

Infrastructure Challenges Caused by Industrial Transformation to Achieve Greenhouse Gas Neutrality

Ammonia Production in the Antwerp-Rotterdam-Rhine-Ruhr Area

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Several pathways for potentially greenhouse gas neutral production of ammonia have been investigated compared to today's conventional ammonia production at chemical sites in Antwerp, Dormagen, and Geleen. These pathways include on-site water electrolysis using grid electricity, off-site production via water electrolysis using renewable electricity and supply of green hydrogen to the site, pyrolysis of natural gas and conventional ammonia production coupled with CO₂-capture on-site and transport to a storage site. All pathways effectively eliminate scope 1 emissions present in conventional production but continue to emit scope 2 emissions from grid electricity consumption. Eventually, a coordinated industry-wide and cross-industry effort is needed to address the transformational changes and develop the common cross-border infrastructures.

Keywords: Ammonia production, Greenhouse gas emissions, Hydrogen, Industrial transformation, Infrastructure

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1 Introduction

The chemical industry has undergone significant changes over time with respect to its feedstock composition and energy sources [1]. Modern chemical sites are highly integrated and rely on a steady supply of different raw materials, energy carriers and feedstock. This supply is facilitated by the respective transport and distribution networks that connect the chemical site to ports, refineries, road and rail transport, natural gas and liquid fuels as well as power grid and sometimes district heat infrastructure.

These infrastructure components play a vital role, even if mostly invisible, in the daily operation of chemical sites. While this infrastructure enables the operation, its size and complexity are also designed for the operations on-site. While there is some room for expansion within most infrastructures, it is not given that a major change in the demand from the site operation could be matched immediately by the existing infrastructures.

The European Union aims for climate neutrality in 2050 [2] in accordance with the Paris Agreement [3]. This commitment will be supported by climate neutrality goals in different sectors and within specific industries. The European chemical industry has signed on this target and currently evaluates technologies [4]. Most recently, national and European roadmaps on the role of hydrogen were published

[5, 6]. While there is broad political consensus for the most part towards this goal, the actual detailed implementation will require significant changes on the process level in order to reduce emissions, the switch of feedstock and the use of alternative energy sources.

Taking a site operator's perspective makes the decision making even more complicated. The chemical industry acts within an international, highly competitive market. Overall, Europe's chemical industry is stagnant or even declining with most of the world's investments currently being placed

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in China, the Middle East or the US. Its competitiveness, especially in base chemicals, depends strongly on existing, depreciated plants, highly integrated and efficient sites, a highly skilled workforce and close proximity to other stakeholders in the value chain.

The transformation to greenhouse gas (GHG) neutrality takes place in a challenging environment of declining market share and high energy prices and existing CO₂ costs compared to other regions of the world.

Within Europe, a large section of the chemical industry is located in Northwestern Europe within the highly densely populated Antwerp-Rotterdam-Rhine-Ruhr area (ARRRA). These locations (see Fig. 1) feature an excellent infrastructure connection with major seaports, complex road, rail, river and canal networks, refineries, natural gas, fuel and industrial gas pipelines as well as a high-capacity power grid with ever increasing renewable contributions from wind power and Europe's highest security of supply.

At the same time, there are significant changes of the energy carrier supply occurring. Natural gas supply is shifting from (Dutch) L-gas to (Russian) H-gas, making the dedicated Dutch infrastructure for L-gas obsolete. Natural gas exploration from the North Sea declines and less and less of the existing infrastructure to transport Dutch natural gas to the Eastern neighbor is needed for this purpose.

The existing power grid on the other hand has been designed for electricity generation by a few large continuously run central power stations and has to make the transition towards more fluctuating and intermitting renewable feed-in while guaranteeing a high security of supply.

Other options and opportunities on the political horizon are still to be unlocked, with hydrogen infrastructure in the region being in its infancy and insufficient for the task ahead and a CO₂ infrastructure for carbon capture and utilization (CCU) or carbon capture and storage (CCS) essentially non-existent.

Within this paper, the authors try to address the following issues for the example of ammonia production at exemplary sites in Belgium, Germany and the Netherlands each:

- What kind of infrastructure change will be required if chemical processes are transformed and will it be a sudden or continuous change?
- What would be the implications for specific sites and for cross-border collaboration?
- Can existing infrastructure be repurposed or retrofitted to make cost-efficient use of these assets in the energy transition?

2 Methodology

2.1 Ammonia Production

The production of ammonia is one of the largest and most important chemical processes in existence. It is of unrivalled importance for the downstream production of nitrogen-based fertilizers and quite literally, feeds the world. However, the conventional Haber-Bosch process is also energy- and emission-intensive, even if based on steam reforming of

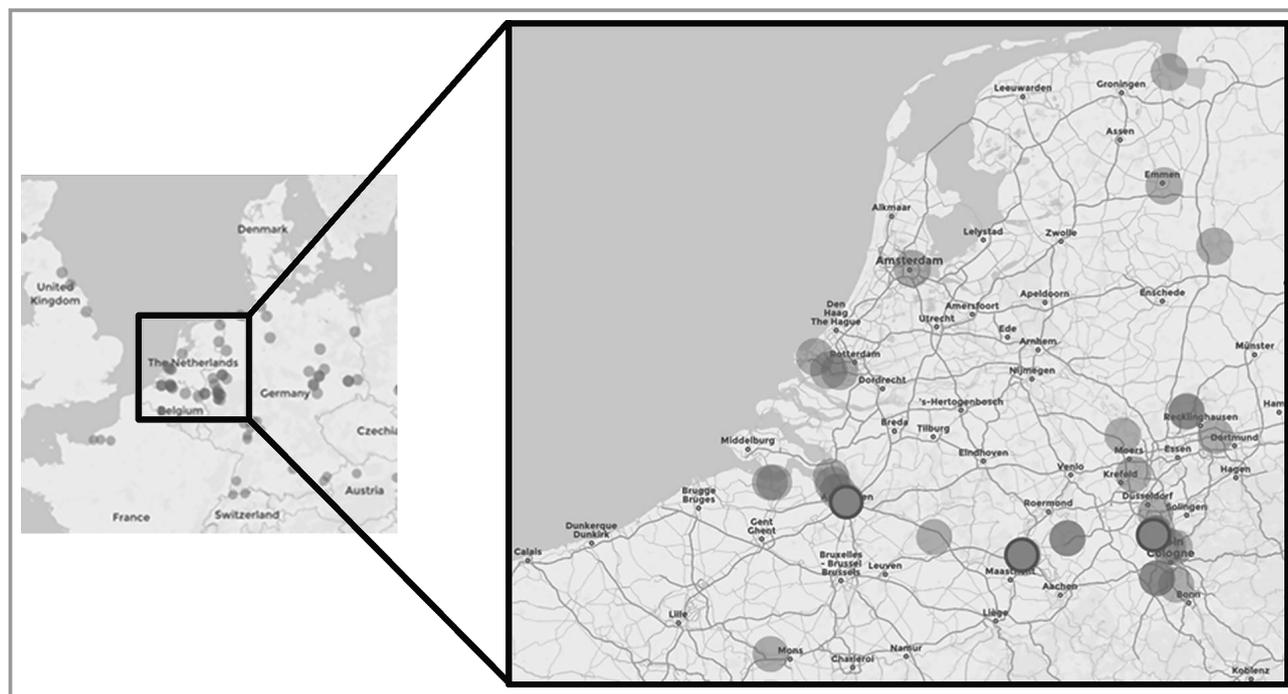


Figure 1. Depiction of main industrial sites in Antwerp-Rotterdam-Rhine-Ruhr area (ARRRA). Emphasized circles represent the three chemical sites under consideration in this study, which contribute an estimated 20 % of European ammonia production in 185 km radius.

natural gas, which produces about 2 t CO₂ for each ton of NH₃ produced [4].

Due to its importance and size, the ammonia production is often the dominant process on a given site. Downstream processes mainly transform ammonia with some of the CO₂ from the water-gas shift reaction to urea to be used as fertilizer or for resins or to nitrates, the latter also mostly used for fertilizers. Ammonia itself, however, does not contain any carbon and the largest part of the CO₂ emission, the feedstock-based emission, could be conceivably avoided by the direct use of hydrogen.

There are several different pathways, each of them with its own impact on infrastructure for greenhouse gas¹⁾ free production of ammonia. Based on the assumptions below, the time-resolved specific production cost for ammonia along each production pathway will be calculated and compared to each other. Infrastructure demand can be derived by the extent of energy carriers or gases needed or produced. This approach is an extension of the one used in a current study on the chemical industry in Germany [7].

2.2 Pathways for Greenhouse Gas Free Ammonia Production

The possible pathways for GHG-free ammonia production under consideration in this study as well as the conventional process are briefly explained below. The different options are schematically displayed in Fig. 2.

