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The role of hydrogen for the defossilization of the German chemical industry

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HIGHLIGHTS

- Defossilization is a stringent constraint in addition to GHG mitigation.
- Non-energetic demand is satisfied by green hydrogen and its derivatives.
- Chemical recycling and the MTO route can be identified as critical technologies.
- Defossilizing the German industry doubles the industrial hydrogen demand in 2050.
- Cumulative costs of transformation of a defossilized energy system increase by 32%.

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ABSTRACT

Within the European Green Deal, the European industry is summoned to transform towards a green and circular economy to reduce CO_2-emissions and reach climate goals. Special focus is on the chemical industry to boost recycling processes for plastics, exploit resource efficiency potentials, and switch to a completely renewable feedstock (defossilization). Despite common understanding that drastic changes have to take place it is yet unknown how the industrial transformation should be accomplished. This work explains how a cost-optimal defossilization of the chemical industry in the context of national greenhouse gas (GHG) mitigation strategies look like. The central part of this investigation is based on a national energy system model to optimize the future energy system design of Germany, as a case study for a highly industrialized country. A replacement of fossil-based feedstocks by renewable feedstocks leads to a significant increase in hydrogen demand by +40% compared to a reference scenario. The resulting demand of hydrogen-based energy carriers, including the demand for renewable raw materials, must be produced domestically or imported. This leads to cumulative additional costs of the transformation that are 32% higher than those of a reference scenario without defossilization of the industry. Fischer-Tropsch synthesis and the methanol-to-olefins route can be identified as key technologies for the defossilization of the chemical industry.

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Introduction

The central concept of this work deals with non-energetic demand. This demand describes energy carriers that are not used as fuels, but as raw material inputs in processes [1]. The largest share of German non-energetic consumption is accounted for by crude oil derivatives and natural gas which are used in basic chemicals, e.g., to produce methanol, ammonia, or plastics. Initially, no direct emissions are emitted through non-energetic demand. However, energy-related emissions can arise from the use of electricity or fuel for the manufacturing processes, as well as process-related emissions from the conversion of the non-energetic sources into end products. Worldwide, non-energetic consumption is responsible for about 15% of industrial CO_2-emissions [2]; the exact share of German CO_2-emissions is not recorded statistically. Since 1990, non-energetic consumption has remained constant at between 250 and 310 TWh [3]. Even though a slight drop in non-energetic demand has been observed in the last three years, the chemical industry expects demand to increase in the future [4].

The German Climate Protection Act calls for greenhouse gas (GHG) neutrality in 2045 [5]. However, since the current national GHG legislation for a future low-carbon Germany does not include non-energetic demand (CO_2 embedded in products), these future emissions (which occur through decomposing or burning at end-of-life) are not accounted for. A GHG-neutral Germany by legislation does not require a fossil-free (defossilized) energy system. This is why in recent national energy scenarios for Germany (e.g. Refs. [6–8]), showing possible transformation paths towards a low-carbon energy system in 2050, defossilization is not at all or insufficiently considered. An assessment of the extent to which defossilization measures are part of cost-optimal and efficient greenhouse gas reduction strategies and what effects their absence implies for the German energy system as a whole has not yet been made [9]. This work analyses the impacts of defossilization strategies in the chemical industry on the transformation towards a low-carbon German energy system.

State of the art

Germany's primary energy consumption was 3580 TWh in 2019 [3]. Although the share of renewable energy sources has risen steadily in recent years, conventional energy sources still account for 85% of primary energy demand. The main contributors are crude oil with more than 33% and natural gas with 25%. Lignite and hard coal each account for about 9% and nuclear energy for another 6%. Approximately 70% of the primary energy input could be converted into 2515 TWh of final energy available to the end-use sectors in 2019. The industrial sector claims a share of 28% of final energy consumption with 704 TWh, making it the sector with the second largest demand in Germany. Only the transport sector has an even larger final energy demand with 770 TWh [10]. About 25% of industrial energy demand is met by electricity, but industry requires an additional 486 TWh of fuels, most of which are fossil fuels. Accordingly, the industrial sector is of great importance when it comes to substituting Germany's demand for fossil fuels with renewable energy sources. Within the industrial sector, it is possible to further break down the final energy demand and allocate it to the individual industries or branches of the economy. Six industries can be identified, which together account for about 2/3 of the total industrial final energy demand. First and foremost, metal production and basic chemicals account for the majority of the energy demand, each with 21%. The importance of these industries for the industrial final energy demand and also the fact that the other industries of other manufacturing sector are characterized by a higher heterogeneity in their processes predestines these six industries for a more detailed and at the same time representative investigation in an energy system model.

In order to analyse how the topic of defossilization is covered in recent studies of the German energy system more than 30 different scenarios in 25 studies over the last years were reviewed. A detailed review of energy system models, which are used for these studies can be found in a previous publication by the authors [9]. A summary of how these studies have considered defossilization strategies can be found in Table 1. In particular the older scenarios have not at all or only insufficiently covered the topic of defossilization. This is mainly due to insufficient coverage of sectoral energy demands and a lack of implementation of specific technology alternatives to produce chemicals with green raw materials. Also, the modeling approach for most of the older scenarios was limited and based on crude balancing of energy flows. No simulation or optimization models for the whole energy system were used, which makes it difficult to include very specific parts of the energy system.

Latest studies focus more on detailed energy sectors. Also, the trend to optimization approaches and more complex models when it comes to analyse future energy system designs can be observed [36]. This explains why in most cases a mix of simulation and optimization models is used to determine the optimal future system. However, non-energetic demand is not considered in most scenarios, so that statements on cost efficiency cannot be made. Only in the study "Climate-neutral Germany" [33] is information provided on process changes in the provision of non-energy demand. However, since these estimates were calculated with a model network (simulation model for the industrial sector) and not with a closed integrated optimization model, no statement can be made about the cost efficiency of defossilization.

Bazzenella et al. [37] analyse the European chemical industry and state that decarbonization is "intrinsically impossible" since many chemical products are based on carbon. For a more sustainable industry carbon has to originate from renewable sources instead (defossilization). The energy demand for the European chemical industry alone amounts to around 600 TWh in 2020. Bazzanella et al. created several scenarios for the transformation of the chemical industry until 2050. Their "maximum ambition" scenario shows an increase of energy demand for the European chemical industry in 2050 by a factor of 2.5 compared to 2015. The industry becomes a net consumer of around 200 Mt CO_2 in 2050 with the methanol-to-olefins route (production of high-value chemicals via methanol instead of processing naphtha in

Table 1 – Analyzed studies with regard to the consideration of defossilization strategies (adapted from Ref. [11]) (-: not considered; number of "x" stands for degree of detail of consideration within study).

Year	Ref.	German energy system scenarios	Defossilization
2009	[12]	Long-term scenarios (2009)	-
2009	[13]	Model Germany	-
2010	[14]	Energy target 2050: 100% from renewable energies	-
2012	[15]	Long-term scenarios (2012)	-
2014	[16]	Development of the energy markets - Energy reference forecast	x
2014	[17]	Energy transition business model	-
2015	[18]	Climate protection scenario 2050	-
2016	[19,20]	Energy system 2050	-
2016	[21]	The energy transition after COP 21 - Current scenarios for German energy supply	-
2016	[22]	Sector coupling through the energy transition	-
2017	[23,24]	Long-term scenarios (2017)	x
2017	[25]	Shaping the path to a greenhouse gas-neutral Germany in a resource-conserving way (2017)	x
2018	[26]	Climate paths for Germany	x
2018	[27]	Cost-efficient sector coupling	-
2018	[28]	dena - Lead study on integrated energy transition	x
2019	[29]	Shaping the path to a greenhouse gas-neutral Germany in a resource-conserving way (2019)	x
2019	[30]	Paths for the energy transition	-
2020	[31]	Paths to a climate-neutral energy system	x
2020	[32]	Hydrogen Roadmap North Rhine-Westphalia	x
2020	[33]	Climate-neutral Germany	x
2021	[7]	Climate-neutral Germany 2045	x
2021	[8]	dena - Lead study departure to climate neutrality	x
2021	[34]	Path to a greenhouse gas-neutral energy system	-
2021	[6]	Germany on the way to climate neutrality	-
2022	[35]	New destinations on old paths?	xx

steam crackers) as the key technology for the transformation towards a sustainable European chemical industry [37].

Williams et al. [38] analyse carbon-neutral pathways for the United States and also consider the need to substitute fossil-based feedstock for the chemical industry. They conclude to produce the required chemical feedstock in 2050 from gasification of biomass with synthesis in Fischer-Tropsch processes and hydrogen from electrolysis based on renewable electricity.

