Hydrogen technologies for a CO_2-neutral chemical industry – a plant-specific bottom-up assessment of pathways to decarbonise the German chemical industry

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Abstract

With approximately 21 % of total emissions in Germany, the industrial sector is one of the major emitting sectors, accounting for almost 30 % of final energy demand and predominantly using fossil fuels.

Hydrogen based on renewable electricity can have a key role in the transition towards a CO_2-neutral industrial production, since its use as an energy carrier as well as a feedstock in various industrial process routes is promising. One of the most important industries with great potential for hydrogen use is the chemical industry, in particular the production of basic chemicals like ammonia and methanol. While many scenarios towards 2050 see an important role for hydrogen in the 2050 supply mix for the industry sector, they are less specific on the path towards 2050 and the role of hydrogen e.g. in 2030.

Here, we assess the role of hydrogen in the mid-term and further detail the possible paths towards 2050 by taking into account the specific replacement and modernisation cycles of the production plant stock and assess today's maturity of hydrogen-based technologies. The analysis includes a thorough literature review as well as the development of a plant-specific database.

By considering the age structure of basic chemical process installations in Germany, 33 % can be replaced by 2030 and 89 % by 2050. This results in 11 % that have to be replaced before the end of their lifetime for getting CO_2-neutral until 2050. A replacement of 100 % would lead to cumulated capital investments of about €26 billion and yearly operating costs of €15 billion. The re-assessment and benchmarking of a scenario taken from the literature for the selected products by integrating results from the analysis of plant modernisation cycles shows, that the plant replacements and market diffusion of alternative production routes could be integrated faster than assumed in the literature.

Introduction

The German Federal Government has set firm mitigation targets in the context of the approval of the Climate Protection Act in November 2019. These include a 55 % reduction in greenhouse gas emissions by 2030 compared to the base year 1990 and climate neutrality by 2050 (BMU 2019). With approx. 21 % of total GHG emissions in Germany in 2017, the industrial sector is one of the largest emitting sectors, accounting for almost 30 % of final energy demand and predominantly using fossil fuels (UBA 2018; UBA 2018b). In particular, energy-intensive industrial sectors such as steel, cement and chemicals represent a particular challenge for achieving the German and European climate targets due to their high specific and absolute emissions in combination with technical restrictions of currently available technologies, as well as emissions from chemical reactions in the production process. Consequently, considerable efforts must be made to avoid the use of fossil fuels and raw materials in the individual process routes and the generation of process emissions. This is difficult or impossible to achieve with currently available technologies.

The direct and indirect use of electricity based on renewable energies can play an important role in the decarbonisation of industry (Möst et al. 2020; Rehfeldt et al. 2020; Lechtenböhmer et al. 2016). Storable electricity-based energy carriers (e.g. methane or hydrogen), which can be integrated into current systems and processes at short notice, can make a major contribution to achieving ambitious 2030 targets. A significant role is attributed to hydrogen, as its use is promising both as an energy carrier and for feedstock use in various industrial process routes. As a storable medium, hydrogen can also be used for energy storage to balance demand and fluctuations in the production of renewable energies in the future (Hartner et al. 2019).

The chemical industry has a great potential for hydrogen use. In particular, the production processes for basic chemicals (e.g. ammonia, methanol and ethylene) show potential for hydrogen-based transformation. This paper examines a possible transformation pathway to alternative process routes. The analyses are based on the knowledge of specific parameters from the literature and notice about the age structure of the existing plant stock in Germany as well as their production capacities.

Methodology

The presented results discuss the transformation of the German chemical industry based on technological approaches relevant in the literature. Statements and sensitivities with regard to energy demand, potential and cost assumptions of available technologies are examined. The potentials for the use of hydrogen and their possible market diffusion for a transformation pathway of the chemical industry are investigated, taking into account the site-specific age structure of the plant stock. Important aspects for the assessment of the diffusion of the technologies are market maturity, costs and energy demand. A final benchmarking with an existing decarbonisation scenario from the literature, which is a 95 % reduction scenario until 2050, helps to classify these results.

TECHNOLOGY EVALUATION (1)

In order to investigate a possible transformation of the chemical industry with regard to CO_2 neutrality, a comprehensive literature research is being conducted for the production routes of ammonia, methanol and ethylene production (via steam cracker). An overview of conventional and possible alternative climate-friendly production processes is compiled. Special attention is given to data on costs, specific emissions, specific energy consumption and hydrogen demand of the different technologies.

Due to the high potentials of the considered products regarding the use of renewable hydrogen, the analysis focuses on hydrogen production and hydrogen use.

SITE SPECIFIC EVALUATION OF THE TRANSFORMATION PATHWAY (2)

Based on a site-specific evaluation of the current technologies and process paths for ammonia, methanol and ethylene production, the status quo of the German plant stock is determined. Information on the age structure of the plant stock in combination with a consideration of the diffusion of technologies that are not yet ready for the market today – using renewable hydrogen – enables the determination of a bottom-up transformation potential of the chemical industry in Germany.

BENCHMARKING WITH DECARBONISATION SCENARIO (3)

Based on the technology evaluation and the transformation path developed, a comparison with an existing decarbonisation scenario (4b Mix95, (Fleiter et al. 2019)) for the basic chemicals ammonia, methanol and ethylene is carried out. The scenario 4b Mix95 used for comparison shows the modelled energy demand of the chemical industry. It was created with the modelling platform FORECAST (https://www.forecast-model.eu), which aims at developing long-term projections for the future energy demand of individual countries until 2050 (Fleiter et al. 2018). The analyses are based on a bottom-up modelling approach that takes into account the dynamics of technologies and socio-economic factors. The change to low-CO_2 production processes in the scenario 4b Mix95 is modelled in FORECAST with a high process resolution and is determined exogenously in the context of the scenario assumptions, whereby the existing plant stock and modernisation cycles, which are analysed in greater detail in this paper, are not explicitly taken into account.

