Decarbonization of the German chemical industry in light of the Paris Agreement

Final Report

Interdisciplinary Project Group

MSc Industrial Ecology

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Preface

This report is the final deliverable of the Interdisciplinary Project Group, a course from the Master of Science in Industrial Ecology a LU and TUD. The project was commissioned by the German Aerospace Center (DLR). Three students from the programme: Sif de Visser, Stefan Lübke, and Yeji Park worked on the project from September 2020 to January 2021.

The research topic on the decarbonization of the German chemical industry is part of a nationwide climate research initiative (HI-CAM) in which DLR is involved in. As part of the initiative, DLR is developing scenarios for the carbon goal of Germany with a focus on the future energy supply of the industrial sector. Among the industries DLR is looking into, the case of the chemical industry was given to the students as a research topic.

The authors want to express sincere gratitude to the project supervisor and commissioners who have provided essential and invaluable support. Special thanks go to Bernand Steubing for providing comprehensive perspective and sharp insight. Many thanks to Carina Harpprecht for full support and detailed guidance, and Sonja Simon for providing research directions and energy-specific insights.

Executive Summary

As a ratifier of the Paris Agreement, Germany aims to be greenhouse gas (GHG) neutral by 2050. The chemical industry is currently responsible for 8% of the final energy demand in Germany. This industry is hard to decarbonize being a complex multisector, where end products are applied in different industries. Supply chains are highly integrated, the diversity of chemical products is large, and the infrastructure has a long lifespan, meaning that changes require long-term planning.

The Helmholtz Climate Initiative (HI-CAM) research project assesses how various industries in Germany can facilitate the transition to a GHG neutral balance. This study contributes to the HI-CAM project by examining the case of the chemical industry. The research question "*How can the German chemical industry transform to comply with the carbon goals set in the Paris Agreement?*", is addressed.

First, a technology table is delivered which shows the identified existing and developing technologies for the chemical product groups of ammonia, urea, chlorine, methanol, and High Value Chemicals (HVC). The consequences of shifts in energy carriers and production technologies are examined for process and energy-related emissions. Specifically, the final energy demand, the energy carriers used and the GHG emissions are considered.

Second, two scenarios are created: a reference (RS) and a normative scenario (NS). The RS serves as a benchmark, while the NS considers an optimal situation for technology production pathways to achieve minimal GHG emissions. Finally, the scenarios are compared with carbon budgets for temperature increases of 1.5 and 1.75 °C.

The results show that the transformation requires the phase-out of conventional technologies and the increase of technologies such as electrolysis, methane pyrolysis, biomass gasification and plastic waste pyrolysis. Electricity demand is expected to increase substantially due to the high share of electrolyzers. The ultimate strategy forward to 2050 is highly dependent on the decarbonization of the energy sector. An unsuccessful transition of the energy system has large implications for the chemical industry and might opt for a different approach favoring other alternatives such as biomass gasification.

Comparing carbon budgets with the scenarios shows that in all cases the carbon budget is exceeded. Low-carbon production technologies are not expected to be sufficiently developed before 2035, leaving no carbon budget for the future. Time is running if Germany wants to comply with the Paris Agreement. Without extending the focus from feedstocks and production technologies switches, the carbon budget will most likely not be met. Circular economy measures, industry-wide and cross-regional cooperation will be essential to further decarbonize the chemical sector. It is recommended to consider potential synergies and trade-offs to see how the chemical sector can transform from an energy-intensive and high emitting sector to a solution-provider to other sectors.

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Abbreviations

BAFA	Bundesamt für Wirtschaft und Ausfuhrkontrolle (Federal Office of Economics and Export Control)
BMUB	Bundesministerium für Umwelt und Bau (Federal Ministry for Environment)
BTX	Benzene, toluene, xylenes
$CB_{global, 2018}$	Global carbon budget from 2018 onwards
$CB_{Germany, 2020}$	German carbon budget from 2020 onwards
$CB_{chemical,scope1}$	Carbon budget of chemical industry in the industry sector
$CB_{chemical,scope2}$	Carbon budget of chemical industry in the energy sector
CCU	Carbon capture and utilization
CEFIC	European Chemical Industry Council
CH_3OH	Methanol
CH_4	Methane
CO_2	Carbon dioxide
CO_2-eq.	Carbon dioxide equivalent
DECHEMA	Deutsche Gesellschaft für chemisches Apparatewesen (German Society for Chemical Apparatus)
DLR	Deutsche Zentrum für Luft- und Raumfahrt e. V. (German Aerospace Center)
$E_{Germany,2018}$	Emissions in Germany in 2018
$E_{Germany,2019}$	Emissions in Germany in 2019
$E_{chemical,scope2,2020}$	Emissions in the energy sector associated with the German chemical industry 2020
EF	Emission Factor
GHG	Greenhouse Gas
Gt	Gigaton

H_2	Hydrogen
H_2O	Water
$[H_2NCOO]NH_4$	Ammonium carbamate
H_2NCONH_2	Urea
HI-CAM	Helmholtz Klimainitiative (Helmholtz Climate Initiative)
HVC	High Value Chemicals
ICCA	International Council of Chemical Associations
IEA	International Energy Associations
IPCC	Intergovernmental Panel on Climate Change
IRENA	International Renewable Energy Agency
LU	Leiden University
MWh	Megawatt hours
Mt	Mega ton
MTA	Methanol-to-Aromatics
MTO	Methanol-to-Olefins
N_2	Atmospheric nitrogen
NDC	Nationally Determined Contributions
NH_3	Ammonia
NS	Normative Scenario
O_2	Oxygen
R&D	Research & Development
RS	Reference Scenario

SRU	Sachverständigenrat für Umweltfragen (Expert council for environmental issues)
TWh	Terawatt hours
TRL	Technology Readiness Level
TUD	Technical University Delft
UNFCCC	United Nations Framework Convention on Climate Change
VCI	Verband der Chemischen Industrie (Association of the chemical industry)
WRI	World Resource Institute
WBCSD	World Business Council for Sustainable Development
%population	Population share
$\%share_{chemical}$	Share of the chemical industry on the German carbon budget
$\%share_{industry}$	Share of the industry sector on the German carbon budget
$\%share_{chemical\ on\ industry\ sector}$	Share of the chemical industry in the industry sector

1 Introduction

Paris Agreement and 2050 carbon neutrality goal of Germany

A historical agreement to limit global warming “well below 2°C, preferably below 1.5°C above pre-industrial level” was made by 190 parties at the Conference of the Parties in Paris in 2015. The Special Report on Global Warming of 1.5°C by the IPCC (2018) again stressed the importance of staying below 1.5°C, by explaining how climate-related risks on both nature and the human system will intensify with a further increase of global temperature. The report points out that a global temperature rise of 2°C would cause 2.6 times worse extreme heat and 10 times more frequent ice-free summers around the globe, compared to 1.5°C.

To jointly achieve the Paris climate goal, countries who are part of the Paris Agreement need to set Nationally Determined Contributions (NDCs) which indicate national contributions for GHG emissions reduction. Germany, as a ratifier of the agreement, has stated its NDCs in the Climate Action Plan 2050. With the plan, Germany draws a long-term strategy to become GHG-neutral by 2050, and a mid-term goal of reducing its overall carbon emissions with 55% by 2030 compared to 1990 (BMUB, 2016).

Decarbonization of the German industry sector

The industry sector is one of the six sectors for which Germany defines a pathway with individual targets and measures toward the goal of decarbonization. Reducing emissions of the industry sector is crucial, in 2017 it was the second-largest emitting sector in Germany (BMUB, 2016) with 200 Mt CO_2 equivalent (CO_2-eq.), representing 22% of the total emissions (Wuppertal Institute, 2020).

Long investment cycles and long lifespans of industrial infrastructure are characteristics of the sector that make its decarbonization more challenging than other sectors. With a lifetime of 20 to 50 years, industrial plants in operation today can continue running in 2050 and beyond (Agora Energiewende & Wuppertal Institute, 2020). For this reason, early prediction remains crucial for the decarbonization of the sector, so that existing plants can be made more compatible with low carbon technologies, or a new infrastructure can be built at the right time.

Transformation of the German chemical industry

i) Relevance of the chemical industry

The chemical industry is one of the major industries within the industry sector. With regard to turnover, it is the third-largest industry representing a share of 10% (DECHEMA, 2019). In the international comparison, Germany is on the 4th rank behind China, the USA, and Japan (VCI, 2019).

The chemical industry is accountable for a significant amount of energy demand in Germany. 20% of the energy consumed in the industry sector is consumed by the chemical industry, representing 8% of the final energy demand in Germany (VCI, 2020). Furthermore, the chemical industry is a major emitter of GHG emissions in Germany. In 2019, 37 Mt CO_2-eq. was emitted directly by the chemical industry, representing 19% of the total direct industrial emissions (Wuppertal Institute, 2020).

ii) Development of energy demand and emissions

Over the past three decades, the chemical industry has seen changes in its energy demand and emissions. While the production volume has grown by 80%, the energy demand has decreased slightly with 20% since 1990. Accordingly, the specific energy demand, which is the energy demand per unit of product, has been reduced as well and currently amounts to half of the demand in 1990 (VCI, 2020). Similarly, GHG emissions of the industry have been mitigated since 1990. The emissions have dropped more significantly than the energy demand. Consequently, specific emissions also showed a notable reduction. Especially non-CO_2 GHG emissions have dropped by about 50%. Such a reduction indicates that there has been a decoupling of energy demand and emissions from the production within the industry. Additionally, the decrease in energy demand and the recent increase in energy generation from renewable energy sources have induced the reduction in emissions of the chemical sector (Wuppertal Institute, 2020).

iii) Complexity of the chemical industry

The chemical industry features complexity from a number of aspects. It can be considered a complex multi-sector (Levi & Cullen, 2018), as the end products are highly diverse with more than 30,000 types of chemicals (VCI, 2020) and supply a wide variety of material and energy services for other sectors. The supply chain is characterized by many intermediate products. Ammonia can be considered both an end product or a basic chemical which is further processed into the intermediate product urea, which again can be further refined into a fertilizer. Furthermore, there are numerous production processes and pathways possible for each product.

As a consequence, the production processes of chemicals are highly integrated. Inputs and outputs of energy and materials are strongly harmonized and interdependent. This becomes visible in the so-called “Verbund-Standorten” of chemical companies. These are production sites of chemical companies that host a variety of highly integrated chemical production plants. Within such a facility, synergies are created to increase efficiencies; energy demand is reduced via heat integration, wastes are avoided, and the primary material demand is reduced. A particularly interesting example of such a process in light of climate change is the use of CO_2. It is increasingly used as an input for chemical processes and thereby substituting fossil carbon sources (DECHEMA, 2017). This is also known as carbon capture and utilization (CCU).

Related to the diversity and the depth of process integration is also the variable characteristic of energy carriers. Energy carriers such as hydrogen (H_2), biomass, oil products, etc. can be used as fuel to supply energy for a process but also as the feedstock of chemical processes. Used as a fuel, the energy carrier is part of an exothermic reaction such as combustion where its energy is used to power a chemical reaction. As a feedstock, the energy carrier becomes part of the reaction product. Often, in a production process, a part of the input energy carrier is fuel and another part is feedstock (DECHEMA, 2017).

Similar to other industries, the chemical industry produces parts of its energy demand on-site themselves. Thus, the source of energy supply is twofold, external source from the energy sector and internal source from the chemical industry’s own production. For heat production energy generated on-site is mainly used. For electricity, one-third of it is sourced internally while two-thirds are supplied from external sources. On-site energy generation is mainly conducted via combined-heat power plants which are mainly fired with natural gas. Emissions from such on-site energy generations result in energy-related emissions of the chemical industry (DECHEMA & FutureCamp, 2019).

Next to energy-related emissions, similar to other industries, process emissions are the other significant part of the emissions. These are emissions arising from non-energy-generation processes. These process emissions are extremely difficult to reduce due to the way they are embedded in the production processes of chemical products.

iv) Transforming the German chemical industry to stay within the carbon budget

As mentioned above, there have been advancements in the past decades with regard to the decoupling of production growth, emissions and energy demand in the chemical industry. However, considering the significant amount of emissions the chemical industry contributes to the entire sector, further transformation of the industry is required to meet the German carbon goal. For this reason, this paper aims to identify ways to transform the German chemical industry to meet Germany's carbon goals and analyze how such a transformation brings changes to its energy demand, energy carrier and emissions.

A few studies have looked into ways of transforming the German chemical industry to meet the carbon neutrality goal of Germany until 2050 (Agora Energiewende & Wuppertal Institute, 2020; DECHEMA, 2017; DECHEMA & FutureCamp, 2019). However, none of the studies has reviewed ways to meet a stricter carbon goal of staying within the industry's carbon budget according to the budget set by the Paris Agreement. This study addressed the research question: "*How can the German chemical industry transform to comply with the carbon goals set in the Paris Agreement?*"

The research steps are guided by the following set of sub-questions:

1. What are the implications of the transformation of technology pathways on the final energy demand, energy carriers and emissions of the German chemical industry?
2. Which technology pathways should be considered in an optimal scenario to transform the German chemical industry?
3. To what extent can the German chemical industry stay within its carbon budget to comply with the Paris Agreement?

2 Methodology

2.1 Scope definition

The scope of the study is chosen in compliance with the goal of the study and the scope of the HI-CAM project.

Geographical and temporal scope

The geographical scope of the study is Germany. To comply with the scope, the majority of emissions and energy data for selected products and identified production pathways are sourced from the case of Germany (Agora Energiewende & Wuppertal Institute, 2020; DECHEMA & FutureCamp, 2019). When German data is not available, data from European studies is used. For a few production pathways where both German or European data is not available, data from other regions is used. Detailed information on the source of energy and emission data of each production pathway can be found in Appendix B.

The temporal scope of the study is from 2020 to 2050, corresponding to the research goal. Therefore, the study considers both current and future technologies that are commonly in operation in the year 2020, and ones that will become available by 2050 with enhanced efficiency or lower emissions. To stay close to up-to-date information, the study used literature published within the last four years (Agora Energiewende & Wuppertal Institute, 2020; DECHEMA, 2017; DECHEMA & FutureCamp, 2019) as the main references.