On a global scale Bataille [39] estimates that the feedstock demand for chemicals will rise by a factor of 1.5 from 2020 until 2050, with ammonia, methanol and olefins being the main feedstock chemicals. Most scenarios predicting the transformation of the global chemical industry consider the reduction of process emissions but not the substitution of fossil-based feedstock, and thus talk about decarbonization rather than defossilization. Mallapragada et al. [40] for example, analyse how the chemical industry can be decarbonized through electrification. They propose four different processes to provide sustainable heat to produce chemicals and thus analyse the CO_2 mitigation potential of these technologies. However, they do not consider the fossil-based feedstock used to produce these chemicals. Eryazici et al. [41] also analyse the potential of electrifying the chemical industry and address the challenge of reducing process related CO_2 emissions. Nevertheless, apart from the use of renewable hydrogen they do not consider or propose alternatives for fossil-based feedstock. There are currently only few scenarios concerning the transformation of the chemical industry on a global scale [42] and none of them assess the defossilization of the chemical feedstock. However, there are several studies concerning possible production routes with renewable-based feedstock for the chemical industry. Melero et al. [43] for example, analyse the use of biomass as renewable feedstock in refinery units to produce sustainable chemicals. Overa et al. [44], Jhong et al. [45] and Schiffer et al. [46] focus on the electrochemical conversion of CO_2 to useful chemicals and thus defossilize certain production routes for the global chemical industry. Luna et al. [47] describe technical challenges of renewable powered electrosynthesis to substitute fossil-based petrochemical processes. All these studies focus on the technical realization of defossilization processes but do not evaluate their techno-economic potential for the global chemical industry.

The aim of this work is to analyse transformation paths of the chemical industries in Germany in the context of the transformation of the overall energy system to achieve the set climate targets in 2050. Coherent scenarios will be developed to evaluate long-term strategies in the industrial sector and their impact on other sectors. For this purpose, it is necessary to consider the industrial sector in a closed integrated overall energy system model. The focus of the implementation is on detailed consideration of material flows in the energy system model, in order to also be able to make statements about strategies for defossilization in the chemical industry with regard to the transformation of the energy system by 2050. The following research question is to be answered. What are the effects of defossilization of the chemical industry on the transformation of the German energy system?

Modeling approach

The *National Energy System model with SecTor coupling* (NESTOR) is an optimization model for the German energy system. It covers a wide range of technologies describing the German energy system. The model is set up as a large interacting network of nodes and edges. A detailed description of how the model works and examples of typical input parameters can be found in the supplementary data of a previous publication by the authors [11]. NESTOR is part of the Energy Transformation Pathway Optimization Suite (ETHOS), which is available open source.[1] The nodes describe all energy and material sources, conversion technologies, energy and material storages, and energy and material sinks, whereas the edges describe energy and material flows between the nodes. The energy system model analyses the future low-carbon energy system design of Germany and the transformation towards it. Under greenhouse gas reduction restrictions, the model derives the energy system design and the transformation pathway based on cost-optimality. During the course of this work the model was developed further. Technologies and processes relevant for the German industrial final energy demand were implemented on a detailed level and parametrized with techno-economic data (capex, opex, lifetime, efficiencies, etc.). This allows processes for defossilization of the chemical industry to be analyzed and evaluated based on cost-efficiency and effectiveness. The cost comparison of the transformation is carried out on the basis of a reference scenario. This ensures that autonomous developments of the energy system, which would occur during the transformation even without increased efforts to reduce greenhouse gas (GHG) emissions, can also be taken into account.

The objective function of this optimization problem requires the minimization of the annual system costs (eq. (1)). $C_{0,y}$ describes the average investment cost of component y, $r_{n,i,y}$ is the annuity factor (using the lifetime n and interest rate i), $m_{fix,y}$ describes the operational costs, and x_y the installed capacity of component y. Summing over all components yields the annual fixed system cost. With $m_{var,k}$ as the variable operating cost of edge k, and $\dot{x}_{k,t}$ as the energy or material flow at a given time t, the annual variable costs can be summed over all edges and time steps. Both parts give the objective function which is to be minimized [48].

$$min f(x)_{LP} = min \sum_{y \epsilon Y} C_{0,y} \cdot (r_{n,i,y} + m_{fix,y}) x_y + \sum_{k \in K} \sum_{t \in T} m_{var,k} \dot{x}_{k,t} \Delta t \qquad \text{eq. 1}$$

Since this objective function defines a linear optimization problem the so-called penny switching effect can occur. One technology is given complete preference over a similar technology just because costs are slightly lower. When several technologies have similar costs, this effect leads to drastic switching of the optimal technology mix, when only marginal cost changes occur. To obtain more robust model results and avoid the penny-switching effect, Lopion et al. [48] added a quadratic part to the objective function (eq. (2)). With this addition, annual costs of a technology depend on a range of investment costs $C_{0,y}*s_y$ (s_y describes the relative maximum deviation from the average costs of that technology) rather than only on a linearized cost part. A more realistic consumer behavior in energy system models is achieved with this extension. The derivation and validation can be found in Lopion et al. [48].

$$min f(x)_{QP} = min \sum_{y \epsilon Y} \left[C_{0,y} \cdot (1 - s_y) \cdot x_y + \frac{C_{0,y} \cdot s_y}{x_{ub,y} - x_{lb,y}} \cdot {x_y}^2 \right] \cdot (r_{n,i,y} + m_{fix,y}) + \sum_{k \in K} \sum_{t \in T} m_{var,k} \cdot \dot{x}_{k,t} \Delta t \qquad \text{eq. 2}$$

The network of components within the energy system model is subject to additional constraints. For example, the limitation of allowed CO_2 emissions of the overall system is defined in a specific constraint (eq. (3)). Summed over all time steps t and edges k, the amount of specific CO_2 emissions ω multiplied by the energy or material flow $\dot{x}$ must not be larger than the total allowed amount of CO_2 emissions Ω in the system.

$$\sum_{k \in K} \sum_{t \in T} \omega_{k,t} \cdot \dot{x}_{k,t} \le \Omega_{max} \qquad \text{eq. 3}$$

Further constraints concern the mathematical formulation of energy and material conservation and can be found in Lopion [49].

The following paragraph briefly describes the implementation of certain production processes in the chemical industry and important input parameters. Methanol synthesis requires hydrogen, which is currently provided by steam reforming from natural gas or partial oxidation of mineral oil. The future use of CO_2-free hydrogen has two major advantages. First, the process-related CO_2 emissions of steam reforming are avoided. On the other hand, process-related CO_2, which was previously captured in other processes, can be used as a raw material. Several carbon capture and utilization options exist within the model ranging from 30€/t_{CO2} to 200€/t_{CO2} e.g., for the production of cement or processing of biomethane. For ammonia synthesis, the Haber-Bosch process is represented in the model, in which natural gas is currently converted to hydrogen in steam reforming and then reacts to form ammonia. Since urea synthesis is usually downstream of the Haber-Bosch synthesis, no additional process heat is required in the conventional case, since the waste heat from steam reforming can be used. In the case of a process conversion for the use of externally supplied CO_2-free hydrogen, similar to the methanol synthesis, not only CO_2 is required as a raw material, but also process heat for the downstream urea synthesis. The following parameters (Table 2) were used to implement the production processes of methanol, ammonia and chlorine.

The production of high-value petrochemicals (HVC) is the most important process chain in terms of non-energetic feedstock consumption. At the beginning of this chain is the production of naphtha. Together with diesel and kerosene, naphtha is produced from mineral oil in refineries and then

[1] https://github.com/FZJ-IEK3-VSA.

Table 2 – Investment costs and specific energy requirements of selected production processes in the chemical industry (adapted from Ref. [11]).

	Invest-costs[a]	Specific energy demand[b]				
	2020 (2050) €/t	Power kWh/kg	Natural gas kWh/kg	Hydrogen kWh/kg	Process heat kWh/kg	Reference value
Chlor-alkali electrolysis	404 (404)	2.35			0.3	Chlorine
Haber-Bosch process	670 (670)	2.07	5.83		1.83	Ammonia
Haber-Bosch process (H_2)	500 (500)	1.72		5.93	1.83	Ammonia
		Power *kWh/kg*	Natural gas *kWh/kg*	Crude oil *kWh/kg*	Process heat *kWh/kg*	
Methanol (steam reforming)	400 (400)	0.17	6.94		3.14	Methanol
Methanol (partial oxidation)	530 (530)	0.18		9.22		Methanol
		Power *kWh/kg*	Hydrogen *kWh/kg*	Biomass *kWh/kg*	Process heat *kWh/kg*	
Methanol (H_2)	197 (197)	1.5	6.33			Methanol
Methanol (biomass)	400 (400)	0.17		10.08	3.33	Methanol

[a] based on [4].
[b] based on [50,51].

refined into fuels (Fig. 1). However, naphtha is also used in the petrochemical industry as the main non-energetic feedstock for the production of HVCs. With biomass gasification and Fischer-Tropsch synthesis, two processes are modeled in addition to the classical refinery processes that will be available for the production of green naphtha in the future.