2.2.1 Conventional Ammonia Production (Gray Hydrogen)

Conventional ammonia production is based on steam-reforming of natural gas followed by a water-gas shift and separation of CO₂ from the product gas to yield hydrogen. Nitrogen is supplied by the reformer if air is used for the reforming process. Nitrogen and hydrogen react to form ammonia. For downstream urea production, if relevant at the specific site, some of the captured CO₂ will be used, while the excess CO₂ is released to the atmosphere.

2.2.2 Blue Hydrogen via Steam Reforming of Natural Gas and CCS

Generally, blue hydrogen is defined by hydrogen produced from a fossil-based energy carrier via reforming with subsequent CCS of the CO₂ produced, thereby making the hydrogen GHG-free. This option is often discussed in the context of a centralized hydrogen production and supplying it via a hydrogen infrastructure. However, in case of ammonia production this option is likely to be slightly different. Conventional ammonia plants already perform nearly all steps of the blue hydrogen process chain, i.e., reforming of natural gas, water gas shift and capture of CO₂. The only parts missing are the transport and storage aspects. In order to make most of existing assets and minimal change to the process, blue hydrogen would be essentially produced on-site from natural gas with the captured CO₂ transported to a storage site. Therefore, this pathway for ammonia

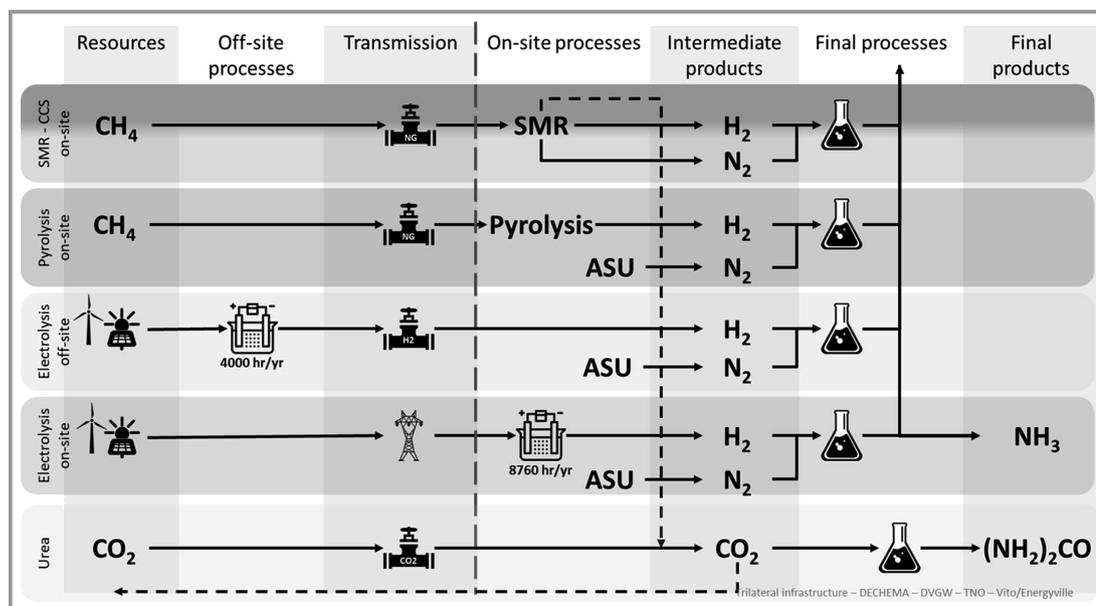


Figure 2. Greenhouse gas neutral pathways for ammonia and urea production considered in this study.

1) This study only considers direct emissions, either by the process (scope 1) or connected to energy used by the process, e.g., electricity (scope 2).

production requires a CO₂ transport and storage infrastructure rather than an external hydrogen supply. Nitrogen is supplied with the air used in the reformer. Some of the CO₂ can be used for downstream urea production. It should be noted that the CO₂ captured from the steam reforming process is of very high purity and can be used for further chemical synthesis without additional purification. Consequences of changes in on-site integration of CO₂ as a by-product of steam reforming have not been considered within this work.

2.2.3 Dark Green Hydrogen via On-site Electrolysis with Grid Electricity

Water electrolysis can be installed on-site to produce hydrogen and oxygen. In order to provide a continuous supply of hydrogen, grid electricity is used and the scope 2 emissions according to the electricity mix considered. The annual operation of the electrolyzer under these assumptions is not limited to intermittent green electricity supply caused by intermittent renewable energy sources in contrast to the assumptions taken under the green hydrogen pathway. Nitrogen is supplied by an air separation unit on-site (ASU). Oxygen produced by both processes might find a use in other processes on-site. Nitrogen and hydrogen react to form ammonia. Greenhouse gas neutrality will successively be reached by the transformation of electricity generation to become more and more renewable. Any downstream urea production would require an additional CO₂ supply.

2.2.4 Green Hydrogen via Hydrogen Pipeline

Green hydrogen is produced off-site by water electrolysis with electricity from renewable power sources, e.g., wind energy. Due to the intermittent and fluctuating characteristics of the electricity supply, hydrogen is fed into a transport infrastructure including buffer and storage facilities, which smoothens the feed-in profile with hydrogen storage facilities. This pathway would also incorporate green hydrogen imports from non-EU countries; however, for reasons of non-domestic added value, this import route has not been made a focus of this research. The same applies for the import routes of green hydrogen products, e.g., green ammo-

nia. For this work, the annual operational hours of the electrolyzer are considered being limited to 4000 h in accordance with Germany's national hydrogen strategy [5]. Ammonia production on-site is utilizing a pipeline connection to access green hydrogen and react it with nitrogen from a local ASU to ammonia. Any downstream urea production would require an additional CO₂ supply.

2.2.5 Turquoise Hydrogen via Pyrolysis of Natural Gas

Methane pyrolysis yields hydrogen and solid carbon with mostly carbon being the desired product. For the investigated pathway, pyrolysis takes place on-site with natural gas supplied by a possibly expanded natural gas infrastructure. Nitrogen is supplied by a local ASU to provide the reactants for ammonia production. Any downstream urea production would require an additional CO₂ supply. The economic impact of use of CO₂ for urea production is not considered in this study.

Of all considered technologies, methane pyrolysis is the process with the lowest technological maturity and hence the greatest uncertainty. The process concepts for methane pyrolysis can be divided into the three categories thermal decomposition, plasma decomposition, and catalytic decomposition. Plasma processes for the production of carbon black from natural gas have been realized on industrial scale (e.g., Kvaerner process, Karbomont plant, TRL 8) and are still being further developed (Olive Creek plant, mechanical completion planned in 2020, TRL 8). In these processes, hydrogen is used as a by-product to produce thermal energy. After successful operation of a pilot plant (Carbonsaver process, TRL 5), a plasma torch for the production of hydrogen-enriching natural gas was not developed further. Process approaches on thermal decomposition (KIT process, TRL 3), catalyst/plasma decomposition (TOMSK-GAZPROM consortium, TRL 3), and catalytic decomposition (e.g., Hazer Group, TRL 3) are still at a very early stage of development. Only BASF's thermal process (carbon granules in a moving bed, TRL 4) is already being further developed for scale-up [8].

The different pathways properties are detailed in Tabs. 1 and 2.

Table 1. Overview of properties of different pathways for ammonia production.

	Conventional NH ₃ production (gray hydrogen)	Blue hydrogen pathway	Dark green hydrogen pathway	Green hydrogen pathway	Turquoise hydrogen pathway
Hydrogen production process	On-site SMR of natural gas	On-site SMR of natural gas with off-site CCS	On-site water electrolysis (grid electricity) ~8760 h a ⁻¹	Off-site water electrolysis (green electricity) ~4000 h a ⁻¹	On-site pyrolysis of natural gas (grid electricity)
Nitrogen production process	Reformer output	Reformer output	ASU (grid electricity)	ASU (grid electricity)	ASU (grid electricity)
Additional infrastructure requirement	None	CO ₂ pipeline, CCS site	Expand power grid connection	H ₂ pipeline	Expand natural gas pipeline and power grid connection
CO ₂ for urea	Available	Available	CO ₂ supply required	CO ₂ supply required	CO ₂ supply required

Table 2. Modeling parameters used for different pathways. Values taken from [7] and [9], sometimes adjusted according to other assumptions.