Data: Review of potential CO_2-neutral production technologies

RESULTS OF THE TECHNOLOGY REVIEW

In this chapter, conventional and alternative methods of hydrogen production are investigated in more detail, as they form the basis for the decarbonisation of the above-mentioned products of the basic chemistry.

With regard to the cost analyses in the following, capital investments and production costs are compared for each product. The concept "capital investment" refers to the actual investments and the concept "production costs" refers to the annualised investments per ton and specific fixed and variable operating costs. An interest rate of 8 % and a depreciation of 20 years are assumed for the annuity of the investments. Sensitivity analyses that had been carried out showed that there is no appreciable impact in the level of the interest rate or the years of depreciation on the production costs because the variable operating costs dominate production costs. The shown figures in this chapter refer to the chosen base year 2020. Estimations for further development of the parameters on the path during 2050 are made at the end of this chapter for the observed technologies in the results. Furthermore for all calculations current electricity price and capacity factors of production facilities and constant production volumes until 2050 have been assumed. All calculations are referring to the LHV of the several products. Table 1 shows the assumed frame parameters used for the calculations of the following results.

Hydrogen production in the chemical industry

The chemical industry in Germany has the largest energy demand of the German industrial sector with approximately 24 % and consumes about 7 % of the total final energy demand in Germany (Eurostat 2019). In Germany, about 1.6 million tons of hydrogen are produced annually. Thereof approx. 40 % are directly used in refineries, 15 % are used for methanol production (whereof most of the methanol is also produced in refineries) and 30 % are used for ammonia production. Today's hydrogen production is based almost exclusively on fossil fuels.

Table 1. Overall frame parameter used for calculations in the present study.

Parameter	Unit	2020	2030	2050
Electricity price	€/kWh	0.05	0.05	0.05
Electricity emission factor	g CO_2-eq/kWh	510*	280	0
FLH	h/y	7,000	5,500	4,000
Depreciation	y	20	20	20
Interest rate	%	8	8	8

** Based on numbers from Umweltbundesamt (UBA) for 2017 (UBA 2018a).*

Approx. 33 % is produced from natural gas, 15 % from coal, 12 % from naphtha and only about 7 % is produced by electrolysis. The remaining 33 % are by-products of the oil refineries (Dena 2016). Ammonia and methanol production are the products with the highest hydrogen demand (Stiller et al. 2010). For this reason, a large part of the transformation of the basic chemicals production relies on the decarbonisation of hydrogen production. The potential technologies are examined more detailed below.

Conventional technologies for hydrogen production

The conventional production of hydrogen from fossil fuels is based on synthesis gas production and can be divided into three processes: steam reforming, partial oxidation and coal gasification. The main fossil sources used are natural gas, heavy fuel oil and distillation residues.

Since steam reforming is the predominant process route for the production of synthesis gas in Germany, it is used as the reference technology in the following.

Alternative technologies for hydrogen production

Conventional fossil-fuel based production methods could be supplemented by alternative renewable energy based methods in the mid-term and completely replaced in the long term. By substituting the existing hydrogen production from steam reforming in Germany, a theoretical emission saving of about 5.6 million tons of CO_2 would be possible (Dena 2016). Approaches for alternative production processes already exist, but not all of them are ready for the market at the present time. In the following, two promising technologies with possible market entry in the next decade in large-scale applications are investigated concerning their economic and environmental parameters.

At first, **water electrolysis** is basically technically mature. In this process, water is broken down into hydrogen and oxygen in an electrolyser using electric current.

Depending on the electrolyte material and the operating temperature, a distinction is made between different electrolysers:

- Alkaline electrolysis (AEL)
- Proton exchange membrane electrolysis (PEMEL)
- High temperature electrolysis (SOEL)

Electrolysis only produces indirect CO_2 emissions for the generation of the required electricity. Thus, if based on CO_2-neutral electricity, the resulting hydrogen is also produced CO_2-free.

Due to the fact, that AEL is the most advanced electrolysis technology in the following "Electrolysis" describes the data for AEL (Smolinka et al. 2018).

The second possible process for alternative hydrogen production is **methane pyrolysis**. Here, natural gas is thermally broken down into its components hydrogen and carbon at over 1,000 °C in a high-temperature reactor. No CO_2 is directly emitted in the process. Instead of CO_2, carbon is produced, which can then be stored as a pure substance in solid form and used in many industrial areas (Dechema 2017).

Table 2 shows the comparison the capital investment (€/kW) and the specific production costs (€/ton) for the conventional hydrogen production via steam reforming and the two already described production processes water electrolysis and methane pyrolysis. The basis for the calculation of the cost estimation for conventional hydrogen production is taken from (Pérez-Fortes et al. 2016; Dechema 2017), for water electrolysis from (Smolinka et al. 2018; Dechema 2017; Bertuccioli et al. 2014; Buttler 2018) and for methane pyrolysis statements from (Machhammer et al. 2016; Dechema 2019) were adapted. The capital investment of the conventional production route and the expected investment of the methane pyrolysis are in a similar range, whereas electrolysis has about a third higher investment. The calculations for the production costs result in nearly the same costs for electrolysis and methane pyrolysis, whereas the conventional hydrogen production costs are two thirds of the alternative production costs, which goes along with the literature (Machhammer et al. 2016; Dechema 2019; Dechema 2017; Ikäheimo et al. 2018).