By using biomass, or hydrogen, CO_2 emissions can be avoided in the production of naphtha. In the further course, naphtha is split into highly refined chemicals in steam crackers. Conventionally, the required process heat is provided by combustion of parts of the naphtha, which results in CO_2 emissions. In the future, however, it will also be possible to provide the required process heat by means of electric heaters. The second process implemented for the production of HVCs is the methanol-to-olefins process. In this process, methanol is used instead of naphtha as a feedstock for the production of HVC. Connected to the production of HVC are recycling processes for the treatment of waste streams composed of HVC. The following parameters (Table 3) were used to implement the production processes of high-value chemicals.

For this work a reference scenario was created, in which GHG emissions have to be reduced by 95% in 2050 compared to 1990 levels. Apart from the phase-out of coal and nuclear power generation (as already stated in national legislation [57,58]), no other limitation is placed on the model. Recycling rates are fixed at today's levels in all industrial sectors until 2050. Novel recycling processes (e.g., chemical recycling of plastic waste) are only available from 2040. Otherwise, no further restrictions are applied. The model starts from 2020 with the current power plant and technology stock in all energy relevant sectors (transport, industry, buildings) and optimizes the operation only (no new technologies can be built), which is used for calibrating the model and validating its result with statistics. Starting from 2020 the transformation path is optimized. The model optimizes the energy system design in 5-year intervals until the target system in 2050 is reached. During these calculation runs the maximum yearly GHG emissions, which can be emitted by the optimized energy system are limited based on German regulations to reach a low-carbon energy system [59]. Another scenario is calculated to analyse the effects of a switch in the chemical industry from a fossil-based to a fully renewable use of raw materials (defossilization). Within this scenario, additionally to restricting the GHG-emissions as in the reference scenario, no fossil energy carriers are allowed. This constraint reveals the additional efforts which are necessary to not only reach a low-carbon but a defossilized German energy system.

Reference Scenario

The following paragraph briefly presents key results of the reference scenario. The reference scenario is the basis for all further calculations and can be seen as a free optimization, taking into account the previously explained boundary conditions and assumptions, up to the year 2050. A more detailed description of the reference scenario can be found in Kullmann et al. [11] and Kullmann [60].

Primary energy demand

In 2020, more than 85% of primary energy consumption comes from fossil fuels (Fig. 2). Crude oil and natural gas together account for a share of more than 50%. By 2050, a drastic reduction in fossil energy sources is necessary, so that their share drops to about 4%. This represents non-renewable waste. In addition to wind energy (approx. 540 TWh), photovoltaics (approx. 350 TWh) and biomass (approx. 440 TWh), which together account for 63% of the primary energy demand in 2050, approx. 300 TWh of hydrogen and 113 TWh of other renewable energy sources (power-to-liquid) will be imported.

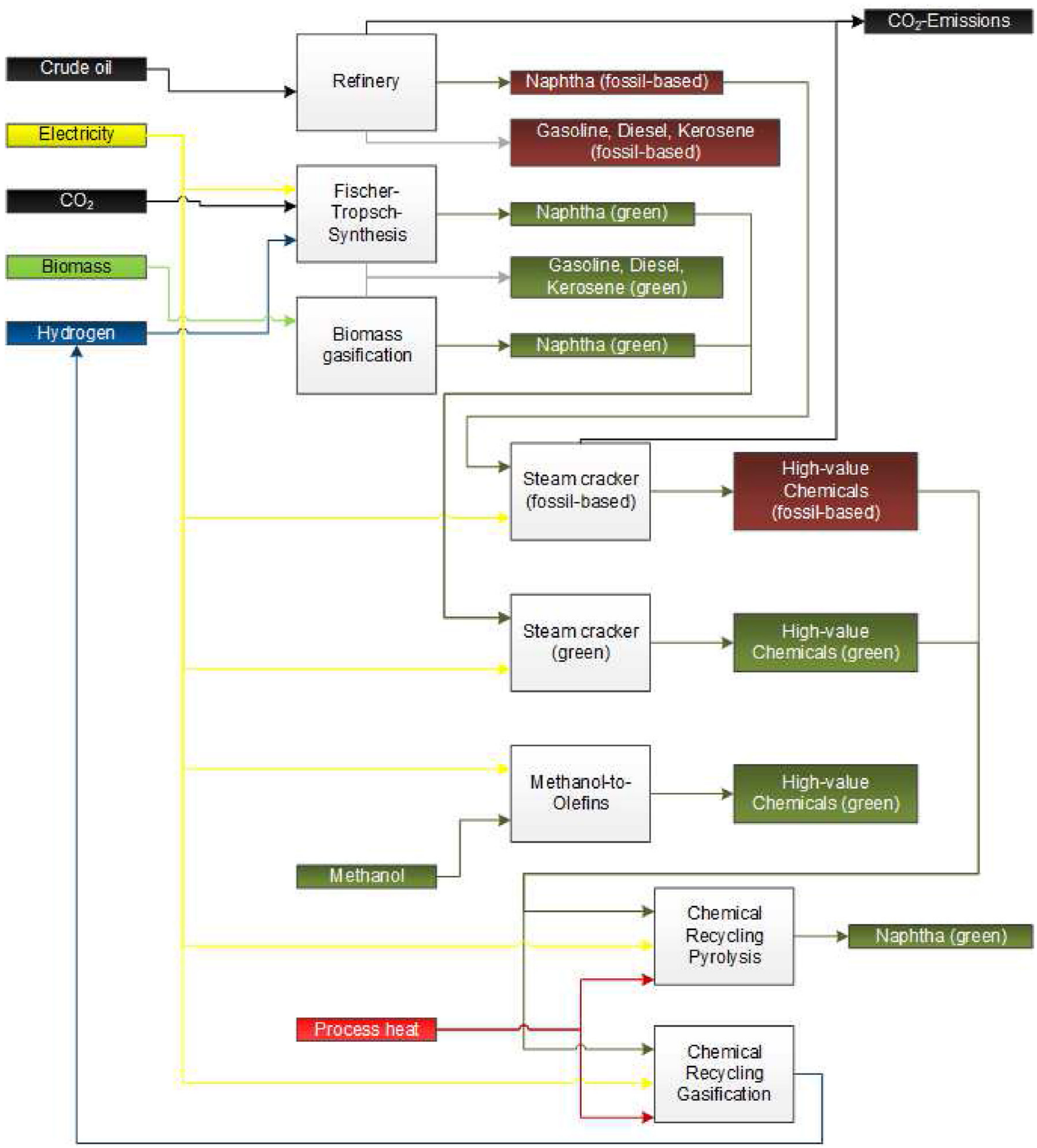

Fig. 1 – Schematic display of how the production of high-value chemicals is embedded in the energy system model.

In summary, except for non-energetic (n-energ.) demand, the energy system design in 2050 does not rely on any other fossil fuels.

Final energy demand

There is a 48% decrease in final energy demand for the Trade, Service & Commerce sector compared to 2020, to approximately 230 TWh. The final energy demand in the transport and building sector is reduced by more than half to 340 TWh, respectively 290 TWh by 2050. Only the industrial sector has an almost constant final energy demand of about 730 TWh (+280 TWh non-energy demand) until 2050. Taking into account an assumed increase in goods production and gross value added of 1.2%/a on average across all sectors until 2050, the final energy demand of industry per total generated gross value added consequently decreases by approx. 43%.

Electricity demand and generation

Increasing electrification can be observed in all final energy sectors until 2050. Net electricity consumption will increase to 970 TWh in 2050. Sector coupling (especially electrolysis as well as power-to-heat) play a decisive role (Fig. 3). The industrial sector has the largest electricity demand and is already partially electrified due to certain industries (e.g. non-ferrous metals). Nevertheless, an increase in electricity demand of 50% to approx. 330 TWh until 2050 can be observed. This is largely (80%) due to new processes that will be available in the future and replace processes based on fossil fuels. High-

Table 3 – Investment costs and specific energy demand of selected processes for the production of high-value chemicals (HVC) and synthetic refinery products (processes that can use secondary raw materials from recycling are marked with *) (adapted from Ref. [11]).

	Invest-costs[a]	Specific energy demand[b]				Reference value
	€/t	Electricity kWh/kg	Methanol kg/kg	Naphtha kg/kg	Hydrogen kWh/kWh	
Methanol-to-Olefins	268 (268)	1,39	2,34			HVC
Steamcracker *	1700 (1700)	0,1		1,22		HVC
Steamcracker (el. heating) *	250 (250)	4,7		1,22		HVC
Fisher-Tropsch-Synthesis	788 (500)	3,5			1,32	Diesel/ Gasoline/ Kerosene

[a] adapted from [52–54].
[b] based on [4,55,56].