Product selection

Five groups of chemical products: ammonia, urea, chlorine, methanol, and HVC are selected as product groups of focus in the study. The selection is made based on the proportion the product groups take up in the energy demand and emissions of the chemical industry. Through literature review, it is found that the selected five product groups plus Butadiene are accountable for about 75% of the GHG emissions of the German chemical industry (DECHEMA & FutureCamp, 2019). The same five product groups were mentioned as products which contribute to more than half of energy demand and CO_2 emissions of the chemical industry in Europe in another study (DECHEMA, 2017). Studies on the global chemical industry (IEA, ICCA & DECHEMA, 2013; IRENA, 2020) also point out similar groups. Butadiene, which is mentioned in the study on the German chemical industry, is exempted from the selected list of product groups due to a lack of data and because it is not mentioned as a major contributing product in other studies.

Technological scope

Conventional and future low carbon technologies for the production of each product group have been selected via a literature review. For future technologies that are not introduced in the market yet, literature has been consulted to find out in which year the technology would be available. In some cases, the Technology Readiness Level (TRL) is used to calculate the market entry year of a technology. The TRL is a concept that allows for the evaluation and comparison of the maturity of innovative technologies in a systematic manner (Buchner et al., 2019).

Once the TRL reaches level 9, the technology is considered ready to enter the market. In the study, it is assumed that it takes 5 years to go up one level on the TRL ladder. According to DECHEMA and FutureCamp (2019), it takes on average 7 years, however, this can be faster when ideal Research and Development (R&D) conditions and funding are assumed. A table which lists the years of when technologies become available plus a detailed description on the TRL approach can be found in Appendix C.

Scope of energy and emissions

A production-based approach is applied to focus on the energy demand and emissions associated with the production within the geographical scope of Germany. The accounting is largely based on the approach of the GHG protocol (WRI, 2014). The German chemical industry is defined as the "reporting entity". Therefore, the system boundaries of the sub-category "chemical industry", as defined in the 'Common Reporting Format for the provision of inventory information' of the UNFCCC (n.d.) are used. For this reporting entity, the scope 1 and scope 2 emissions are considered. Scope 1 covers all emissions that the reporting entity causes and thus controls itself. This covers all direct process emissions but also energy-related emissions when the energy is generated by the reporting entity itself. Opposingly, scope 2 emissions cover indirect emissions of the reporting entity associated with energy purchased from external sources.

Not considered are scope 3 emissions, which cover all emissions upstream and downstream of the reporting entity (WRI & WBCSD, 2011). Thus, emissions associated with the feedstock supply, the use phase and the waste management are out of scope. As the feedstock and the fuel are partly the same energy carrier (e.g., natural gas), it has been attempted to define the proportion of energy carriers that is used as fuel and to exclude the part used as feedstock.

Moreover, not only CO_2 but all GHG emissions are accounted for within the scope of this study. Opposingly, the carbon budget is only taking CO_2 emissions into account. How the comparison between the modeled scenario with a GHG scope and the carbon budget with a CO_2 scope has been conducted is discussed in chapter 2.3 more thoroughly.

Of high importance is the accounting of CCU by chemical products. The carbon capturing at the primary emitter and the use of the captured carbon in a CO_2-conversion plant (e.g., Fischer Tropsch plant) represent a multi-functional process (see Fig. 1). Therefore, multi-functionality has to be solved for proper accounting. For this, a simple form of allocation between the primary emitter and CO_2 conversion plant, where captured carbon is used, is conducted. According to Ramirez et al. (2020), for CCU technologies with a low TRL an allocation of negative emissions to the primary emitter should be applied (known as 0:100 allocation) to avoid double-counting of emissions. Emissions occurring from the carbon capturing process and subsequent steps such as the transport are subtracted from the negative emissions. Hence, the net negative emissions associated with capturing the CO_2 are allocated to the primary emitter instead of the chemical conversion process.

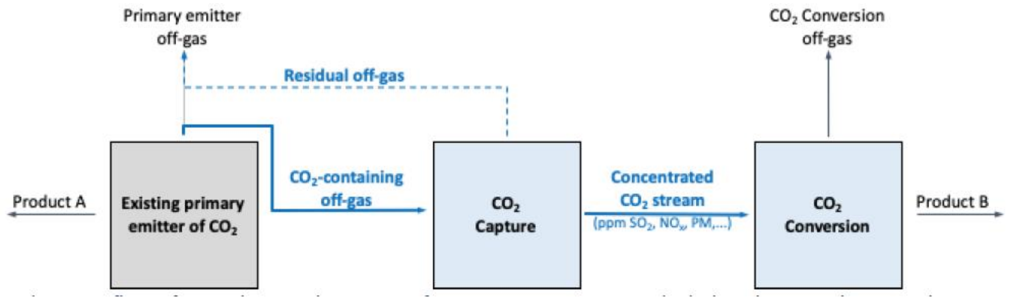

Fig. 1. Flow diagram showing the multi-functionality between primary emitter with carbon capturing and CO_2 conversion plant fed with captured carbon from Ramirez et al. (2020)

With regard to the energy carriers considered, the energy carriers listed by BAFA are used. To avoid double-counting, the primary energy carriers that are used for electricity production are not accounted for. This approach is taken because the particular compositions of the electricity mix for the future are missing. Similarly, hydrogen that is produced in processes of the chemical industry is separately accounted for to avoid double-counting. An important assumption is that all the supplied energy is generated domestically, as discussed in chapter 4.4.

2.2 Product pathway identification

System boundaries

Based on the scope defined in chapter 2.1, the system boundaries of the study are drawn. The overarching boundary of the system is depicted in Fig. 2, where the system boundary is encapsulating the production pathways of all product groups. Production pathways are the core of the system and describe the order and the combination of process steps needed for the production of each chemical product group. The study will look into the energy input into the system from different types of energy carriers, and the GHG emissions resulting from the production processes and energy use.

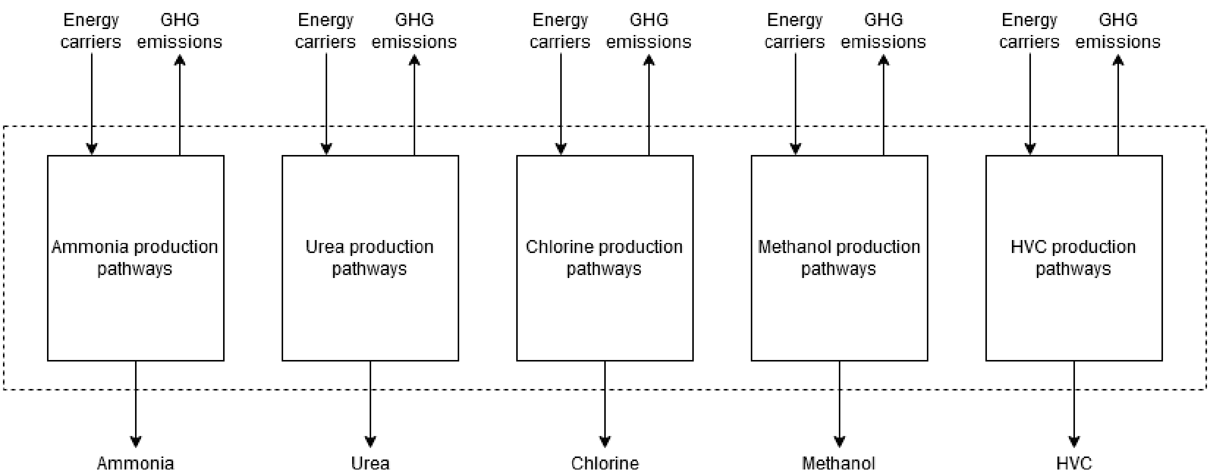

Fig. 2. System boundaries of the study

Production pathway of selected products

Multiple production pathways exist for the production of each chemical product group. By means of a review of production processes described in literature (Agora Energiewende & Wuppertal Institute, 2020; DECHEMA, 2017; DECHEMA & FutureCamp, 2019), a set of main production pathways with a chain of production processes have been identified for each product group. The complexity and types of the available production pathway differ per product group. A detailed explanation and flow diagram of production pathways for each product group can be found in Appendix A.

Technology table

Energy and emissions data for production pathways of each product group is put into a technology table, as can be seen in Table 1. In case an aggregated data for one entire production pathway is available, the collected value is put in for the corresponding production pathway. However, in the case of production pathways of HVC, the aggregated data was not available due to data gaps for individual production processes and inconsistent system boundaries and scopes of reference studies. For HVC first energy demand and emissions data are collected on a disaggregated level, namely for the production process that consists of each production pathway. Then this data is aggregated into data on the production pathway level. By aggregating the data of individual production process steps into one data point, a higher level of consistency could be achieved, and double counting or data gaps could be avoided. The aggregated data of each production pathway is put together in the 'Technology table_default' sheet of Appendix B, while the disaggregated data for HVC production processes are put in the 'HVC data_disaggregated_default' sheet of the same appendix.

Table 1. Technology table of production pathways

	Emissions	Energy carriers				
Production pathway	**Process emissions [t CO2/t product]**	**Oil [MWh/t product]**	**Gas [MWh/t product]**	**Electricity [MWh/t product]**	**Biomass [MWh/t product]**	**Hydrogen [t/t product]***
Ammonia via H2 from steam reformation	1.17E+00		5.83E+00	2.07E+00		1.78E-01
Ammonia via H2 from electrolysis			0.00E+00	1.07E+01		1.78E-01
Ammonia via H2 from methane pyrolysis			4.17E-01	3.40E+00		1.78E-01
Urea via H2 from steam reformation	1.70E+00		3.30E+00	2.14E+00		1.00E-01
Urea via H2 from electrolysis	7.00E-02			8.10E+00		1.00E-01
Urea via H2 from methane pyrolysis			2.40E-01	2.87E+00		1.00E-01
Chlorine via mercury cell				3.60E+00		
Chlorine via diaphragma cell				3.00E+00		
Chlorine via membrane cell				2.80E+00		
Methanol via steam reformation	1.49E+00		3.86E+00	1.67E-01		1.89E-01
Methanol via biomass gasification	6.40E-01			1.70E-01	4.06E+00	
Methanol via H2 from electrolysis	0.00E+00			1.10E+01		1.89E-01
Methanol via H2 from methane pyrolysis	5.00E-02			3.29E+00		1.89E-01

HVC via Methanol-to HVC (with H2 from electrolyzer)	1.53E+00		1.38E+00	3.58E+01		6.14E-01
HVC via crude oil-based naphtha in thermal cracker	1.06E+00	3.25E-01		1.35E-01		
HVC via crude oil-based naphtha in electrical cracker	2.00E-01	2.50E-01		4.73E+00		
HVC via plastic waste pyrolysis in thermal cracker	8.00E-01		8.32E-02	6.58E-01		
HVC via plastic waste pyrolysis in electrical cracker			6.40E-02	5.13E+00		
HVC via Fischer-Tropsch from gasified biomass in thermal cracker	8.00E-01			3.60E-01	1.03E+01	
HVC via Fischer-Tropsch from gasified biomass in electrical cracker				4.90E+00	7.91E+00	
HVC via Fischer-Tropsch from H2 from electrolysis in thermal cracker	8.00E-01			4.56E+01		3.72E-01
HVC via Fischer-Tropsch from H2 from electrolysis in electrical cracker				3.97E+01		2.86E-01

*Calculation & data source can be found in Appendix B. (*Hydrogen is an intermediate energy carrier produced within the chemical industry and not considered as an input to the chemical industry)*

2.3 Modeling approach

Leaning on the approach applied for similar studies for other sectors related to the HI-CAM project, the modeling is based on four essential core steps. This four-step approach has been adjusted to the research questions of this study and therefore, the steps have been adjusted and three steps have been added (Fig. 3). The modeling has been conducted in Microsoft Excel and the model can be found in Appendix G.

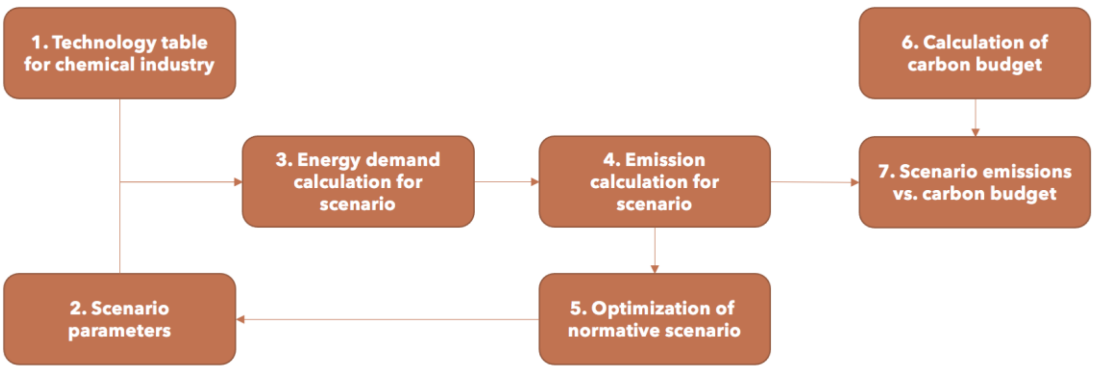

Fig. 3. Modeling steps of the scenarios

The foundation of the model is the technology table mentioned in the previous chapter. The technology table contains all considered pathways for producing each product group under study and their specific energy demand per energy carrier and process emissions. An integrated data collection approach has been applied combining aggregated data for each production pathway, and aggregation of disaggregated data per individual production processes.

The second step is the development of scenario parameters. Scenario parameters are the technology shares of production pathways for the individual products and energy efficiencies. Time steps of 5 years are chosen for the scenario parameters from 2020-2050. The technology shares are developed for two scenarios: the Reference Scenario (RS) and the Normative Scenario (NS), see chapter 2.3.1. The energy efficiency rates are obtained from DECHEMA and FutureCamp (2019) and are diminishing asymptotically to zero over time.

In step 3, the technology table and the scenario parameters are merged. Thus, the demand per energy carrier is calculated by multiplying the production volume per production pathway with the respective energy demand in the technology table.

Subsequently, in step 4, the associated emissions for the scenario time steps are calculated. Therefore, the process emissions and the energy-related emissions are summed up. For the energy-related emissions, emission factors (EF) from BAFA as well as annual EFs for electricity provided by DLR are used. The DLR provided lower-end and upper-end EFs for electricity production from a not yet published study by Naegler et al. (n.d.). Since Germany committed to having a carbon-neutral electricity production by 2050, the lower-end EFs are used for both scenarios.