Conventional hydrogen production with CCS technology is not considered in this paper, as we focused on new technologies for green hydrogen without producing any CO_2. The production of renewable hydrogen from biomass is likely to play a subordinate role on a large scale due to its limited potential and is therefore not considered further.

The results presented for hydrogen production serve as basis for the calculations of the cost data of the production chains for ammonia, methanol and ethylene carried out in the following.

As the synthesis of the several products are already at TRL 9 the limiting factor for the market entry of the alternative technologies for ammonia, methanol and ethylene is the TRL and possible market readiness of the hydrogen production unit. According to (Agora 2019) and (Dechema 2017), market entry for electrolysis is expected from 2025 (but first large-scale electrolyser are already going to be installed) and for methane pyrolysis from 2030.

Ammonia

Ammonia, one of the most important inorganic basic materials, is used in Germany to about 80 % for the production of fertilizers (ISPT 2017). Thus, the development of ammonia demand is strongly dependent on the fertilizer market and is slightly declining in Germany, since the demand for fertilizers has also been declining for some years despite increasing agricultural production (Agora 2019). In 2017, ammonia production in Germany amounted to about 2.9 million tons (Agora 2019; VCI. 2019). With a specific hydrogen demand of 0.178 tons per ton of ammonia, this corresponds to a hydrogen consumption of 516 kt and an energy consumption of about 27.5 TWh (Dechema 2017; Agora 2019; VCI 2019).

Conventional Ammonia production technologies

The production of ammonia consists of two integrated process stages, the synthesis gas process and the ammonia synthesis according to the Haber-Bosch process (Dechema 2017; Smith et al. 2004).

In Germany, 70 % of conventional ammonia production is carried out by steam reforming of natural gas and, at one site that accounts for about 30 % of the production capacity, by partial oxidation of heavy oil and oil residues (Fleiter 2013).

Alternative Ammonia production technologies

Taking into account the scale of application, potential alternatives for green hydrogen are water electrolysis using renewable energy (Power-to-Ammonia) and methane pyrolysis.

For the production of ammonia from electricity, carbon-free hydrogen is obtained by means of water electrolysis (power-to-ammonia). No direct CO_2 emissions are produced, and the coupling of hydrogen production by water electrolysis and the subsequent Haber-Bosch process makes it possible to avoid the use of fossil fuels (Ikäheimo et al. 2018).

Due to the higher electrical efficiency of high-temperature electrolysis and the possibility of heat integration with ammonia synthesis for better heat utilization, high-temperature electrolysis may have the best potential for coupling with ammonia synthesis in the future (Cinti et al. 2017). But as mentioned above, here low-temperature electrolysis has been taken for the analyses because of uncertainties in the data for high-temperature electrolysis.

The difference between the alternative and conventional ammonia production is only the provision of the hydrogen required for the ammonia synthesis. However, due to the development stage of methane pyrolysis, large-scale use and market entry is expected later than water electrolysis.

Technology comparison

The capital investment and the calculated ammonia production costs of ammonia production are also shown in Table 2 for the conventional hydrogen supply and for the processes using hydrogen from electrolysis or methane pyrolysis. The different process steps for the various modes of hydrogen production and the ammonia synthesis have been calculated separately. Knowledge about the cost data and correspondingly adapted assumptions for the ammonia synthesis from (Ikäheimo et al. 2018) provided a basis for the calculations carried out.

For the production of ammonia with electrolysis hydrogen literature values of (Sánchez 2018) are about €100/ton higher not explaining their assumptions in detail. By conducting a sensitivity analysis in our calculations these production costs are obtained with minor changes in full load hours or efficiencies. Additionally assumptions of increasing electricity costs because of higher percentage of renewables in the electricity mix lead to higher production costs.

Conventional production costs can be found in (Boulamanti 2017), where the European average is €337/ton. Their production costs have been defined differently and take no annualised investments into account but only include feedstock, credits due to valuable co-products , electricity, thermal energy, other materials (chemicals and catalysts) and labour and others (salaries, maintenance costs, property tax etc.). So ongoing and fixed operating costs are taken into account, which correspond to the variable and fixed operating costs in this paper below. According to the current status, the investments can be expected to decrease by 2050.

Methanol

Methanol is widely used in the chemical industry as an intermediate for a variety of industrial chemicals (Olah et al. 2009). In addition, methanol has excellent combustion properties, which allows its use as a fuel or fuel additive in vehicles.

In 2017, 1.05 million tons of methanol were produced in Germany, which, with a specific hydrogen demand of 0.189 tons of hydrogen per ton of methanol, results in a total hydrogen demand of about 200 kt. This leads to a total energy demand of approx. 9 TWh.

Conventional Methanol production technologies

Methanol production can basically be divided into three steps: Synthesis gas production, raw methanol production and methanol processing (Menrad 1982).

Most of the methanol produced industrially today comes from the catalytic conversion of synthesis gas. The production of synthesis gas is analogous to that occurring in the production of ammonia by means of steam reforming or partial oxidation (Dechema 2019; Agora 2019).