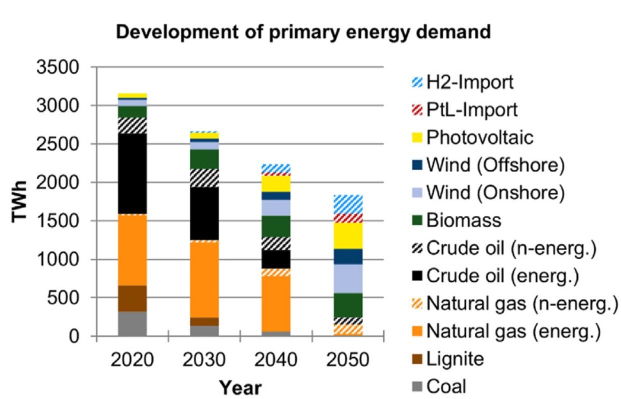

Fig. 2 – Development of primary energy demand of the reference scenario until 2050 in TWh (energ.: energetic; n-energ.: non-energetic).

temperature process heat pumps and electric boilers, power-to-heat technologies are responsible for another 20% of the increase (23 TWh) in the industrial sector.

However, electrolysers will make the biggest difference to today's electricity consumption in the future. In 2050 they claim 245 TWh, more than a quarter of total electricity demand. They are the largest driver of the significant increase in electricity demand by 2050, accounting for 58% of the increase.

While renewables account for only about 45% of electricity generation in 2020, their share rises to 100% by 2050. Consequently, a shift to fully renewable power generation is of great importance for the success of the transformation of the entire energy system. Electricity generation increases by two-thirds from about 600 TWh in 2020 to 1000 TWh. Despite accounting for more than 50% of installed electricity generation capacity, rooftop and ground-mounted photovoltaics account

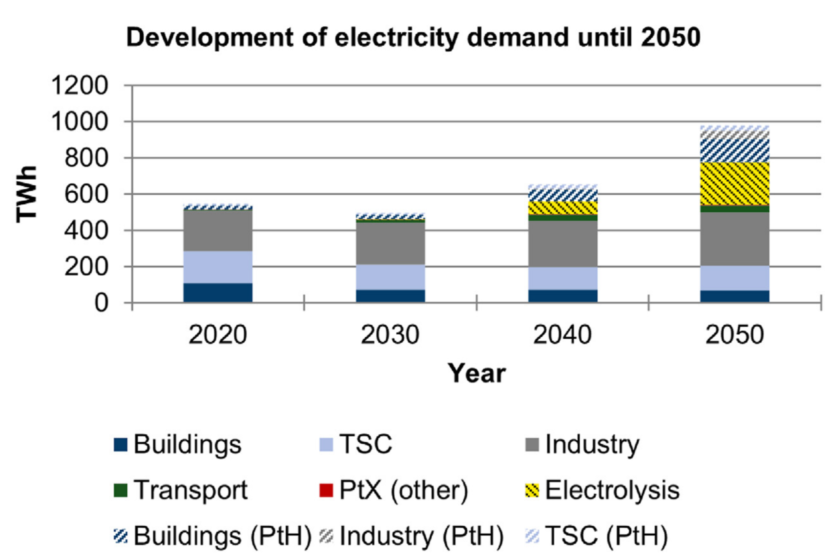

Fig. 3 – Development of electricity demand of the reference scenario until 2050 in TWh (TSC.: Trade, Service & Commerce sector; PtH: Power-to-heat).

for only 35% of electricity generation at 350 TWh. This results in 1090 full load hours (FLH) for rooftop photovoltaic systems and 1133 FLH for ground-mounted photovoltaic systems. Wind turbines account for the largest share of electricity generation in 2050 (54%). With 1850 VLS and a generation of about 360 TWh, onshore wind turbines contribute 36% to the total electricity generation. Offshore wind turbines have 4600 VLS in 2050. The electricity generation is about 180 TWh, which is 18% of the total electricity generation.

Ambitious measures are needed in the conversion of power generation. While in 2020 there is still a total installed capacity of about 220 GW in total, this value will increase by almost three times to about 600 GW by 2050. Roof-mounted and ground-mounted photovoltaic systems with an installed capacity of approx. 310 GW are the main contributors to this. They thus account for more than 50% of the total installed capacity in 2050. Onshore wind power plants (194 GW) and offshore wind power plants (40 GW) will also play a significant role in power supply in the future. By contrast, generation plants based on fossil fuels will be completely phased out by 2050. In 2050, there will still be residual capacities of natural gas power plants amounting to 17 GW. However, these will be operated exclusively with biogas and can therefore also be counted as renewable electricity generation.

Hydrogen production and consumption

The increased electricity demand for electrolysis can be attributed to increasing hydrogen demand in 2050. While there is no significant capacity in 2020 (outside of industrial sites for direct use in the respective processes, which are not explicitly shown here), more than 58 GW of electrolysis capacity will be needed in 2050. These produce about 163 TWh of hydrogen at 2800 FLH. Domestic hydrogen production accounts for about 40% of total demand. Most of the required hydrogen amount will be imported. Hydrogen demand in 2050 results mainly from industrial and transport sector demands (47%, and 35%, respectively). The industrial sector requires approximately 190 TWh of hydrogen in 2050.

Finally, Fig. 4 shows the total industrial hydrogen demand, broken down by sector. Steel production and methanol synthesis are the two sectors with the highest demand. Almost one third of the industrial hydrogen demand, 62 TWh, is required in steel production. It is used in the direct reduction plants. With 51 TWh (non-energetic), methanol synthesis requires more than 25% of total industrial hydrogen demand in 2050. The cement industry requires 28 TWh of hydrogen for process heat supply, which is listed separately in the chart due to its significant amount. Another 32 TWh hydrogen are needed for process heat supply for the rest of the industry in industrial kilns/furnaces. The Haber-Bosch process also requires about 20 TWh of green hydrogen (non-energy) in 2050. In summary, the steel industry, through its energetic demand, and methanol synthesis, through its non-energetic demand, can be identified as the two most significant industries for future hydrogen demand.

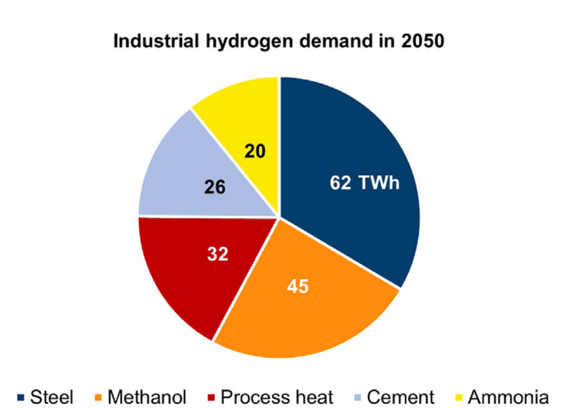

Fig. 4 – Industrial hydrogen demand of the reference scenario in 2050 in TWh.

Results and discussion of defossilization scenario

This chapter describes the results of the defossilization scenario, which is used to investigate the transformation of the German chemical industry from fossil-based to a fully renewable raw material supply. A reference scenario serves as a basis for comparison. Since defossilization implies an additional demand for renewable energies as well as green hydrogen, the question of supply (domestic production/import) arises. In addition to the 95% reduction target in 2050, the chemical industry is completely converted to a use with renewable raw materials (defossilization). The focus of this paper is placed on the industrial sector, and here in particular on the chemical industry. Further analyses and background information can be found in Kullmann et al. [9,11] and Kullmann [60].

Fig. 5 shows the development of primary energy consumption of the defossilization scenario and the change compared to the reference scenario. In 2050, no major absolute change in primary energy consumption can be seen; additional 80 TWh primary energy are required in the defossilization scenario, and it can be observed that non-energetic crude oil and natural gas are completely substituted by hydrogen.

In 2050, about 160 TWh more hydrogen is needed compared to the reference scenario, substituting 91 TWh crude oil and 125 TWh natural gas, resulting in a total demand of 560 TWh hydrogen for the whole energy system. In addition, there is a small additional consumption of natural gas used for electricity generation (59 TWh). This can be explained by the released CO_2 budget in the chemical industry. By forcing the chemical processes to switch to renewable raw materials, fewer CO_2-emissions are generated in this sector, which can be emitted more in other sectors, e.g., power generation, and still meet the overall GHG-reduction target.

Fig. 6 shows that a change in final energy consumption occurs almost exclusively in the industrial sector. On the one hand, 30 TWh less fuels are used for non-energy purposes and, on the other hand, 115 TWh more for energy purposes.