In the 5th step, optimized technology shares aiming at emission mitigation are developed via an optimization algorithm. This step is only applicable to the NS. All the data until step 4 is fed into the optimization algorithm. The optimization provides scenario parameters that can be used to calculate the energy demand and emissions of the NS, via repeating step 2, 3, and 4. Details about the optimization is explained in chapter 2.3.1.

In step 6, the carbon budget for the German chemical industry is calculated. The calculation approach is described in chapter 2.3.2.

Finally, in step 7, the cumulative emissions of both scenarios are calculated. Therefore, the emissions of the intermediate years between the timesteps are interpolated linearly. Afterwards, the cumulative emissions are compared with the carbon budget. There are two issues with the comparison of the carbon budget and cumulative emissions, which are assumed to cancel each other out. The carbon budget is underestimated in the sense that it covers CO_2 emissions only, while the cumulative emissions account for all GHG emissions. The cumulative emissions are also underestimated since they only cover the 5 main product groups, which are responsible for about 75% of the chemical industry's GHG emissions (DECHEMA & FutureCamp, 2019).

2.3.1 Reference and normative scenario

The RS serves as a benchmark to compare against the results of the NS. The NS describes the pathway for the decarbonization of the chemical industry. The scenario calculations are based on scenario parameters, which form step 2 and step 5. The scenario parameter production volume is equal for both scenarios, meaning that the differences between the scenarios are caused by the technology shares of production pathways.

Globally, the production volume is expected to grow, however, Germany and the EU are saturated markets and potential increases are considered neglectable (expert Agora Energiewende, personal communication, December 11, 2020). Therefore, the production volumes are assumed to remain constant over time. The quantities are based on DECHEMA and FutureCamp (2019), and the same trend of constant production is also observed by other studies such as Agora Energiewende and Wupptertal Institute (2020).

Technology shares reference scenario

For the RS, the technology shares are based on the report by DECHEMA and FutureCamp (2019). The authors developed a set of shares for three different scenarios, this report draws upon the “Technology Path” shares specifically. The scenario is considered the closest to a business-as-usual scenario since it is not limited to today’s technologies only, but it does take into account economic factors. New technologies are only introduced once these are economically competitive and have reached a TRL of 9. Furthermore, an R&D budget of 8.5 bn € is assumed and the amount of renewable electricity available in the future is limited to 235 TWh per year. Another point to keep in mind is that carbon capture and storage is excluded from the technology pathways.

Technology shares normative scenario

For the NS, the technology shares are derived using an optimization algorithm. This way, it is possible to determine the optimal set of shares which ensures the minimum quantity of cumulative emissions within a dynamic system, subjected to a set of constraints. The Microsoft Excel add-in program Solver has been used to this end. The optimization problem is formulated in separate sheets for each product group (refer to Appendix G), since the shares of the different product groups are independent of each other.

The formulation requires the definition of three elements: (I) the objective function; (II) degrees of freedom and (III) constraints. The method Simplex LP is selected as the solver method. This method is suitable since only linear constraints are used (Encyclopedia Britannica, 2017). The inequality constraints define a polygonal region which contains all the feasible solutions. The optimal solution can be found at one of the intersections, for which the optimal values are compared and the best one is reported by the solver.

The objective function refers to a function that calculates the cumulative emissions for a product, based on all the technology pathways in place to produce this product. For the degrees of freedom, the algorithm will determine the optimal values for these cells which minimize the objective function. The result of the optimal values forms the basis of the technology shares of production pathways which is used in step 2 of Fig. 3. for further scenario development.

The constraints are a crucial element which ensure that the scenario remains ‘realistic’. In Appendix D there is a detailed description of the constraints applied. The constraints are applied in different sets in a specified order. For example, in the first set, a balance equation ensures that all production pathways sum up to 100% for all products at each timestep. Other constraints ensure a realistic market introduction or phase out.

2.3.2 Carbon budget

Carbon budget of the chemical industry

In the following, the approach for deriving the carbon budget for step 6 of the modeling is described.

To define targets for climate protection policies, different metrics can be used. The most well-known agreement on climate change mitigation, the Paris Accord from 2015, uses the temperature increase as the metric. Due to a strong linear correlation between the CO_2 concentration in the atmosphere and the temperature, this temperature target can be converted to a target of total CO_2 emissions. The Paris Accord's defined target is *"[...] holding the increase in the global average temperature to well below 2°C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5°C above pre-industrial levels"* (UNFCCC, 2015).

Different global carbon budgets for different temperatures increases and different probabilities to reach these goals exist to account for the complexity and sensitivity of the climate system (SRU, 2020). Furthermore, the carbon budget solely covers CO_2 emissions, other GHG emissions are not considered. This is because of the longevity of CO_2 compared with other GHG. This longevity of CO_2 is responsible for the fact that the carbon budget is independent of when the emissions occur as long as the cumulative emissions over time do not surpass the budget. Thus, the carbon budget aims at defining a climate science-based amount of cumulative CO_2 emissions to the atmosphere that is in accordance with defined temperature increase targets (SRU, 2020).

From the global carbon budget, different sub budgets for different entities such as countries, sectors or companies can be derived. For this, an allocation of the global budget to the specific entity is needed. There are a variety of allocation concepts available, which are based on different references such as the share of the global population, relative economic performance, historical emissions, or "grandfathering" of today's emission shares. The European Union and Germany define their carbon budget based on the share of the global population (SRU, 2020).

Basis for the calculation are two global carbon budgets – 420 Gt CO_2 to stay within the 1.5°C limit and 800 Gt CO_2, each starting from 2018 ($CB_{global,\ 2018}$) and with a chance of 67% probability to meet the target (SRU, 2020). These two budgets are chosen as they ensure a high chance to meet the goals of the Paris agreement. To derive the German carbon budget from 2020 onwards ($CB_{Germany,\ 2020}$) an allocation based on the population share (%population) is applied. The emissions that arose in Germany in 2018 ($E_{Germany,2018}$) and 2019 ($E_{Germany,2019}$) are assumed to be constant to the emissions from 2017.

$$CB_{Germany,2020} = CB_{global,2018} * \%population - E_{Germany,2018} - E_{Germany,2019}$$

Equation 1: Calculation of national carbon budget for Germany from 2020 onwards

This national carbon budget is used as the basis for the subsequent calculation of the carbon budget for CO_2 emissions associated with the chemical industry. For this, both emissions from the chemical industry and the on-site energy generation (scope 1) and emissions from externally purchased energy (scope 2) are considered. Consequently, two different sectors, the industry sector and the energy sector are taken into account. The allocation of emissions is based on the grandfathering concept, giving the chemical industry the same share on the carbon budget as it has on the annual emissions.

Firstly, the carbon budget of emissions of the chemical industry in the industry sector ($CB_{chemical,scope1}$) is calculated (see Fig. 4). Therefore the emission share of 2017 is applied as the basis. The emission share of the chemical industry on the German carbon budget ($\%share_{chemical}$) is calculated based on the emission share of the industry sector on the German carbon budget ($\%share_{industry}$) and the emission share of the chemical industry on the industry sector ($\%share_{chemical\ on\ industry\ sector}$). Subsequently, the derived share is multiplied with the German carbon budget to obtain the carbon budget of the scope 1 emissions of the chemical industry.

$$\%share_{chemical,scope1} = \%share_{industry} * \%share_{chemical\ on\ industry\ sector}$$

Equation 2: Calculation of emissions share of the chemical industry on the national carbon budget

$$CB_{chemical,scope1} = CB_{Germany,2020} * \%share_{chemical,scope1}$$

Equation 3: Carbon budget of the German chemical industry

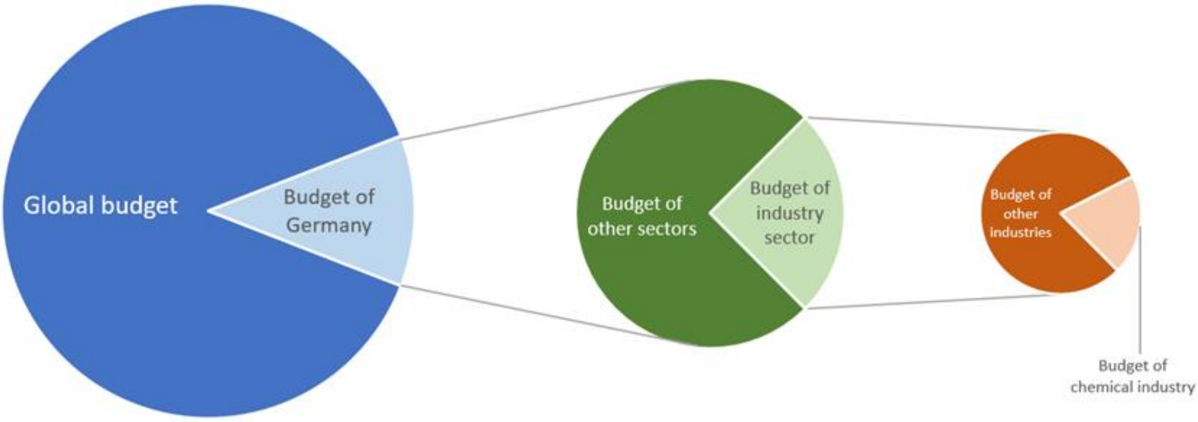

Fig. 4. Calculating the carbon budget of the chemical industry in the industry sector

Secondly, the carbon budget of emissions of the chemical industry in the energy sector ($CB_{chemical,scope2}$) is calculated (see Fig. 5). It is derived via the German carbon budget and the ratio of the scope 2 emissions of the German chemical industry 2020 ($E_{chemical,scope2,2020}$) and total emissions of Germany in 2019 ($E_{Germany,2019}$).

$$CB_{chemical,scope2} = CB_{Germany,2020} * \frac{E_{chemical,scope2,2020}}{E_{Germany,2019}}$$

Equation 4: Carbon budget in the German energy sector associated with the chemical sector

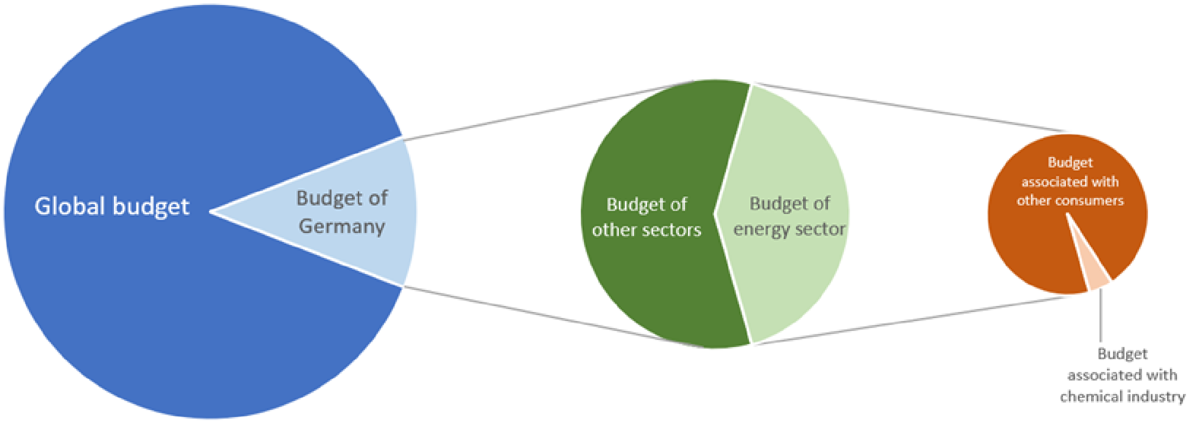

Fig. 5. Calculating the carbon budget of the chemical industry in the energy sector

In order to calculate the total carbon budget of the chemical industry, the scope 1 budget and the carbon budget in the energy associated with the chemical industry, the scope 2 budget are added up.

3 Results

3.1 Technology shares of production pathways

As described in chapter 2.3.1, different technology shares are given to production pathways of each scenario to calculate their energy demand and emissions. Details of the technology shares can be found in Appendix E, table E1 for RS and E2 for NS.

As seen in Fig. 6, the technology shares of the four predominant, fossil-based production pathways decrease to a level of 40% to 60% by 2050 in the RS. In the NS the shares of the conventional pathways decrease more significantly than the RS, even reaching a complete phase-out in 2050, as visualized in Fig. 7. Moreover, the starting point of the phase-out is at an earlier point in time in the NS, which can be attributed to the optimistic assumptions regarding the R&D of technologies.