Alternative Methanol production technologies

The production of methanol via alternative routes differs from ammonia production only in the appropriation of the synthesis gas for methanol synthesis. CO_2 sources for mixing with hydrogen to produce synthesis gas can be the flue gases from power plants or factories that produce steel, cement and other large CO_2-intensive products. The required hydrogen can be provided by water electrolysis (power-to-methanol) or methane pyrolysis as described before.

Technology comparison

Analogous to ammonia production, Table 2 shows the results of the calculations for the capital investment and production costs of methanol production for the conventional and the two alternative hydrogen supply technologies. Hydrogen supply processes and methanol synthesis have been calculated separately similarly to ammonia, too. The basis for the methanol synthesis is provided by (Pérez-Fortes et al. 2016). This results in the shown capital investment and production costs, which goes in line with (Pérez-Fortes et al. 2016). (Boulamanti 2017) name the average operating costs for methanol at about €408/ton.

Ethylene

Ethylene is produced in the petrochemical industry by thermal cracking of long-chain hydrocarbons (usually naphtha) in a so-called steam cracker as a partial product of the process. In addition to ethylene other HVC (high value chemicals) such as propylene and butene are also produced. The following discussion is limited to ethylene, whose production volume in 2017 was approximately 5.2 million metric tons in Germany (VCI 2019).

Conventional Ethylene production technologies
Ethylene is conventionally produced by fossil heat generation for thermal cracking in steam cracker. The composition of the product components can vary depending on the feedstock to be cracked (Dechema 2019; Agora 2019).

Alternative Ethylene production technologies
Compared to ammonia and methanol, the possibility of transforming ethylene production via hydrogen is much more complex, since no hydrogen is used in conventional ethylene production. In addition to the substitution of fossil-fired steam cracker by electrically heated boilers for steam generation, ethylene production via methanol (methanol-to-olefins) as an intermediate product represents a further variation for decarbonisation.

Technology comparison
Similarly to ammonia and methanol before, Table 2 shows the comparison of the capital investment (€/kW) and the specific production costs (€/ton) for the conventional ethylene production via steam cracker and the alternative MtO process by way of both already described production processes, namely water electrolysis and methane pyrolysis. The MtO production is a process with high potential for hydrogen and the literature mentions that 2.8 tons methanol per ton ethylene are needed (Dechema 2017). (Boulamanti 2017) estimated EU total average operating costs for conventional ethylene production to about €748/ton when ethylene is the only main product.

The specific total energy requirement of hydrogen-based ethylene production via methanol-to-olefins (MtO) is, about factor 5 higher than the conventional route. For the calculations the required methanol is produced hydrogen via electrolysis. Another alternative for ethylene production with less energy demand could be the production via steam crackers with electrical steam generation. This variant will not be considered in more detail in the following, as this technology has an expected market entry due to its Technology Readiness Level (TRL) (1–3) after 2050 and possible hydrogen potentials are examined in this paper (Agora 2019). According to the current state of the art, the specific emissions of the MtO process are also far above (factor 8–10) those of conventional technology today due to the indirect emissions of the electricity used in the electrolyser. A potential market entry of the hydrogen route is conceivable from 2025.

Chosen Technologies for a possible transformation pathway

From the technology evaluation carried out it is clear that the implementation of alternative technologies is only meaningful if a supply of renewable electricity can be guaranteed, due to the current high indirect CO_2 emissions.

Altogether, due to the uncertainties concerning methane pyrolysis, for the following calculations water electrolysis (AEL) is chosen as technology for the alternative production routes and the costs on the path until 2050 are only estimated for the following alternative technologies.

- Ammonia: Ammonia via water electrolysis (AEL)/Power-to-Ammonia
- Methanol: Methanol via water electrolysis (AEL)/Power-to-Methanol
- Ethylene: Ethylene via methanol/Methanol-to-Olefins

The specific energy consumptions and emission factors of the respective technologies are also adapted from and based on several literature studies such as (Dechema 2017; Ikäheimo et al. 2018; Dechema 2019; Olah et al. 2009).

Taking into account current electricity emissions, the specific emissions from water electrolysis are significantly higher than the emissions of the other technologies. Regarding to ammonia, the emissions for electrolysis are doubled compared to steam reforming and tripled compared to methane pyrolysis. Methanol has significant lower emissions using the conventional process due to the use of CO_2 produced in the steam reformer unit by the following methanol synthesis unit.

Table 2 summarises first results on the assumed parameter used for the several technologies on which the following calculations and results are based on.

Results

TRANSFORMATION PATHWAY DUE TO THE AGE OF THE PLANT STOCK

Figure 1 shows all ammonia, methanol and ethylene production sites in Germany. Size ranges are given to which the respective production capacity of the respective site corresponds. Based on the age structure of the plant stock and the production capacity, the transformation of the chemical industry and an estimation of the dimension of necessary investments can be made. In the literature, a theoretical lifetime of such chemical plants of 40–60 (Fleiter 2013) or 50 years (Dechema 2019; Agora 2019) is given. We calculate possible diffusion pathways for alternative low-carbon processes based on the assumption that no pre-mature capital replacement takes place and that reinvestment is conducted after the end of life.

Taking into account the age structure of the plants with an average theoretical lifetime of 60 years, Figure 2 shows that a total of 20 % of ammonia plants, 50 % of methanol plants and 33 % of ethylene capacities will be subject to renewal by 2030. By 2040, 80 % of ammonia, 75 % of methanol and 55 % of ethylene plants will have reached the end of their service life, which accounts for about 80 % of the production for the three products of the base year 2017. Finally, 100 % of the ammonia and methanol plants and 78 % of the ethylene plants will have to be replaced by 2050.