	Conventional NH ₃ production (gray hydrogen)	Blue hydrogen pathway	Dark green hydrogen pathway	Green hydrogen pathway	Turquoise hydrogen pathway
Technology available (TRL 9)	Existing technology	Existing technology	2031	2031	2040
Full load hours (hydrogen production) [h]	8300	8300	8300	8300 (4000)	8300
Investment cost (excluding electrolyzer) [€ t _{cap} NH ₃]	670	500	500	622	670
Electricity demand, electrolyzer [MWh t ⁻¹ NH ₃]	Not applicable	Not applicable	8.96 time-dependent	8.96 time-dependent	Not applicable
Electricity demand, other [MWh t ⁻¹ NH ₃]	2.07	2.07	1.72	1.72	3.41
Natural gas demand [GJ t ⁻¹ NH ₃]	27.6	27.6	0	0	75.48
Additional transport costs	None	100 € t ⁻¹ CO ₂	None	300 € t ⁻¹ H ₂	None

2.3 Other Parameters

The following parameters were used for the calculations of specific cost of production of ammonia, Tab. 3.

Table 3. Assumptions for economic evaluation.

Parameter	Value
Ammonia production volume [kt a ⁻¹]	Constant for each site on 2017 values
Depreciation time plant [a]	20
Technical lifetime electrolyzer [h]	Time-dependent
ROI [%]	8
OPEX estimated as percentage of investment [%]	5

2.3.1 Time-Dependent Parameters

While little change in the efficiency of the conventional ammonia production is foreseen, water electrolysis is expected to undergo significant improvement with time as summarized in Tab. 4 [9].

Table 4. Time-dependent parameters for the water electrolyzer [9].

Parameter	2020	2030	2040	2050	2075	Comment
Investment cost [€ kW ⁻¹]	1.200	950	850	750	500	
Efficiency [%]	70	75	78	80	85	HHV
Investment cost [€ t _{cap} ⁻¹ H ₂]	7707	5695	4931	4215	2645	
OPEX [€ t ⁻¹ H ₂]	231	171	148	126	108	Without electricity
Technical lifetime [h]	50 000	60 000	70 000	80 000	100 000	

2.3.2 Energy Cost

The cost for different energy carriers and feedstock will change over time. Certain assumptions are taken into account to describe the time-dependent development of energy and feedstock cost.

The cost for natural gas is considered to be constant at 6300 € TJ⁻¹ (LHV) in order to reduce the complexity of the study and to single out the effect of the renewable pathways compared to the conventional one.

The cost for grid electricity is set constant at 45 € MWh⁻¹ for industrial consumers, which is very low compared with the average industrial electricity price [11]. However, this value will be adjusted by the additional cost for CO₂ (EUA) according to the emission intensity of the electricity in a given country and year. With ongoing decarbonization of the electricity sector, this value remains higher in the long run than the value used for green electricity to compensate for the need to provide continuous supply. This approach is consistent with Geres et al. [7]. Grid electricity used for water electrolysis is likely to fall under the category of genuine risk of carbon leakage due to indirect emission cost and might be eligible for compensation of its indirect emission costs [12].

Renewable electricity from intermitting and fluctuating renewable sources is expected to become cheaper with time, starting at 72 € MWh⁻¹ in 2020 down to around 30 € MWh⁻¹ in 2075. The full load hours of an electrolyzer for the production of green hydrogen from renewable electricity are set to 4000 h a⁻¹ in agreement with Germany's national hydrogen strategy [5]. Green hydrogen will not be produced on-site and a 300 € t⁻¹ H₂ transport fee will be added to the cost of hydrogen production.

CO₂ costs (EUA) are assumed to rise linearly within EU ETS trading periods from 25 € t⁻¹ CO₂ in 2020 to nearly 200 € t⁻¹ CO₂ in 2075. Currently, no CCS infrastructure exists for blue hydrogen. Transport and storage cost of 100 € t⁻¹ CO₂ are assumed in this study. The developments are summarized in Tab. 5 and displayed in Fig. 3. The specific hydrogen production costs for the different technologies is displayed in Fig. 4.

Table 5. Time-dependent energy cost parameters.

Parameter	2020	2030	2040	2050	2075	Comment
Natural gas price [€ TJ ⁻¹]	6300	6300	6300	6300	6300	
Grid electricity [€ MWh ⁻¹]	45	45	45	45	45	Continuous supply, without cost of CO ₂
Green electricity [€ MWh ⁻¹]	72	62	52	42	30	Intermitting and fluctuating supply
CO ₂ -price (EUA) [€ t ⁻¹ CO ₂]	25	85	119	152	195	

2.3.3 Specific Emissions for Grid Electricity

The overall emissions caused by electrolytic processes strongly depend on the electricity used. Emissions caused by using grid electricity (scope 2 emissions) will decrease over time as the electricity systems become more and more based on renewables. It is, however, important to take only the emissions into account that are related to power generation. Generally, specific emission factors are reported for heat and power generation [10]. These factors have to be adjusted, since heat generation is more efficient than electricity generation by thermal power plants. Only Germany reports an electricity-only emission factor.

Being aware of introducing a systematic error, for the sake of consistency the following approach was applied: historical CO₂ emission intensity from electricity generation as reported by the European Environmental Agency (EEA) up

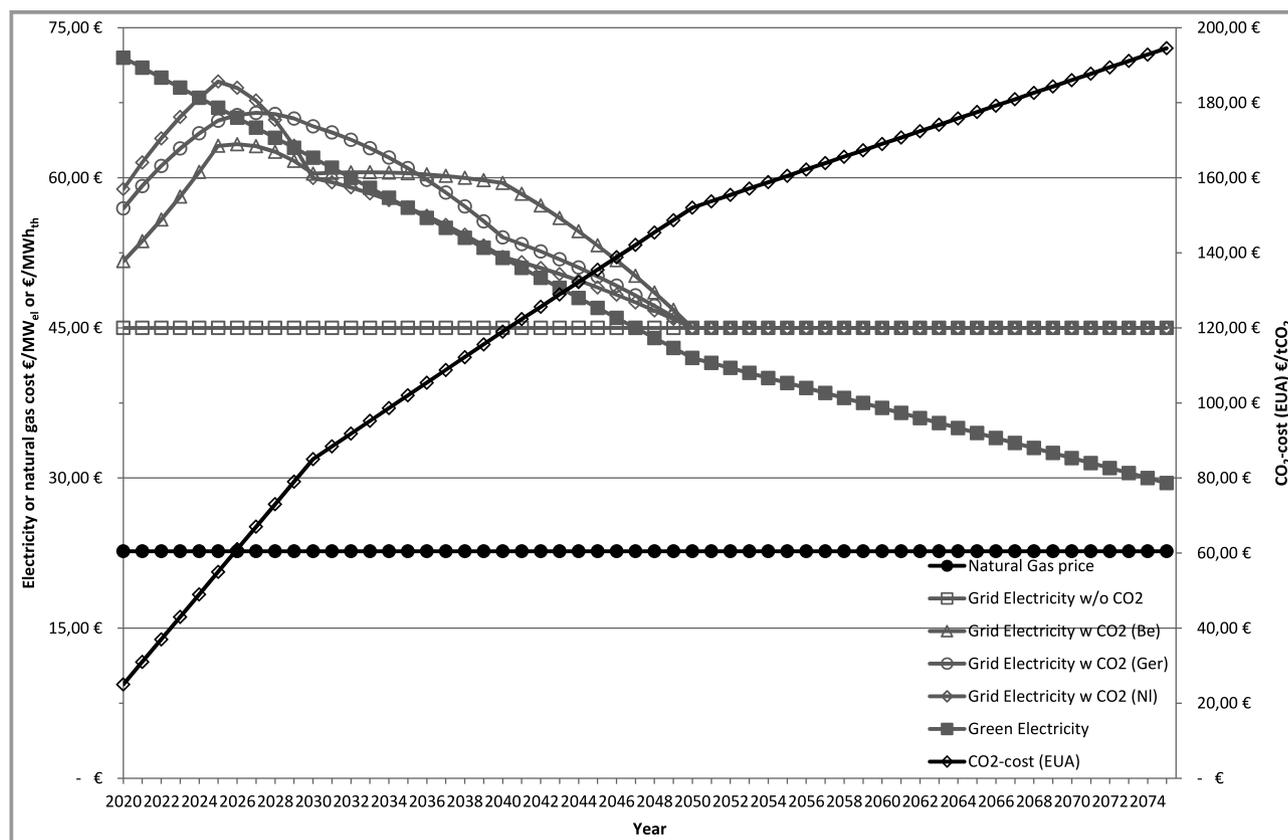


Figure 3. Assumed development in costs for energy carriers, feedstock and CO₂.