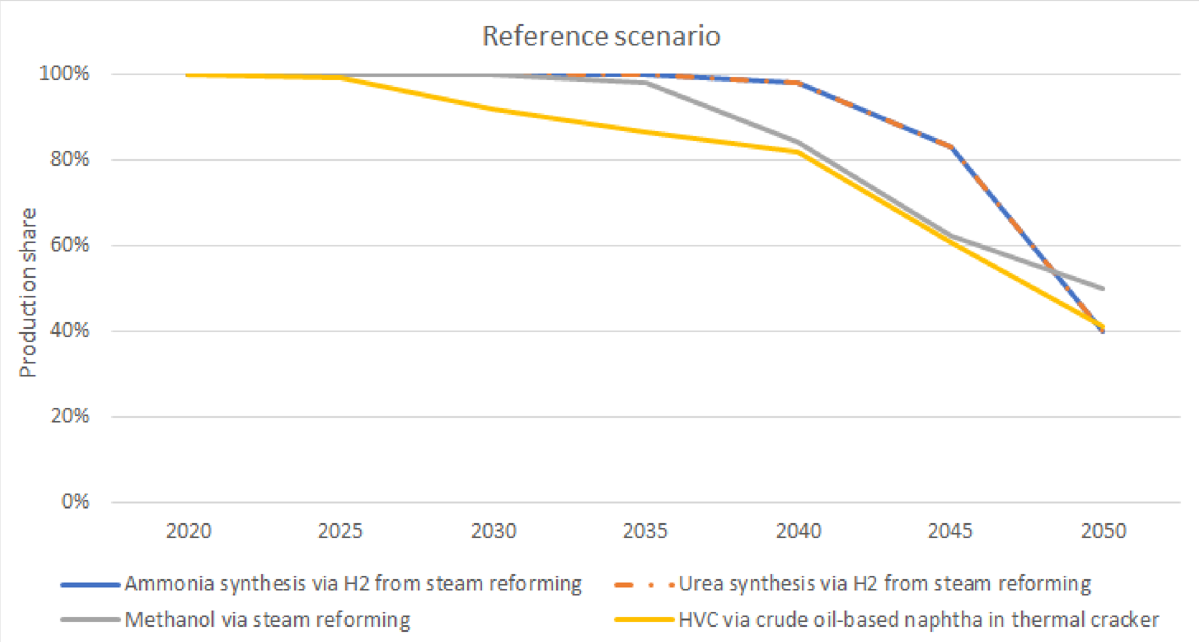

Fig. 6. Decrease in fossil-based production pathways in the RS

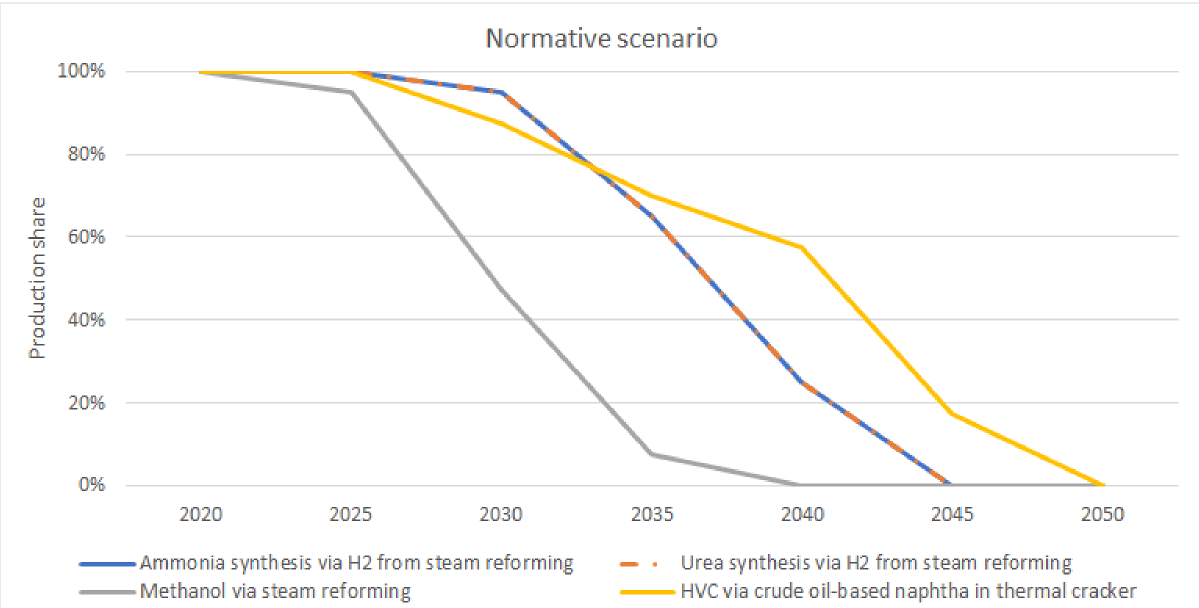

Fig. 7. Phase-out of fossil-based production pathways in the NS

3.2 Comparison between reference and normative scenario

Energy demand

As can be seen in Fig. 8, the energy demand of the RS shows a rapid growth after 2040, mainly in electricity demand. The demand for fossil-based fuel shows a notable decrease after 2045.

The NS reveals a significant increase in energy demand and a drop in fossil-based fuel demand from 2040, which is substituted by electricity. Before 2040, changes in energy demand and proportion between energy carriers remain minor. The rapid growth in energy demand after 2040 is caused by electricity substituting other fossil-based energy with higher EFs, which are used as fuel and feedstock. As the share of renewables grows in the energy mix of electricity, the EFs of electricity becomes lower than the EFs of other energy carriers. In the end, via electricity it is possible to produce products with lower emissions, however, this requires more energy than via other types of energy carriers which leads to a higher total energy demand.

Another notable part of the NS is the change in biomass demand. The demand shows a constant growth until 2045, and then decreases as part of it is substituted by electricity. This indicates that biomass works as a transition technology that bridges the time from fossil-based fuel to renewable-based electricity, until the energy mix of electricity is transformed sufficiently to bring down the EF of electricity lower than other energy carriers.

Overall, an increase in their energy demand by 2050 appears in both scenarios, especially in electricity demand. However, the NS shows a much bigger growth in energy demand, with a more significant increase in electricity and a drop in fossil-based fuel demand. The energy demand of the NS in 2050 shows a growth of 342 TWh compared to its demand in 2020. The demand is also found to be 175 TWh higher than that of the RS in 2050. 92% of the energy demand of the NS in 2050 is for electricity, while the share of electricity in the RS stays at 87%. The NS shows a significant drop in natural gas demand and a phase-out of oil in 2050. However, the demand for both natural gas and oil remains in the RS in 2050, with the natural gas demand being 18 times higher than in the NS. The notable increase in electricity demand and drop in other energy carriers demand of the NS is derived from the lower EF of electricity.

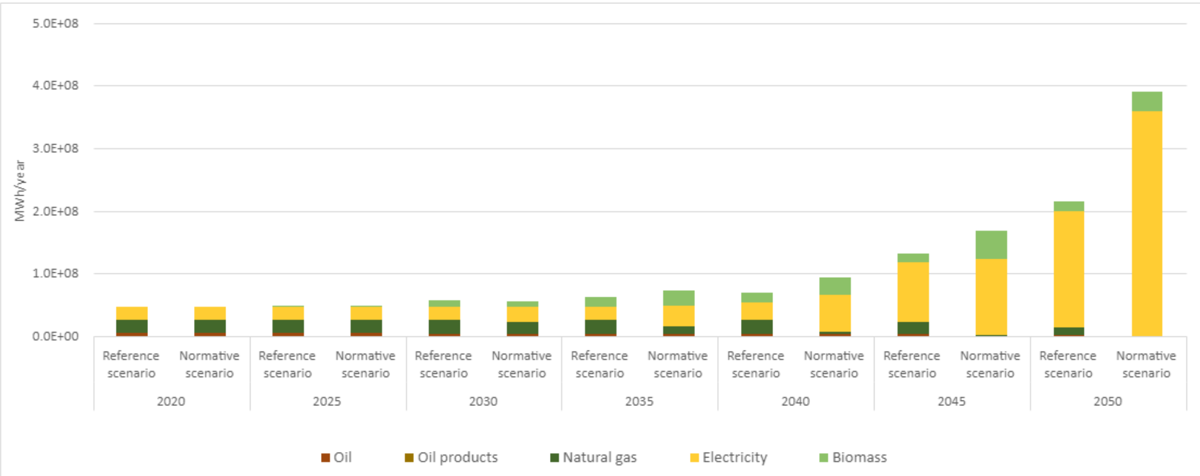

Fig 8. Change in energy demand per energy carrier

Energy demand per product is analyzed for both scenarios as can be seen in Fig. 9. In the RS, HVC is found to be the major contributor to the increase in energy demand especially after 2040. HVC also causes the majority of energy demand (88% of the total energy demand in 2050) in the NS. The high energy demand of HVC in both scenarios is derived from the growth of electrical cracking and hydrogen production via electrolysis for the production of HVC, which have a high electricity demand.

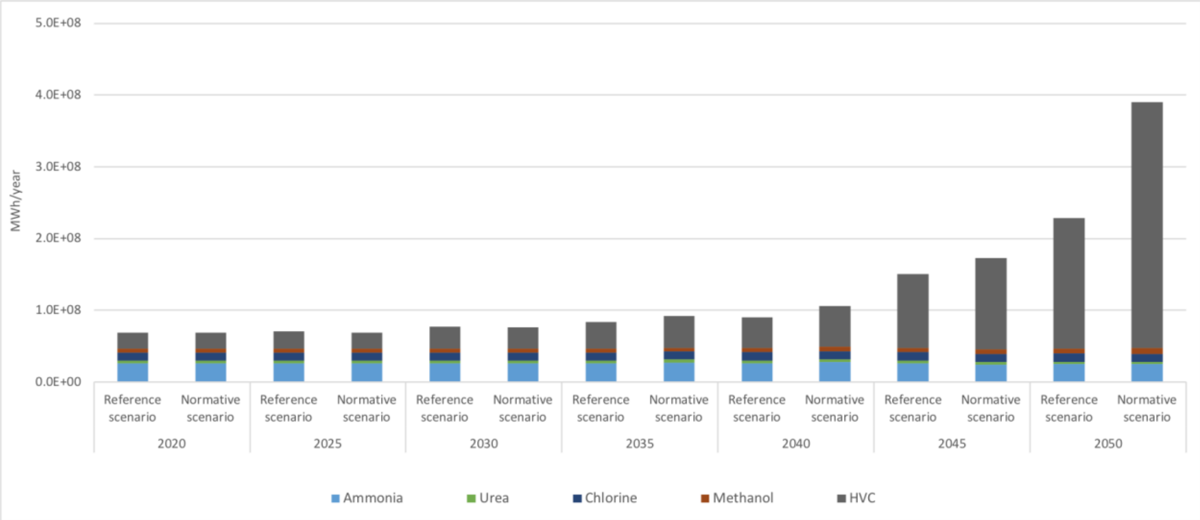

Fig. 9. Change in energy demand per product

Energy demand per production pathway

In this section, cumulative energy demand per production pathway of each product group from 2020 to 2050 is described. This gives an indication of how much of the individual energy carriers are used for each production pathway in the two scenarios.

Ammonia

Energy demand per production pathway of ammonia is depicted in Fig. 10. Electricity is the only energy carrier used for the pathway with H2 electrolysis, while the other two pathways require both natural gas and electricity. In terms of energy demand, electrolysis has the highest and methane pyrolysis has the lowest demand.

The energy demand of the pathways with methane pyrolysis and electrolysis turns out to be higher in the NS, while the energy demand of the steam reforming pathway is predominant in the RS. This is due to a higher technology share of the first two production pathways in the NS compared to the RS.

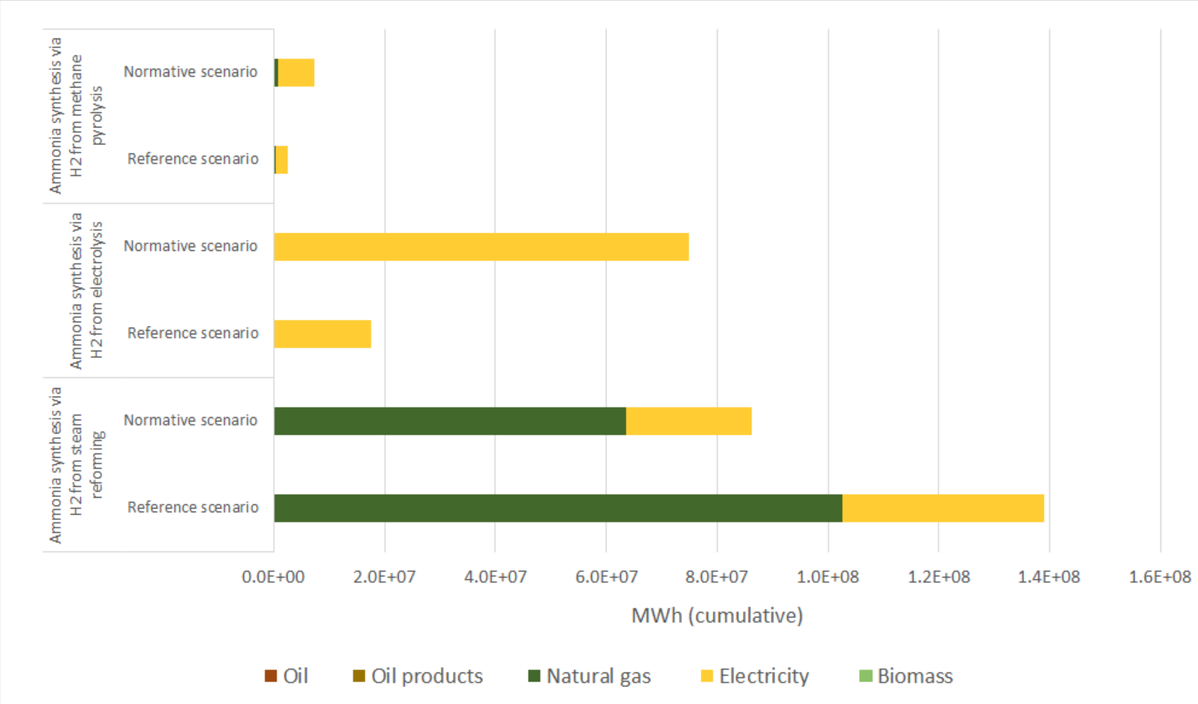

Fig. 10. Cumulative energy demand per production pathway of ammonia

Urea

As can be seen in the below Fig. 11, production pathways of urea show a similar trend in energy demand with ammonia. This is due to the similarity in production pathways of the two product groups: urea is produced by feeding ammonia into the urea synthesis process.

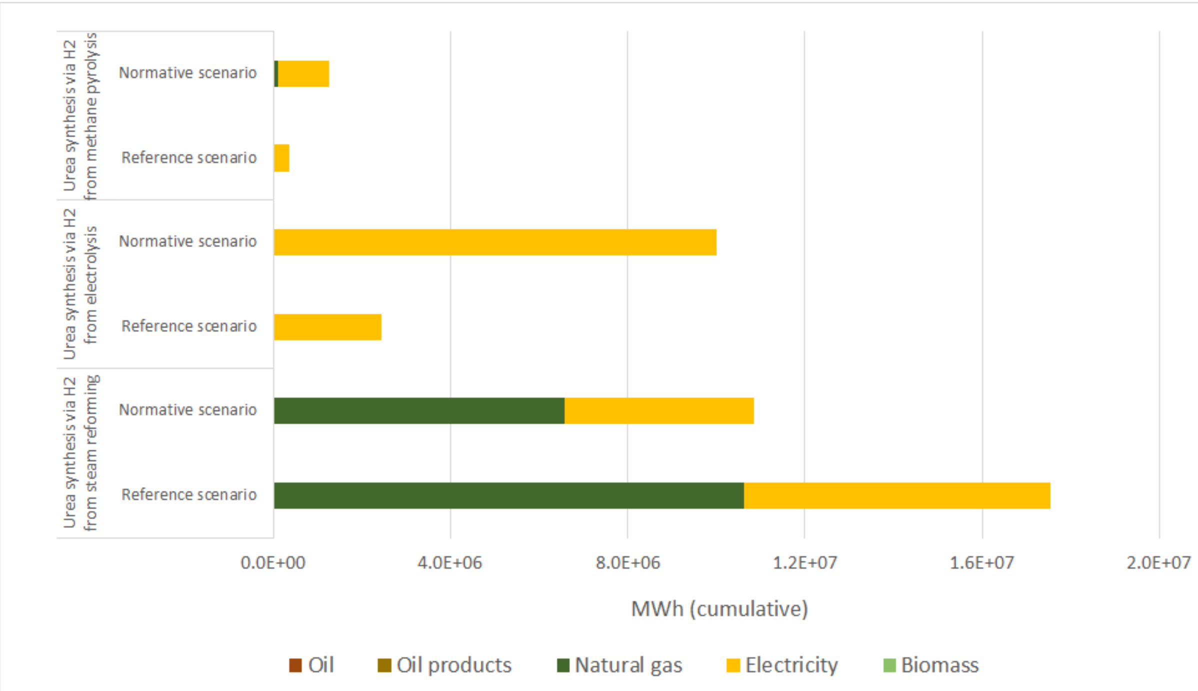

Fig. 11. Cumulative energy demand per production pathway of urea

Chlorine

The three production pathways of chlorine share similarity in that all use electricity as their energy carrier, as seen in Fig. 12. The membrane cell technology is the most efficient and requires the lowest amount of electricity compared to the other two technologies.