A slight change of final energy demand also occurs in the building sector. This is due to the increased demand for hydrogen in industry, as a result of which 13 TWh are withdrawn from the building sector (cf. Fig. 10) and instead compensated for by other measures (e.g. use of heat pumps instead of H_2 condensing boilers).

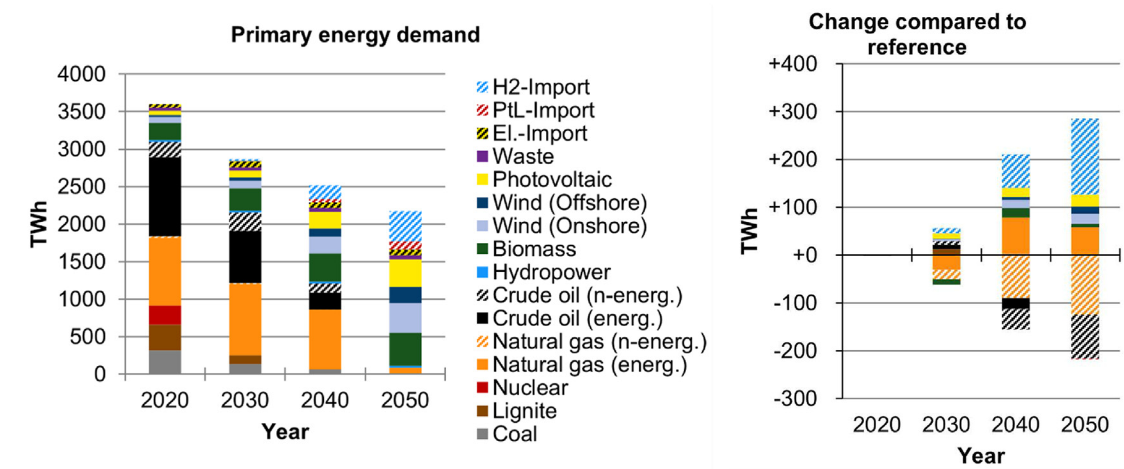

Fig. 5 – Development of primary energy demand of the defossilization scenario until 2050 (left) and the change compared to reference scenario in TWh (right) (energ.: energetic; n-energ.: non-energetic).

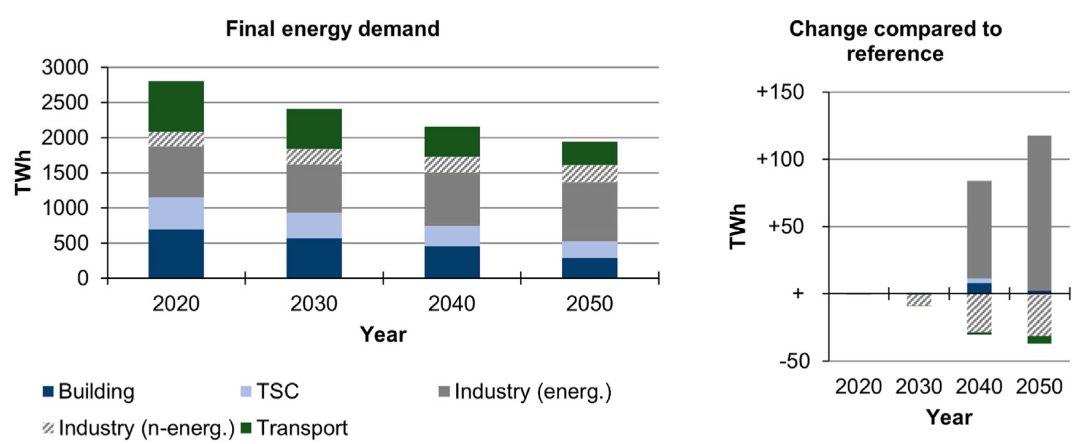

Fig. 6 – Development of the final energy demand of the defossilization scenario until 2050 (left) and the change compared to reference scenario (right) (energ.: energetic; n-energ.: non-energetic; TSC: trade, service, commerce).

Fig. 7 illustrates that in 2050, approximately 70 TWh more electricity will be needed in the industry sector. Of this, power-to-heat technologies for process heat supply account for more than 55% (about 40 TWh). In addition, 10 TWh of additional electricity will be needed in 2050 for the production of green naphtha in Fischer-Tropsch synthesis (Power-to-X, see Fig. 14).

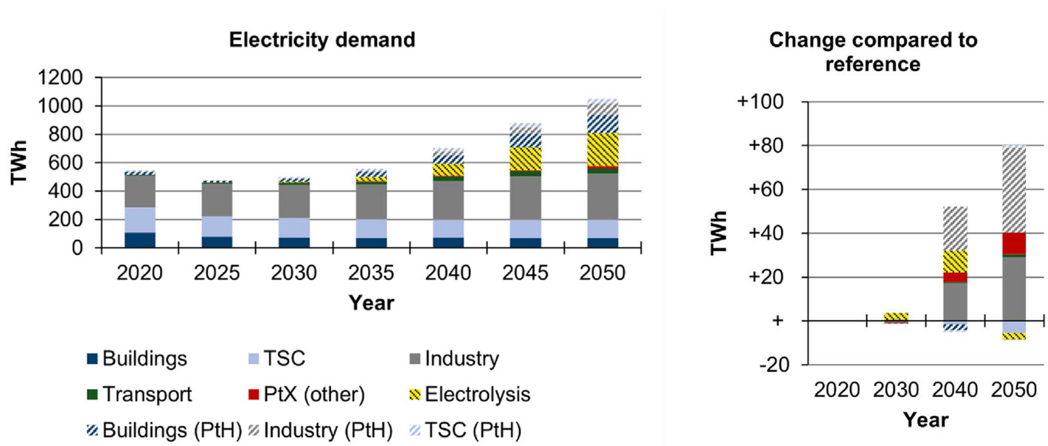

Fig. 7 – Development of the electricity demand of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh (TSC: trade, service, commerce; PtH: power-to-heat).

The development of electricity generation is shown in Fig. 8. In 2050, the total electricity generation in the defossilization scenario increases by about 8%, or about 80 TWh, compared to reference.

The reason for the changes in electricity generation is an increased demand for electricity in the industrial sector. Both wind turbines and photovoltaic plants generate about 25 TWh more electricity in 2050. The lower hydrogen reconversion (−12 TWh) is substituted by natural gas power plants.

The conversion of the chemical industry also has an impact on electricity generation capacity (see Fig. 9). In total, about 45 GW more capacity needs to be installed (including 16 GW of wind power and 25 GW of photovoltaics). As mentioned above, shifting the CO_2 budget out of the chemical industry results in 10 GW more natural gas-fired power plants being installed. However, these will be run at peak load and will largely replace hydrogen reconversion.

Overall, installed capacity in 2050 thus increases to 661 GW, which is about 9% higher than the total capacity in the Reference Scenario.

The hydrogen demand divided among the different sectors is shown in Fig. 10. Overall, the industrial sector requires more than 185 TWh of additional hydrogen in 2050.

This brings the total demand in the industrial sector to 371 TWh and accounts for about 66% of the total hydrogen demand. Compared to the reference scenario, the hydrogen demand of the industrial sector is thus about twice as high.

Larger changes can be observed in hydrogen production and demand. From Fig. 11, it can be seen that about 560 TWh of hydrogen will be produced by 2050 in the defossilization scenario. The import of hydrogen accounts for more than 70% with 400 TWh.

Compared to the reference scenario, an additional 160 TWh (40%) of hydrogen will be required in 2050. The additional demand is covered exclusively by imports. This indicates that a defossilization of the chemical industry cannot be achieved cost-efficiently under the given boundary conditions by exclusively domestic hydrogen production.

A deeper dive in the model results of the chemical industry reveals that of the 16.5 Mt of plastics produced in 2050, 50% will be supplied via the methanol-to-olefins route and the other half via the use of green naphtha in steam crackers, either via hydrogen in Fischer-Tropsch processes or the use of pyrolysis oil from chemical recycling (see Fig. 12).

Methanol production in the defossilization scenario shows significant differences compared to the reference scenario (see Fig. 13). In 2050, methanol production is based exclusively on the use of green hydrogen and, to a lesser extent, on electricity. A total of 134 TWh of hydrogen is required and 122 TWh of natural gas is substituted.

Compared to the reference scenario, defossilization results in an additional hydrogen demand of 89 TWh in 2050. At the same time, 122 TWh of natural gas are substituted. The methanol-to-olefins route in 2050 is by definition based entirely on the use of green methanol. This means that about 10 Mt of fossil methanol have to be substituted compared to reference. The driver for the switch is the need for green high-value chemicals for plastics production.

This feedstock switch also implies a change in naphtha production (Fig. 14). In 2050, about 10 Mt of naphtha will be produced. Of this, more than 3 Mt (30%) is based on pyrolysis oil from chemical recycling and about 7 Mt from Fischer-Tropsch synthesis. Compared to reference, the introduction of Fischer-Tropsch synthesis in this way replaces the entire crude oil input for naphtha production in 2050.