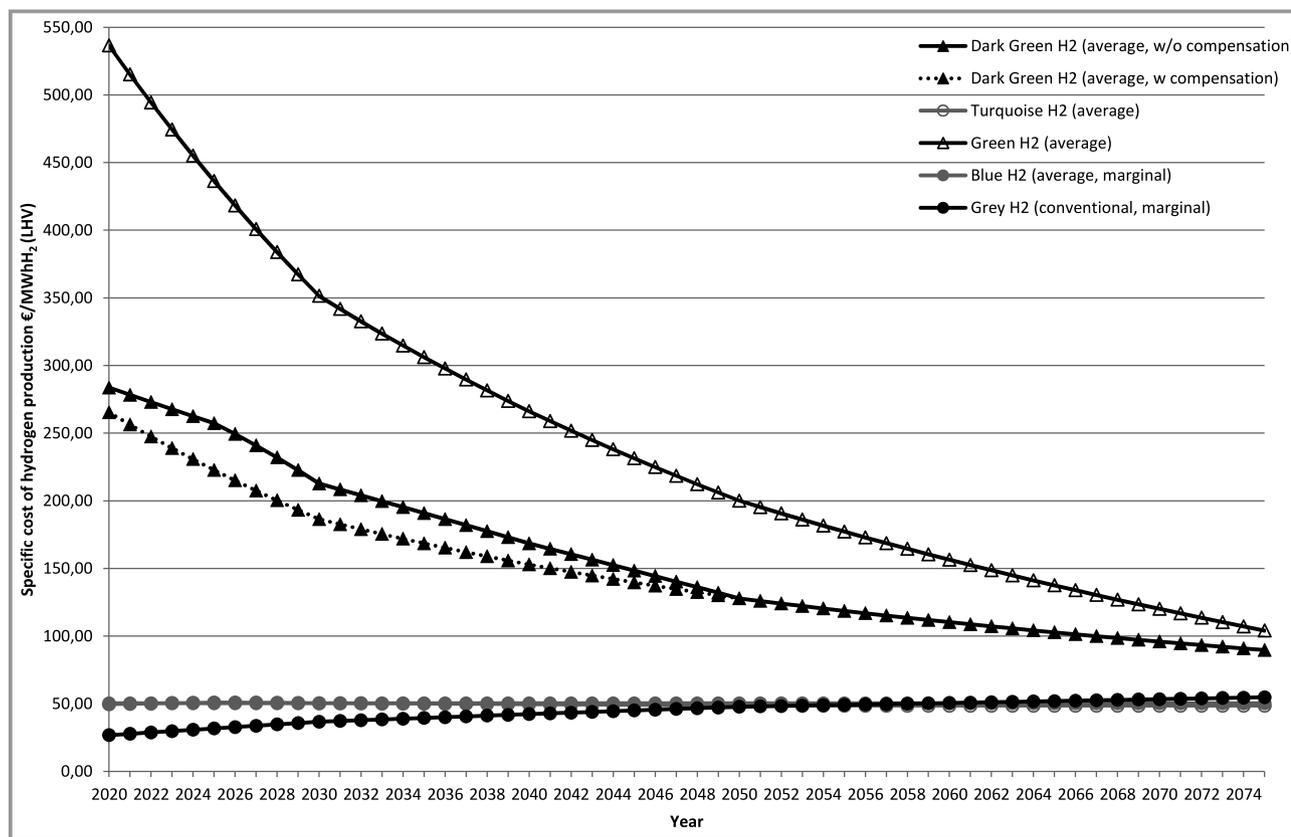


Figure 4. Development of specific production cost for hydrogen for the different pathways. Green hydrogen is much more expensive due to only 4000 full load hours for the electrolyzer. Gray hydrogen and blue hydrogen are produced with existing depreciated plants, while all other technologies require additional investment. The effect of compensation of CO₂-cost related to external electricity is shown in the dotted line for dark green hydrogen production.

to the latest reporting year 2016 [12], for future projections 2025, 2030 and 2040 benchmark values were used based on the National Trends Scenario as applied in the Ten-Year Network Development Plans (TYNDPs), published by ENTSO-E and ENTSO-G [12]. By 2050 the grid electricity supply in all three countries is assumed to be carbon-free, according to EU political goals. This development is displayed in Fig. 5.

All electricity considered in the pathways is grid electricity with the exception of electricity used for water electrolysis in the green hydrogen case.

2.3.4 Specific CO₂ Emission Intensity and Production Cost

Based on the above assumptions and values, the yearly specific CO₂ emissions, scope 1 (direct emissions) and scope 2 (emissions from electricity used) for the production of 1 t ammonia are calculated for each pathway. This allows to determine from what moment in time a specific pathway is more favorable in terms of overall emissions than the conventional ammonia production route.

Yearly specific ammonia production costs are also calculated for each pathway to determine at what point in time

the new pathway might be competing with the existing conventional production. The generalized equation is:

$$\begin{aligned} \text{Cost}(\text{tNH}_3) = & \text{CAPEX} + \text{OPEX} \\ & + \text{Feedstock and Energy}(\text{NG, H}_2) + \text{Electricity}(\text{grid}) \\ & + \text{EUA}(\text{CO}_2) + \text{Transport and Storage}(\text{H}_2, \text{CO}_2) \\ & + \text{Water} - \text{Revenue}(\text{O}_2) \end{aligned} \quad (1)$$

Not all terms come into effect for all pathways. Notably, conventional production and the blue hydrogen pathway are based on existing plants and do not have a CAPEX term.

At the moment in time when the specific ammonia production cost from an alternative pathway is equal or lower than the specific ammonia production cost of the conventional process, it would be favorable for the operator to switch to the alternative pathway, which would then be more competitive than the conventional production.

2.3.5 Sensitivity Analysis

In order to gain insight into sensitivities of individual of individual parameters, the cost parameters for electricity (green and grid), natural gas, CO₂ (EUA), ROI, deprecia-

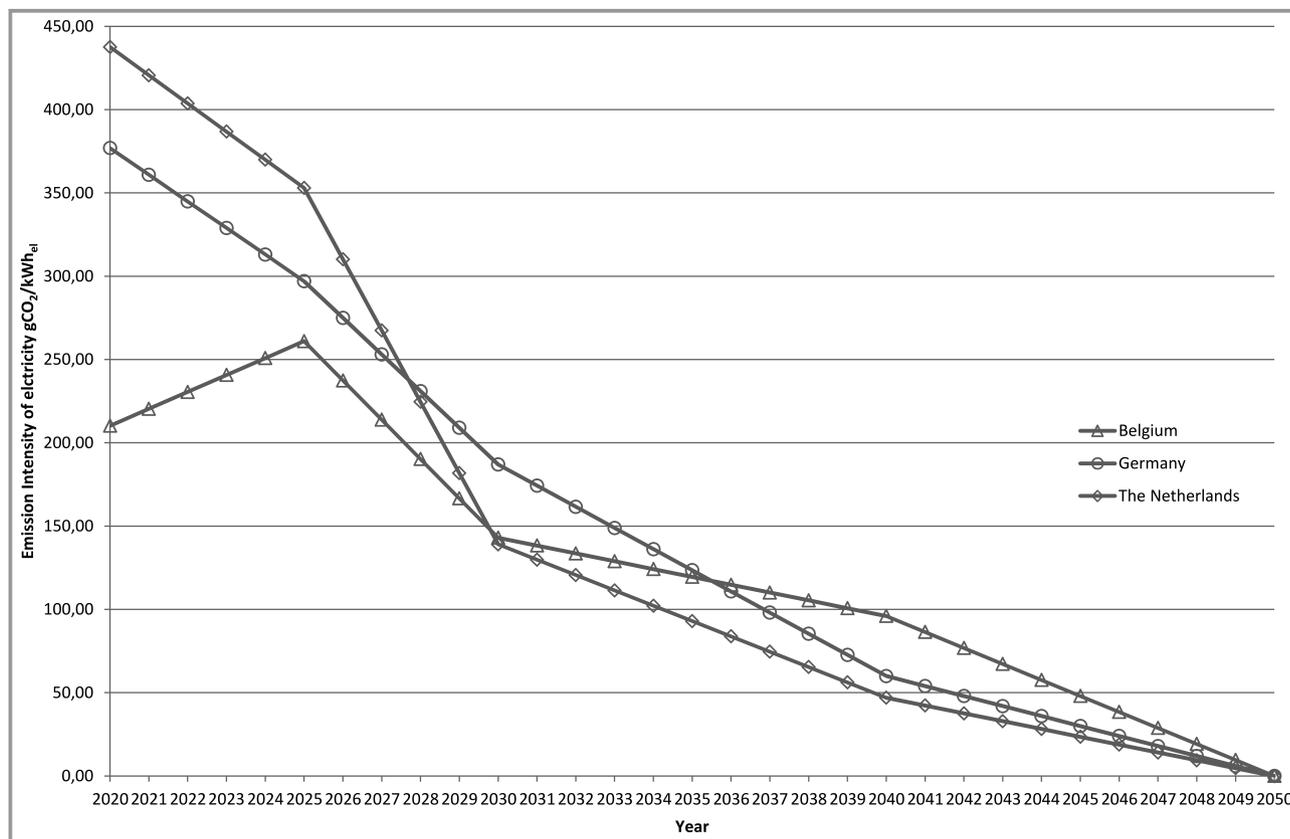


Figure 5. Development of emission factors for grid electricity.

tion time and CAPEX were independently varied in the range from 50 % to 150 % of the set value.