The capital investment in the respective time intervals (decades) is compared on the left side in Figure 3, divided into "Electrolyser Unit" and "Synthesis Unit" of the particular chemicals. This means necessary total (cumulative) investments (including investments for hydrogen production) of 8 billion euros by 2030, 16.4 billion euros by 2040 and 22.3 billion euros by 2050 have to be made as shown in right part of Figure 3, if each of the plants will be replaced totally after the assumed lifetime of 60 years. Until 2050, 22 % of the ethylene plants will still not have been replaced, representing additional investments of 3.7 billion euros.

Figure 4 indicates that based on today's production volume of these products an annual hydrogen demand of 3.45 million tons

Table 2. Data overview and first results used for further calculations for the following transformation pathway.

Product	Parameter	Technology	Unit	2020	2030	2050
		Steam Reforming	€/kW	710	710	710
	Capital investment	Electrolysis	€/kW	1,100	700	300
		Methane Pyrolysis	€/kW	780	650	450
		Steam Reforming	%	80	82	85
	Efficiency (LHV)	Electrolysis	%	70	73	80
		Methane Pyrolysis	%	70	73	80
		Steam Reforming	kWh/kg	39.6	39.6	39.6
Hydrogen	Specific energy consumption	Electrolysis	kWh/kg	53	51	48
		Methane Pyrolysis	kWh/kg	67	65	60
		Steam Reforming	€/kg	2	2	2
	Production costs	Electrolysis	€/kg	3.4	3.2	2.75
		Methane Pyrolysis	€/kg	3.1	2.95	2.65
		Steam Reforming	kg CO_2/kg H_2	11	11	11
	Emission factor	Electrolysis	kg CO_2/kg H_2	27	14,8	0
		Methane Pyrolysis	kg CO_2/kg H_2	9,1	5	0,3
	Capital investment	Ammonia Synthesis	€/kW	870	830	750
	Efficiency	Ammonia Synthesis	%	70	73	80
	Specific energy consumption	Ammonia Synthesis	kWh/kg	2	2	2
		via Steam Reforming	€/kg	0.96	0.96	0.96
Ammonia	Production costs	via Electrolysis	€/kg	1.25	1.17	1.03
		via Methane Pyrolysis	€/kg	1.19	1.16	1.13
		via Steam Reforming	kg CO_2/kg NH_3	2,5	2,5	2,5
	Emission factor	via Electrolysis	kg CO_2/kg NH_3	5,1	2,8	0
		via Methane Pyrolysis	kg CO_2/kg NH_3	1,7	1	0,5
	Capital investment	Methanol Synthesis	€/kW	750	730	700
	Efficiency	Methanol Synthesis	%	70	73	80
	Specific energy consumption	Methanol Synthesis	kWh/kg	1.7	1.7	1.7
		via Steam Reforming	€/kg	1.12	1.12	1.12
	Production costs	via Electrolysis	€/kg	1.34	1.28	1.12
Methanol		via Methane Pyrolysis	€/kg	1.30	1.28	1.17
		via Steam Reforming	kg CO_2/kg MeOH	0,5	0,5	0,5
	Emission factor	via Electrolysis	kg CO_2/kg MeOH	5,2	2,8	0
		via Methane Pyrolysis	kg CO_2/kg MeOH	1,7	1	0,5
	Capital investment	MtO Synthesis	€/kW	150	120	75
	Efficiency	MtO Synthesis	%	75	78	83
	Specific energy consumption	MtO Synthesis	kWh/kg	–	–	–
		via Steam Cracker	€/kg	0.78	0.78	0.78
Ethylene	Production costs	via Electrolysis	€/kg	3.86	3.59	3.15
		via Methane Pyrolysis	€/kg	3.7	3.58	3.29
		via Steam Cracking	kg CO_2/kg Eth	2	2	2
	Emission factor	via Electrolysis	kg CO_2/kg Eth	20	11	0
		via Methane Pyrolysis	kg CO_2/kg Eth	6,7	3,7	0,8

has to be provided (left). This results in an electricity demand for the production of hydrogen as a raw material of about 180 TWh per year. Overall, 100 % implementation of the alternative production routes represents a potential saving of up to 16 million tons of CO_2 in the production of the three basic chemicals under the constraint of 100 % renewable electricity (right).

As it can be seen in Figure 5 convenient to the plant renewal in Figure 2, the total share of renewed plants influences the share on capital investment and operating costs. Figure 5 shows furthermore, that the operating costs increase from about €5 billion/year in 2030 to about €15 billion/year in 2050, which goes in line with the increase of the annuity from about €6 billion/year in 2030 to nearly €18 billion/year in 2050, taking into account a depreciation of the capital investments of 20 years. The operating costs would increase between 15 and 20 % compared to existing plants.

The modernisation cycles mentioned in the literature and used in this analysis are theoretical values. In reality, significantly longer lifetimes of the plants can often be observed, as usually only individual plant components get replaced or modernised. Thus the basic structure of a plant as well as individual plant components can exist significantly longer than the assumed 60 years and make it difficult to assess well-founded statements about possible reference investments. Therefore, the investments of the alternative technologies presented are to be understood as total investments.

