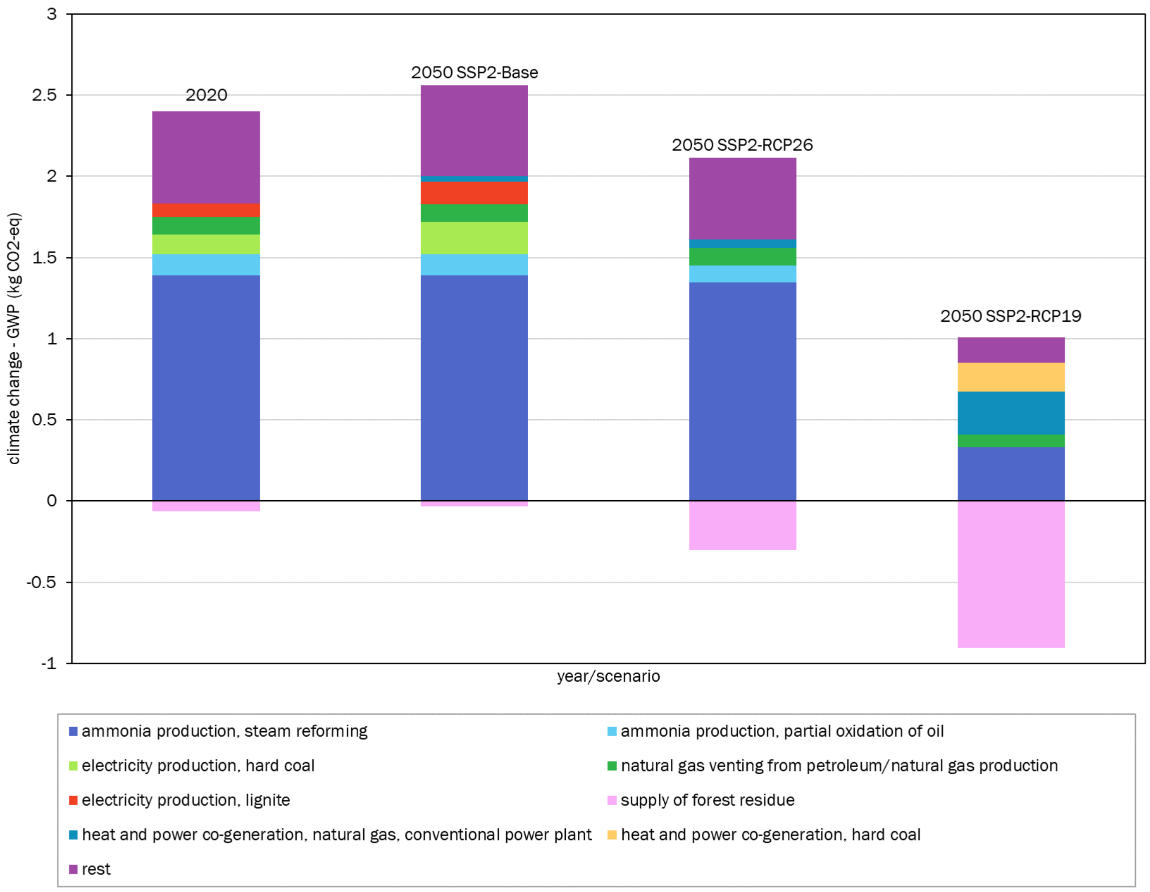


Figure 3-5 GWP contribution analysis of 1 kg ammonia (new market for ammonia (WEU))

As expected, coal has a much smaller contribution to these results while steam reforming dominates. The 2050 RCP19 impact of SMR is much lower, since Europe is modelled to have a lot of electrolysis in this scenario. This is visible in the higher contribution of heat and power co-generation in the RCP19 column. The other significant finding from the RCP19 2050 column is that the negative contribution forest residue (biomass) almost completely offsets the positive contribution from the other activities.

3.1.7 Impact of Steam Reforming and Natural Gas Production

Energy plays a major role in the background of production processes. Instead of looking at the market level, this section looks at ammonia from steam reforming alone in order to highlight the influence of natural gas production on the SMR impact.

The global warming potential of 1 kg ammonia production by steam methane reforming varies per region (from 1.9 kg CO2-eq in Canada to 3.2 kg CO2-eq in India in 2020). The SMR unit process itself produces about 1.5 kg emissions (in this model, it is the same for each region) while the difference is made up of emissions due to background electricity production, transportation, coal mining, natural gas extraction/processing, etc. depending on the location in question. Natural gas production (and its associated methane emissions) varies globally. The GWP of ammonia from steam reforming for the top producers is shown in Figure A2- 13 in Appendix 2.

Figure 3-6 and Figure 3-7 show the grouped process contributions to the GWP of 1 kg ammonia from steam reforming for Russia and Western Europe respectively. Although steam reforming is modelled the same for both regions, Russia has higher emissions due to natural gas venting or flaring in particular, as well as other processes such as heat and power co-generation.

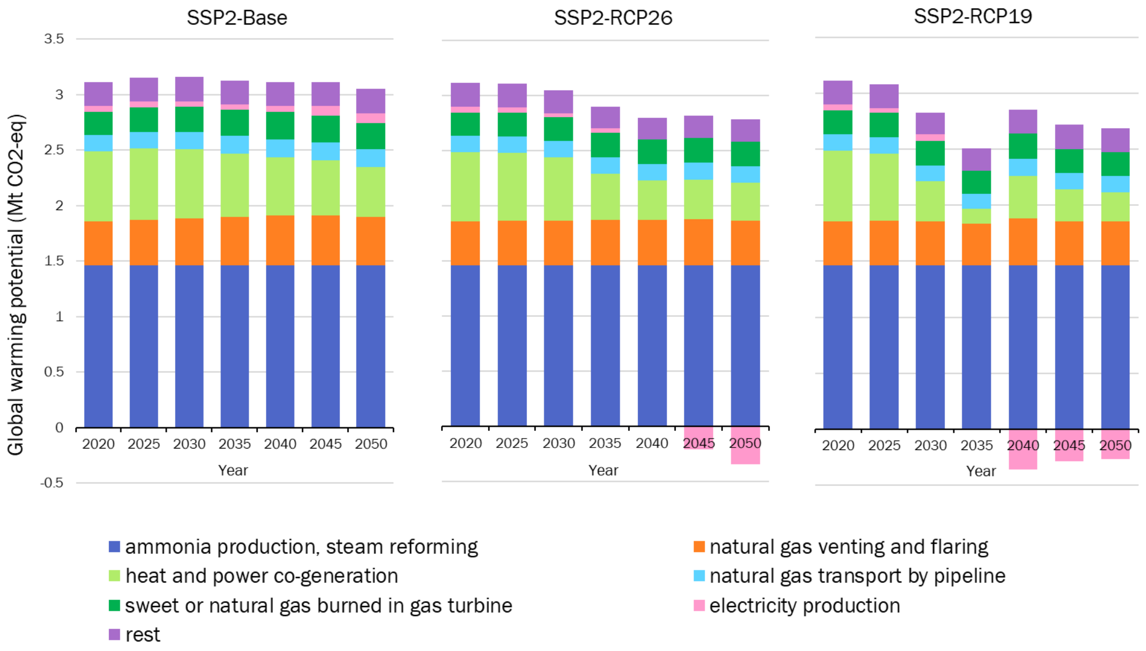


Figure 3-6 Grouped process contributions to 1 kg ammonia from SMR (Russia)

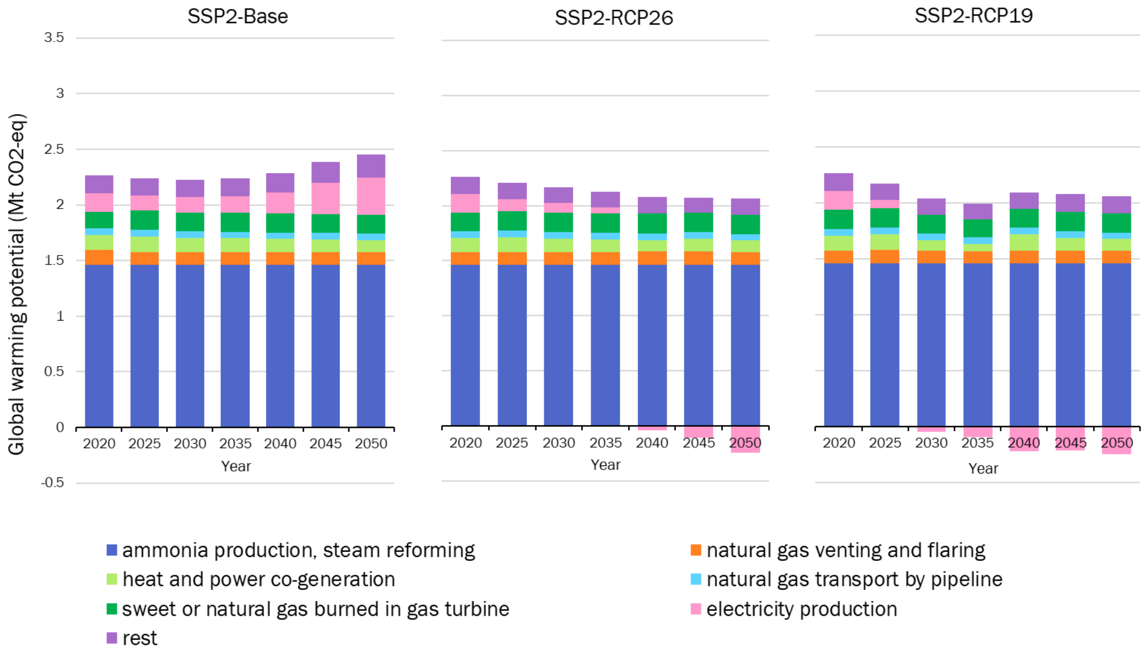


Figure 3-7 Grouped process contributions to 1 kg ammonia from SMR (WEU)

Ecoinvent 3.8 does differentiate natural gas into 27 regional markets, though many are European countries leaving several of the IMAGE regions uncovered. Where possible, SMR in a particular region pulls from the natural gas market of the same region. Where the regions are not covered, the initial default region remains (in this model, the US). The electricity update from *premise* also includes updated natural gas inventories to improve coverage of venting and fugitive natural gas emissions (Meili et al., 2021), so these natural gas production markets are better estimates than the 10-20 year old ecoinvent data. Using the prospective LCI database created in this research (with the electricity/natural gas and ammonia updates), a comparative LCA shows Hungary and Greece as the worst emitters for natural gas production, with a global warming potential of 1.4 kg CO2-eq per cubic metre (m3) natural gas, and the Canadian province Alberta and Denmark as the lowest emitters at 0.2 kg CO2-eq/m3 natural gas.

While CO_2 is often the most talked about greenhouse gas, methane is also a major contributor to global warming. Methane is the main component of natural gas, and during production and transport methane is released (intentionally and through leaks) into the atmosphere (Rutherford et al., 2021). The leaks, or “fugitive” methane emissions, are difficult to measure and have often been underestimated (Kemfert et al., 2022). The IEA agrees that energy sector methane emissions are about 70% higher than reported by national governments (IEA, 2022).

Natural gas has often been presented as a green alternative to coal or other fossil fuels, but expansion of natural gas infrastructure is causing a lock-in which slows the transition to renewable energy sources (Kemfert et al., 2022). In fact, Howarth (2014) found that conventional natural gas and shale gas both have larger greenhouse gas footprints than coal or oil when focusing on a 20-year time scale. Methane leaks also vary in severity by region, depending on local regulations. Satellites have captured images of large methane releases, representing about 8 megatonnes of methane annually, which are not presently counted in inventory estimates (Lauvaux et al., 2022). The worst regions of those measured were Turkmenistan, Russia, and the United States. Plugging the largest leaks will save billions of US dollars and help cut methane emissions (Lauvaux et al., 2022). Emissions from methane leaks could be cut in half if all countries implement the best abatement policies which include banning flaring except in emergencies, mandatory leak detection and repair, and equipment standards (IEA, 2022).

For these reasons, the relative impacts of the technologies in this study should be considered critically. Since they rely on continued use of natural gas, turquoise and blue ammonia should be approached with caution not be considered silver bullet solutions. Despite their relatively low GWP (compared to grey ammonia), they still risk large amounts of fugitive emissions in the upstream processes.

3.1.8 Comparison to ecoinvent 3.8

To illustrate the value of future background scenarios in prospective LCA, a comparison between the existing ecoinvent inventories and the scenario inventories is shown in Figure 3-8. Using the World market, the change in global warming potential (per kg NH_3) due to the three scenarios can be seen. Since no overall World market previously existed in ecoinvent, the IEA 2020 production mix was used to approximate the global average impact. This red line represents the outcome if a prospective LCA is done *without* background scenarios and no improvements were assumed for the future (i.e. the GWP of ammonia production would not change).

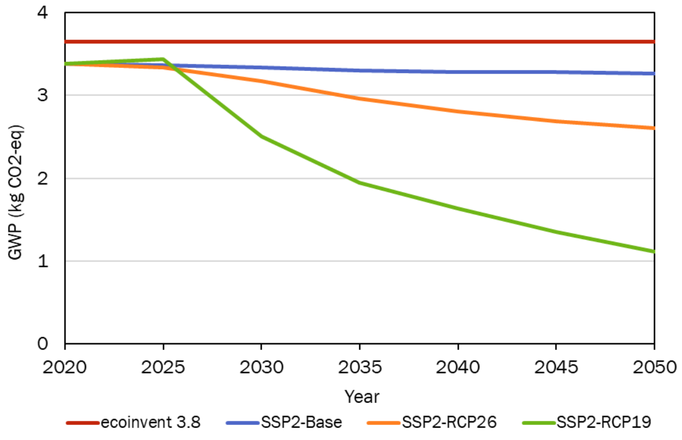


Figure 3-8 Climate change impacts of global ammonia production with and without future background scenarios

In 2020 the difference between the red line and the others is based only on the adjustments/additions to the ammonia production inventories. At that time, ecoinvent 3.8 is only 7% greater than the updated inventories. However, by 2050 the “old” ecoinvent overestimates the climate change impact by 11%, 28%, and 70% respectively against the three scenarios. This can have a major impact on the results of a prospective LCA which has electricity or ammonia used in the background, as many of them do. Figure 3-8 also shows the benefit of (and need for) ambitious climate action. Strong policies such as those modelled in IMAGE SSP2-RCP19 and the IEA’s Sustainable Development Scenario can lead to climate change impacts which are 3.3 times lower per kilogram ammonia than the current state of ammonia production.