The energy demand for the membrane cell production pathway is higher in the NS, while the demand for the other two technologies is higher in the RS. This is because a higher share is attributed to the more energy efficient membrane cell technology in the NS.

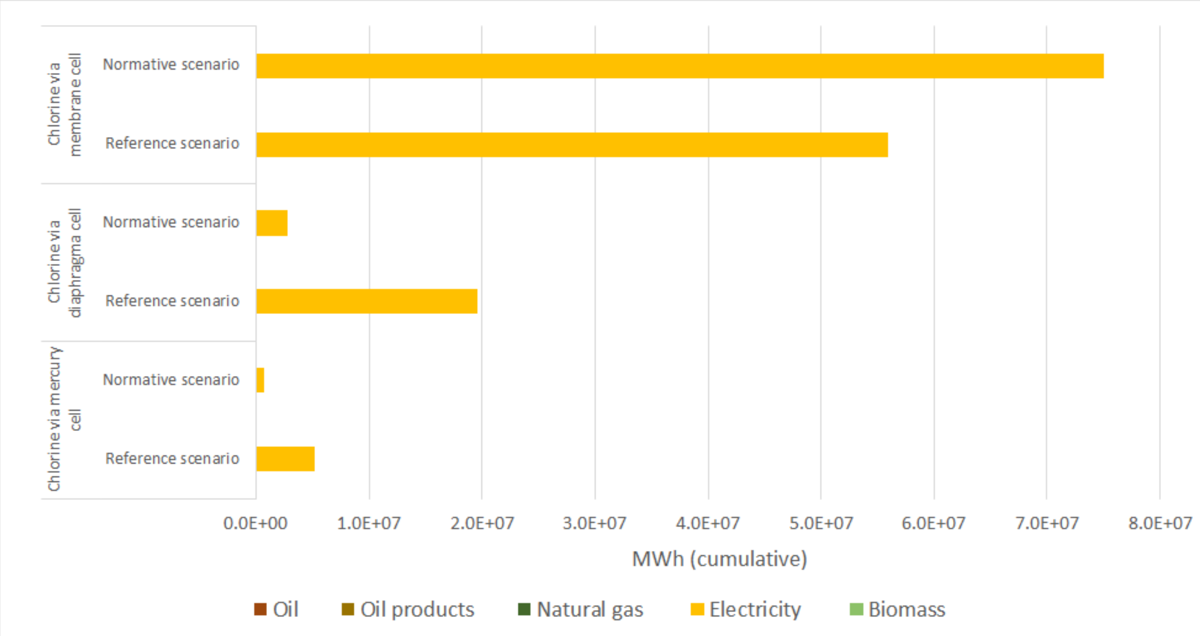

Fig. 12. Cumulative energy demand per production pathway of chlorine

Methanol

Methanol can be produced via four production pathways: two low-carbon hydrogen production pathways of electrolysis and methane pyrolysis, biomass gasification, and conventional steam reforming.

A clear difference between the energy carrier demand of the two scenarios is shown in Fig. 13. The NS has a lower energy demand from the steam reforming pathway which is based on natural gas, while it shows a higher demand in the other three pathways of methane pyrolysis, electrolysis, and biomass gasification. This reflects the growing preference for electricity-based technologies, and the preference of biomass over natural gas as energy carriers in the NS.

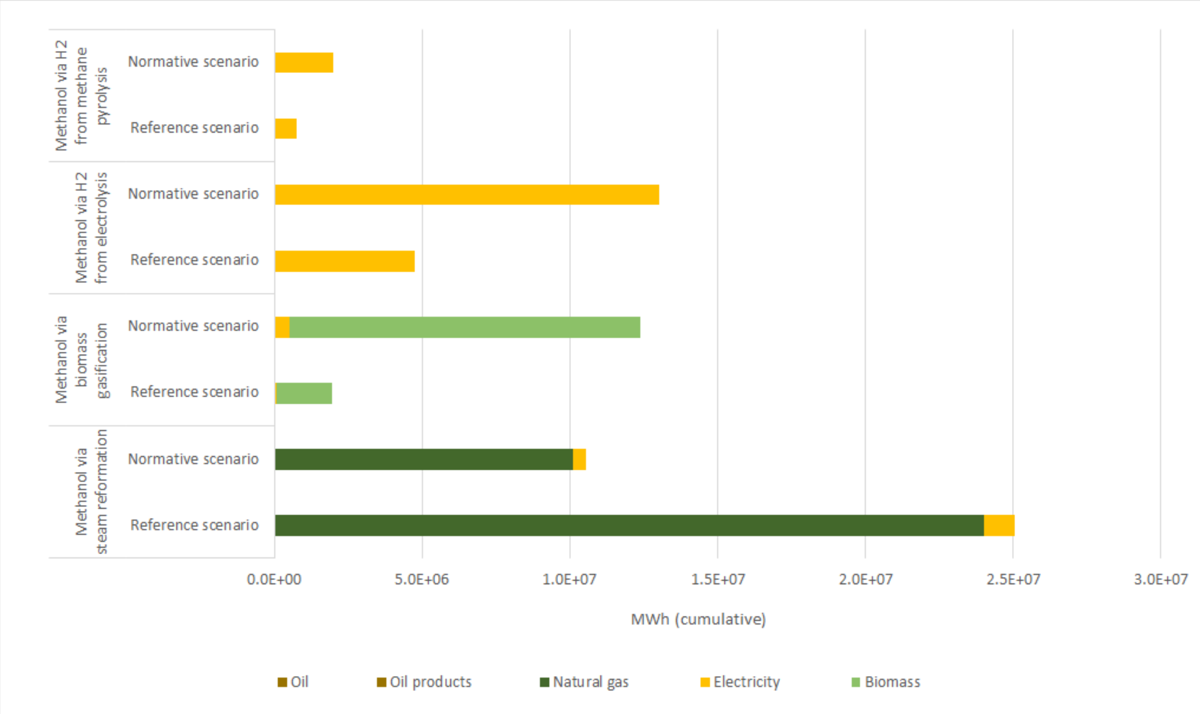

Fig. 13. Cumulative energy demand per production pathway of methanol

HVC

Production pathways of HVC are manifold, with a diversity of energy carriers in use. In terms of energy demand, the electricity demand of pathways containing electrolysis and electrical cracking turn out to be higher than other pathways.

The RS has a tendency of showing higher energy demand in crude-oil and thermal cracking-based pathways than the NS as seen in Fig. 14. The NS shows a higher energy demand in pathways using electrical cracking, especially in the pathway combining Fischer-Tropsch with electrolysis and electrical cracking. This can be reasoned back to two factors: the higher share of electrical cracking given to the NS, and the high electricity demand for electrolysis and electrical cracking technologies.

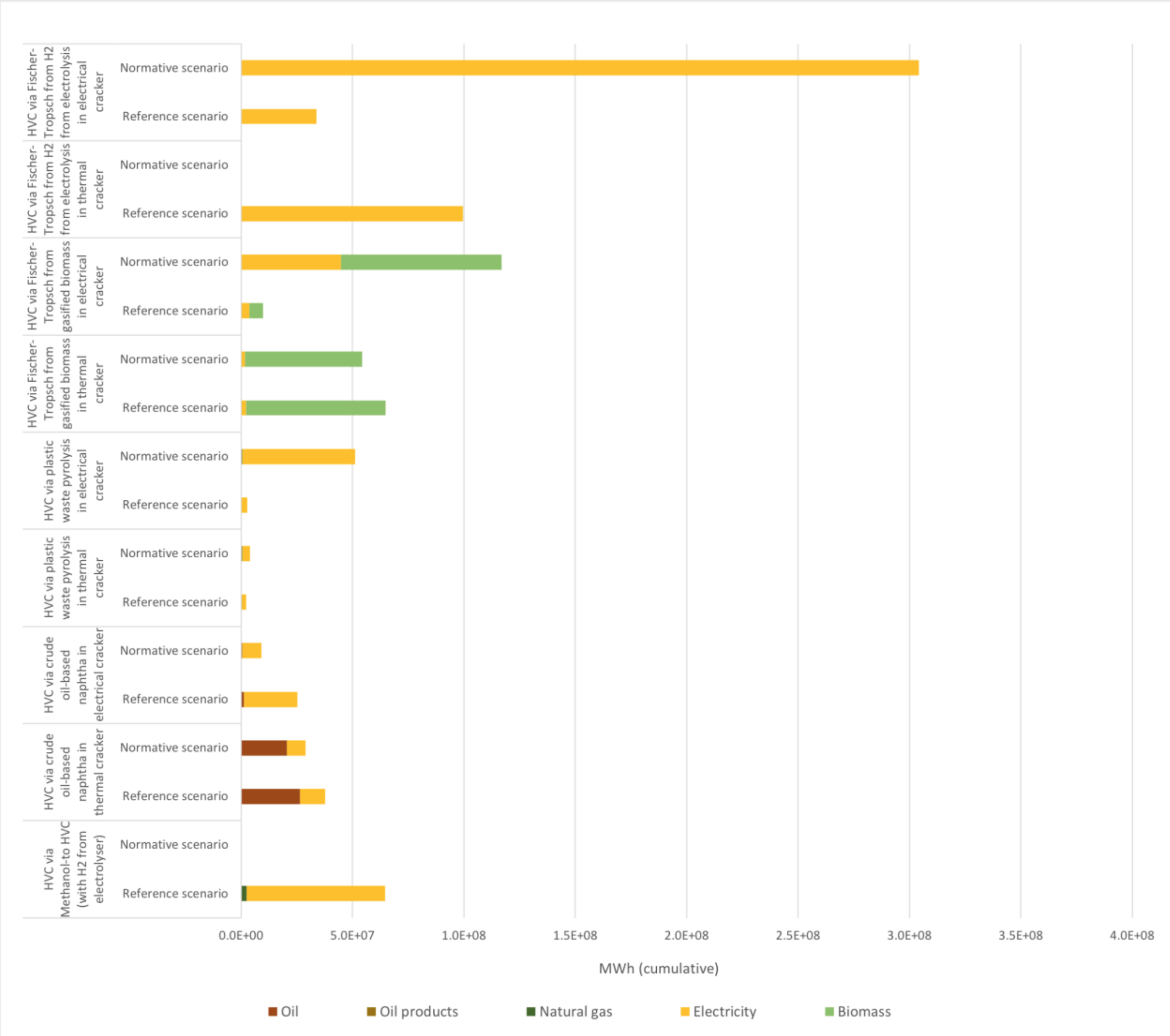

Fig. 14. Cumulative energy demand per production pathway of HVC

Emissions

Changes in total emissions of each scenario per energy carrier are depicted in Fig. 15. The RS shows a constant reduction in its emissions, especially where the emissions from electricity significantly reduce in 2050.

Emissions of the NS drop drastically by 96% in 2050 compared to 2020. Process emissions have dropped significantly since 2040, which is due to the increased share of electricity-based production pathways. The emissions from electricity disappear in 2050, as the EF of electricity reaches 0. As other energy carriers are substituted by electricity with the EF of zero, total emissions result in a significantly low amount in 2050.

Overall, both scenarios show a constant reduction in their emissions, while the NS shows a much bigger drop in total emissions and process emissions.

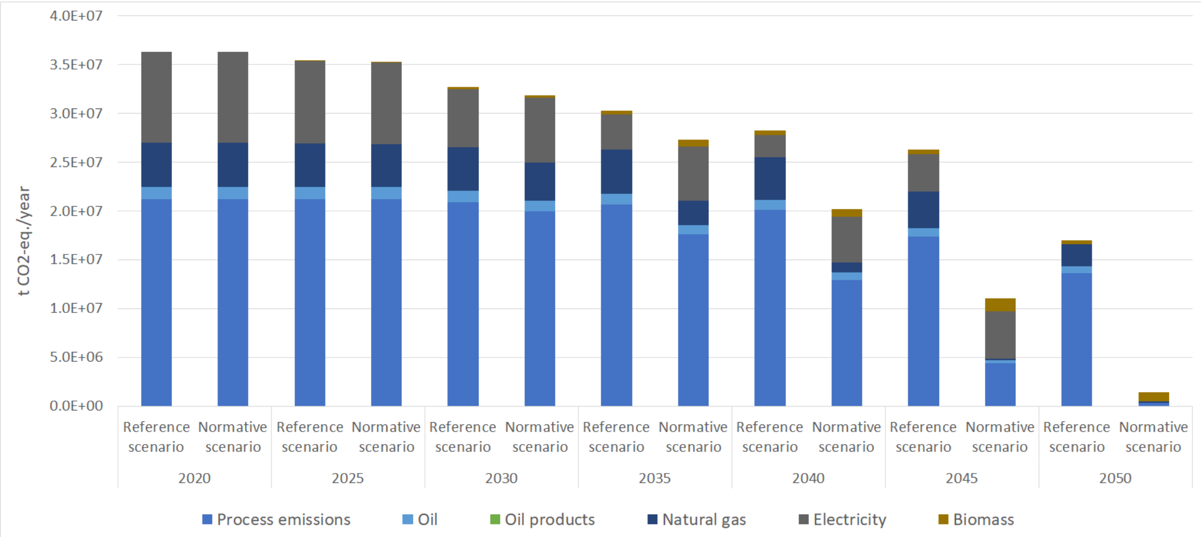

Fig. 15. Change in emissions per energy carrier

Fig. 16 shows the change in total emissions per product. In the RS, emissions from HVC, ammonia, and urea show a notable reduction in 2050.