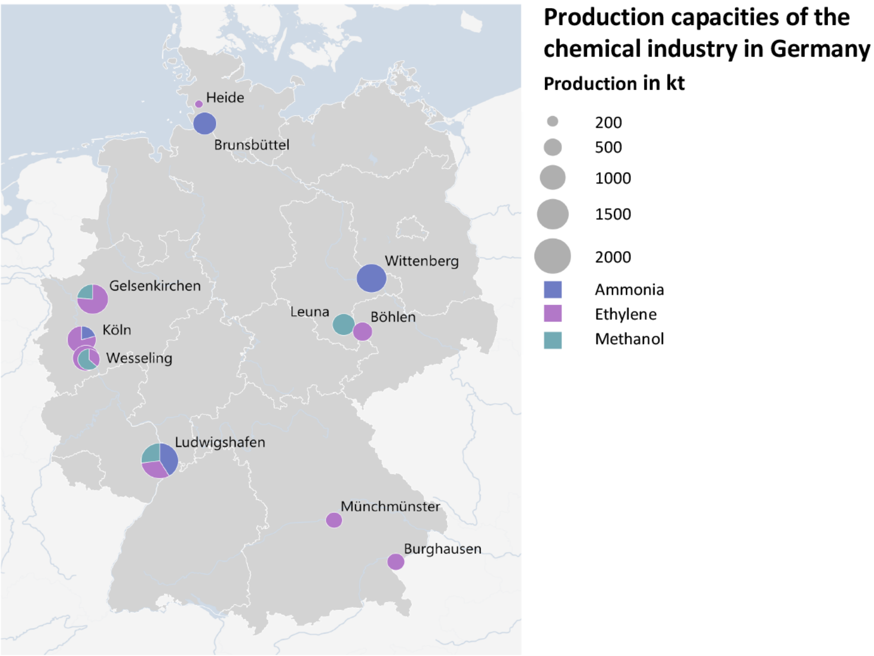


Figure 1. Ammonia, methanol and ethylene production sites in Germany and their site-specific production capacities.

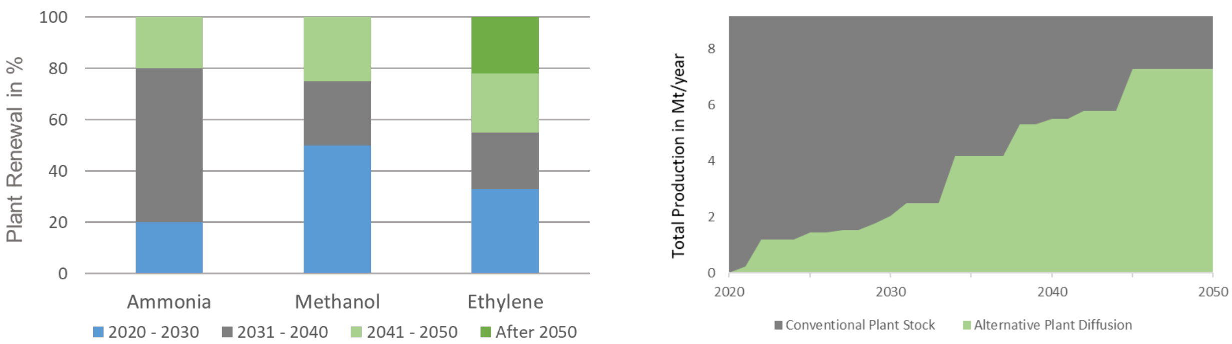


Figure 2. Possible plant renewals taking into account the age structure of the current plant stock of the ammonia, methanol and ethylene production (left) and amount of the total cumulated production (right).

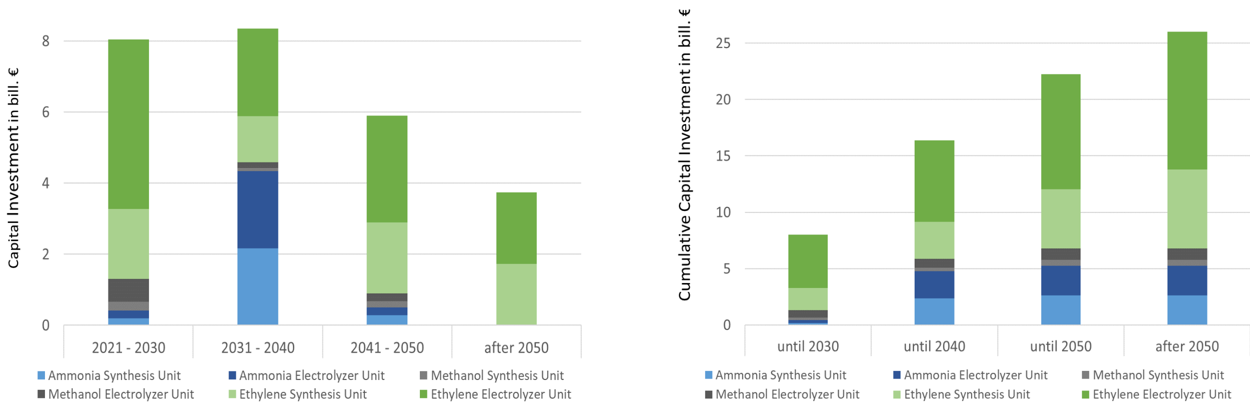


Figure 3. Total capital investments in the several decades for ammonia, methanol and ethylene (left) and cumulative capital investments (right) divided into synthesis and electrolyser unit for the particular products.