Evaluating future technologies based on past data can lead to several missteps such as investing in the wrong technology and ending up with sunk costs or missing the potential of a future “green” technology because it is not the most sustainable option today. While results based on models of the future must always be taken with caution, they can provide valuable insight. It would be wrong to take the 2020 results as true for 2050, but it would also be wrong to assume the RCP19 pathway will become reality without a lot of policy changes and global effort. However, these results are a promising indicator that there is hope for partial decarbonisation of the ammonia industry by 2050.

3.2 Total Ammonia Production Impact

The relative impacts of the different technologies and regions can be used to shed light on the overall ammonia industry impact. Figure 3-9 shows the climate change impact of global ammonia production. The influence of the top producers (which was determined using the regional production volumes and their respective GWPs per kilogram ammonia) is also shown.

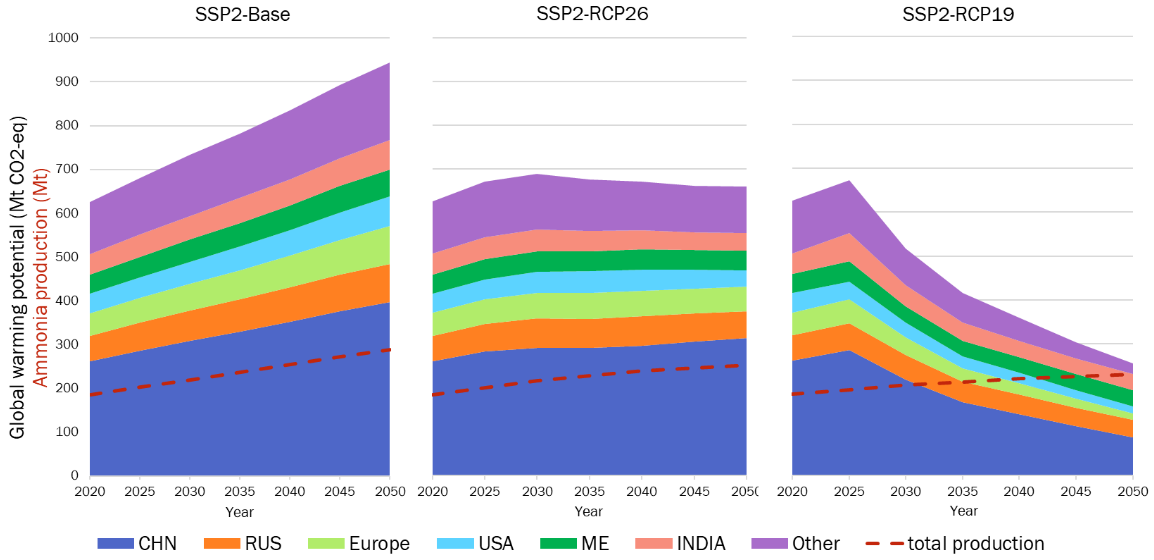


Figure 3-9 Overall ammonia industry GWP (including relative contributions of the top producers), compared to total ammonia production volume

Under the scenarios and assumptions used in this analysis, the ammonia industry will not be fully decarbonised by 2050. In the most ambitious storyline (of the three studied here), SSP2-RCP19, ammonia production will still be responsible for 255 Mt CO2-eq emissions in 2050. However, this still illustrates the value of strong climate policy, because left unchecked (as in the Base scenario) the emissions could reach almost 950 Mt CO2-eq in 2050 (over 3.5 times as much as the RCP19/IEA SDS scenario). The RCP26/IEA STEPS scenario has 660 Mt CO2-eq in 2050 (over 2.5 times the amount in RCP19).

In order to limit global warming to 1.5 °C (67% likelihood), the remaining carbon budget (from the start of 2020) is 400 gigatonnes (Gt or billion tonnes) CO_2 (IPCC, 2021). The cumulative impact of ammonia production from 2020 through 2050 will use 6%, 5%, and 4% of this carbon budget for SSP2 Base, RCP26, and RCP19 respectively (24, 21, and 15 Gt). For 1.7 °C (67% likelihood), which matches a bit more closely to the IEA Sustainable Development Scenario, the remaining budget is 700 Gt.

The main impact comes from the continued use of coal gasification and steam reforming. If green ammonia displaces a larger share of the market and stricter policy measures are put in place, reducing the total amount of fossil ammonia, this number could potentially be lowered. Figure 3-10 shows the amount of ammonia produced globally by each production technology type, classified in their ammonia colours. Here electrolysis is shown as yellow ammonia, as that is how it was modelled in this research, but much of this could be green ammonia in reality.

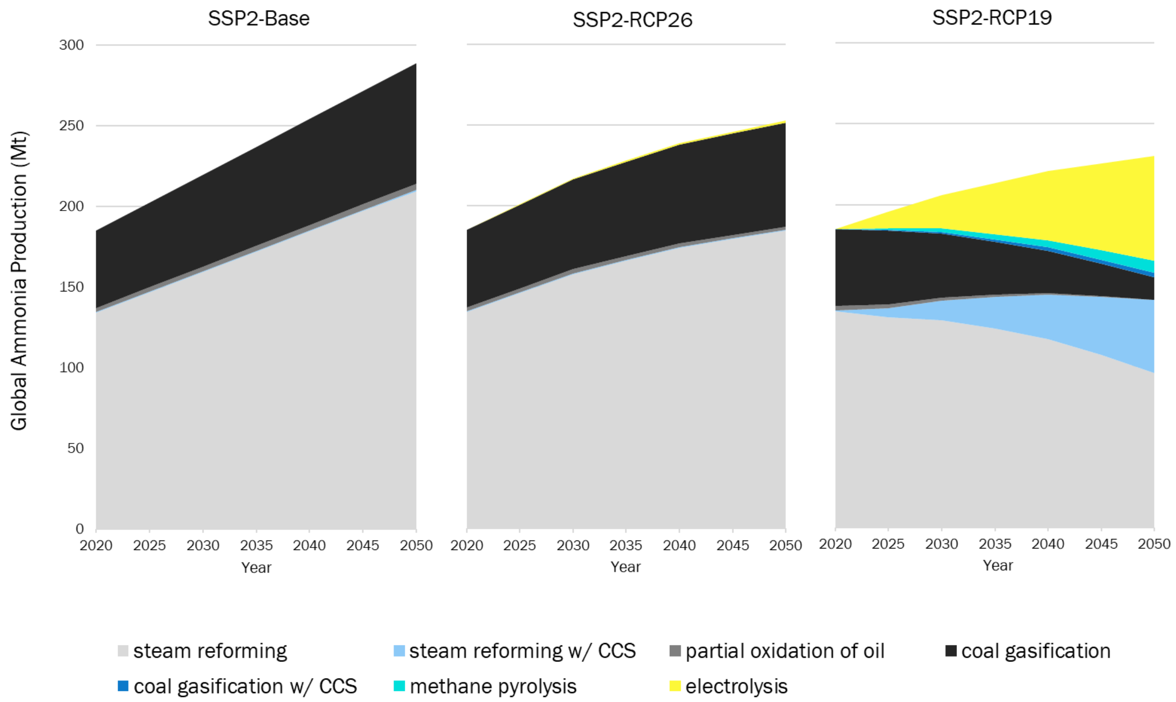


Figure 3-10 Global ammonia production volume by technology type

One of the main reasons that SMR and coal gasification still play a significant role in 2050, is for the production of urea. While some black or grey ammonia plants may be retrofit with CCS, this major fertiliser requires the convenient source of CO_2, which wouldn't be available from electrolysis, methane pyrolysis, or the CCS technologies. This model used the same handling of steam reforming CO_2 emissions as ecoinvent 3.8, where all the CO_2 produced is shown as an emission, whether or not it will be used downstream for urea. While using CO_2 for urea might seem like it is preventing emissions, they are eventually released during the fertiliser's use phase, and should not be considered "stored" CO_2.

This will remain necessary until there is a demand decrease and/or shift to alternative fertilisers. More than half of the ammonia currently produced globally is used for urea, so fossil ammonia (with its source of CO_2) cannot be easily substituted with green ammonia, although biomass gasification is an potential alternative (IRENA & AEA, 2022). The IEA's sustainable development scenario (matched with RCP19) does show a 28% reduction of urea fertiliser use by 2050, with a shift to ammonium nitrate and calcium ammonium nitrate (IEA, 2021a).

The IRENA report anticipates that all new ammonia production capacity will be renewable after 2025 and that it will be cost competitive with blue ammonia after 2030 (IRENA & AEA, 2022). Even with this promising outlook, there is still the issue of existing ammonia plants. They are unlikely to be decommissioned early and become stranded assets. Chinese plants in particular (average age 12 years) are not yet close to their normal “lifetime” (50 years) (IEA, 2021a).

3.2.1 Other Impact Categories

As touched upon in section 3.1.3, the land use impact category (soil quality index) increases for electrolysis in the RCP19 scenario due to the increased use of bioenergy. In contrast, water use for electrolysis was found to be lower than that of steam reforming. Rather than looking at the technologies separately, the impact for the market for ammonia (World) can be combined with production volumes to determine the total impact of the industry.

Figure 3-11 shows the percent difference between the total global impact in a particular year/scenario versus the total global impact in 2020. As expected, land use impact has the greatest increase in RCP19, but water use has the greatest impact increase in the Base scenario.

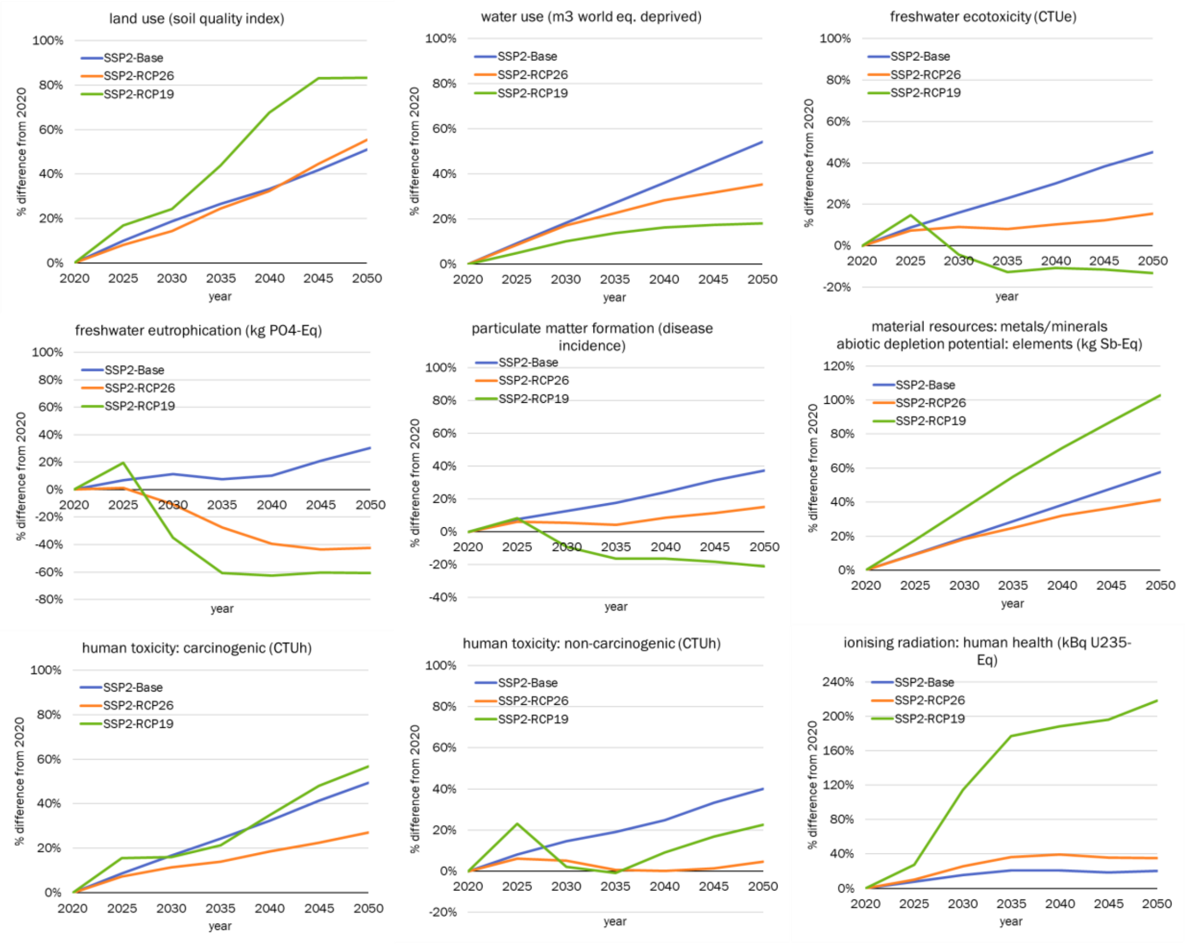


Figure 3-11 Percent difference (against 2020) of total global impacts over time for all scenarios (multiple impact categories)

Many categories follow the same pattern as climate change and water (Base = worst, RCP19 = best), but there are exceptions. Material depletion of metals/minerals rises the most in the sustainable scenario, driven mainly by copper mining. Due to its high electrical conductivity and low substitution potential, copper demand is tied to the growth of renewable energy systems (Schipper et al., 2018). Copper smelting also contributes to the growth of carcinogenic and non-carcinogenic human toxicity impacts in the RCP19 scenario, though the Base scenario has the highest growth for non-carcinogenic due to hard coal ash treatment combined with the higher total volume of ammonia. Finally, ionising radiation increases by over 200% in the sustainable scenario due to the growth of nuclear energy (and the corresponding treatment of tailings and nuclear waste).