For the energy demand for naphtha production, this results in an additional demand of 94 TWh hydrogen in 2050 compared to reference (Fig. 15). Both the Fischer-Tropsch synthesis and the methanol-to-olefins route can be identified as key technologies for the success of the defossilization of the chemical industry.

Together with methanol production (+89 TWh), these two areas are mainly responsible for the increase in hydrogen demand in the industrial sector. The chemical industry uses more than 250 TWh hydrogen in 2050.

The goal of defossilizing the chemical industry in addition to reducing greenhouse gases by 95% by 2050 represents an additional restriction and leads to a significant increase in additional costs compared to the reference scenario (Fig. 16). The largest additional costs are caused by

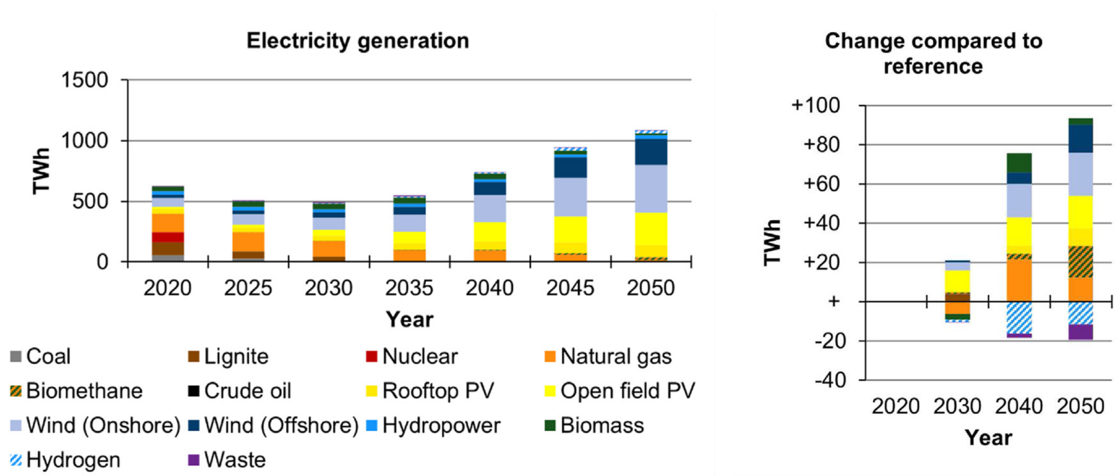

Fig. 8 – Development of the electricity generation of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh.

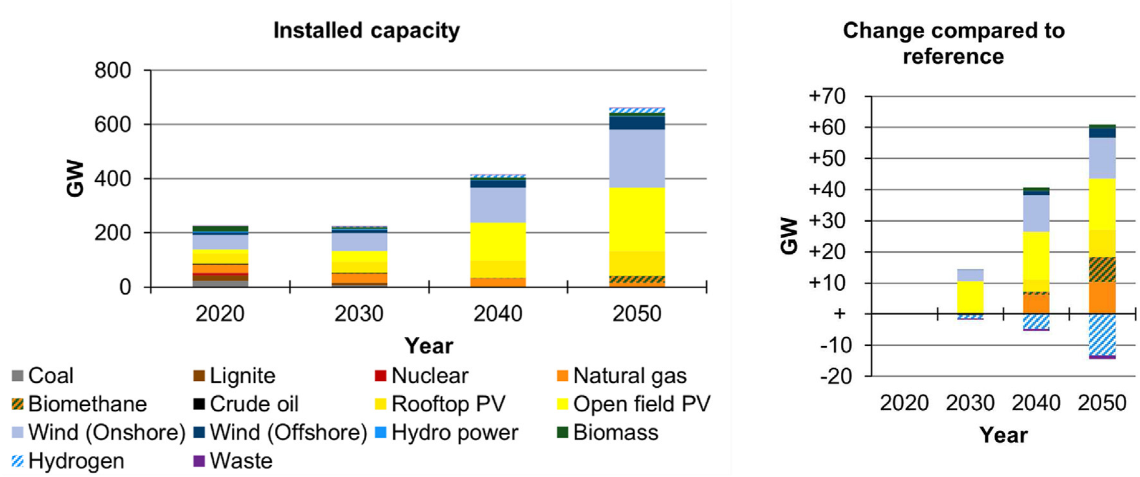

Fig. 9 – Development of the installed capacity of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh.

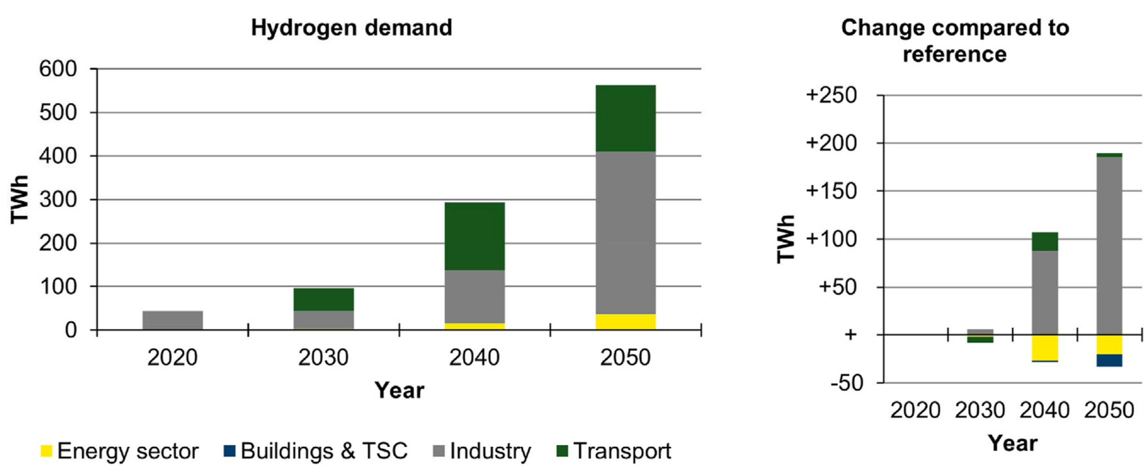

Fig. 10 – Development of the hydrogen demand of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh (TSC: trade, service, commerce).

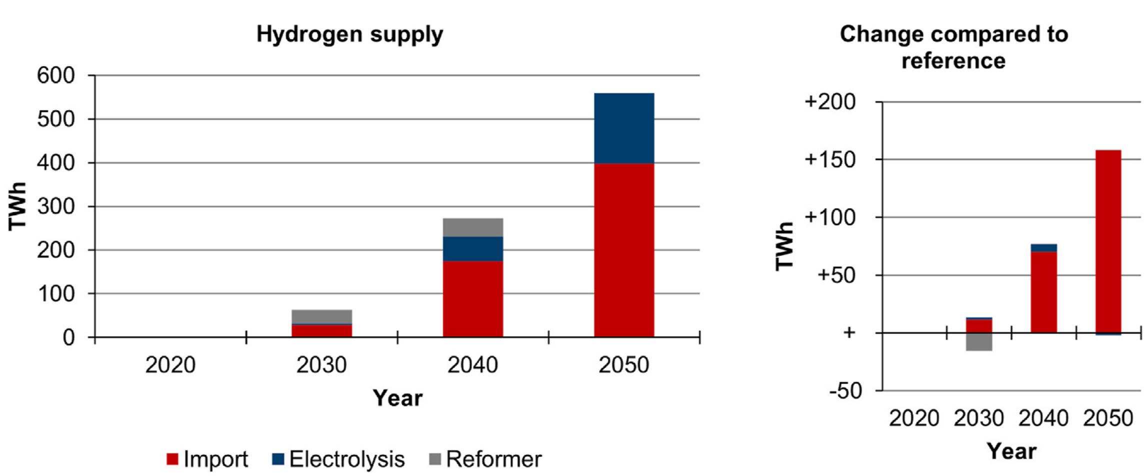

Fig. 11 – Development of the hydrogen supply of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh.