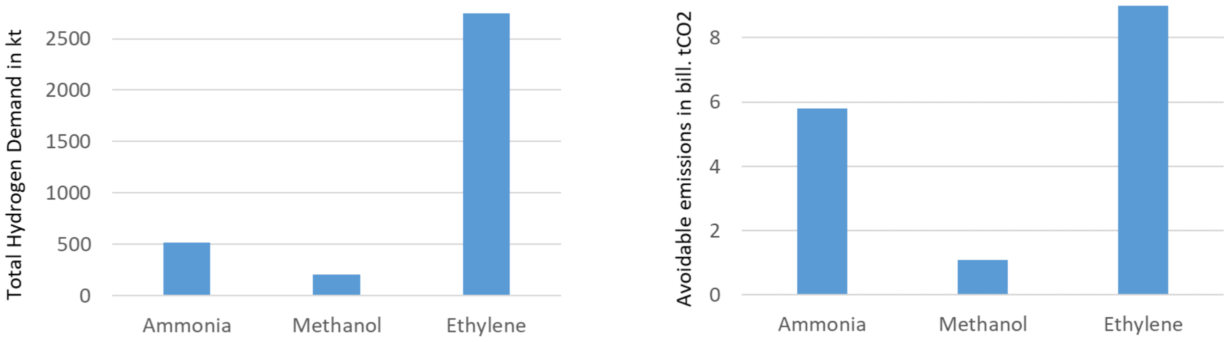


Figure 4. Total annual hydrogen demand for 100 % plant replacement towards alternative technologies based on the production of the year 2017 (which is assumed to be constant over the whole transformation period) (left) and avoidable CO_2-emissions by implementing the alternative processes under the constraint of 100 % renewable electricity (right) for ammonia, methanol and ethylene.

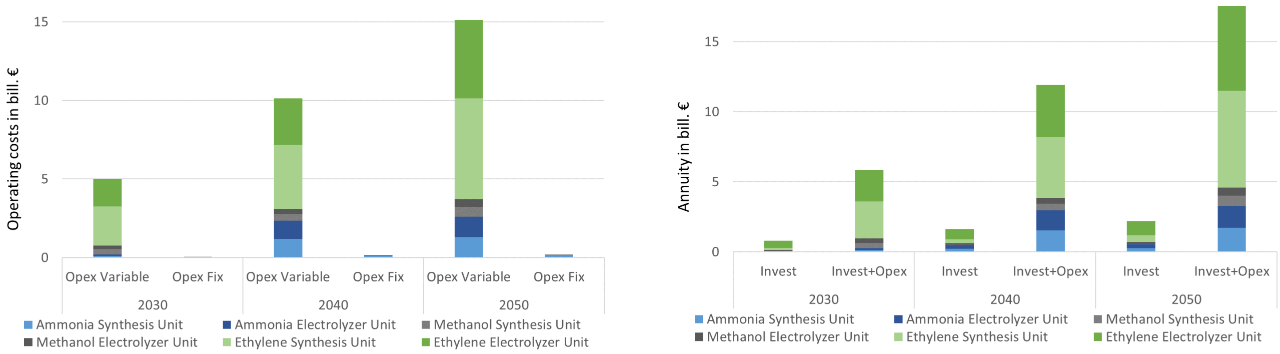


Figure 5. Annualised variable and fixed operating costs (left) and annualised capital investments and total production costs (capital investments + operating costs) (right) of the synthesis and electrolyser units for ammonia, methanol and ethylene.

BENCHMARKING WITH SCENARIO TAKEN OUT OF LITERATURE

We take our plant specific bottom-up assessment of a possible transformation pathway considering the age structure of the plant stock and compare it to the assumed pathway in the scenario study (Fleiter et al. 2019). The scenario "4b Mix95" from the study presents an ambitious decarbonisation scenario reducing GHG emissions for the EU industry by about 95 % in 2050 compared to 1990. New low-carbon processes are exogenously introduced in this scenario. It is based on the core assumption that the market diffusion of innovative CO_2-free production technologies in the chemical sector will be 100 % by 2050 and will start around 2030.

Figure 6 shows the results for the development of energy demand in the chemical industry in Germany. Overall, an increase in electricity demand from 53 TWh in 2015 to 286 TWh in 2050 can be observed. The year 2030 shows an electricity demand for hydrogen as feedstock of 8.4 TWh. Taking into account the age of the plant stock, substantial replacements can take place earlier and the energy demand for hydrogen supply is significant higher than in the scenario 4b Mix95, which is due to the very energy-intensive MtO route for ethylene production. In 2040, scenario 4b Mix95 shows an electricity demand for hydrogen as feedstock of 60.5 TWh. In comparison, the electricity requirement for hydrogen production is about 42 TWh higher in the present paper. Assuming full implementation of the technologies by 2050, the 4b Mix95 scenario shows a use of 163.4 TWh for hydrogen production. In comparison, the calculations performed in the present paper show an electricity demand for hydrogen production of 146.4 TWh in 2050. Assuming full implementation by 2050, this results in an electricity demand of 180 TWh.

The denomination "electricity for clean gas" in 4b Mix95 specifies the electricity demand for the production of synthetic methane in the scenario.

The decarbonisation scenario from the literature shows hydrogen in 2050 as the most important energy carrier (main production for use as feedstock) in the chemical industry. The comparison carried out indicates that the age of the existing plants may result earlier replacements than assumed in the scenario 4b Mix95. This might lead to a faster diffusion of new techniques or involves a high danger of long-term lock-in, if the re-investment is favoring the conventional fossil-based routes. With lifetimes of 60 years, the new plants will reach their lifetimes long after 2050 or will need to be replaced before they reach the end of life, which involves uneconomically higher system costs.