While these are important side effects to keep in mind, these impact categories are less well defined and reviewed than climate change, and the results should always be taken with caution. Besides metal depletion, which will be discussed again briefly in section 3.4.1, these categories will not be explored more deeply in this thesis.

3.2.2 Regional Total Impact by Technology

To look closer at the main drivers of the regional emissions, the contribution of each technology to its total impact can be explored. Figure 3-12 shows these results for China. As expected, coal gasification is responsible for most of the emissions of China's ammonia industry.

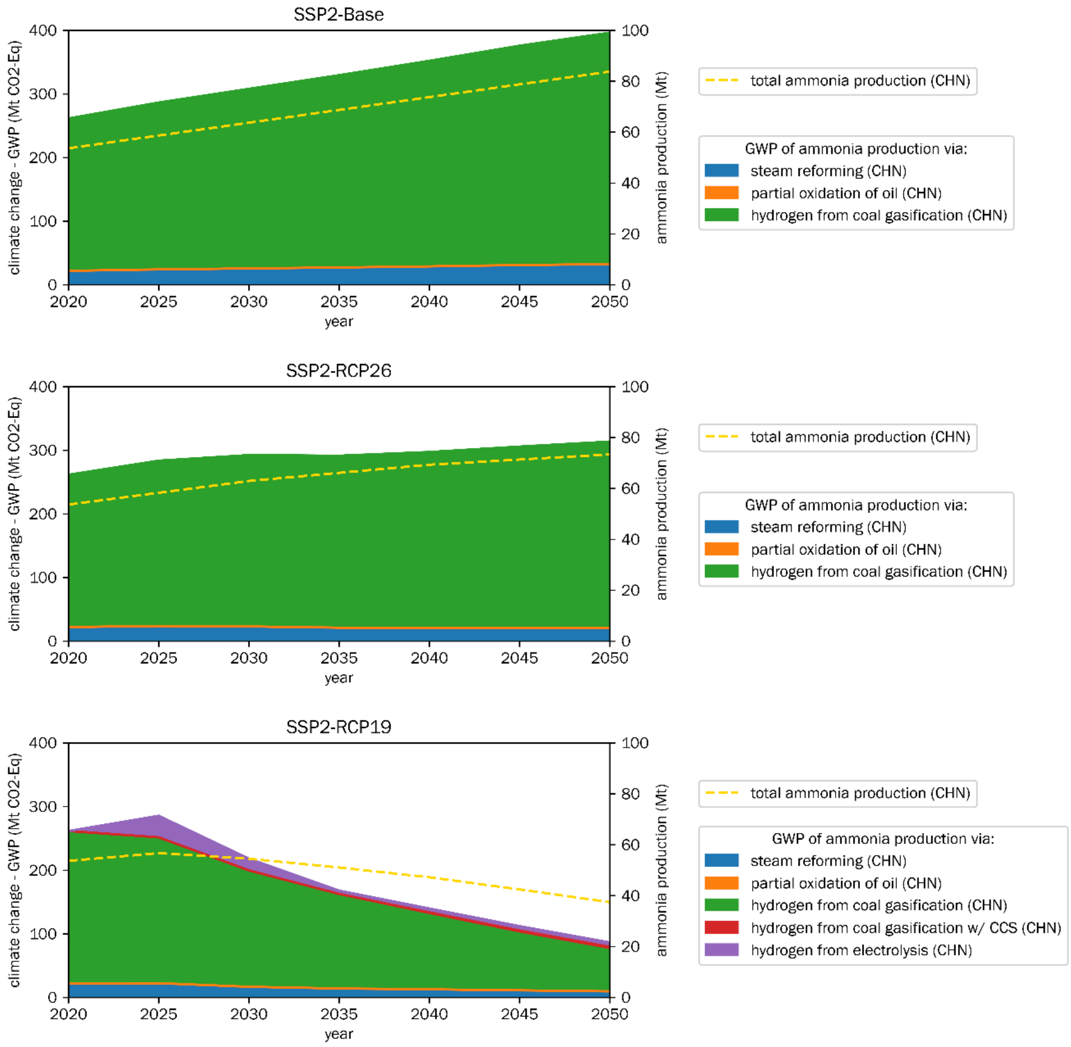


Figure 3-12 Overall GWP from ammonia production (China); contribution by technology type

When looking at this chart, it's important to understand that it shows the GWP contributed by each technology, rather than production shares. For example, the purple electrolysis area in RCP19 remains small because its relative impact is small, not because the production volume of ammonia via electrolysis hydrogen is small (on the contrary, in China in 2050 (RCP19) more ammonia is produced via electrolysis than by coal gasification). As discussed at the start of this section (3.2), the impact of ammonia from electrolysis does not make a very significant contribution to the overall GWP. The total GWP of Chinese ammonia production goes from over 260 Mt CO2-eq to below 90 Mt in the sustainable scenario.

The total ammonia production is shown as a dashed yellow line, in order to illustrate the connection between the production volume and the change in total impact (particularly in the Base scenario where they are closely linked).

Some regions show a greater decoupling between the total ammonia production and the total climate change impact. See, for example, India in the RCP19 scenario in Figure 3-13.

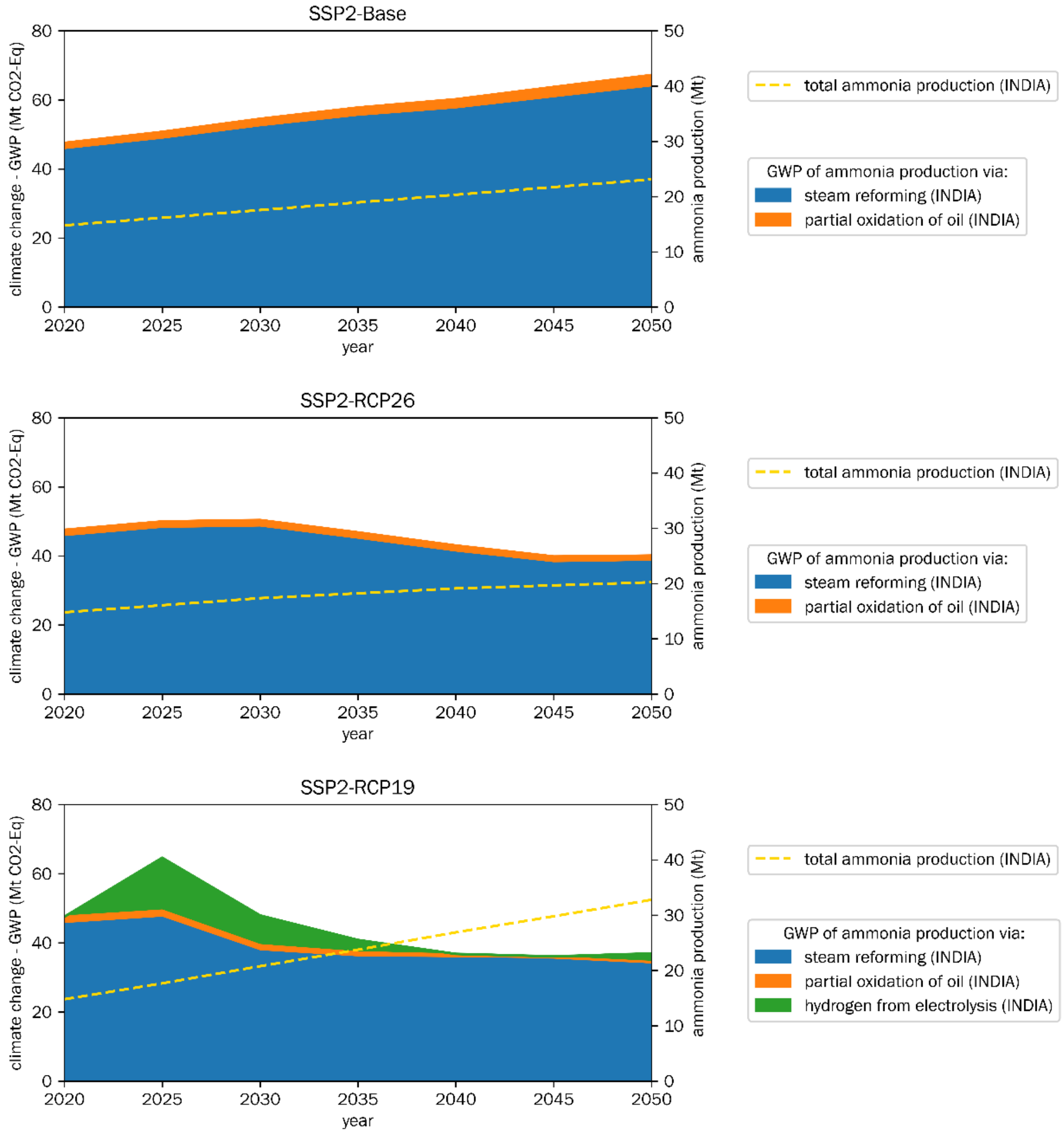


Figure 3-13 Overall GWP from ammonia production (India); contribution by technology type

Here the total ammonia production continues to grow steadily, while the industry's emissions plateau after 2035. The 2025 emissions spike from both China and India also highlight the need to use designated renewables for electrolysis ammonia, rather than connecting to the grid.

3.3 Model Limitations

This model is meant to improve the future background coverage of ammonia in the chemical industry. While it meets this goal, there are still several limitations due to simplifications and assumptions. First, as discussed previously, the background IMAGE electricity storylines and IEA ammonia scenarios do not align perfectly. Comparability can be an issue when scenarios of different sources are mixed. However, even with a slightly different scenario alignment (e.g. the IEA Sustainable Development Scenario matched to RCP26 instead of RCP19), this would still be a better result that having no background scenario at all, as was demonstrated in Figure 3-8 at the start of this section.

When looking at data quality, some of the inventories (particularly partial oxidation of heavy fuel oil) are weaker than others due to availability of information. A more accurate inventory would improve the model, but since this technology represents less than 2% of global ammonia production and is being phased out in the sustainable scenario, it is not a critical issue.

This thesis focused on ammonia in the chemical industry, but there is also potential for major growth in ammonia as a fuel, energy carrier, or storage medium. Ammonia produces no CO_2 emissions when combusted, has a high energy density, and is easier to transport and store than pure hydrogen (IEA, 2021a). These emerging uses of ammonia are excluded from the main scope of the IEA Roadmap, but they are important to keep in mind. The SDS 2050 ammonia demand could almost double from 230 Mt for existing agricultural/industrial uses (as used in this model) to over 400 Mt if maritime fuel and power generation are added (IEA, 2021a).

Some forecast even greater growth of emerging ammonia sectors. The IRENA 1.5°C scenario expects almost 200 Mt and 130 Mt of new (renewable) ammonia demand by 2050 due to the maritime sector and trade of ammonia as a hydrogen carrier respectively (IRENA & AEA, 2022). Their 2050 projection of ammonia demand for existing applications (334 Mt) is higher than the IEA's and results in a 2050 total ammonia demand of 688 Mt (566 Mt of which would come from renewable energy sources) (IRENA & AEA, 2022). Since these applications for ammonia do not require any CO_2 downstream, as with urea, it's makes sense that electrolysis would be used to cover this new demand. This means that the markets for ammonia *as a fuel* would have a different technology mix than the markets for ammonia (as a chemical) produced in this thesis. The total climate change impact will depend on both the overall mix of production technologies and the type of electricity used for electrolysis ammonia. If this new volume is completely covered by renewables, it's possible that there will be no additional direct emissions, and the total global impact would not change significantly. Only indirect or background emissions would be added, and if BECCS are used, the amount could even decrease.

These outlooks are not without challenges. In order to use green hydrogen (or ammonia) to decarbonise the chemical industry, other hard-to-abate sectors, and emerging applications such as fuels, there will need to be a huge and rapid increase in green energy installations to meet the demand (Collins, 2020).

Another limitation is that ammonia plant sizes will likely change when moving to electrolyser-based H2 since these will be smaller operations (Brown, 2018). This is not reflected in the inventories but would be worth investigating in future work. In addition, an average ammonia transport distance was given to all new ammonia markets, based on those from ecoinvent 3.8. This means that transport distances can be over- or under-estimated and are not regionally differentiated, which is a drawback. Transportation may become more significant in the overall impact of ammonia in the future, especially if plants are more distributed and sources of renewable energy need to be nearby. This should be improved in later models.

Finally, green ammonia is not considered separately in this model. If they can overcome issues of intermittency, hydrogen and ammonia producers may move towards an off-grid supply of electricity, choosing to power electrolysers by on-site renewable energy. This course of action will be very beneficial in terms of environmental impact, because it doesn't require waiting for the grid mix to become more sustainable. It does however make it more complex to standardise these plants in an LCA. Individual inventories can be created for hydrogen produced from different renewable electricity sources, but predicting the future “average” mix of these will be a major undertaking. Alternatively, LCA practitioners completing site-specific LCAs can choose to manually adjust their electricity inputs, rather than using the electricity markets.

3.4 Sensitivity Analysis

3.4.1 Electrolysis and Critical Raw Materials

To test the robustness of the chosen inventories and scenarios, an input is modified and the change in the output is measured (sensitivity analysis).

One of the weakest assumptions during the setup of the scenario files was that the ratio of alkaline and PEM electrolysis would remain static over time. This assumption was made due to lack of other forecasts, and due to the notion that most of the final impact (particularly in terms of climate change) would come from the electricity used rather than the electrolyser itself.