2.3.6 Infrastructure Demand

Grid electricity as well as other energy carriers required and direct CO₂ emitted in case of blue hydrogen for each pathway is adjusted for overall production volume and the full load hours of the plant to derive the overall required yearly supply, from which the required respective load is then calculated.

3 Results

3.1 CO₂ Emission Intensity

The conventional ammonia production process has direct emissions on-site (scope 1) both from feedstock, i.e., hydrogen production from natural gas via steam reforming (SMR) and energy, as well as emissions caused by grid electricity use (scope 2).

All other pathways avoid direct emissions on-site or apply CCS and only cause emissions by the use of grid electricity (scope 2). Scope 2 emissions are decreasing in line with the decarbonization of the respective power sector.

With the notable exception of gray hydrogen being produced by water electrolysis powered by grid electricity, all alternative pathways lead to significant instant reductions of CO₂ emissions by ammonia production in comparison to the conventional process. Dark green hydrogen achieves specific emission parity with the conventional process around 2030–2034, depending on the decarbonization progress of the grid electricity.

A comparison of the specific emission intensity development for the different ammonia production pathways is provided in Fig. 6. It also clearly shows the convergence of specific emissions between different countries as electricity generation becomes more and more CO₂-neutral with time and achieves full convergence by 2050.

3.2 Specific Production Cost

While most alternative pathways allow for rapid reduction of specific CO₂ emissions compared to the conventional production, the same relation does not hold for specific production costs. Fig. 7 provides the development of specific production costs for NH₃ for the different pathways under investigation. The current reference value is given by the partially-filled black columns, which represent a depreciated conventional plant.

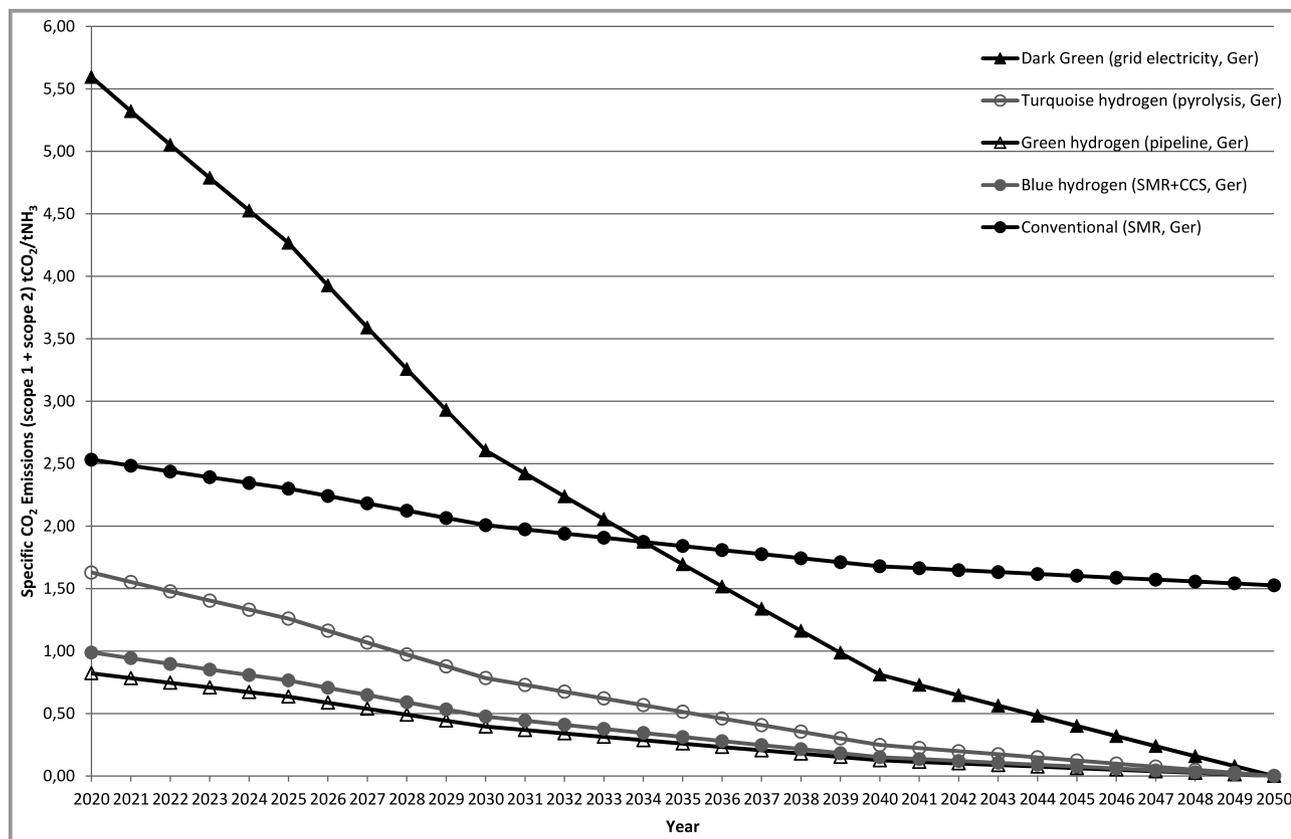


Figure 6. Comparison of specific emission intensity of different ammonia production pathways for the Dormagen site. Variations between different countries in the dark green hydrogen would reflect different emission intensity in the electricity grid and disappear once electricity generation is CO₂-neutral in 2050. The resulting emission intensity is mainly caused by residual use of grid electricity, e.g., for air separation, pumps, etc.

Production of ammonia via green hydrogen is by far the most expensive option due to the full load hours limitations and therefore relatively expensive hydrogen. Grid hydrogen does not suffer this penalty and sees a strong decrease in specific production costs due to improved electrolyzers. Specific production costs for turquoise and blue hydrogen remain essentially constant over time but become more competitive due to increasing CO₂ emission costs for the conventional pathway.

Variations between different sites are marginal and therefore not displayed in Fig. 7. They do exist pre-2050 when emission intensity of the grid electricity still contributes to differences. The blue hydrogen option becomes slightly less costly when CCU is considered on-site, i.e., urea production at Geleen, NL.

3.3 Cost Parity with Conventional Production

One crucial question is at what point in time a (non-depreciated) alternative pathway reaches cost parity with the (depreciated) conventional process, i.e., when would a company consider replacing the existing plant by the new tech-

nology? As displayed in Tab. 6, only the blue hydrogen pathway achieves cost parity for the considered set of assumptions and within the chosen timeline for all possible combinations.

3.4 Cumulative CO₂ Emissions

The answer to the question when a specific technical solution might be implemented has a strong impact on the cumulated emissions of ammonia production of a given plant over the investigated period of time. Assuming a constant production, Fig. 8 displays the effect of implementing different pathways as incremental substitution as soon as the criterion is met. Early adoption of alternative pathways might lead to significant reduction of cumulated emissions over the period.

3.5 Sensitivity Analysis

The results strongly depend on the assumptions taken for each of the parameters taken. Each of these values might be