The NS shows a similar trend of emissions reduction in the three product groups, however at a much larger scale. The emissions from HVC are especially notable, with a reduction of 90% from 2045 to 2050.

Such a reduction in both scenarios is induced by the increase in the share of electricity-based production pathways of each product. Increased use of electrolysis and electrical cracking causes the emissions reduction of HVC, while increased use of electrolysis lowers emissions from ammonia and urea.

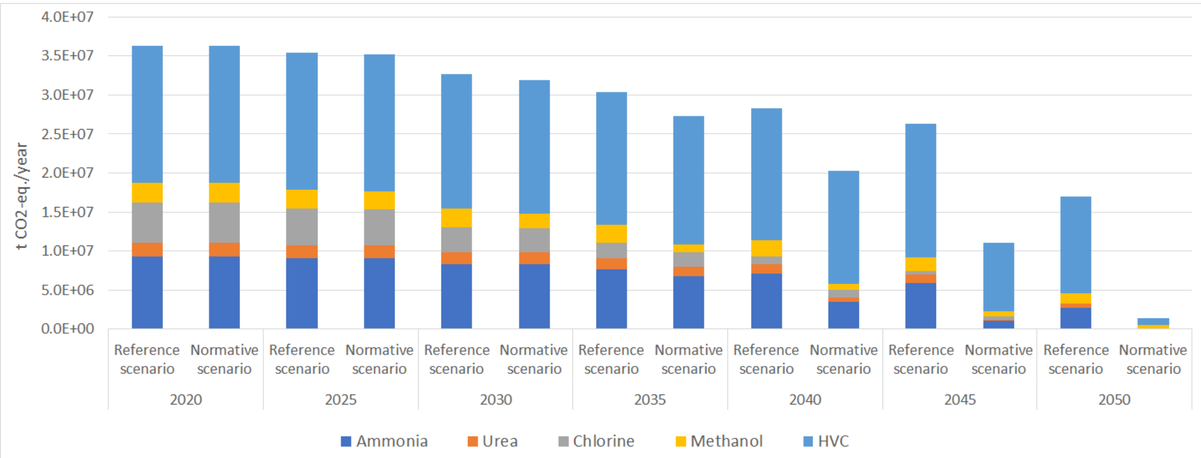

Fig. 16. Change in emissions per product

Differences in the technology shares for each scenario bring differences in their energy demands and emissions. Such a difference results in the annual emissions of each scenario in Fig. 17.

The RS shows a constant decrease in annual emissions, with a bigger drop from 2045. The annual emissions of the NS stay similar to the RS until 2030, and the gap between the two becomes larger as emissions of the NS drop rapidly from 2035.

In the end, with higher technology shares given to low-emissions production pathways, the NS results in a more significant drop than the RS, with its annual emissions at 1.4 Mt CO_2-eq. in 2050. This value amounts to 4% of annual emissions in 2020 and 8% of emissions of the RS in 2050.

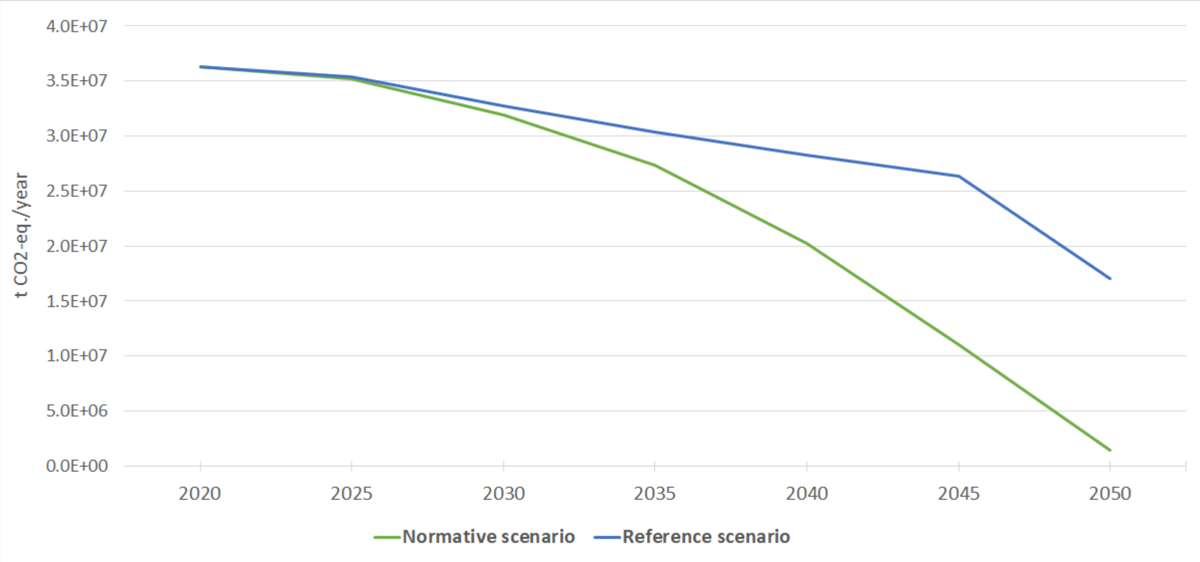

Fig. 17. Change in annual emissions

3.3 Comparison of cumulative emissions with carbon budget

The German carbon budget from 2020 onwards to stay below 1.5°C and 1.75°C with a chance of 67% are 2.5 Gt and 6.7 Gt, respectively. For the 1.5°C goal, the total carbon budget (scope 1 & 2) amounts to 0.167 Gt, whereas the 1.75°C-compatible carbon budget lies at 0.45 Gt. About 62% of this budget is assigned to emissions in the chemical industry itself (scope 1), covering the emissions of the processes but also of on-site energy generation. The remaining 38% of the carbon budget is associated with the emissions related to the energy production in the energy sector to supply external power to the chemical industry (scope 2). The chemical industry has thus a share of about 6.7% on the German carbon budget.

As seen in Fig. 18, the cumulative emissions of each scenario are compared with the defined carbon budget. The cumulative emissions of the RS and the NS result in 0.9 Gt and 0.7 Gt respectively.

The gap between the scenarios and the carbon budget becomes smaller with the 1.75°C goal. However, still with the 1.75°C goal the gap between the scenarios and the carbon budget remains significant. With the NS for which the study optimized the technology shares to result in the least emissions, it is not possible to stay within the carbon budget for either 1.5°C or 1.75°C, with a respective gap of 0.6 Gt and 0.3 Gt. The results indicate that the NS is not sufficient to meet the carbon budget of the chemical industry.

Furthermore, both scenarios are surpassing the carbon budgets in the early years in Fig. 18. This shows that the technologies currently in place are consuming the carbon budget even before the emission curve starts to be flattened.

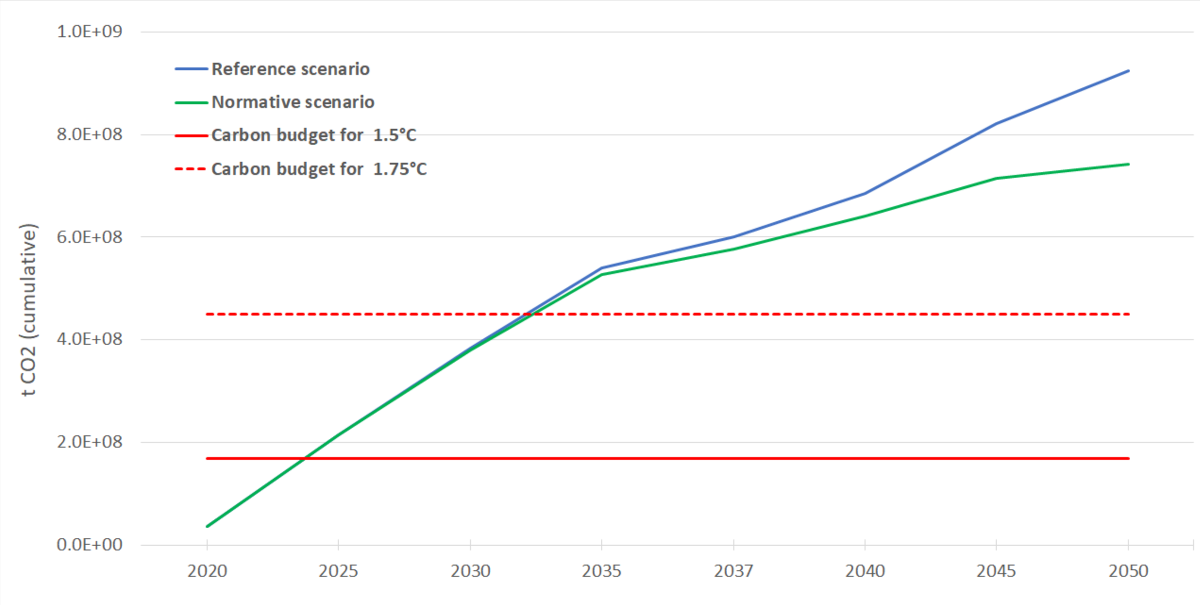

Fig. 18. Cumulative emissions of two scenarios and carbon budget

4 Discussion

4.1 Sensitivity analysis

Sensitivity analysis with higher electricity emission factors

This sensitivity analysis shows what happens if the renewable energy transition is not as successful as expected. It is of pivotal importance to address this scenario, as electrification may no longer be the best option when the electricity EFs will not reach zero in 2050, as is the case in the set of lower electricity EFs.

In the RS, the energy demand composition stays equal, as the technology shares for the production pathways are fixed. In the NS, the optimization method has been redone using the alternative set of higher electricity EFs (Appendix F). Drastic changes in technology shares (Appendix E, Table E3) can be found for methanol and HVC, and to a certain extent also for ammonia and urea. Electrolyzers become less important, while biomass gasification and plastic waste pyrolysis jump in the gap. It can be seen in Fig. 19 that the energy demand for electricity becomes substantially lower in this case, while it increases for biomass.

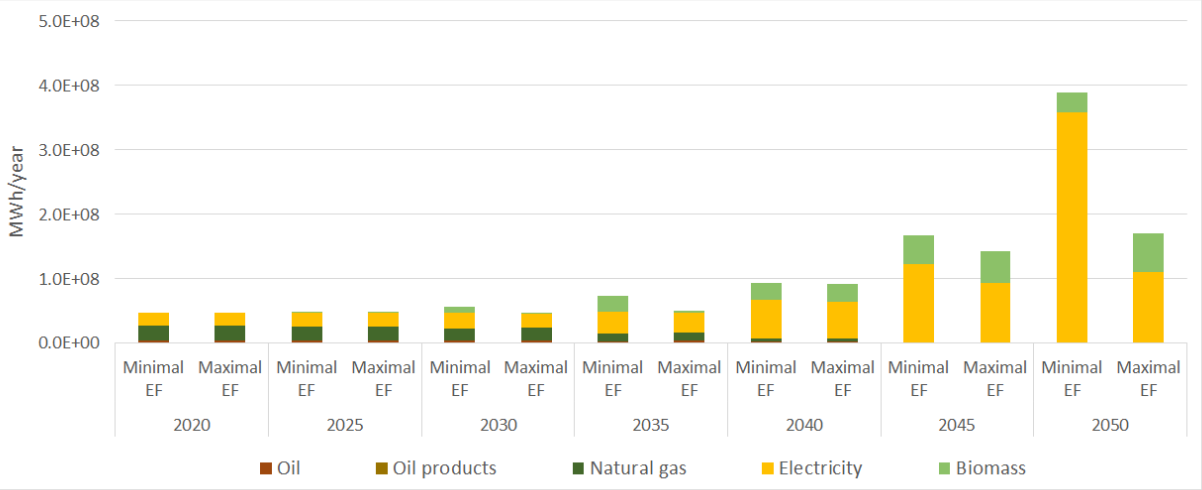

Fig. 19. Sensitivity analysis comparing the energy demand for a set of lower and higher electricity EFs in the **NS**

In Fig. 20 and Fig. 21, the CO_2 emissions are substantially higher for both the RS and NS when the higher electricity EFs are applied. The increase in biomass is clearly visible. Especially towards 2050, the results are more sensitive to the EFs.

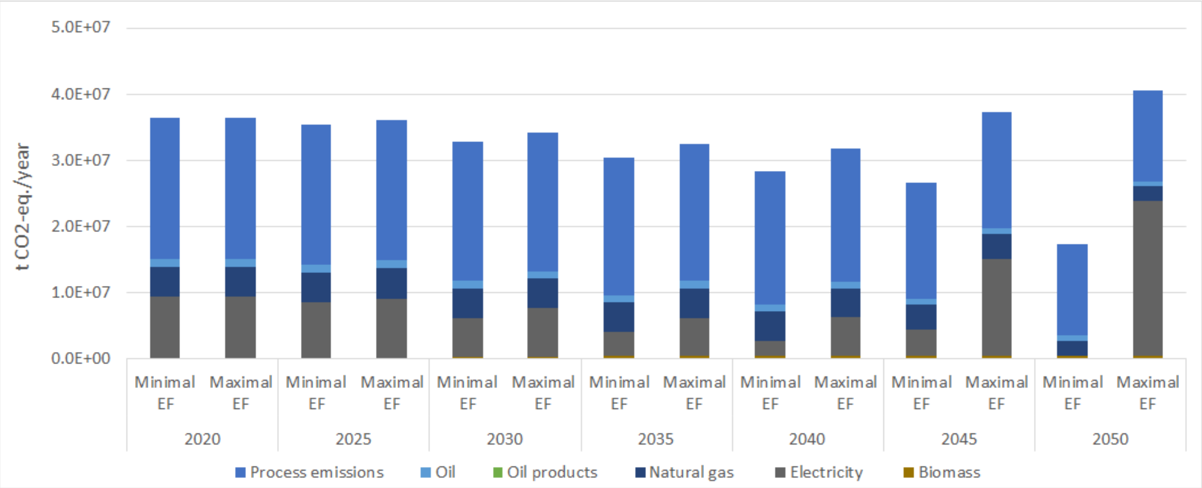

Fig. 20. Sensitivity analysis comparing the CO_2-equivalent emissions for a set of lower and higher electricity EFs in the **RS**.