A comparison of 1 kg hydrogen produced by each electrolyser type (in China) revealed that they differ only slightly in global warming potential. This is likely due to the small difference in electricity input required (50 vs. 55 kWh for 1 kg hydrogen from AE vs. PEM). This difference becomes less significant in later years as the electricity mix gets cleaner in RCP26 and RCP19.

To compare the overall impact on the ammonia industry of the choice of AE or PEM, two new scenario files were constructed. One where AE represents 100% of the ammonia from electrolysis hydrogen, and the other with 100% PEM. The full database was constructed for each of these scenario files. The final results can be compared in order to test how sensitive they are to a change in electrolysis type. The climate change impacts of 1 kg produced from the global market for ammonia under the three situations (original mix, 100% AE, 100% PEM) were almost identical. This means that the choice of electrolyser type has not skewed the results. Plots of these results can be seen in Appendix 2, Figures A2- 14 and A2- 15.

In an LCA of proton exchange membrane water electrolysis and steam methane reforming, Bareiß et al. (2019) also found that electrolysis is a low-emission alternative to SMR when renewable electricity is used. This sensitivity analysis was also consistent with their findings that the components of the electrolyser itself are negligible when compared to the impact of the electricity used. With respect to the choice of electrolyser, this model is quite robust.

While it is an advantage that the results will not change dramatically if the future mix of PEM vs AE is not correctly estimated, this also means that the differences between the two technologies may need to be assessed through a different method than LCA. In some cases, such as to gain an understanding of material criticality, a global material flow analysis may be better suited.

For example in Figure 3-14, the metals/minerals resource depletion results for the two electrolysis types are shown (given in Abiotic Depletion Potential (ADP) of kg antimony-equivalent (Sb-eq) as recommended by the JRC (Fazio et al., 2018)).

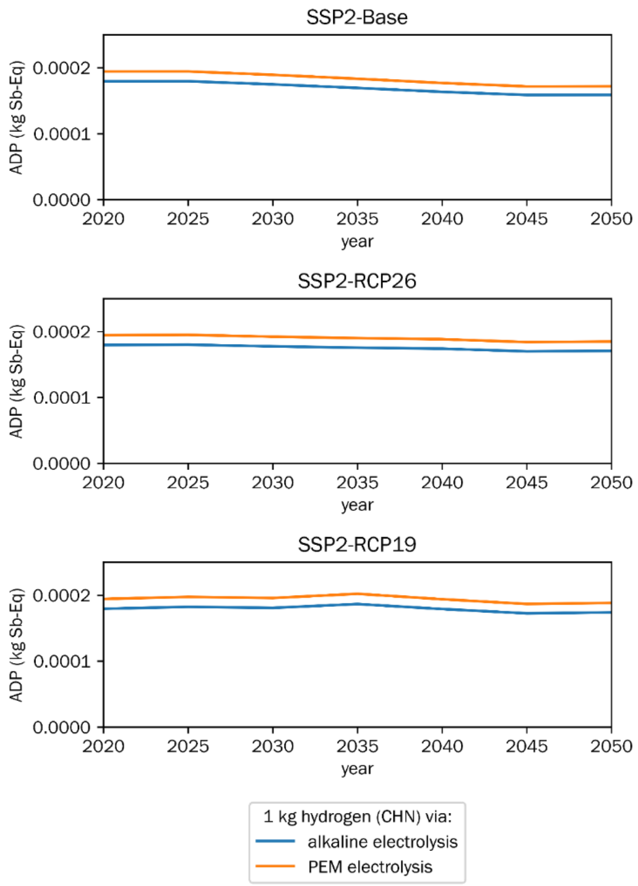


Figure 3-14 ADP of 1 kg hydrogen produced by alkaline and PEM electrolysis (China)

The ADP model includes characterisation factors for many metals and elements such as iridium and platinum (van Oers et al., 2020), though in this case their impacts are almost completely drowned out by copper mining. While there is a slight difference between the two electrolysis types (PEM is 8% higher than AE), this does not provide much insight into supply issues or depletion of specific resources.

The scarcity of iridium, which will limit the growth of PEM technology unless there is a sharp decrease in PEM cell iridium loading and a sharp increase in recycling rates (Minke et al., 2021), is not visible in these results. Looking at the ADP alone, it's not clear that without technological improvements PEM will be restricted by its raw material demand.

These improvements may be feasible. Bareiß et al. (2019) assume a major reduction of the required amount of platinum and iridium is possible in the near future (from 0.075 to 0.010 kg platinum and from 0.75 to 0.037 kg iridium for a 1 MW PEM stack), which will help both with the cost of the electrolyser stacks and slowing the depletion of these metals.

In a study focusing on the manufacturing and end-of-life phases of alkaline and PEM electrolysers, Lotrič et al. (2021) also find that PEM has a larger environmental impact than AE on average due to the use of platinum. They also conclude that closed-loop critical raw material recycling can lower the abiotic depletion potential can by 70% for PEM electrolysers and 62% for alkaline electrolysers (Lotrič et al., 2021).

Practitioners also need to remember that LCA is not a test of feasibility. It doesn't *limit* the amount of an electricity/fossil fuel/steel that you can use, it simply quantifies the theoretical impact of the system being studied.

3.4.2 Methane Pyrolysis Multifunctionality

Methane pyrolysis has the potential to significantly reduce CO_2 emissions from ammonia, but it will need to be developed further before it is viable (Ausfelder et al., 2022). This also means that the methane pyrolysis inventory could change drastically when the technology has scaled up. The new inventory added to this model is preliminary and doesn't contain the same level of detail (of inputs or emissions) as the other inventories. For this reason, the methane pyrolysis results are considered less reliable than those of the more established technologies.

In addition to that, methane pyrolysis is a multifunctional process which produces 1 kg hydrogen and 3 kg solid carbon. In the modelling stage, the decision was made to allocate the burden on an economic basis by a factor of 0.71 to H2 and 0.29 to carbon (calculated on $1.11/kg H2 and $0.15/kg C (von Wald et al., 2020)). However, this assumes that there is a future market for all the carbon co-produced by methane pyrolysis. In order to understand the influence of this modelling choice, another database was created where the entire environmental burden is allocated to the hydrogen production (i.e. the carbon has a $0 value and no allocation is performed).

In the IEA SDS scenario, North America is expected to have the highest share of methane pyrolysis compared to the other regions. Figure 3-15 therefore shows the USA results for the original model (red line) compared to the new model (dashed red line) with hydrogen "responsible" for the full burden of methane pyrolysis.

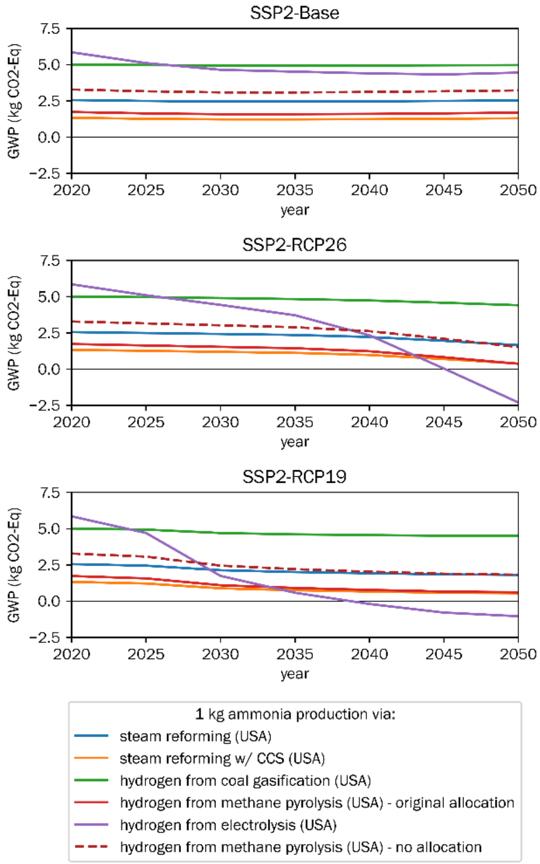


Figure 3-15 GWP per ammonia production technology (USA) – original model (solid red line) vs. methane pyrolysis with no allocation (dashed red line)

The dashed red line representing 1 kg ammonia produced by methane pyrolysis is now higher than SMR (blue line) for almost the whole time period and all scenarios. It remains the lower emitter than coal gasification and early (grid) electrolysis. This reinforces the point that no final decisions should be made about methane pyrolysis based on this model alone.

Another interesting region to look into is Russia, shown in Figure 3-16 below. Based on the original model (orange line), methane pyrolysis has the lowest global warming potential across all scenarios and years. With the new allocation (dashed orange line), steam reforming performs better (as does electrolysis by 2050 in RCP26 and by 2035 in RCP19).

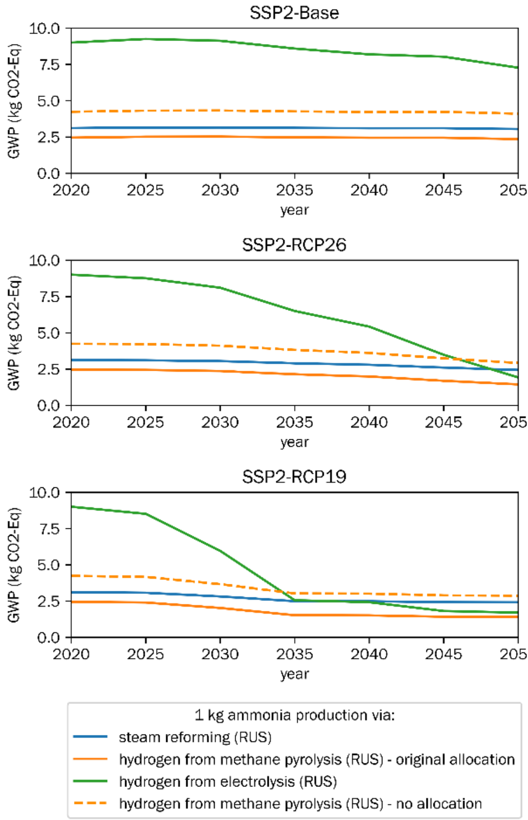


Figure 3-16 GWP per ammonia production technology (RUS) – original model (solid orange line) vs. methane pyrolysis with no allocation (dashed orange line)

In terms of the allocation method for methane pyrolysis, the model is not as robust as it was for electrolysis. Since the ranking of the technologies changes when the allocation changes, the results are less reliable. A better understanding on if there will be future demand for the carbon co-product will help determine the best allocation method for this process. More research should be done into methane pyrolysis before final decisions are made about this technology.

In addition, while not measurable in an LCA, the continued reliance on non-renewable resources such as natural gas may also be a reason to avoid choosing turquoise ammonia over green. This is in part for environmental conservation, but also for social and economic reasons which have become increasingly relevant in recent months (i.e. the European gas crisis due to dependence on Russian supply).

3.4.3 Flexibility of Ammonia Database

In order to assess the flexibility of this method, the chosen scenarios were applied to the REMIND Integrated Assessment Model. Since their SSP2 storylines can easily be matched to the IMAGE ones (as in Table 2-1), the main task was to update the production volumes to the new regions. The geographical divisions were slightly different, and didn't align as closely to the original IEA regions. Table 3-1 shows the 12 REMIND categories and their corresponding IMAGE categories. The total production volumes for each REMIND region came from combining the total of the

IMAGE regions as listed in the second column. However, because the production shares came from the IEA regional groups, some assumptions were made to find the REMIND region's production shares. For example, MEA region includes the Middle East, North Africa, and Turkey so the production technology mix was an average of the IEA's Middle East, Africa, and Europe.

Table 3-1 REMIND regional divisions compared to IMAGE and IEA

REMIND	IMAGE	IEA production mix
Canada, Australia, New Zealand (CAZ)	CAN + OCE	North America, Asia Pacific (≈Africa)
China (CHA)	CHN	China
European Union (EUR)	WEU + CEU	Europe
India (IND)	INDIA	India
Japan (JPN)	JAP	Asia Pacific (≈Africa)
Latin America (LAM)	BRA + RSAM + RCAM + MEX	Central & South America (3/4), North America (1/4)
Middle East, North Africa, Turkey (MEA)	ME + NAF + TUR	Middle East, Africa, Europe
(Non-EU member states) NEU	*excluded from scenario file*	-
Other Asia (OAS)	INDO + SEAS + RSAS + KOR	Asia Pacific (≈Africa)
Russian Federation (REF)	RUS + STAN + UKR	Russia (2/3), Europe (1/3)
Sub-Saharan Africa (SSA)	WAF + SAF + EAF + RSAF	Africa
United States of America (USA)	USA	North America

NEU (non-EU member states) was excluded from the scenario file in order to simplify the conversion between the two IAMs. Technically, EUR (European Union) does not match perfectly with the IMAGE or IEA Europe regions, which cover EU and non-EU states.

With the new scenario and yaml files, the Custom Scenario Tool produced a database with the three storylines (SSP2-Base, SSP2-PkBudg900, PkBudg1100) and 11 regional markets.

The impact of 1 kg ammonia production from the top producers' markets for ammonia can be compared in Figure A3- 1. The overall results are not very different from the outcomes of the IMAGE database. The matching scenarios can be seen in Figure 3-17.