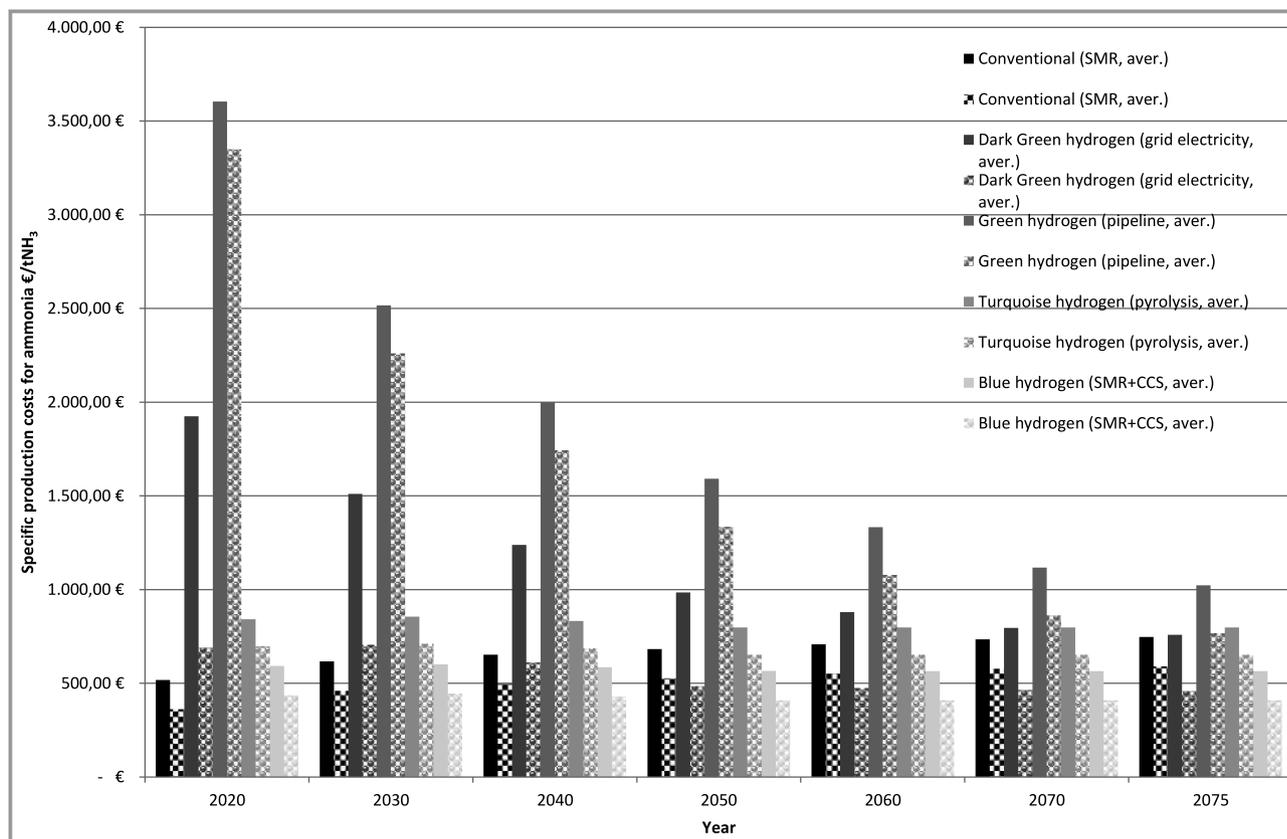


Figure 7. Development of specific NH_3 production costs for different pathways over time. Solid bars represent the non-depreciated plant, while the plaid columns represent depreciated plants.

Table 6. Overview when cost parity of new production technology with conventional production is reached. Blue hydrogen reaches earlier cost parity in Geleen due to urea production on-site, for which some of the CO_2 can be used (depr. = depreciated).

	Dark green hydrogen		Green hydrogen		Turquoise hydrogen		Blue hydrogen	
	Non-depr.	Depr.	Non-depr.	Depr.	Non-depr.	Depr.	Non-depr.	Depr.
<i>Antwerp, Belgium</i>								
CO ₂ -parity	2032		2020		2020		2020	
Non-depr.	–	2040	–	–	–	2046	2030	2020
Depr.	–	2049	–	–	–	–	2070	2030
<i>Dormagen, Germany</i>								
CO ₂ -parity	2035		2020		2020		2020	
Non-depr.	–	2038	–	–	–	2046	2030	2020
Depr.	–	2048	–	–	–	–	2070	2030
<i>Geleen, The Netherlands</i>								
CO ₂ -parity	2031		2020		2020		2020	
Non-depr.	–	2038	–	–	–	2046	2026	2020
Depr.	–	2048	–	–	–	–	2057	2026

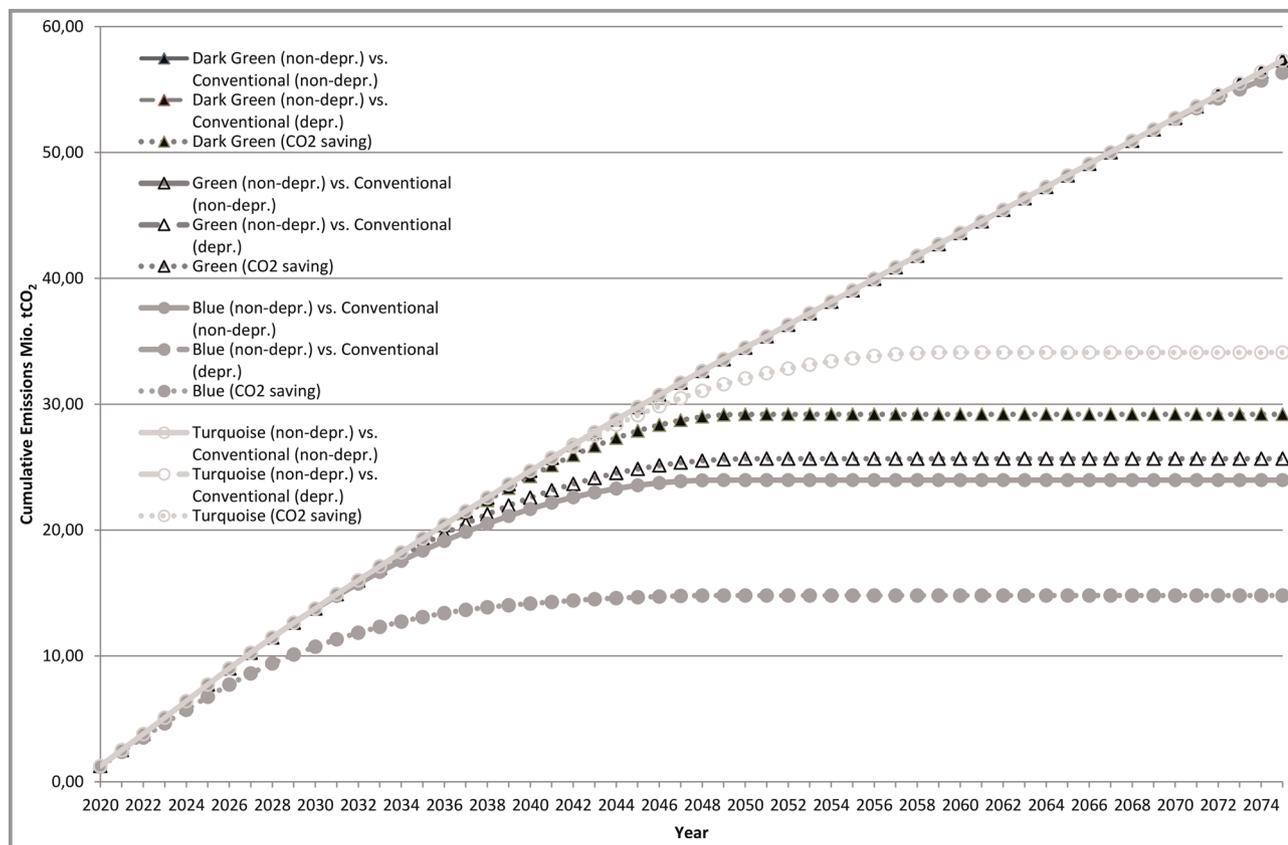


Figure 8. Cumulative emissions by ammonia production at the Antwerp site. Greenhouse gas neutrality is reached once the lines become horizontal. Implementation of new technology substitutes conventional production incrementally at a rate of 5 % per year from the moment when the technology is available or meets the criterion below. Solid lines refer to alternative pathways being implemented when they reach cost parity versus non-depreciated conventional production, dashed lines when cost parity of non-depreciated alternative pathways against depreciated conventional production is reached, dotted lines display the effect when CO₂ parity with conventional production is reached.

scrutinized and other values may be taken for a more “realistic” result. The robustness of the calculations can be evaluated with a sensitivity analysis.

Each of the parameters (depreciation period, ROI, CAPEX (electrolyzer), CO₂ cost (EUA), natural gas price and electricity price) was independently varied between 50 % and 150 % of the standard value. The results can be displayed in graphs similar to Fig. 9, which summarizes the sensitivity results.

This approach is in accordance with the sensitivity analysis of Geres et al. [5] to describe the transformation of the chemical industry in Germany.

3.6 Infrastructure Needs

Each possible pathway has significant implications on the infrastructure required on-site in order to supply the required energy carrier or remove CO₂ emitted by the plant. Conventional production requires natural gas as feedstock and for energy purpose as well as some electricity for compressors, etc. Dark green hydrogen would be produced

on-site via water electrolysis and requires a much more prominent connection to the power grid in order to provide the electricity. Green hydrogen would be produced elsewhere and then supplied by a hydrogen pipeline. Turquoise hydrogen would require more natural gas than the conventional process and the natural gas pipeline capacity may need to be expanded. Finally, in the blue hydrogen pathway, in the special case of ammonia production, the hydrogen would be produced on-site by SMR and the captured CO₂ would be transported to a storage site with a CO₂ pipeline.