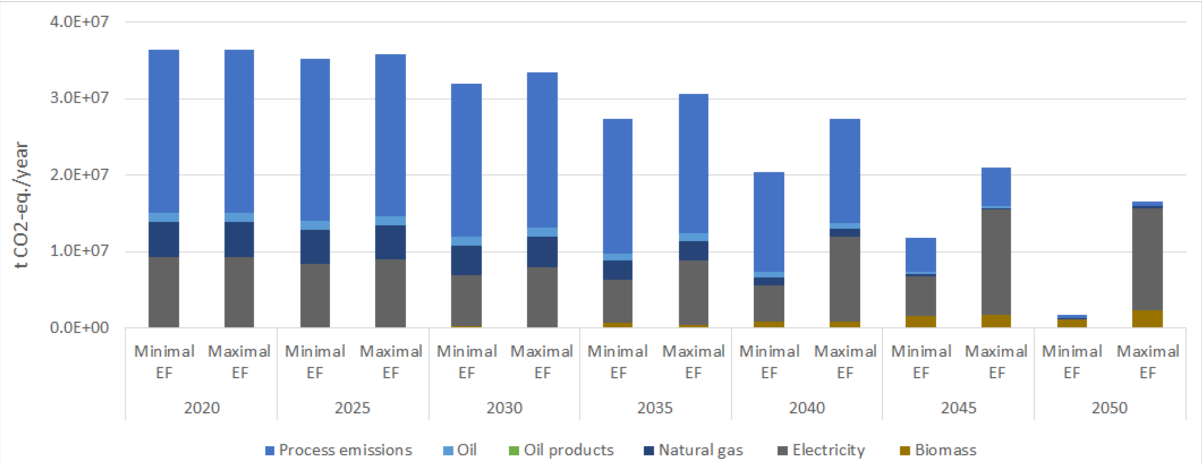

Fig. 21. Sensitivity analysis comparing the CO_2-equivalent emissions for a set of lower and higher electricity EsF in the **NS**.

In Fig. 22 it becomes evident that the influence of higher electricity EFs will be visible after crossing the carbon budget for the 1.75 degrees scenario. This sensitivity analysis concludes that having higher electricity EFs requires a different strategy to abate emissions. It also shows how tightly coupled the chemical and energy sector are.

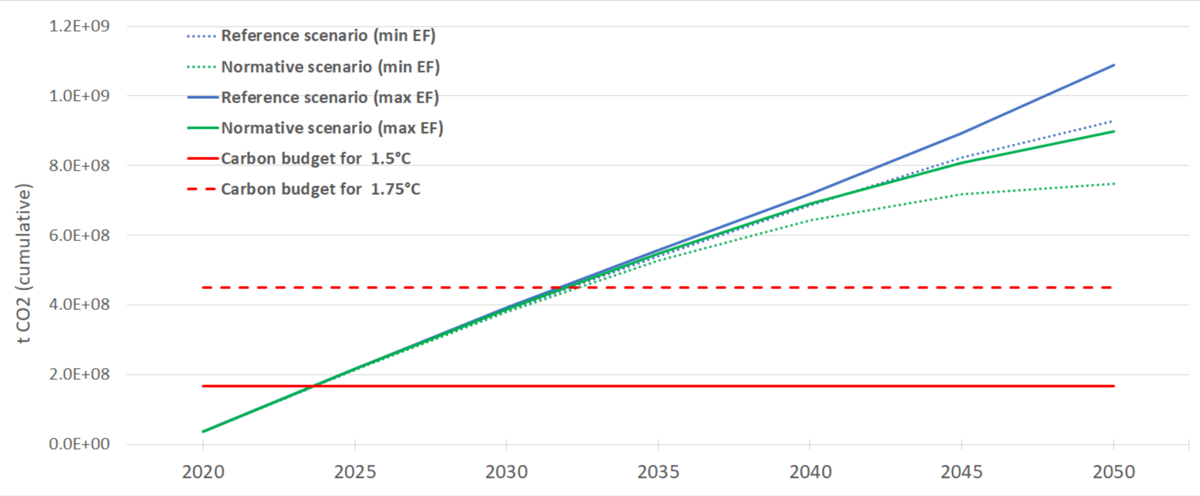

Fig. 22. Cumulative CO_2-equivalent emissions for the RS and NS.
Both the set of lower and higher electricity EFs and the carbon budgets are depicted.

Sensitivity analysis with 100:0 allocation of CCU emissions

This sensitivity analysis studies the effect of the allocation of emissions. As discussed in chapter 2.1, negative emissions occurring due to CCU are allocated to the primary emitter (0:100). For the sensitivity analysis, the allocation is flipped to a 100:0 basis, so that the negative emissions are allocated to the use process of captured carbon, the so-called CO_2 conversion process. The technology table with 100:0 emissions allocation is optimized leading to the technology shares in Appendix E, Table E4. The optimization of the technology shares dedicates significantly larger shares to electrolyzer processes, especially for methanol and HVC. This is evident in Fig. 23, where a tremendous increase in energy demand is observed for the 100:0 allocation approach.

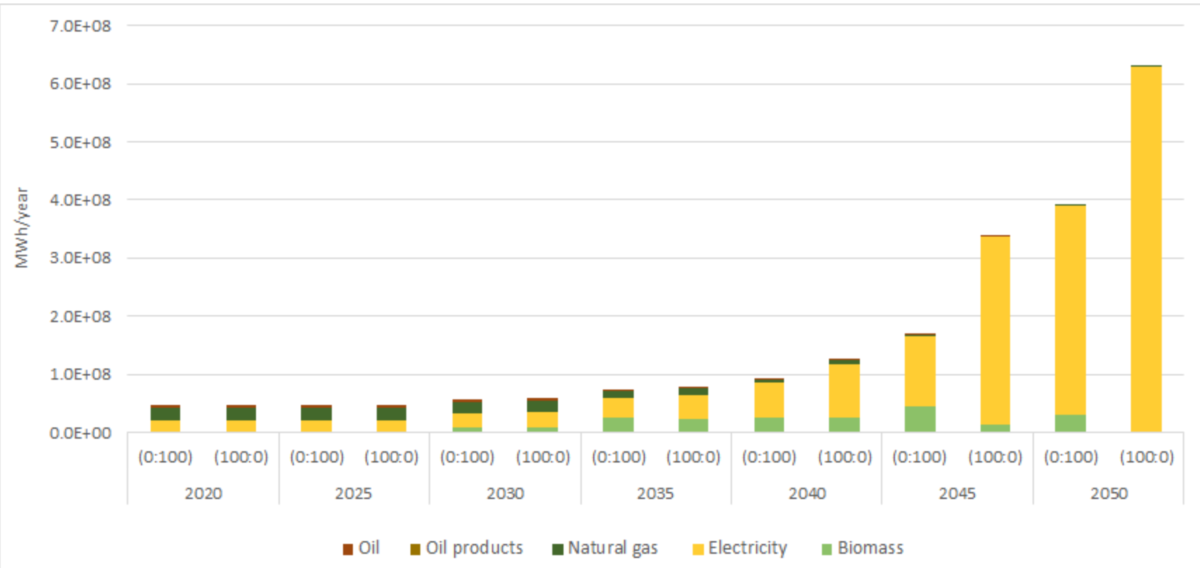

Fig. 23. Energy demand for the NS showing a 0:100 and 100:0 emission allocation approach.

As expected, the emissions occurring after 2035 are reduced for the 100:0 approach in both the RS (Fig. 24) and the NS (Fig. 25). For the RS, the reduction is steeper. The process emissions even become negative in 2045 in the NS. In 2050, the high electricity demand is assumed to be supplied by clean electricity, which explains why the total emissions become negative.

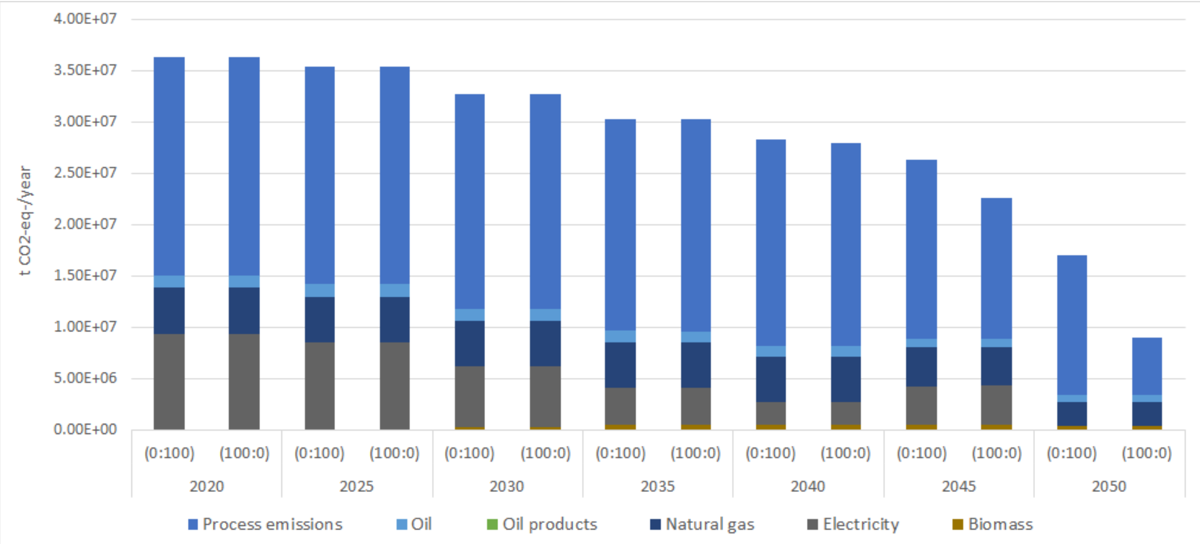

Fig. 24. CO_2-equivalent emissions for the RS showing a 0:100 and 100:0 emission allocation approach

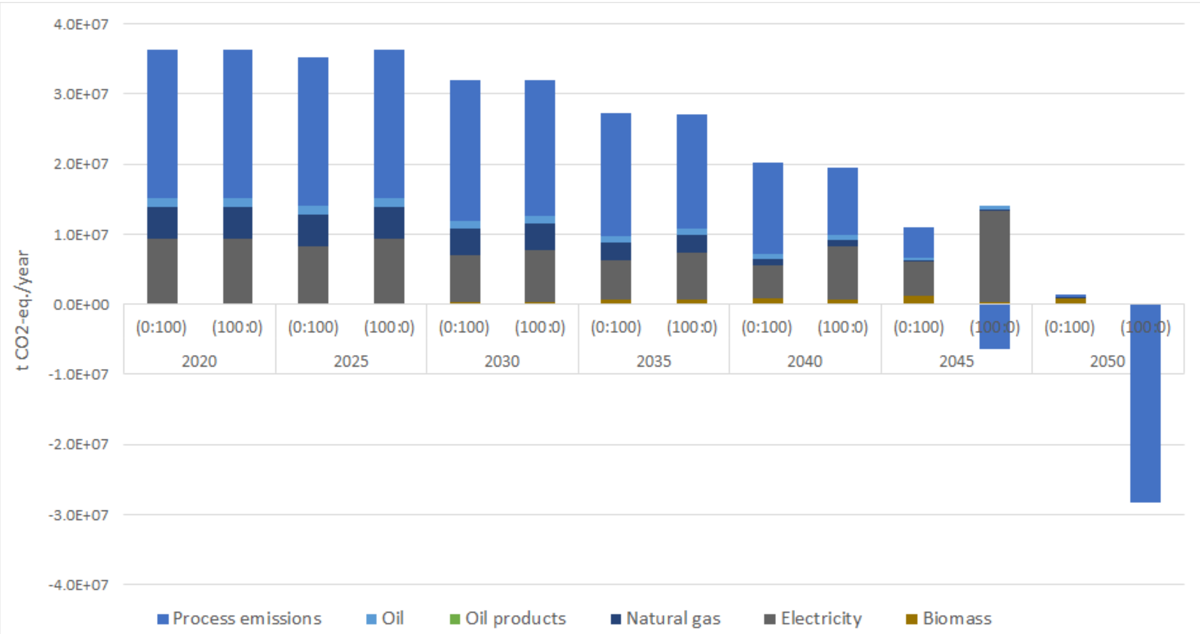

Fig. 25. CO_2-equivalent emissions for the NS showing a 0:100 and 100:0 emission allocation approach.

Fig. 26 shows that the graphs adopting the 100:0 allocation bend down around 2045, which is where the negative emissions can be expected to be dominating. The cumulative emissions are reduced in the RS and become negative in the NS. The NS is especially sensitive to the allocation approach, but the overarching message remains the same. Changing the allocation approach is not sufficient for the chemical industry to remain within the carbon budget.

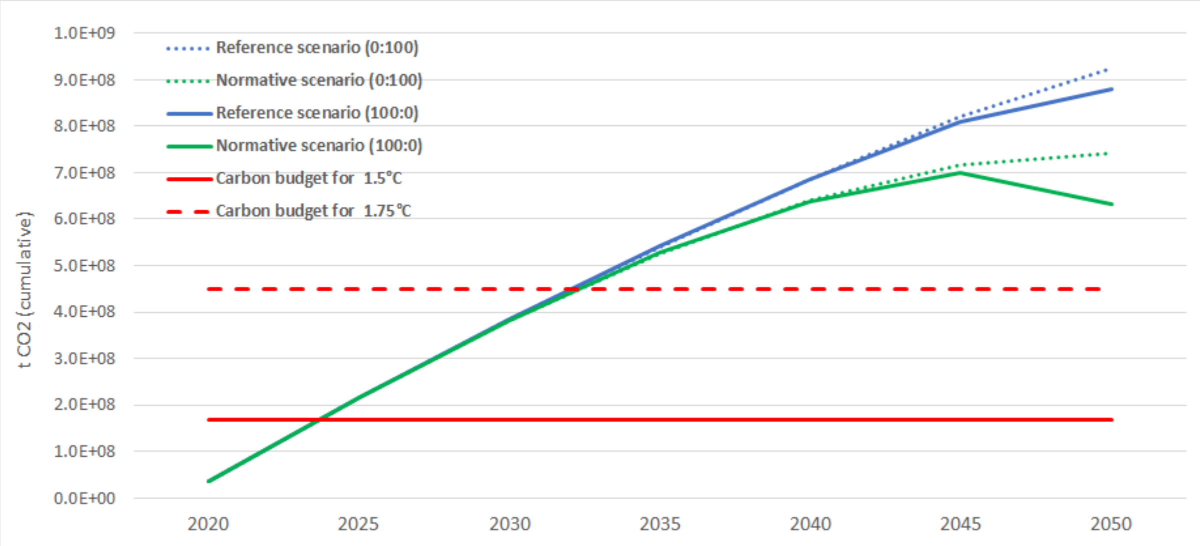

Fig. 26. Cumulative CO_2-equivalent emissions for the scenario and two different allocation approaches, 0:100 and 100:0.