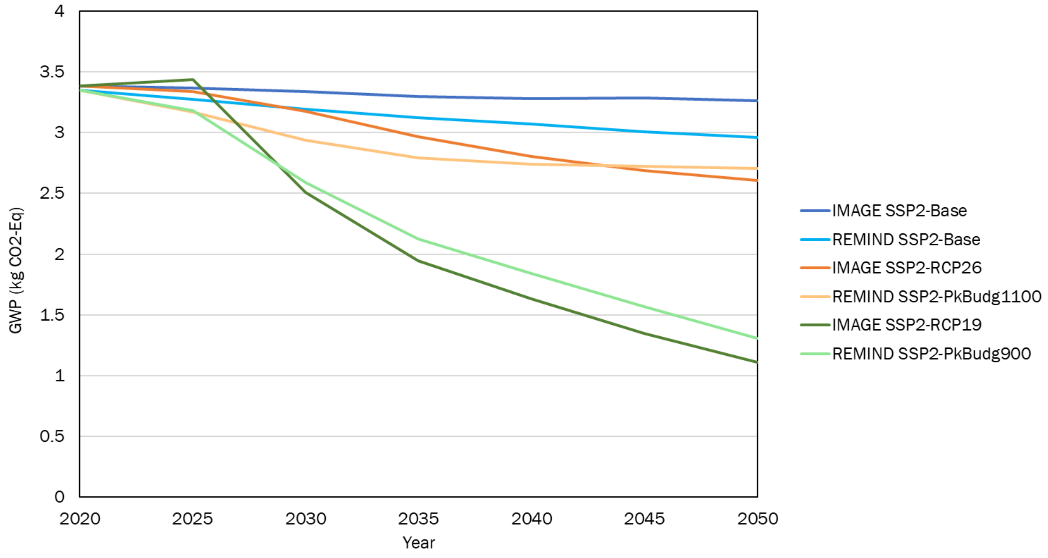


Figure 3-17 GWP of 1 kg from the market for ammonia (World) of each corresponding IMAGE and REMIND storyline

For the World market, the GWP of 1 kg ammonia from REMIND differs by less than 10% from IMAGE at each corresponding year and scenario.

One of the key differences between the two IAMs is more noticeable at the regional technology level. In the REMIND storylines, the GWP for ammonia from electrolysis remains positive for all of the top producers, except the REF region (Russian Federation plus Eastern Europe and Central Asia) in 2040 in PkBudg900. In the IMAGE scenarios, the GWP for ammonia from electrolysis goes below zero in the RCP26 and RCP19 storylines for Western Europe, the Middle East, and the USA. This indicates that REMIND places less reliance on BECCS to meet the warming targets.

REMIND's SSP2-Base scenario also seems to decarbonate electricity more significantly than IMAGE's SSP2-Base. For several regions electrolysis becomes a contender in terms of lower environmental impact after 2040 or 2045, whereas with IMAGE, electrolysis remains one of the worst emitters in the base scenarios.

The REMIND technology comparison graphs for the top producers can be seen in Appendix 3, Figures A3- 2 through A3- 7.

This analysis shows that the method is flexible enough to move between IAMs, *if* the IAMs have corresponding storylines. The only modification needed for conversion from one IAM to the other is the regional regrouping. An understanding of the underlying model is also important when drawing conclusions based on the results.

4 Conclusions and Recommendations

This thesis aimed to answer the overarching research question: ***How will the scale and technology mix of ammonia production for existing applications develop in the future, and what will that mean for the climate?*** Using the IEA Ammonia Roadmap aligned with the IMAGE electricity scenarios, an extensive prospective LCI database was produced allowing for scenario LCAs across three storylines from 2020 to 2050.

Regionally, China produces the largest volume of ammonia as well as the ammonia with the largest climate change impact, due to the dominance of coal gasification technology. While Chinese production peaks by 2030 in the sustainable development scenario, and coal gasification is gradually decreased and offset by electricity, the region's per-kg impact and production volume is still the highest in 2050.

Regional differences in background processes such as natural gas production and electricity production have a major impact on the foreground technology processes. For example, steam reforming in Russia produces 1.4 times the life cycle emissions of steam reforming in Western Europe, despite the SMR process itself being the same.

For many regions, electrolysis (yellow) ammonia becomes the technology with the lowest global warming potential by around 2045 in the RCP26 storyline and 2035 in RCP19. Until the regional electricity mixes are cleaner, SMR, SMR with CCS, or methane pyrolysis offer lower emission options. However, electrolysis using on-site or designated renewable energy creates emission-free green ammonia, removing the need to wait years for a cleaner regional grid. This means that electrolysis is the best choice for new plants if a producer is not making urea on-site (or has an alternative source of CO_2 if they are). The type of electrolyser should be chosen carefully, with a look at future material scarcity.

Reduction in urea demand will be important for reducing reliance on SMR with CCU, and a swift uptake of electrolysis with designated renewables must be the focus.

Overall, under the scenarios and assumptions used in this analysis, the ammonia industry will not be decarbonised by 2050. In the most ambitious storyline, SSP2-RCP19, ammonia production will still be responsible for 255 Mt CO2-eq of yearly emissions in 2050. However, without the strong climate policies in the RCP19/IEA SDS scenario, the 2050 emissions would be more than 2.5 or 3.5 times worse (RCP26/IEA STEPS or the Base scenario respectively).

If green ammonia plays a larger role or stricter policy measures are put in place, this number could potentially be lowered. The cumulative impact of ammonia production from 2020 through 2050 will be 24, 21, and 15 *giga*tonnes CO2-eq for SSP2 Base, RCP26, and RCP19 respectively. This will use 6%, 5%, and 4% respectively of the remaining carbon budget (from start of 2020, to limit global warming to 1.5°C with a 67% likelihood).

The RCP19 storyline requires a sufficiently high carbon price to drive the growth of renewable ammonia alternatives (IEA, 2021a). The current lack of emissions regulations restricts the growth of green ammonia since it is not yet cost-competitive, and strong policies are needed to accelerate it (IRENA & AEA, 2022).

While the sustainable scenario is the best option in terms of climate change, the increased use of BECCS and renewable electricity installations can lead to some burden shifting. RCP19 has the lowest impact for some key categories such as global warming potential, water use, freshwater ecotoxicity, freshwater eutrophication, and particulate matter formation. It has the highest impact for land use (due to BECCS), metal depletion (due to renewable electricity), ionising radiation (due to nuclear power). These other impact categories are not as well modelled as climate change, but it’s still important to keep this side effects in mind and work to minimise them as much as possible.

Material criticality or scarcity could also be a constraint for massive expansion of electrolysis technology, but that is less well captured in LCA. Other methods such as material flow analysis would be better suited to assessing critical raw materials in the green hydrogen/ammonia supply chain.

The model used in this analysis is robust enough to handle changes in electrolysis type, because their relative impacts are fairly similar in terms of global warming potential (since they depend mainly on the electricity used). However, it is less robust in terms of the allocation method for methane pyrolysis since the ranking of the technologies changed when the allocation changed. In general, more research should be done into methane pyrolysis before final decisions are made about this technology.

The method is flexible enough to be used with other IAMs, providing that the storylines still line up and the regions are regrouped.

Based on the outcomes of this thesis, there are some recommendations which would add to the reliability and robustness of the results and some opportunities for further research. First, the transport values added to the ammonia markets could be improved to be regionally specific. If this is not feasible on a global level, then individual LCA practitioners could improve their studies with more accurate location data for their specific case. Plant size changes could also be incorporated into the inventories, as they would have different infrastructure and transportation.

Second, the electrolysis inventories should be revised and the emerging technology solid oxide electrolysis should be added. Their relative shares over the next 30 years should be made dynamic rather than static, as was the assumption in this research. Electrolysis with flexible inputs (such as local renewable electricity) will also allow the studies to include green ammonia, rather than just yellow.

Finally, better quantification of secondary impacts, such as criticality of raw materials and land competition, could be investigated for LCAs.

Even without these improvements, the method used in this thesis can easily be repeated for other products such as chlorine and methanol. This will increase the future background scenario coverage for the major polluters in the chemical industry. As discussed in the introduction, methanol is the next major industrial user of hydrogen after ammonia, so the hydrogen inventories built for this thesis can be applied to a methanol scenario without much difficulty.

Another next step to expand the coverage of these prospective LCI databases would be to model the future of fuels. Beyond its existing applications, ammonia is expected to be used in the future as a fuel and as an energy carrier. This could result in triple the total volume of annual ammonia production than modelled in this thesis. However, this difference should be covered by green ammonia and not by the market mixes used here (for “chemical” ammonia). The development of new future fuel markets for background ecoinvent databases would include ammonia in the mix, and can therefore build upon the inventories created in this thesis. The hydrogen technologies can also be used for future hydrogen databases, though the technology (market) mixes will again be different.

As more information becomes available, the inventories should be kept up to date, particularly for the emerging technologies such as methane pyrolysis.

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In addition to my two supervisors, I would like to thank anyone who took the time to chat with me and discuss their work, provide data, or offer insights. In particular, this research wouldn’t have been possible without the help and patience of Romain Sacchi (Paul Scherrer Institute) who, in addition to developing the Custom Scenario Tool to simplify the integration of our scenarios via *premise*, provided troubleshooting advice and answered many questions along the way. Thanks also to Sebastiano Carlo d’Angelo for the extra insight into the ammonia inventories, Amelie and Maria for the weekly “future scenario” discussions, and Bart for the Python (and emotional) help. Finally, thank you to my dad and to my friends who supported me (and listened to me talk about ammonia) for the past seven months.

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Appendix 1 – Model Assumptions

Table A1- 1 Inventory modelling choices and assumptions

IEA Category	Technology	Source	Details and Assumptions
gas (& gas w/ CCU)	ammonia production, steam reforming	Carlo d'Angelo et al., 2021	Hydrogen production through SMR followed by ammonia production by the Haber-Bosch process are both covered within this inventory. Business-as-usual ammonia production (H2 from steam methane reforming (SMR) and autothermal reforming (ATR) plant) (Carlo D'Angelo et al., 2021). Assuming that the CO_2 is vented OR that it is used downstream for e.g. urea. Water volumes are calculated when needed based on density @ 20C (998.19 kg/m3). In ecoinvent 3.8, SMR also had a steam co-product and the impact was allocated 95.7% to ammonia, 4.3% to steam. However, this process uses any excess steam to offset some electricity needs, so no steam co-product is created (Carlo D'Angelo et al., 2021).
gas w/ CCS	ammonia production, steam reforming w/ CCS	Carlo d'Angelo et al., 2021 IEA, 2021a	Hydrogen production through SMR followed by ammonia production by the Haber-Bosch process are both covered within this inventory. Technologies "steam reforming w/ syngas CCS" and "steam reforming w/ syngas and flue gas CCS" provide an 82% and 98% CO_2 emission reduction respectively, versus the standard steam reforming process (Carlo d'Angelo et al., 2021). The IEA Ammonia Technology Roadmap indicates that CCS-equipped routes have a 90% CO_2 capture rate (IEA, 2021a). This process, "steam reforming w/ CCS", is therefore assumed to consist of half "syngas CCS" and half "syngas + flue gas CCS" (82*0.5 + 98*0.5 = 90).
oil	ammonia production, partial oxidation of oil	Al-Qahtani et al., 2021 Reed & Kuhre, 1980 Fertilizers Europe, 2000 Carlo d'Angelo et al., 2021	Hydrogen production through POX followed by ammonia production by the Haber-Bosch process are both covered within this inventory. The 1.5 kg of coal required for 1kg NH3 (Al-Qahtani et al., 2021) was modified to have a heavy fuel oil feedstock of 88.2 wt% carbon (Reed & Kuhre, 1980) meaning that instead of 1.5 kg coal, 1.7 kg heavy fuel oil is used. CO2 emissions for 1 kg NH3 are 2-2.6 kg for POX of heavy oil. 700 mg/Nm3 NOx = 0.00224 kg/kg NH3. 0.3 ppmv H2S = 1.46e-6 kg/kg NH3. 100 ppmv methanol = 4.58e-4 kg/kg NH3. 30 ppmv CO = 1.2e-4 kg/kg NH3 (Fertilizers Europe, 2000). Chemical factory, nitrogen, NH3 catalyst, tap water, spent catalyst, water biosphere flows, from Carlo d'Angelo et al. (2021) Haber-Bosch of biomass gasification hydrogen.