Depending on the pathway of choice, existing infrastructure may continue to be used, may have to be expanded or may be obsolete. New infrastructure might be required. The required infrastructure for the different ammonia production technology options are summarized in Tab.7 for Antwerp, Tab. 8 for Dormagen and Tab. 9 for Geleen.

Overall, the infrastructure requirements for the different pathways and all sites considered can be summarized as in Fig. 10. A rough evaluation of the infrastructure readiness of the different sites under investigation for the different pathways reveals Fig. 11, with some additional remarks.

Table 7. Infrastructure implications derived from the different pathways for the ammonia production at the Antwerp, Belgium site with 630 kt a⁻¹ production capacity. Additional energy requirements for compression for CO₂ and green hydrogen have been omitted.

Antwerp, Belgium		Conventional	Dark green hydrogen	Green hydrogen	Turquoise hydrogen	Blue hydrogen
Natural gas	[PJ a ⁻¹]	16.5	0	0	45.2	16.5
	[MW]	551	0	0	1508	551
Electricity	[GWh a ⁻¹]	1239	6201	982	1945	1239
	[MW]	149	745	118	234	149
Hydrogen	[PJ a ⁻¹]	0	0	12.8	0	0
	[MW]	0	0	426	0	0
CO ₂	[kt a ⁻¹]	0	0	0	0	-877
	[th ⁻¹]	0	0	0	0	-100

Table 8. Infrastructure implications derived from the different pathways for the ammonia production at the Dormagen, Germany, site with 300 kt a⁻¹ production capacity. Additional energy requirements for compression for CO₂ and green hydrogen have been omitted.

Dormagen, Germany		Conventional	Dark green hydrogen	Green hydrogen	Turquoise hydrogen	Blue hydrogen
Natural gas	[PJ a ⁻¹]	7.9	0	0	21.5	7.9
	[MW]	263	0	0	718	263
Electricity	[GWh a ⁻¹]	590	2934	468	926	590
	[MW]	71	353	56	111	71
Hydrogen	[PJ a ⁻¹]	0	0	6.1	0	0
	[MW]	0	0	203	0	0
CO ₂	[kt a ⁻¹]	0	0	0	0	-440
	[th ⁻¹]	0	0	0	0	-50

Table 9. Infrastructure implications derived from the different pathways for the ammonia production at the Geleen, The Netherlands site with 1180 kt a⁻¹ ammonia production capacity and 525 kt a⁻¹ urea production capacity. For those pathways that emit CO₂ on-site, CO₂ needs to be provided for urea production via pipeline, indicated by the negative numbers. Additional energy requirements for compression for CO₂ and green hydrogen have been omitted.

Geleen, The Netherlands		Conventional	Dark green hydrogen	Green hydrogen	Turquoise hydrogen	Blue hydrogen
Natural gas	[PJ a ⁻¹]	29.4	0	0	81.5	29.4
	[MW]	1033	0	0	2824	1033
Electricity	[GWh a ⁻¹]	2223	11 126	1762	3489	2223
	[MW]	279	1396	221	438	279
Hydrogen	[PJ a ⁻¹]	0	0	22.9	0	0
	[MW]	0	0	797	0	0
CO ₂	[kt a ⁻¹]	0	348	348	348	-1,298
	[th ⁻¹]	0	40	40	40	-148

4 Conclusions

Ammonia production has several options for eventually GHG-neutral production pathways. All of these alternative pathways essentially eliminate on-site scope 1 emissions that are present in the conventional process. Scope 2 emis-

sions caused by the use of externally supplied electricity remain and vary strongly depending on the specific pathway. Greenhouse gas neutrality for ammonia production can, therefore, only be achieved when scope 2 emissions are also eliminated, e.g., by purchasing green electricity or by general decarbonization of the power grid from 2050 onwards.

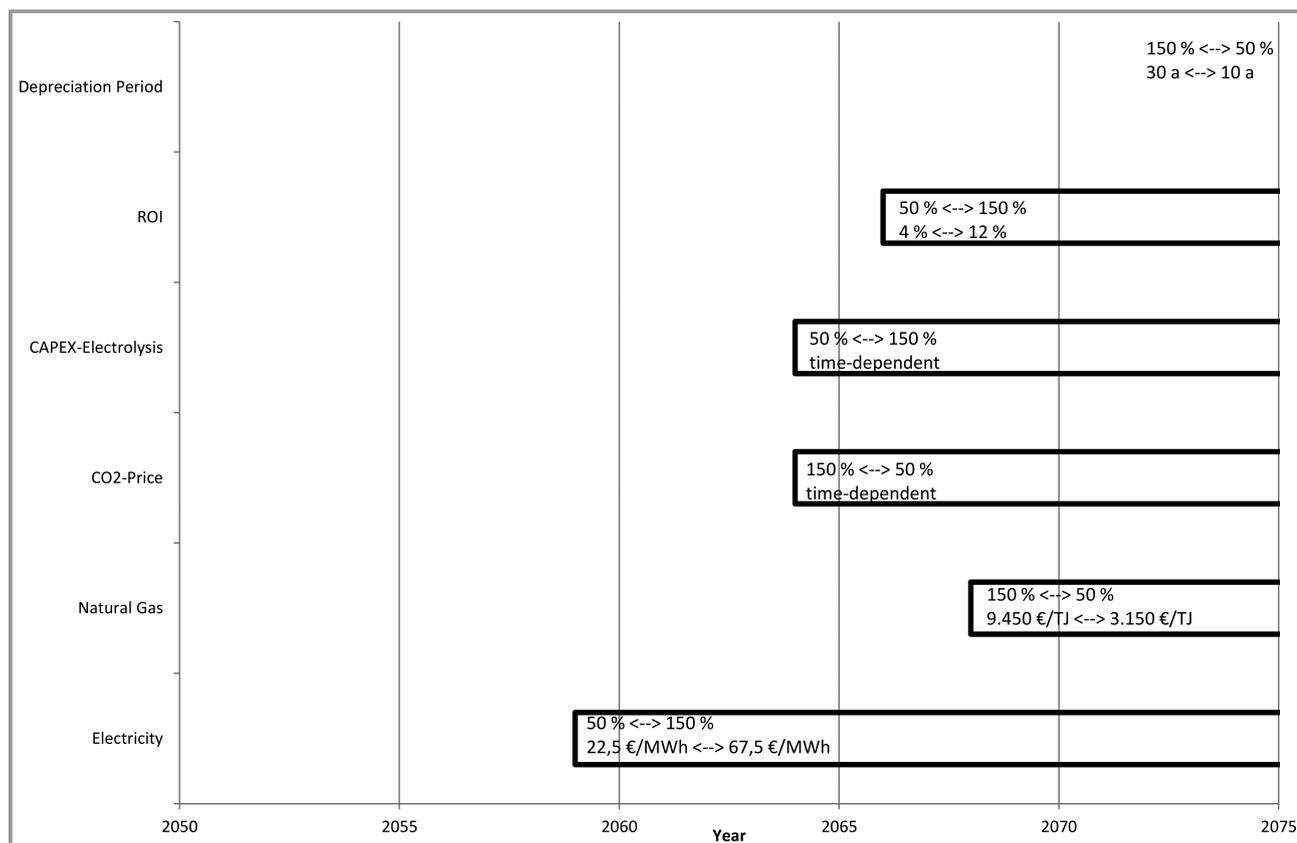


Figure 9. Results of sensitivity analysis for a non-depreciated gray hydrogen plant vs. a non-depreciated conventional plant in Geleen, The Netherlands. In case of electricity cost being half of the standard value ($45 \text{ € MWh}_{\text{el}}^{-1}$ after 2050) cost parity with a new conventional ammonia plant would be reached in 2059, with all other parameters at their standard values. These values represent the variations for the solid gray and black columns in Fig. 7.

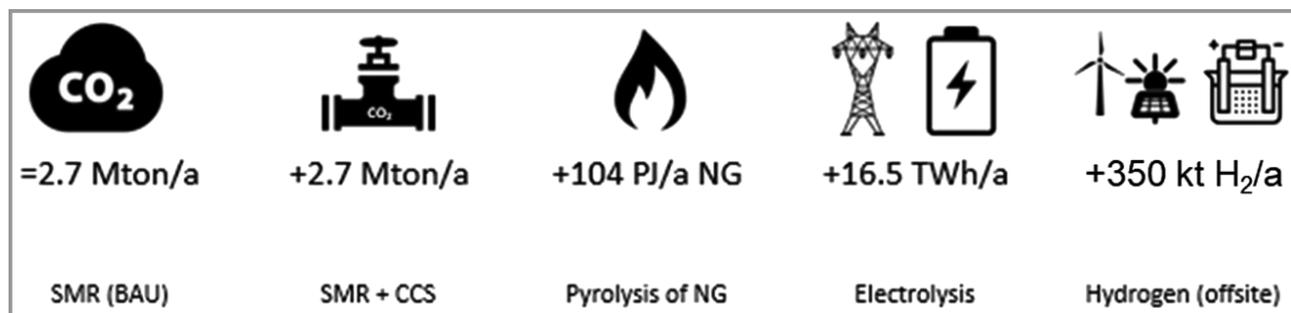


Figure 10. A summary of infrastructure requirements for the different methods for achieving CO₂ neutrality on the investigated sites.