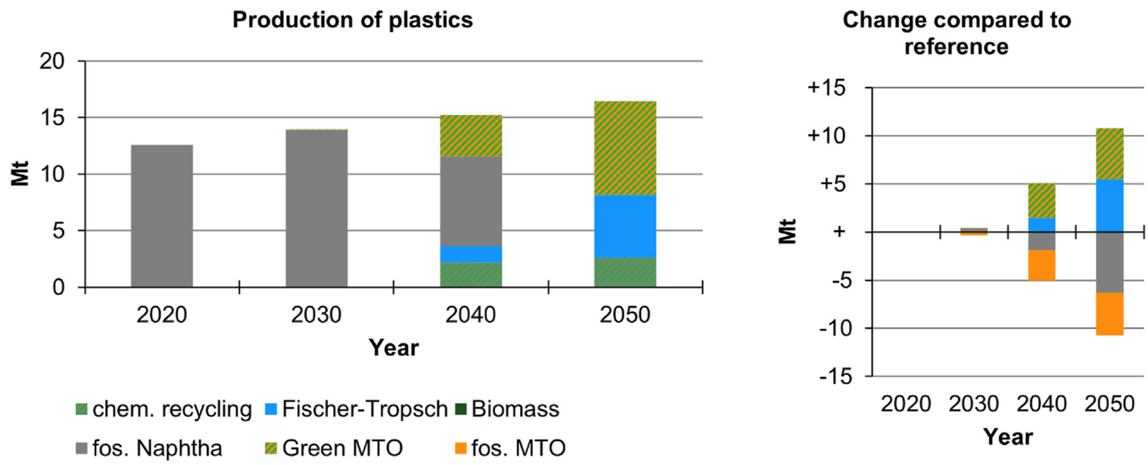

Fig. 12 – Development of the plastics production of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in Mt (MTO: methanol-to-olefins; fos.: fossil-based).

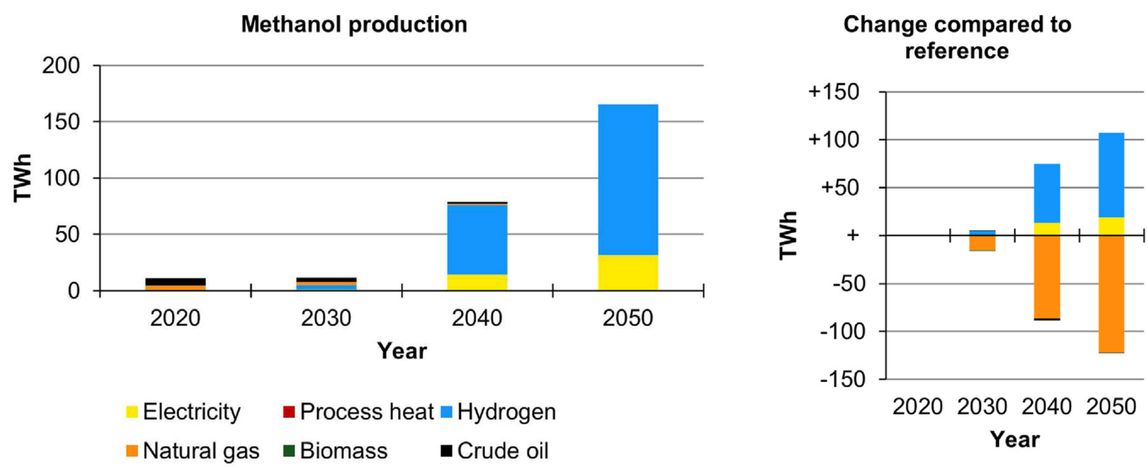

Fig. 13 – Development of the methanol production of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh.

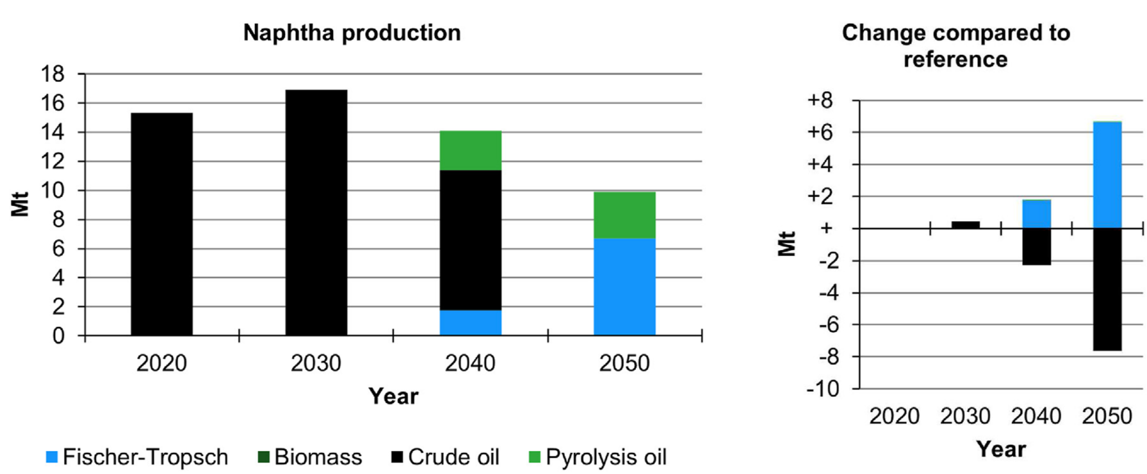

Fig. 14 – Development of the naphtha production of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in Mt.

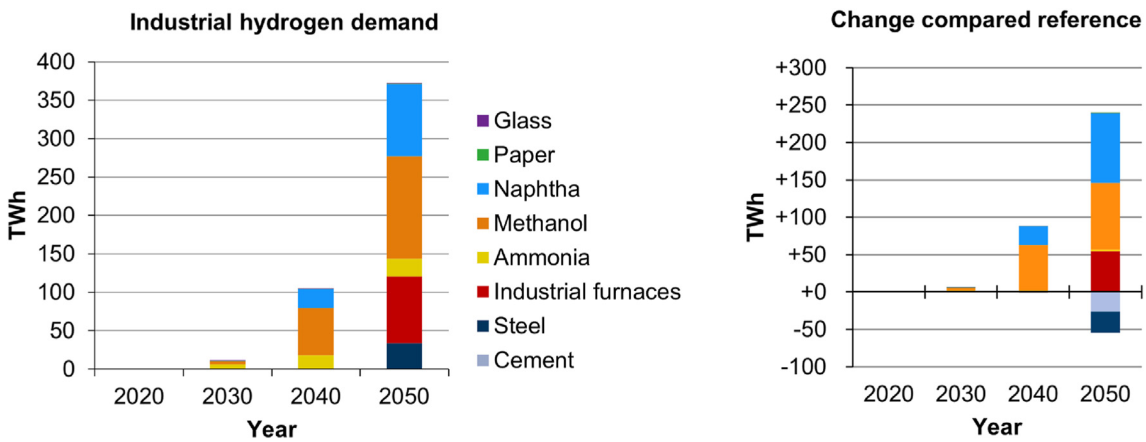

Fig. 15 – Industrial hydrogen demand of the defossilization scenario (left) and the change compared to scenario reference (right) in TWh.

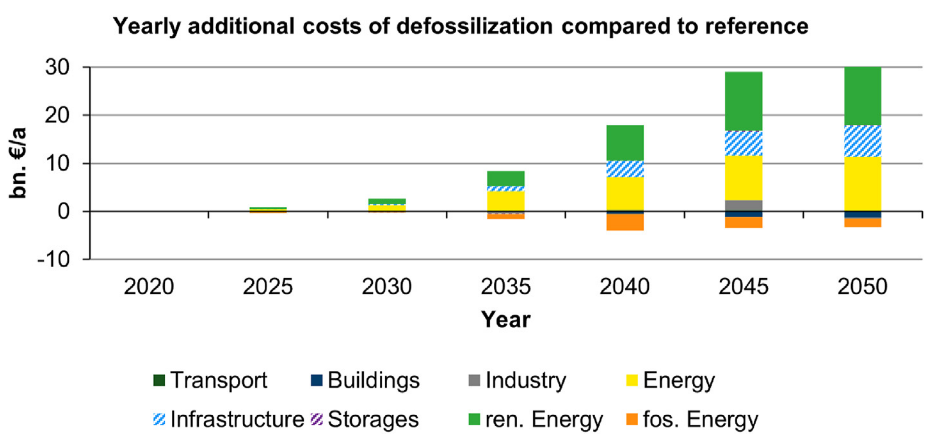

Fig. 16 – Development of yearly additional costs of the defossilization scenario compared to the reference scenario until 2050 in bn. €/a (ren.: renewable; fos.: fossil-based).

hydrogen imports, which are included in the additional costs for renewable energy sources. In 2050, hydrogen imports require more than €15 bn./a additional compared to reference. The substitution of fossil energy sources can only compensate for a small part of the annual additional costs over the entire transformation.