			Liquid oxygen (23.1% of 4 kg air (Fertilizers Europe, 2000)) from cryogenic air separation is added as an input, which could result in an over-estimation of electricity, since compression to liquid form might not be needed if the air separation is done on-site.
coal (& coal w/ CCU)	ammonia production, hydrogen from coal gasification	Carlo d'Angelo et al., 2021	Haber-Bosch process, using hydrogen (from coal gasification) and nitrogen to produce ammonia. Electricity input same as for H-B from electrolysis hydrogen (Carlo d'Angelo et al., 2021). The hydrogen from coal gasification and its electricity co-product are separate inventories (below).
coal w/ CCS	ammonia production, hydrogen from coal gasification w/ CCS	Carlo d'Angelo et al., 2021	Haber-Bosch process, using hydrogen and nitrogen to produce ammonia. Same as H-B for H2 from coal gasification, changed to have input of H2 from coal gasification w/ CCS (below).
pyrolysis	ammonia production, hydrogen from methane pyrolysis	Carlo d'Angelo et al., 2021 Al-Qahtani et al., 2021 Machhammer et al., 2016	Haber-Bosch process, using hydrogen and nitrogen to produce ammonia. Same as H-B for H2 from coal gasification, changed to have input of H2 from methane pyrolysis (inventories below).
electrolysis	ammonia production, hydrogen from electrolysis	Carlo d'Angelo et al., 2021	Haber-Bosch process, using hydrogen and nitrogen to produce ammonia (Carlo d'Angelo et al., 2021). Hydrogen from electrolysis inventories are below.
	average ammonia transport	ecoinvent 3.8	Average transport distances based on the old ecoinvent "market for ammonia" activities. These are added to the new individual ammonia production processes, since the custom scenario tool cannot easily add them to the new markets. Europe did not originally have transport by sea, so this can lead to over-estimation for some regions.
	CO2 from ammonia production, steam reforming	ecoinvent 3.8	By-product of ammonia from SMR, this CO_2 is vented or used in the chemical industry (primarily for urea) in the case of CCU. Based on ecoinvent 3.8, which includes "carbon dioxide, in industry" for tracking purposes. No impact is allocated to the CO_2 (so the production of the ammonia is assumed responsible for the full burden). There are no values given to technosphere or biosphere flows.
	ammonia production, steam reforming w/ syngas CCS	Carlo d'Angelo et al., 2021	50% contribution to "ammonia production, steam reforming w/ CCS" process

	ammonia production, steam reforming w/ syngas and flue gas CCS	Carlo d'Angelo et al., 2021	50% contribution to "ammonia production, steam reforming w/ CCS" process
	multifunctional coal gasification	*premise* (Wokaun & Wilhelm, 2011) Al-Qahtani et al., 2021	Expansion of *premise* generated inventory: hydrogen production, gaseous, 30 bar, from hard coal gasification and reforming, at coal gasification plant (product Hydrogen, gaseous, 30 bar). Some location changes to fit China/RoW better. New emissions (CH_4, N_2O) and updated values (coal, water, CO_2) (Al-Qahtani et al., 2021). Made waste values (hard coal ash, waste gypsum) negative. Originally in megajoule. LHV: 120 MJ/kg. Coal gasification has a net output of electricity. Multifunctional activity that produces 1 kg hydrogen (H_2) and 3.18 kWh electricity (Al-Qahtani et al., 2021). Economic allocation based on $1.11/kg H_2 and $0.04/kWh electricity (Von Wald et al., 2020)
	hydrogen production, multifunctional coal gasification	Von Wald et al., 2020	Co-product from multifunctional process. Economic allocation by base case prices of Von Wald et al. (2020): $40/MWh electricity and $1.11/kg H_2. hydrogen: $1.11/kg * 1 kg = $1.11 electricity: $0.04/kWh * 3.18 kWh = $0.13 1.11+0.13 = $1.24 Allocation factor hydrogen: 1.11/1.24 = 0.90
	electricity co-production, multifunctional coal gasification	Von Wald et al., 2020	Co-product from multifunctional process. Economic allocation by base case prices of Von Wald et al. (2020): $40/MWh electricity and $1.11/kg H_2. hydrogen: $1.11/kg * 1 kg = $1.11 electricity: $0.04/kWh * 3.18 kWh = $0.13 1.11+0.13 = $1.24 Allocation factor electricity: 0.13/1.24 = 0.10
	CO_2 from hydrogen production, coal gasification	ecoinvent 3.8	By-product of ammonia from CG, this CO_2 is vented or used in the chemical industry (primarily for urea) in the case of CCU. Based on ecoinvent 3.8, which includes "carbon dioxide, in industry" for tracking purposes. No impact is allocated to the CO_2 (so the production of the ammonia is assumed responsible for the full burden). There are no values given to technosphere or biosphere flows.

	hydrogen production, coal gasification w/ CCS	*premise* (Wokaun & Wilhelm, 2011) Al-Qahtani et al., 2021	Expansion of *premise* generated inventory: hydrogen production, gaseous, 30 bar, from hard coal gasification and reforming, at coal gasification plant (product Hydrogen, gaseous, 30 bar). Some location changes to fit China/RoW better. New emissions (CH4, N2O) and updated values (coal, water, CO_2) (Al-Qahtani et al., 2021).
	CO2 capture/at H2 production plant, pre, pipeline 200km, storage 1000m	*premise* (Volkart et al., 2013)	Inventory copied from *premise* with electricity removed, since the increased electricity is handled in the coal gasification w/ CCS inventory.
	multifunctional methane pyrolysis	Al-Qahtani et al., 2021 Machhammer et al., 2016	Hydrogen production by methane pyrolysis from Al-Qahtani et al. (2021), electricity from Machhammer et al. (2016). Multifunctional activity that produces 1 kg hydrogen (H2) and 3 kg carbon black (C). Economic allocation based on $1.11/kg H2 and $0.15/kg C (Von Wald et al., 2020)
	hydrogen production, multifunctional methane pyrolysis	Von Wald et al., 2020	Co-product from multifunctional process. Economic allocation based on $1.11/kg H2 and $0.15/kg C (Von Wald et al., 2020). hydrogen: $1.11/kg * 1 kg = $1.11 carbon black: $0.15/kg * 3 kg = $0.45 1.11+0.45 = $1.56 Allocation factor hydrogen: 1.11/1.56 = 0.71
	carbon black co-production, multifunctional methane pyrolysis	Von Wald et al., 2020	Co-product from multifunctional process. Economic allocation based on $1.11/kg H2 and $0.15/kg C (Von Wald et al., 2020). hydrogen: $1.11/kg * 1 kg = $1.11 carbon black: $0.15/kg * 3 kg = $0.45 1.11+0.45 = $1.56 Allocation factor carbon: 0.45/1.56 = 0.29

	hydrogen production, electrolysis	IEA, 2021e Ausfelder et al., 2022	IEA Global Hydrogen Review 2021: Alkaline electrolysers dominate with 61% of installed capacity in 2020, while PEMs have a 31% share. The remaining capacity is of unspecified electrolyser technology and SOEs (installed capacity of 0.8 MW). Since SOEs are still in the research and development phase (Ausfelder et al., 2022), this market will include only the two commercialised technologies (assuming a dominance of alkaline with 61+8=69% and 31% PEM). This division of electrolysis technologies is static in this model but can be improved later with better forecasts for the electrolyser technology mix to 2050 and the addition of SOE.
	hydrogen production, alkaline electrolysis	Carlo d'Angelo et al., 2021	Combined cell stack fraction and electrolyser operation (Carlo d'Angelo et al., 2021).
	hydrogen production, gaseous, 25 bar, from electrolysis	*premise* (Bareiß et al., 2019)	PEM electrolysis: directly using existing inventory in *premise* which is recent, complete, and uses the same source as Carlo d'Angelo et al. (2021). This inventory is not in the "new_activities" database but is linked to the other processes during the creation of the superstructure database.

Appendix 2 – Supporting Figures

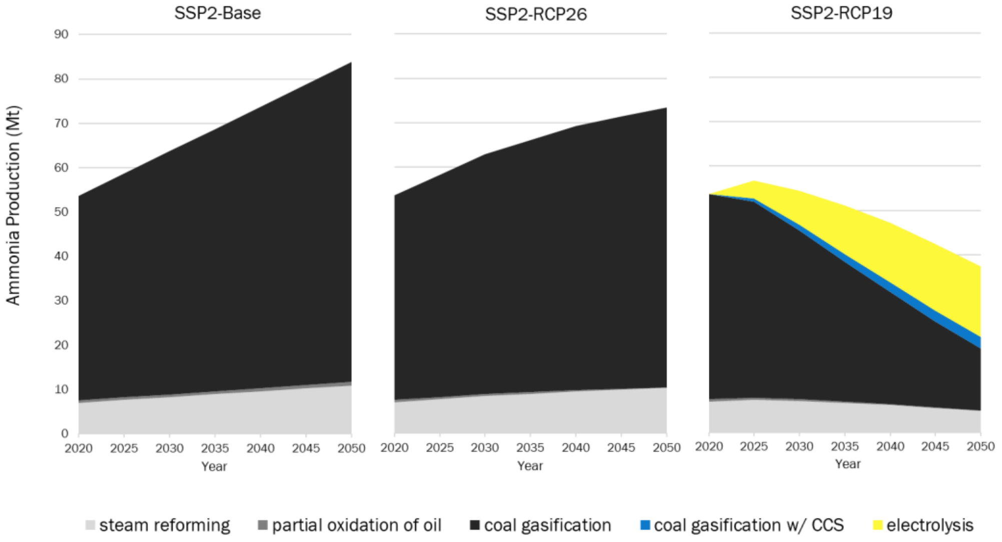


Figure A2- 1 Ammonia production by technology type (China)

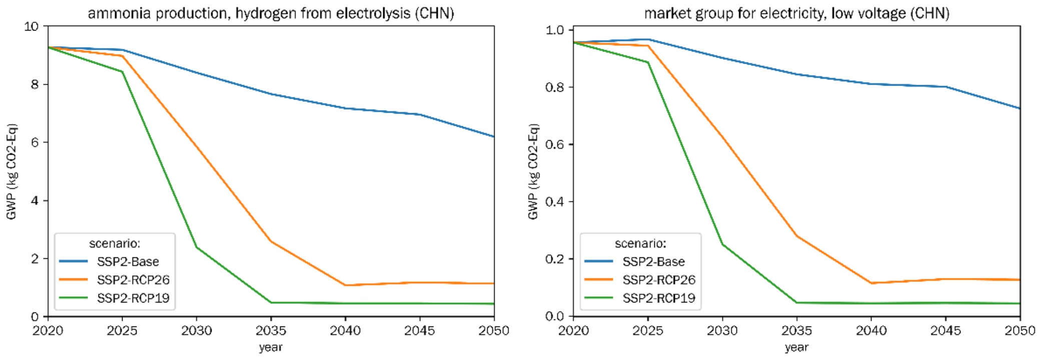


Figure A2- 2 Global warming potential of 1 kg ammonia from electrolysis hydrogen (left) and 1 kWh market for low voltage electricity (right) for China

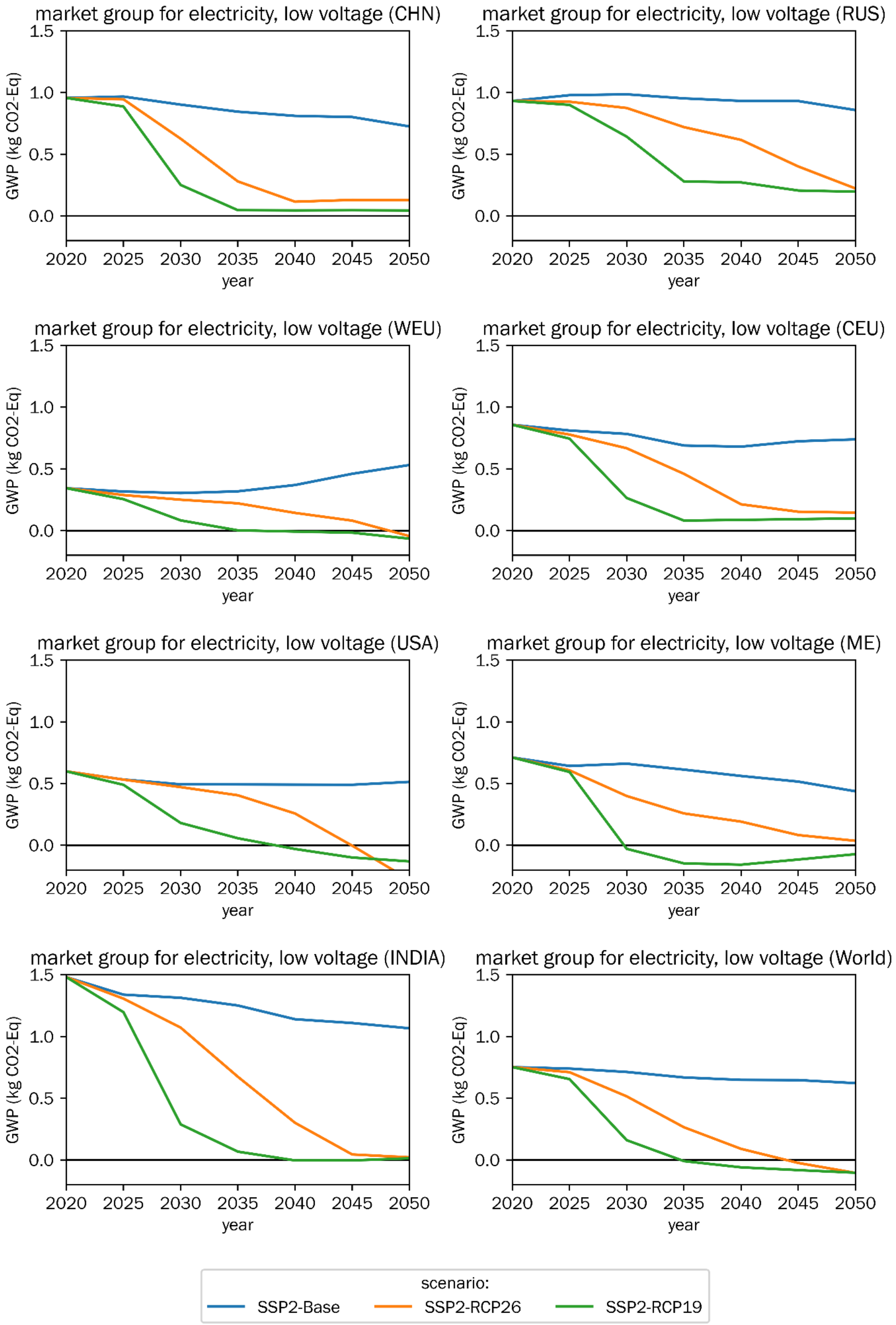


Figure A2- 3 Global warming potential of 1 kWh low voltage electricity from each regional market

Other impact categories, WEU:

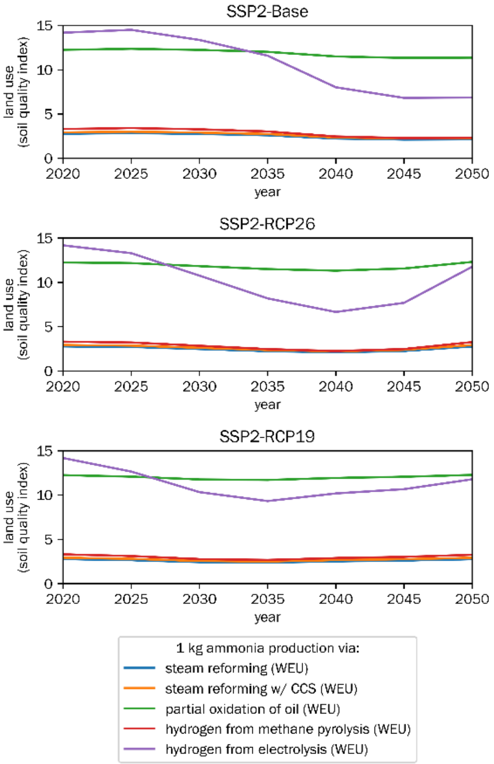


Figure A2- 4 Land use impact per ammonia production technology (Western Europe)