With the exception of the dark green hydrogen pathway, i.e., on-site electrolysis with grid electricity, all other pathways lead to significant instantaneous reduction of overall CO₂ emissions. These pathways allow to some extent for incremental drop-in options to complement the existing process, thereby leading to a smoother transition. In addition, due to the highly integrated nature of conventional ammonia production, even pursuing a simple drop-in strategy would still require significant changes to the existing plant configurations, as they are in general currently not able to accommodate an external hydrogen supply.

However, all pathways struggle to be competitive against depreciated conventional production, which is the current status quo in Europe. Conventional production benefits from relatively low prices for natural gas compared to electricity prices for the electrolytic pathways. This gap is not sufficiently compensated by increasing CO₂ (EUA) cost. Electrolyzers remain a relatively expensive technology even assuming a strong decrease in investment cost over time.

Cost competitiveness remains the dominant challenge to implement new technologies within a globally competing

	Antwerp (BE)	Dormagen (DE)	Geleen (NL)	comments
Conventional	Existing Production	Existing Production	Existing Production	
SMR + CCS (blue H₂)	Harbor location advantageous for CO ₂ export via shipping	CCS currently not legally possible in Germany	Offshore storage potential in empty gas fields	CO ₂ -infrastructure required --> repurposing NG pipelines
Green H₂ (pipeline or shipping)	Hydrogen pipeline but limited capacity; Harbor location with potential for direct H ₂ terminal	Hydrogen pipeline but no connection to port	Natural gas pipelines could be converted to hydrogen	Existing hydrogen infrastructure not sufficient
Electrolysis on-site	Coastal location could lead to easy access to North Sea offshore wind park,	Good grid connection (Power plant on-site, powered by natural gas)	Existing transmission network from coast to site, although far from shore	May be limited by grid capacity and large amount of green electricity (offshore?)
	6 TWh/a would require cross-border grid improvement		11 TWh/a would require grid improvement to site	
Pyrolysis of natural gas	Strong natural gas connection	Natural gas connection with 320 000 cubic meters per hour sufficient	Existing gas infrastructure insufficient	Continuous natural gas supply required

Figure 11. Infrastructure preparedness of the three sites under investigation sites for different pathways. Light shade implies no strong limitations, intermediate shade implies some limitations and dark shade implies strong limitations foreseen at the site to implement a given technology.

industry. Carbon border adjustment mechanisms, such as currently investigated by the European Commission, could be a game changer compensate for higher production cost at European sites. Alternatively, emission-free ammonia hydrogen could be imported from regions with cheaper supply of hydrogen, applying any of the pathways outlined above. The disappearance of ammonia production on any of these sites would have a strong impact on the remaining processes, most likely leading to a complete reorganization of the site configuration or even permanent shut-down of chemical production on the site. However, if ammonia would play a future role as fuel rather than chemical, current European production is unlikely to meet respective future demands.

The assumptions used in this study were taken to the best of the authors' knowledge and may not reflect the future developments sufficiently. But if these assumptions are a relatively close description of the future situation, transformation of basic chemicals production, presents a significant entrepreneurial risk.

Pyrolysis is a technology with a relatively low technological maturity that requires further research and development. Application of CCS to existing ammonia plants seems to be the most promising pathway, since it can be readily implemented on a plant level with little effect on ongoing production and is the technology to become competitive against conventional production the earliest.

Addressing climate change requires an early adoption of alternative pathways, as today's available technologies can already significantly reduce the overall emissions of the site and thereby its contribution to climate change.

However, all alternative pathways require adjustment of existing infrastructures to allow for their implementation. The additional demand of energy carriers can reach up to a significant fraction of the overall national demand and is unlikely to be met by existing infrastructures. It is worth keeping in mind that ammonia production is not the only chemical process that needs to be adapted to achieve greenhouse gas neutrality for the chemical sector. Furthermore, this argument also applies to other industrial sectors, e.g., steel or refineries.

Energy amounts required in the process industries are commonly underestimated. This occurs even more often for energy carriers which are used in non-energy terms, i.e., feedstock, reducing agents. They are, however, responsible for most of the energy demand and greenhouse gas emissions of the industrial sector.

The urgency of the challenge and its implications on the required infrastructures can only be met by a coordinated and common effort beyond national borders. All three sites discussed in this paper are connected to the same energy infrastructures and changes at one site will affect the other sites irrespective of the national borders. Since different pathways lead to different infrastructure requirements, a close industry-overarching cooperation is needed to avoid stranded assets, both on the infrastructure and site level. In the future, it is desirable to compare the cost of competing infrastructure which can provide the industries in this region a long-term license to operate. A position which caters to employing changes, while at the same time ensuring a security of supply for feedstock and energy, zero CO₂ impact, minimum ecological impact and competitive position

in global markets would be securing a long-term perspective for the European heavy industries. This needs to be provided as general input into the European process of energy transition.

The presented methodology also allows a detailed investigation of processes at a given site rather than the same process at different sites, in order to establish the possible transformation pathways and the respective infrastructure requirements.

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References

- [1] J.-D. Arndt, S. Freyer, R. Geier, O. Machhammer, J. Schwartz, M. Volland, R. Diercks, Rohstoffwandel in der chemischen Industrie, *Chem. Ing. Tech.* **2007**, 79, 521–528. DOI: <https://doi.org/10.1002/cite.200700025>
- [2] *A Clean Planet for all A European strategic long-term vision for a prosperous, modern, competitive and climate neutral economy*, COM(2018) 773 final, Communication from the commission to the European Parliament and the European Council, the European Economic and Social Committee, the Committee of Regions and the European Investment Bank, Brussels, November 28, **2018**.
- [3] United Nations, *Paris Agreement*, Paris **2015**.
- [4] A. M. Bazzanella, F. Ausfelder, *Low carbon energy and feedstock for the European chemical industry*, DECHEMA, Frankfurt **2017**.
- [5] *The National Hydrogen Strategy*, Federal Ministry for Economic Affairs and Energy, Berlin, **2020**. www.bmbf.de/files/bmwi_Nationale%20Wasserstoffstrategie_Eng_s01.pdf
- [6] *A hydrogen strategy for a climate-neutral Europe*, COM(2020) 301 final, Communication from the commission to the European Parliament and the European Council, the European Economic and Social Committee, the Committee of Regions, Brussels, July 08, **2020**,
- [7] R. Geres, A. Kohn, S. Lenz, F. Ausfelder, A. M. Bazzanella, A. Möller, *Roadmap 2050, FutureCamp*, DECHEMA, Munich, Frankfurt **2019**.
- [8] S. Schneider, S. Bajohr, F. Graf, T. Kolb, State of the Art of Hydrogen Production via Pyrolysis of Natural Gas, *ChemBioEng Rev.* **2020**, 7 (5), 150–158. DOI: <https://doi.org/10.1002/cben.202000014>
- [9] H. Blanco, N. Wouter, J. Ruf, F. Faaij, Potential of Power-to-Methane in the EU energy transition to a low carbon system using cost optimization, *Appl. Energy* **2018**, 232, 323–340. DOI: <https://doi.org/10.1016/j.apenergy.2018.08.027>
- [10] *CO₂ Emission Intensity*, European Environment Agency, Copenhagen **2020**. www.eea.europa.eu/ds_resolveuid/0EKWQC5FRZ (accessed on July 24, 2020)
- [11] *Energiedaten Gesamtausgabe*, Bundesministerium für Wirtschaft und Energie, Berlin **2020**. www.bmwi.de/Redaktion/DE/Artikel/Energie/energiedaten-gesamtausgabe.html (accessed on August 31, 2020)
- [12] *Guidelines on certain State aid measures in the context of the system for greenhouse gas emission allowance trading post 2021*, C(2020) 6400 final, Communication from the commission, Brussels, September 21, **2020**.
- [13] *CO₂-emission intensity from electricity generation*, European Environment Agency, Copenhagen **2020**. www.eea.europa.eu/data-and-maps/data/co2-intensity-of-electricity-generation (accessed on August 31, 2020)
- [14] *TYNDP 2020 Scenario Report*, ENTSO-E, ENTSOG, Brussels **2019**. www.entsog.eu/sites/default/files/2019-11/TYNDP_2020_Joint_ScenarioReport_web.pdf (accessed on August 31, 2020)