4.2 Comparison with other studies

This section compares similar studies with the reported findings. While final results may not be comparable due to differences in scope, the main trends can be compared.

IRENA (2020) identifies the best available deep decarbonization options with the aim to stay within a 1.5 °C global temperature rise in a scenario called Transforming Energy Scenario. The focus is on energy-intensive industrial sectors, including the chemical sector, and energy-intensive freight and long-haul transport sectors which are hard to decarbonize. This scenario depicts a significant increase in energy demand due to the electrification of many processes in the chemical sector, which resonates with the findings of this study. It also states that 29% of the emission reduction will be achieved by demand reduction, energy efficiency improvements and reuse and recycling through circular economy concepts. This suggests that the NS can potentially be improved by including more circular economy concepts.

IEA (2012) developed the Energy Technology Perspectives. It is a target-oriented approach, aiming at a 50% cut of emissions by 2050 across all sectors globally. The most significant reductions of scope 1 emissions globally can be achieved by thermal energy efficiency improvements. CCS is another important solution to reduce scope 1 emissions, especially for ammonia plants. In the NS, energy efficiency is not the major contributor to scope 1 emission reductions. This can be explained by the difference in geographical scope since the energy efficiency potential in Germany is well developed already (DECHEMA & FutureCamp, 2019).

A more ambitious roadmap in terms of GHG emissions reductions has been developed by Ecofys and Berenschot (2018) for the Netherlands. It brings down GHG emissions by 80-95% in 2050 relative to 1990. Interesting here is that besides scope 1 and 2 emissions, the roadmap also considers part of the scope 3 emissions, namely the end-of-life treatment of sold products. Ecofys and Berenschot (2018) stress the need for speed as a key success factor. It is shown that earlier innovation leads to accelerated cost reductions as well. The NS comparison with the carbon budget also points out the need for speed as a key take away. Besides, the authors stress the importance of having a broad mix of measures (including bio-based and hydrogen-based route) to maintain a broader basis for future feedstock availability. In a similar vein, the sensitivity analysis observed that biomass is more important in the case of higher electricity EFs.

The study by DECHEMA and FutureCamp (2019) has the most common ground in comparison with this study. Both consider Germany and focus on specific processes for individual chemical products for energy and emissions reduction improvements. Furthermore, the technology shares adopted in the RS are based on their Technology Pathway scenario. DECHEMA and FutureCamp (2019) found a 4-to-14-fold increase in electricity demand up to 700 TWh per year. Thereby the stronger the emission reduction, the higher the growth in electricity demand. Until 2040, the electricity demand is relatively constant, but it starts increasing rapidly afterwards. The growth is particularly predominated by the HVC production. These developments and characteristics are reflected in the results of this study as well.

However, significant differences in results for the GHG emissions can be observed. The emissions in 2020 are significantly higher with 100 Mt CO_2 in the Technology Pathway scenario, compared to the 37 Mt CO_2 found in this study. This gap can be explained by the fact that DECHEMA and FutureCamp (2019) covered scope 3 emissions, which highlights their relevance. Both studies confirm that HVC is the dominating product group causing CO_2 emissions and that significant emission reduction only starts after 2035.

4.3 Limitations

Scope

Related to the scope of the study, there are limitations embedded in this study. In order to comply with the HI-CAM project, scope 3, i.e., up- and downstream processes, are not considered in this study. This means that a life cycle perspective cannot be applied, which has twofold consequences. Neglecting downstream processes omits the end-of-life of the chemical products. According to Agora Energiewende and Wuppertal Institute (2020), this can play a major role for HVC when it is incinerated, as this is responsible for more than 50% of the life cycle emissions. At the same time, higher recycling rates would reduce these emissions, which is also not considered.

Neglecting upstream processes on the other hand has the consequence that emissions related to feedstock production are not considered either, as the *2006 Guidelines for National Greenhouse Gas Inventories* account these as part of the energy sector and not the chemical industry. Low-carbon processes that produce feedstock, such as the Fischer-Tropsch process are accounted as processes of the chemical industry and are thus covered.

Another limitation is connected to the energy provision. The distinction between energy produced on-site and off-site could not be considered with regard to the applied EFs due to a lack of data. Nevertheless, it is expected that a distinction would lead to a reduced EF of on-site energy generation in the present, as the share of natural gas is high leading to a lower EF than the German electricity mix. How this develops in the future is difficult to assess. Moreover, the increase in electricity demand is likely to be supplied by external energy (Dechema & FutureCamp, 2019).

Moreover, the production volume is kept constant over time. The production volume is influenced both by supply and demand factors. Some factors which might influence the supply side have been neglected, such as recycling and material efficiency of the chemical products in the use-phase (IEA, 2018). These are again affected by demand-influencing megatrends, such as the rise of a circular economy, urbanization, an aging population or increased prosperity (Ecofys & Berenschot, 2018).

Finally, the scope narrowed down to a limited number of product groups and production pathways is considered a limitation. Other product groups could potentially become more important and other innovative production processes might break through. However, these cannot be foreseen and long investment cycles and research and development time make this unlikely.

Carbon budget calculation

The quantification of the carbon budget itself contains different shortcomings.

Firstly, allocating by the share of inhabitants for deriving the national carbon budget is highly disputed. There is no global consensus on which carbon budget allocation should be applied, consequently, countries apply the concept that assigns them the highest budget. This fact, however, causes that the entirety of NDCs based on the national carbon budgets significantly surpasses the 2°C target and leads to a 3.2°C global carbon budget (SRU, 2020).

Secondly, the allocation based on grandfathering of the national carbon budget to the chemical industry is a subject of dispute. This grandfathering assumes a proportional reduction of all sectors. The German Climate Action Plan 2050, however, draws a sectoral decarbonization pathway assuming different speeds in the reduction of emissions among the sectors. Particularly, the agricultural and the industry sector will according to the decarbonization pathway be slower (SRU, 2020). While today's share of the industry sector on the annual GHG emissions in Germany is about 21%, the share in 2030 will amount to 31% (SRU, 2020). This indicates that the actual carbon budget allocated to the chemical industry could be higher than the calculated budget in this study.

Thirdly, the comparison between the carbon budget and the cumulative scenario emissions suffers from limitations. This is because the comparison of bottom-up data like the scenario emissions and top-down data as the carbon budget can lead to inconsistencies. While the carbon budget only covers CO_2, the scenario emissions cover all GHG emissions. This is adjusted by the fact that the selected product groups only cover a share of products. Such an assumption is sensitive and the fact that non-GHG emissions tend to be harder to reduce (DECHEMA & FutureCamp, 2019), may cause that the comparability is limited.

Scenario development

The extent to which the NS is realistic remains disputable. Since socio-economic factors are neglected, the scenario cannot be considered realistic. The results are valuable in the sense that the scenario gives an indication of the technical feasibility of emission reduction in light of the carbon budget. A technological focus can be considered optimistic and marks the minimum.

The scenario development of the NS focuses on mitigating emissions to create the most optimal scenario with the lowest cumulative emissions possible, based on data from the technology table. The quality of the scenario inherently depends on the quality of this data.

Underestimated quantities of process emissions or energy carriers required can result in an overestimation of the potential of certain technologies, and vice versa. The chemical sector is criticized for its transparency of reported data, which leads to uncertainties about the scope and accounting mechanisms for the data found in literature. Levi and Cullen (2018, p. 1726) state the data in the chemical sector is “few and far too costly”.

Besides reliance on the quality of data, the optimization approach suffers from the simplified level of constraints. Especially if a constraint is active, i.e., the constraint is satisfied as an equality constraint, the provided minimum or maximum value can be traced back in the results. Since the various production pathways consist of very different processes, it is preferable to implement technology-specific constraints rather than a generalized set.

Other implications on the environment

In this analysis, solely GHG emissions and thus impacts in the impact category “climate change” were taken into consideration. Thus, implications associated with other impact categories were not considered. In a transformation heavily relying on electrolyzers and with growing shares of biomass, this can be of relevance as electrolyzers are known for their demand for abiotic resources such as platinum (Kleijn & Van der Voet, 2010) and biomass can depending on its type also be associated with significant environmental and social consequences (Tonini & Astrup, 2012).

4.4 The German chemical industry in a bigger picture

The German context for decarbonizing the chemical sector is different from other regions, especially developing countries where an increase in chemical product demand is expected (expert Agora Energiewende, personal communication, December 11, 2020). The IEA (2012) measured the energy savings potential across different regions and showed that there are large differences. The largest savings can be achieved in China, for process heat specifically. Significant potential is also estimated for Europe in a wide variety of measures (e.g co-generation, recycling and energy recovery and process heat). It is expected that access to renewable energy will influence decisions on the future locations of chemical production (IRENA, 2020).

In regional scenarios, it is important to consider how allocation choices can affect other regions as well. Whether a consumption- or production-based approach is taken has large implications for the result. The EU is the largest chemicals exporting region in the world (CEFIC, 2020); thus, a product-based approach is likely to attribute higher quantities of emissions to the German chemical industry.

This report follows a production-based approach, which cannot preclude carbon leakage. Carbon leakage is defined as the process in which GHG emissions increase in one country following the reduction of emissions in another country (IRENA, 2020), e.g., due to outsourcing activities. It is acknowledged that feedstock products and the import of hydrogen possibly yield carbon leakage.

As evident from the results, the chemical industry is tightly coupled to the energy sector. In fact, the chemical industry interacts with many other sectors as well. Chemical products have a wide variety of applications in other sectors, both as intermediate and end-use applications.

This means that decarbonization in the chemical sector can reduce emissions in other sectors and vice versa.

Ecofys and Berenschot (2018) have described the chemical industry as a “solution provider”. They reason that the chemical sector can potentially introduce new opportunities in other sectors, if strong collaboration with value chain partners is achieved. An example mentioned by Ecofys and Berenschot (2018) is that the chemical industry and other industries can jointly invest in common infrastructure such as CCS to enable low-cost deployment.

On the contrary, various sector-specific decarbonization scenarios also show trade-offs between different sectors. The demand for sustainable biomass pressures the available sustainable resources and competes with other sectors (Ecofys and Berenschot, 2018). Similarly, the trend of electrification is observed in other sectors as well, e.g. due to the adoption of electric arc furnaces in the iron and steel sector and electric vehicles in the road frights sector (IRENA, 2020). Van Wijk and Wouters (2020) expect that Europe cannot produce the future demand for renewable energy domestically. They suggest developing a joint hydrogen strategy with North-Africa since there is a large potential for solar conversion technologies to produce hydrogen sustainability while utilizing existing infrastructure.

5 Conclusion

This study revolves around the question of how the German chemical industry can transform to comply with the carbon goals set in the Paris Agreement. For the chemical product groups ammonia, urea, chlorine, methanol and HVC, existing and developing production technologies are identified. It is shown how a switch in feedstocks and production technologies can reduce both process and energy-related emissions. The switch in production technologies is assessed via two scenarios: the RS serves as a benchmark and the NS is optimized to achieve minimal GHG emissions. The scenarios are compared with carbon budgets for temperature increases of 1.5 and 1.75 °C.

The industry’s transformation will require a transition of production technologies towards non-fossil production processes such as electrolysis, methane pyrolysis, biomass gasification or plastic waste pyrolysis. An increase in electricity demand will be necessary in order to phase-out fossil fuels and feedstocks that form the basis of the chemical industry today. A trend of an increase in final energy demand is observed concurrent with a decrease in GHG emissions, which is only possible due to future electricity having an EF of zero. The final energy demand of the NS is 342 TWh higher in 2050 compared to 2020, and 175 TWh higher than the RS in 2050. Next to electricity, the energy carriers biomass and plastic waste are expected to become more relevant.

The technical feasibility of production technologies transformation is assessed by means of the scenarios. GHG emission reduction is notably higher for the NS, in 2050 the GHG emissions for the NS are equal to 8% of those in the RF. It is observed that the ultimate pathway forward to 2050 is highly dependent on the decarbonization of the energy sector. An unsuccessful transition of the energy system does not only inhibit the emission reduction in the chemical industry, but it may also limit the role of electrolyzers and favor other alternatives such as biomass gasification.

Comparing the cumulative emissions in the scenario with the carbon budgets shows that in all cases the carbon budget is exceeded. Even for the NS, a gap with the cumulative emissions remains respectively 0.6 and 0.3 Gt with the 1.5°C or 1.75°C carbon budget. Since low-carbon production technologies are likely not sufficiently developed before 2035, strong emission reductions are only expected after 2035. Even when CCU benefits are allocated to the chemical industry, future negative emissions occur only after exceeding the carbon budget. Time is crucial, as introducing new technologies and phasing out conventional technologies is time-consuming. This study confirms the statement of IRENA (2020) that the "*window of opportunity is closing fast.*" Therefore, R&D is identified as a crucial lever for the decarbonization of the chemical industry to pave the way for a fast introduction of low-carbon technologies. To incentivise and subsidise the transformation of the chemical industry, policy is of importance. Since this study did not look into the policy-dimension, the question of how policies can support the transformation provides research potential for consecutive studies.

The next steps of the HI-CAM project will place the results in the larger system context by connecting other industries. This allows for examination of the effects on up- and downstream processes. Outside of the project, a more holistic perspective can be obtained if the end-of-life emissions are considered by taking a life cycle perspective. Furthermore, it can be noteworthy to consider other regions as well, especially with respect to EU wide efforts in the energy transition.

In conclusion, the German chemical industry cannot comply with the Paris Agreement if the transition is only focused on switching feedstocks and production technologies. The scenario is considered technology-orientated and optimistic, which emphasizes the challenge ahead. Despite methodological limitations, the results show a convincing gap between the NS and the carbon budget from which it can be concluded that more efforts are needed to decarbonize. Circular economy measures, industry-wide and cross-regional cooperation will be needed as well. Potential synergies and trade-offs require more attention to see how the chemical sector can transform from an energy-intensive high emitting sector to a solution-provider.

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