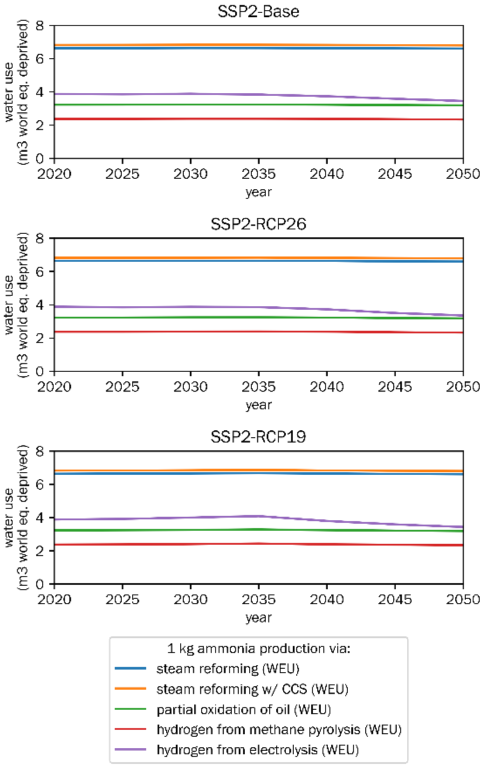


Figure A2- 5 Water use impact per ammonia production technology (Western Europe)

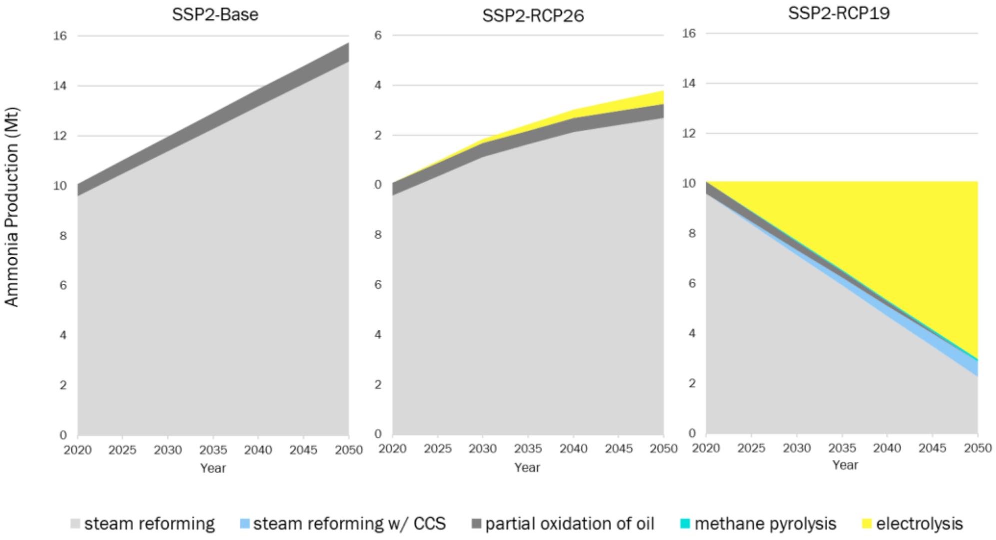


Figure A2- 6 Ammonia production by technology type (WEU)

Comparisons of 1 kg ammonia produced by each technology type (used in that region) for the remaining top producers:

Figure A2- 7 Global warming potential per technology type (Russia)

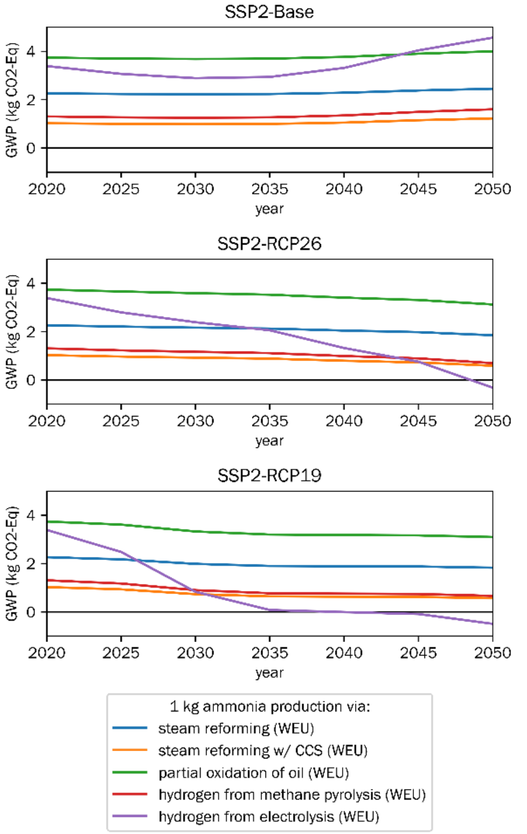


Figure A2- 8 Global warming potential per technology type (Western Europe)

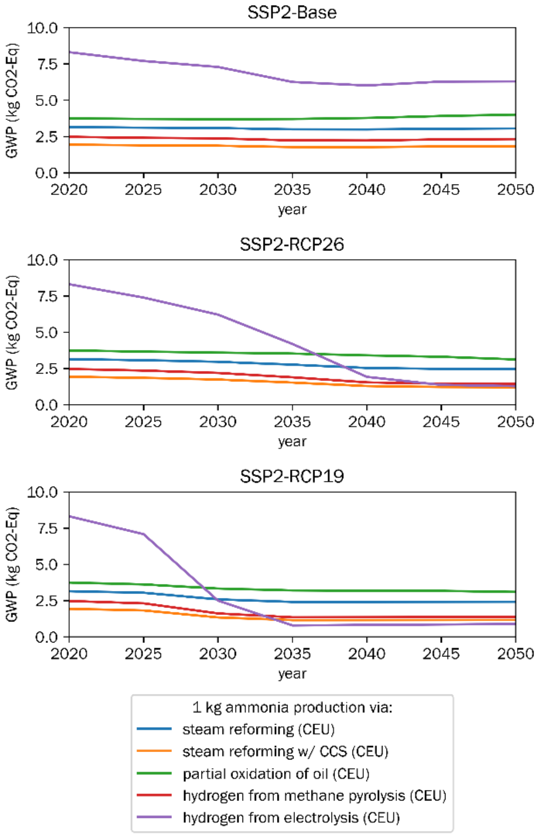


Figure A2- 9 Global warming potential per technology type (Central Europe)

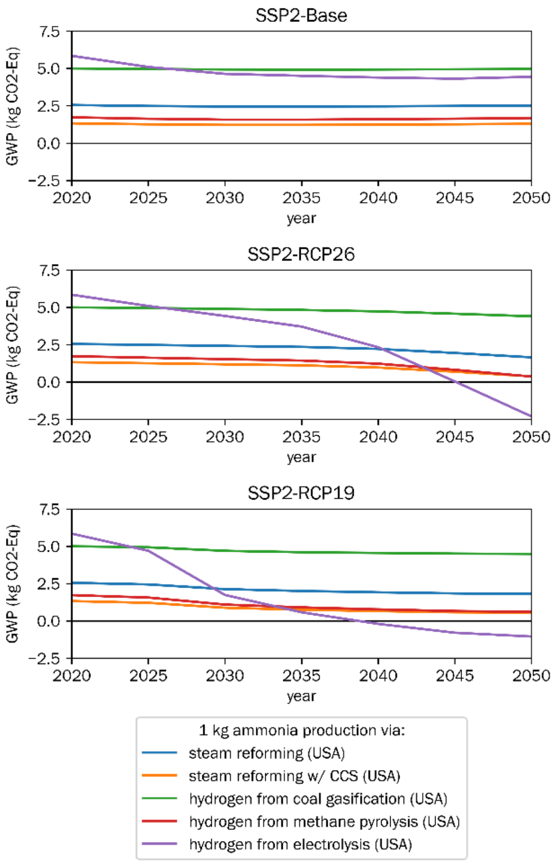


Figure A2- 10 Global warming potential per technology type (USA)

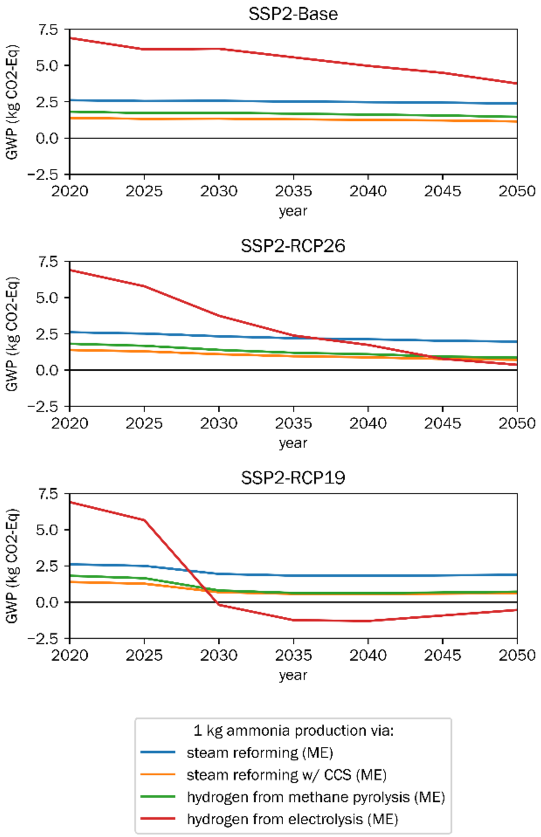


Figure A2- 11 Global warming potential per technology type (Middle East)

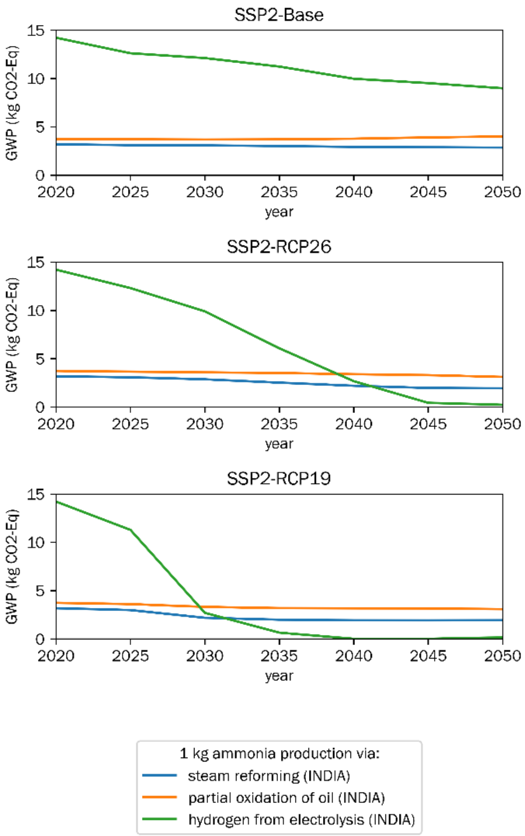


Figure A2- 12 Global warming potential per technology type (India)

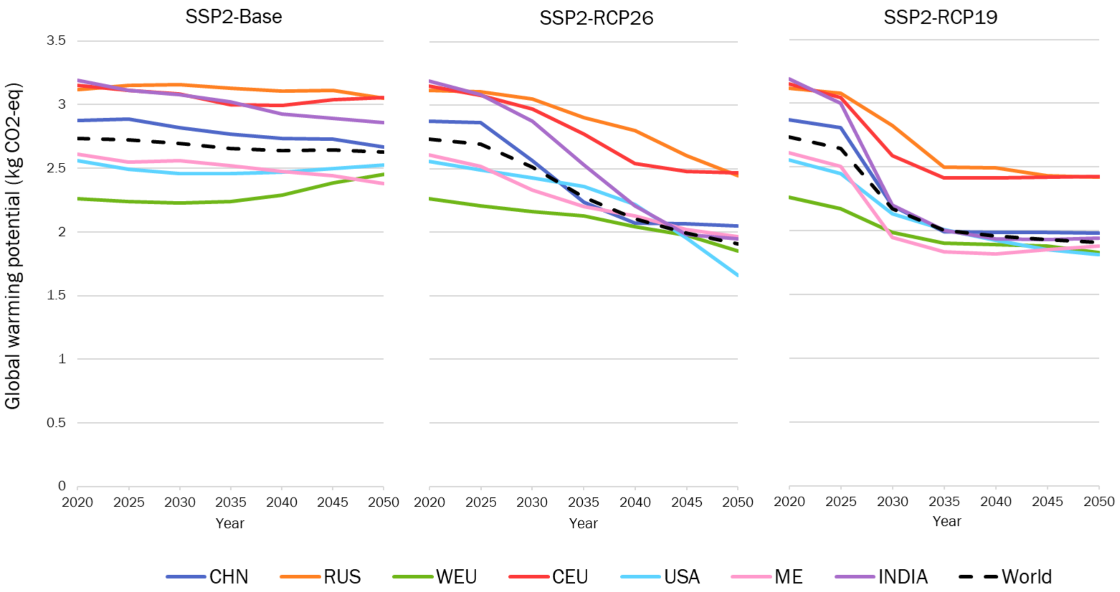


Figure A2- 13 GWP of 1 kg ammonia via steam reforming in the top producing regions (solid lines) and the World market (dashed line)