Overall, the additional annual cost compared to the reference case in 2050 is about €30 billion/a. Compared to the costs of the reference scenarios, the share of additional costs for defossilization is about 33%. This corresponds to a share of almost 0.6% of GDP2050. As can be seen in Fig. 17, the majority of the additional financial expenditure will only become due

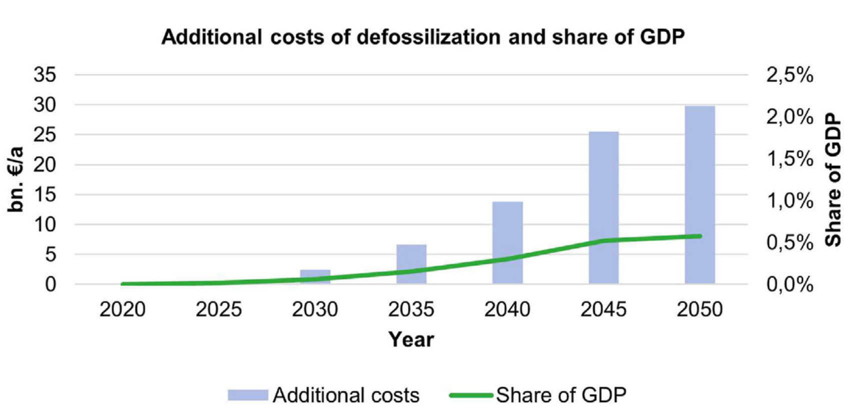

Fig. 17 – Development of yearly additional costs of the defossilization scenario compared to the reference scenario until 2050 in bn. €/a and the corresponding share of GDP (GDP.: gross domestic product).

in the last ten years of the transformation due to the increasingly stringent targets.

Cumulated over the entire transformation, this results in additional costs of €879 billion, which corresponds to additional costs of €212 billion (+32%) compared with the reference case (see Table 4). The average specific CO_2 abatement costs increase by €81/t CO_2 to €333/t CO_2 in the defossilization scenario in 2050.

In addition to an increased demand for hydrogen, process changes can also be observed in other industrial sectors. In steel production in 2050, direct reduction is not operated with hydrogen to the same extent as in reference. Instead of green hydrogen, natural gas and biogas will be used for direct reduction. The share of hydrogen direct reduction thus falls to 18% in 2050.

Around 13% of the steel volume will be produced by natural gas and 21% by biogas in direct reduction (Fig. 18). This also has an impact on the energy demand of steel production (Fig. 19). In 2050, about 29 TWh less hydrogen is used compared to the reference scenario. In return, natural gas demand increases by 17 TWh and biogas demand by 16 TWh.

Since all sectors are integrated in the optimization model, each technology over every sector competes for the cost optimal system design. When one sector uses less hydrogen so another sector can utilize more, this means, by definition of the optimization algorithm, that this state is the more cost-

Table 4 – Selected system costs of the defossilization scenario and change compared to the reference scenario.

	Defossilization	Change compared to reference
Cumulative costs of transformation 2020–2050	879 billion €	+€212 billion
Cumulative CO_2 savings 2020–2050	5699 Mt CO_2	-
Average specific CO_2 abatement costs from 2020–2050	154 €/t CO_2	+37 €/t CO_2
Average specific CO_2 abatement costs in 2050	333 €/t CO_2	+81 €/t CO_2

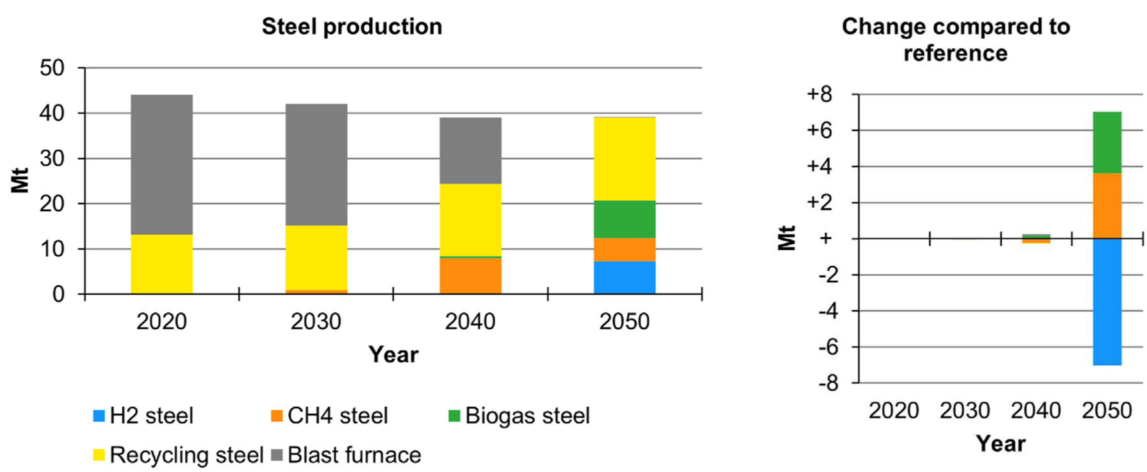

Fig. 18 – Development of the steel production of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in Mt.

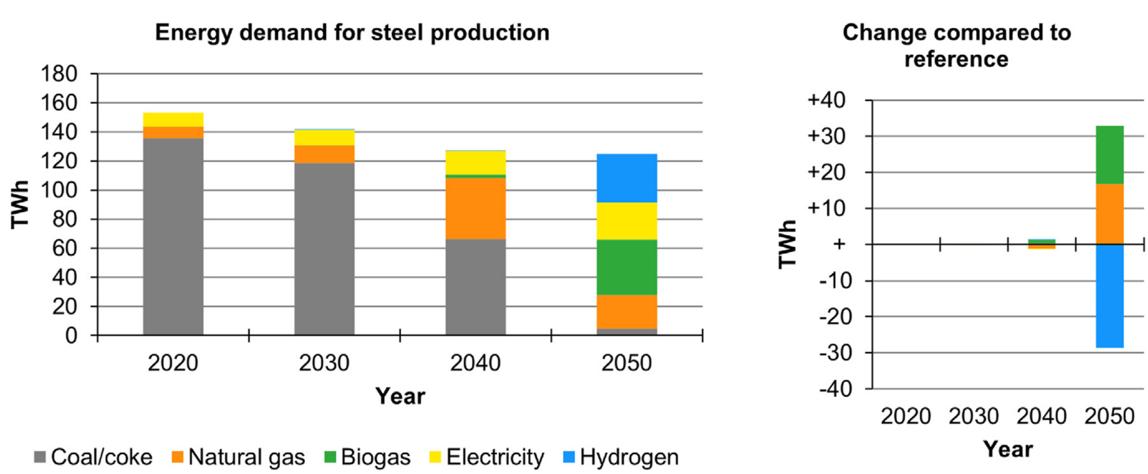

Fig. 19 – Development of the energy demand for steel production of the defossilization scenario up to the year 2050 (left) and the change compared to the reference scenario (right) in TWh.

efficient allocation of hydrogen. Therefore, the results illustrate that it is more cost-effective to use hydrogen for defossilization in the chemical industry and to switch to other energy sources in other industries (e.g., biogas in steel production). These findings suggest that different industry branches will compete for the most cost-efficient hydrogen supply in the future.

Conclusion

Since a significant part of the potential CO_2 emissions in the chemical industry is bound as carbon in the final product, these emissions only occur again during energy recovery (e.g. incineration of plastic waste) or utilization (e.g. ammonia as fertilizer). A new system boundary of national energy system models is therefore necessary to fully account for the emissions contained in products, regardless of where and when they are used in the future. These potential emissions, which are released at some point in the future, are not considered by the typical national accounting methodology. Thus, CO_2 emissions embedded in chemical end products are not affected by national greenhouse gas reduction legislation. Since these emissions will be released at the end-of-life of the products it is crucial to consider strategies to replace fossil CO_2 with renewable CO_2 (defossilization) in national energy system design analyses. Through the implementation of new and innovative industrial processes, it is now possible to evaluate the effects of defossilization on the German energy system design, including the non-energetic demand. This also includes the analysis of suitable defossilization strategies. The following results can be stressed.

- Defossilization is an additional stringent constraint in addition to GHG mitigation.
- There is a significant impact on the overall energy system.
- The majority of non-energetic demand is replaced by hydrogen and its derivatives (green hydrogen is essential).
- Chemical recycling and the methanol-to-olefins route can be identified as critical technologies.
- A defossilized methanol production in 2050 requires 165 TWh hydrogen, which corresponds to an additional 89 TWh hydrogen compared to a reference scenario, in which only GHG emissions are reduced. 19 Mt methanol are used to produce highly refined chemicals.
- The industry sector in a low-carbon German energy system demands 185 TWh hydrogen in 2050. An additional defossilization of the industry doubles the hydrogen demand (370 TWh).

A 95% reduction in CO_2 emissions in 2050 with additional defossilization of the chemical industry leads to increased additional costs. In contrast to the reference case, the cumulative costs of the transformation increase by an additional 32%, or €212 billion. This additional cost is mainly due to the increased hydrogen import.

In the course of a holistic consideration of the transformation of the energy system, the defossilization of the chemical industry should be taken into account by policy makers. In particular, the future supply of hydrogen is decisive for the associated additional costs.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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