SUMMARY OF THE KEY FINDINGS

The comparison on the capital investments indicates that those of alternative hydrogen production equals the capital investment of Steam Reforming (SMR) around 2030. Including the operating costs into the calculation, it can be seen that the production costs of alternative hydrogen production decreases about 20 % until 2050 referred to the base year 2020. This results in alternative hydrogen production costs still 37.5 % and 32.5 % above the conventional technology (SMR) for electrolysis and for methane pyrolysis in 2050.

Concerning ammonia and methanol, the production costs via SMR and via water electrolysis converge to similar values until 2050. Regarding the assumed development of the electricity mix until 2050, the emission factor for ammonia from alternative production technologies equals conventional emission factors around 2035, whereas equality for methanol is given near to 2050, due to the use of CO_2 in the synthesis gas. Ethylene production costs via MtO route is still quadrupled in 2050 compared to steam cracking. This results out of the high energy demand.

Taking into account the current electricity mix the specific emissions per kg of produced hydrogen are more than doubled by water electrolysis compared to SMR, whereas the emission factor of methane pyrolysis may be in a similar range as SMR. Furthermore the emission factor for water electrolysis is about ten times higher in the base year 2020 and equals late around 2045, due to the assumed electricity mix.

For calculating a possible transformation pathway on these results and considering the age structure of the plant stock for a most efficient transformation by assuming a lifetime of 60 years, 33 % can be replaced until 2030, 66 % until 2040 and 89 % until 2050. For compatibility with the political target of CO_2-neutrality until 2050, 11 % must be replaced before their have reached theoretical lifetime.

A 100 % replacement for the German ammonia, methanol and ethylene plants in line with the policies would result in cumulative capital investments of €26 billion until 2050 and operating costs of about €15 billion per year in 2050. The total hydrogen demand would be around 3,475 kt per year and 16 million tons CO_2 are avoidable if 100 % renewable electricity is provided.

Comparing the pathway for these basic chemicals with the scenario 4b Mix95 from Fleiter et al. 2019, the transformation considering the age structure could be much faster in until 2040. The electricity demand for hydrogen as feedstock for full implementation of alternative process routes until 2050 goes in line with the electricity demand calculated in the present paper for restructuring the individual sites.

Conclusion

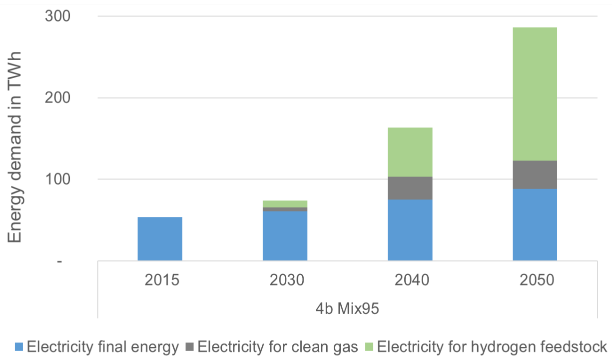
This paper examines the role of hydrogen technologies as climate-neutral alternatives to conventional production processes in the manufacture of energy-intensive basic chemicals with high CO_2 emissions. It is shown, that hydrogen production via electrolysis is the by far most important technology for CO_2-neutral production until 2050. Due to age structure, the conversion to alternative production routes could be faster than assumed. If new investments in conventional technologies will be executed, this results in lock-in dangers with CO_2-intensive plants having again a lifetime of 40 to 60 years.

In order to avoid CO_2-emissions by replacing conventional plants with alternative processes it gets clear that much higher shares of renewable electricity have to be implemented in the electricity mix earlier than in the expected developments. Especially in early years problems due to limited availability of green electricity can occur.

Also infrastructural aspects can play an important role when thinking about hydrogen-based technologies. As the potentials for renewable electricity differ a lot in Europe, solutions for either electricity or hydrogen transportation options have to be found. Furthermore transport of CO_2, which is needed for methanol production and the MtO route, has to be taken into account. In general the import of electricity or hydrogen and their corresponding prices or following effects for the energy system could have impacts on the costs and competitiveness of internal alternative production.

As the alternative process routes are less economical as the conventional technologies (which are developed over decades), implementations of political instruments such as CO_2 taxes are conceivable to ensure competitiveness of domestic production. Also international agreements or instruments like Border Tax Adjustments have to be discussed, as different political requirements lead to economic imbalances.

In addition, more sensitivity analyses could be useful in the future to get more detailed information on the behavior of some parameter on the cost estimates and statements for the



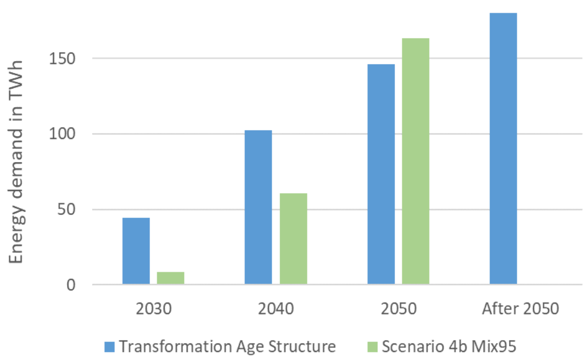


Figure 6. Electricity demand of the chemical industry (left, taken from Fleiter et al. 2019) and comparison of the electricity demand for hydrogen production of the possible transformation pathway considered in this paper and the scenario 4b Mix95 in Fleiter et al. 2019.

relation to the conventional processes in total, e.g. the impact on the future electricity prices.

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