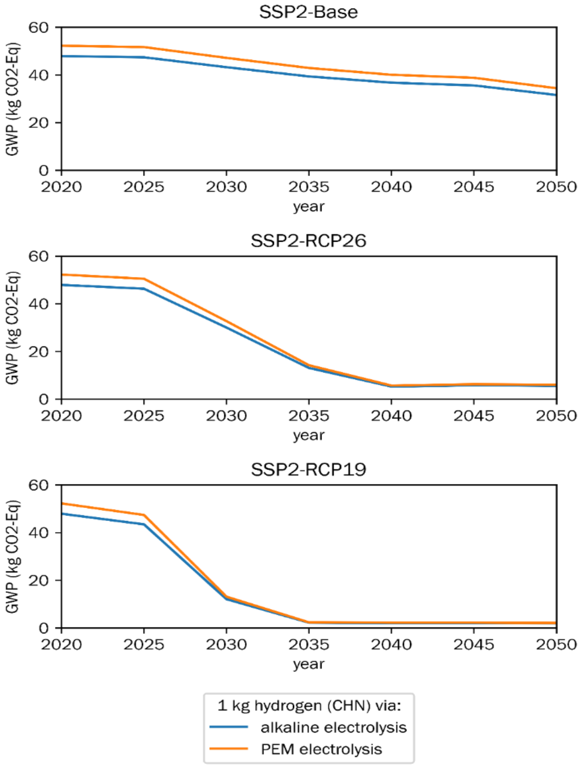


Figure A2- 14 GWP of 1 kg hydrogen produced by alkaline and PEM electrolysis (China)

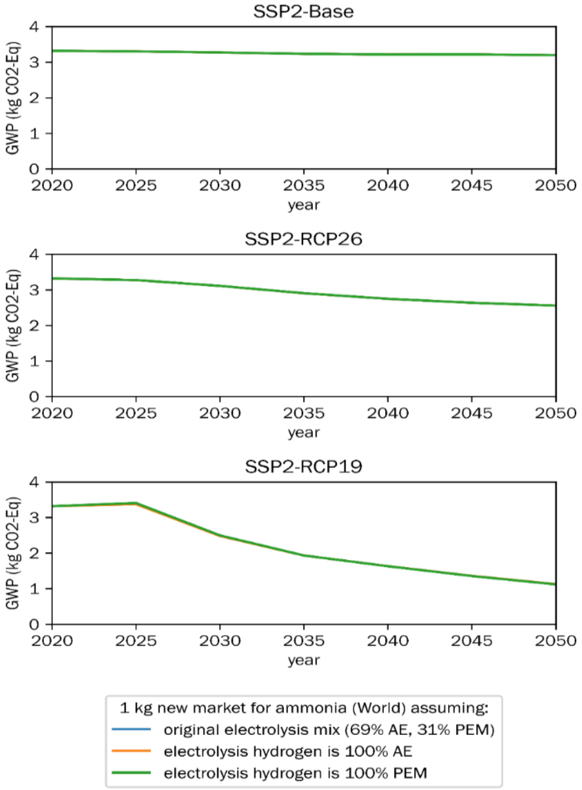


Figure A2- 15 GWP of 1 kg ammonia (new market for ammonia (World)) with different ratios of electrolyser type

*The three lines are almost completely overlayed.

Appendix 3 – Supporting Figures (REMIND)

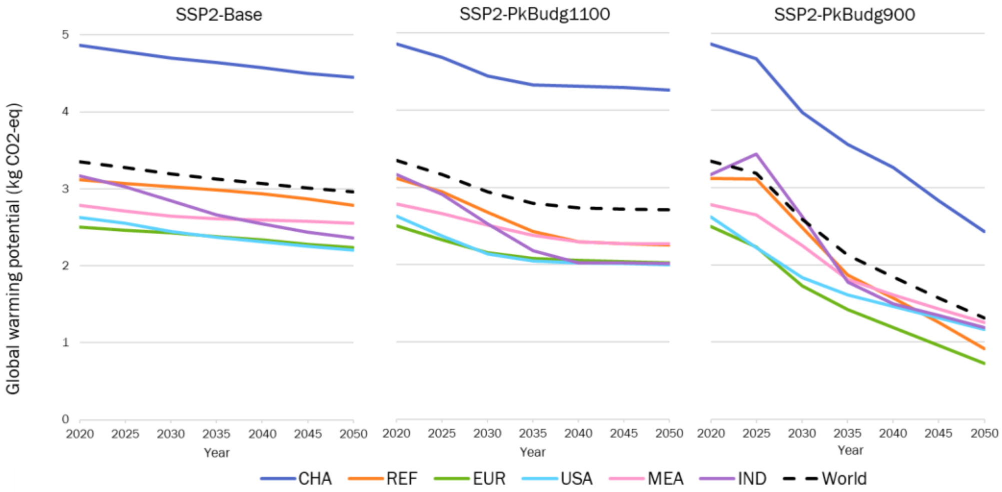


Figure A3- 1 GWP of 1 kg ammonia from the top producers' ammonia markets – REMIND

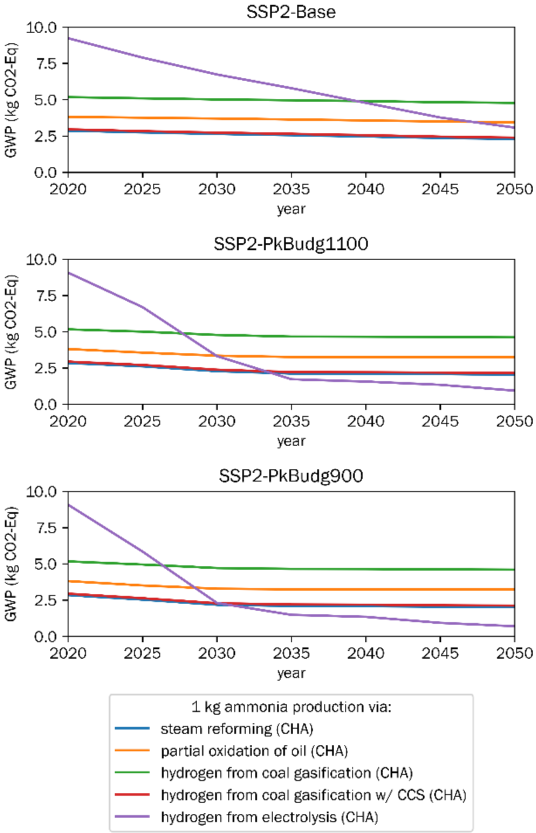


Figure A3- 2 Global warming potential of per technology type (China) – REMIND

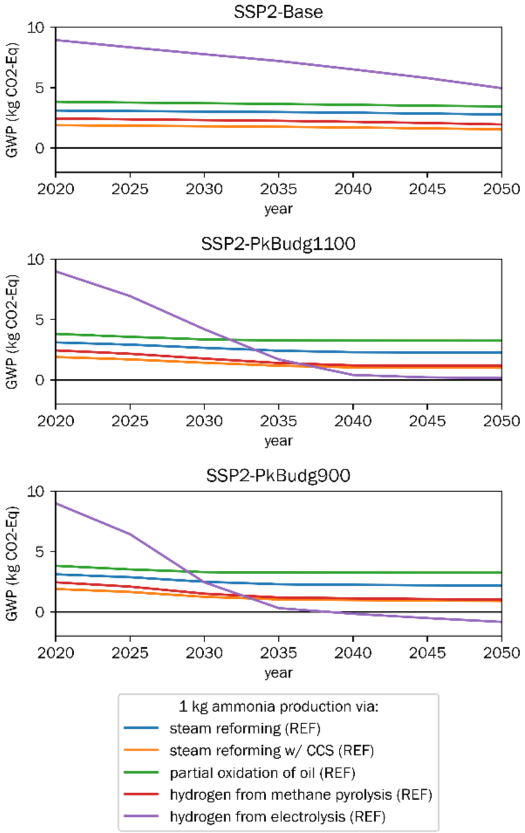


Figure A3- 3 Global warming potential of per technology type (REF) – REMIND

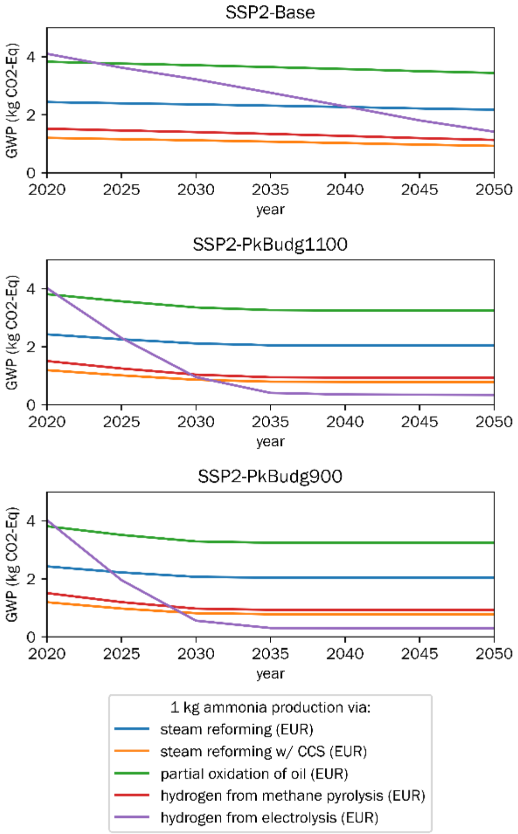
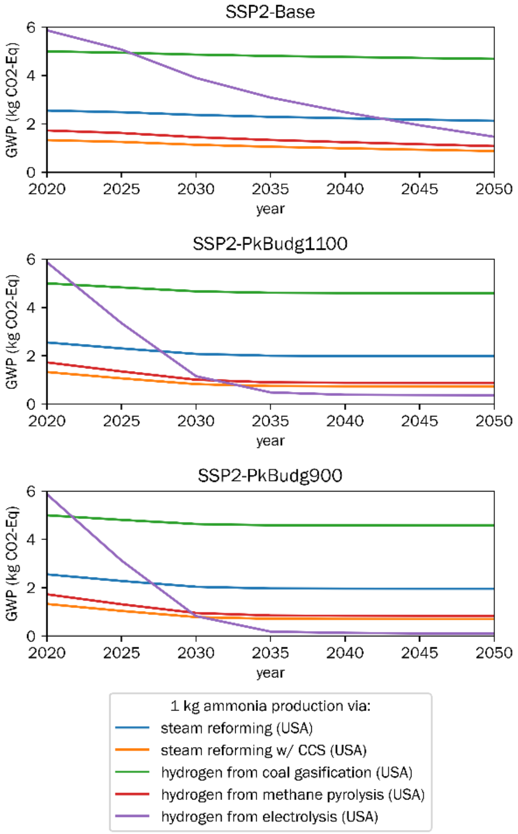


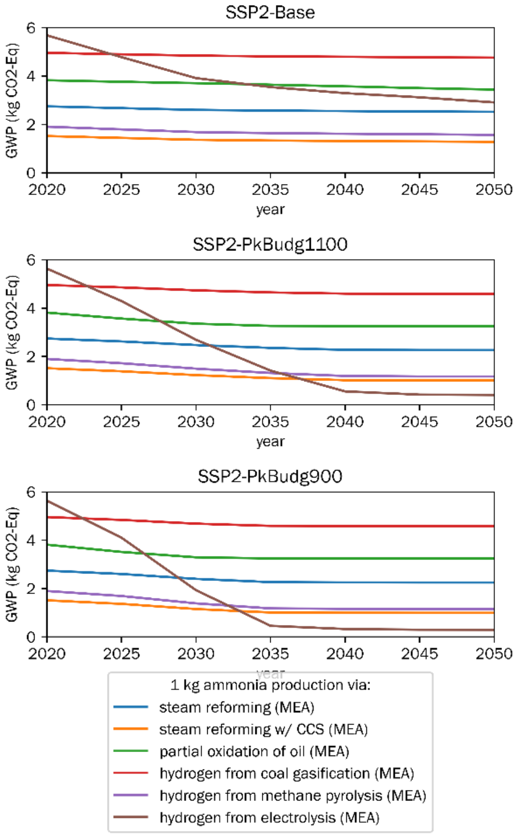
Figure A3- 4 Global warming potential of per technology type (EUR) – REMIND


SSP2-Base

SSP2-PkBudg1100

SSP2-PkBudg900

Figure A3- 5 Global warming potential of per technology type (USA) – REMIND


SSP2-Base

SSP2-PkBudg1100

SSP2-PkBudg900

Figure A3- 6 Global warming potential of per technology type (MEA) – REMIND

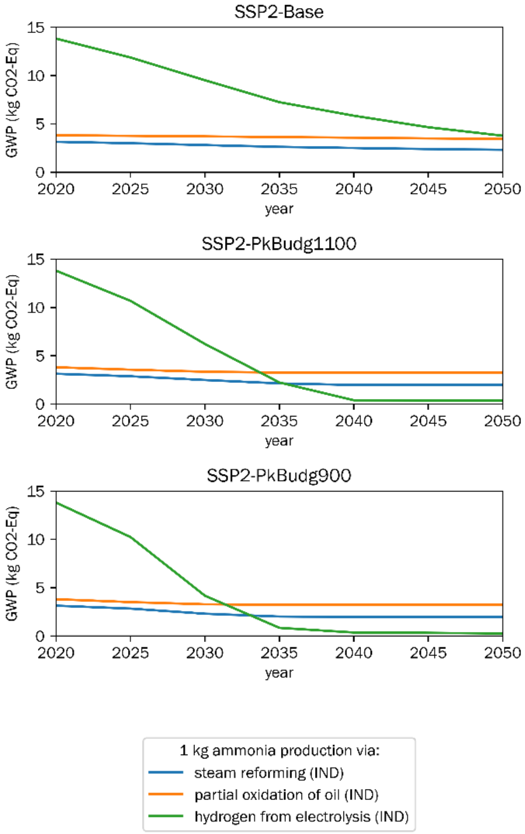


Figure A3- 7 Global warming potential of per technology type (India) – REMIND