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Energy system implications of demand scenarios and supply strategies for renewable transportation fuels

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ABSTRACT

Reducing greenhouse gas emissions in the transport sector is among the hardest challenges in transforming energy systems to zero emissions. Transport energy demands are driven by an interplay of social behavioral, technical factors, political decisions and economic conditions, motivating detailed transport demand modeling.

In Germany, transport energy supply – increasingly from electricity – is expected to challenge the energy supply infrastructure. Recent studies assume large shares of imported clean energy carriers and proclaim global renewable fuel import potentials. Simultaneously, sustainable biofuels' impacts on required electricity supply infrastructure is yet not well understood.

We assess the impact of climate ambition, indirect electrification shares and biofuel availability on energy supply infrastructure in 8 demand scenarios. Coupling the European energy system model REMix with the biofuel allocation model BENOPTex, we calculate cost-minimal energy supply infrastructure for each scenario. This high detail of integrated transport sector and biofuel modeling is novel to energy system analysis.

We find that incorporating user preferences in sales decisions clearly narrows the range of transport energy demand. As the German renewable energy potential is exhausted, higher clean fuel demand is covered by imports. Still, the use of these fuels drives the required power grid expansion, and especially electrolysis and fuel production capacities. Biofuel availability may significantly reduce e-fuel demand reducing cost-optimal hydrogen production capacity in the medium term and necessary grid expansion within Germany beyond 2030.

The model outcome is limited by assumptions on costs and availability of import options. Future work should further address modal shift transport scenarios.

1. Introduction

Cutting Greenhouse Gas (GHG) emissions in the transport sector is among the greatest challenges of clean energy supply [1]. The high energy densities of fossil fuels are a perceived requirement due to range expectancies, limited vehicle space and individual travel patterns. The associated habituation to the technical and economic possibilities of today's mobility leads to a reluctance towards behavioral changes, especially sufficiency. In addition, there is generally no option to carry out carbon dioxide (CO_2) capture, except for large ships, where anthropogenic carbon cycles are being discussed in research. Large parts of transport sector final energy demands are likely to be transformed to electricity based on RES. However, some modes of transport require the chemical-physical properties of hydrocarbons, such as aviation and shipping [2].

Final energy demand shares between electricity, H_2 and hydrocarbons are shaped by political choices. Vehicle stock mainly depends on fleet emission limits and support schemes. Infrastructure expansion is often managed by natural monopolies largely affected by policy-making and international trade relationships are limited or enabled by trade regulations on national or regional level. For hydrocarbons, sustainably produced biofuels may be important alternatives to electricity-based liquid or gaseous fuels referred to as e-fuels. Especially in industrialized

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Nomenclature

AC	Alternating Current
AEL	Alkaline ELectrolysis
BAU	Business-as-usual
BBS	Berlin, Brandenburg Saxony-Anhalt
BEV	Battery Electric Vehicle
BESS	Battery Energy Storage Systems
BECCS	Bioenergy with CCS
BLS	Bremen, Lower-Saxony
CCGT	Combined-cycle gas turbine power plant
CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilization
CH_4	Methane
CHP	Combined Heat and Power
CO_2	Carbon dioxide
CSP	Concentrating Solar Power
DAC	Direct Air Capture
DC	Direct Current
DEL	Direct electrification scenario
DEL_bio	DEL with biofuel availability
DH	District heating grid
EU	European Union
ExCCGT	Backpressure combined cycle gas turbine with heat extraction
FCEV	Fuel Cell Electric Vehicle
FT	Fischer Tropsch fuel production facility
GHG	Greenhouse Gas
GT	Gas turbine power plant fired by various fuels
H_2	Hydrogen
HSH	Hamburg, Schleswig-Holstein
HVAC	High-voltage alternating current transmission line
HVDC	High-voltage direct current transmission line
HYD	Hydrogen scenario
HYD_bio	HYD with biofuel availability
ICE	Internal Combustion Engine
Ind	Industrial
LIB	Lithium-Ion Battery
LP	Linear Programming
MENA	Middle East and North Africa
MVP	Mecklenburg-Vorpommern
NRW	North Rhine-Westfalia
OM	Operation and maintenance
PEMEL	Proton Exchange Membrane
PHEV	Plugin Hybrid Electric Vehicle
PtX	Power-to-X
PV	Photovoltaics
RED	Renewable Energy Directive
REF	Reference scenario
RES	Renewable Energy Sources
RFNBO	Renewable Fuels of Non-Biological Origin
SAF	Sustainable Aviation Fuel
ST	Steam turbine power plant fired by different primary energy carriers
SYN	Synthetic fuel scenario
SYN_bio	SYN with biofuel availability
TFC	Total Final Consumption
TH	Town heating grid
WACC	Weighted Average Capital Costs

countries with high population densities and limited solar and wind power potential, biomass may provide an additional source of primary energy.

The supply of electricity, hydrogen and other energy carriers requires different conversion stages from primary energy sources such as wind and solar energy. Increasing use of synthetic fuels, first hydrogen and then downstream synthetic products, which we refer to as increasing conversion depth, implies efficiency losses due to the second law of thermodynamics [3]. These energy losses are highly relevant in the assessment of different options, as the integration of the conversion steps into the energy system requires different infrastructure development. However, the techno-economic challenges and required fuel properties might demand pursuing deeper pathways.

Additionally, technical, political and user-specific factors interact and can result in varying fuel demand developments. As this also places various demands on the supply structure, integrated modeling must provide important insights into cost-relevant effects and the possible solutions at system level. To investigate the systemic impacts, the modeling for this paper focuses on the replacement of fossil fuels with the low-emission alternatives hydrogen, biogenic or electricity-based hydrocarbons based on RES complementary to direct electrification.

1.1. Motivation

Three transport sub-sectors have particular challenges in the transformation to carbon-neutrality: Road, aviation and navigation. The road sector, and specifically passenger cars, have the greatest share in transportation energy demand and emissions [4,5]. Aviation contributes less to final energy demands but is among the hardest to abate because direct electrification and hydrogen use can only substitute limited shares of persons and goods transported and respective technological concepts have not yet been introduced on a commercial scale [2]. Navigation also faces major challenges when switching to green fuels due to the high energy density required for heavy-duty and long-distance transport and high investments in propulsion systems with a long service life. Thus, shipping is also a candidate for the utilization of considerable quantities of clean synthetic fuels.

Different strategies for GHG reduction in transport are discussed. Decarbonization through direct electrification describes a replacement of internal combustion engines by Battery Electric Vehicle (BEV). Defossilization on the other hand means a change of primary energy source from fossil crude oil to RES based H_2. Also referred to as indirect electrification [6], this strategy requires electricity based on RES for supplying gaseous or liquid clean fuels, unless biomass is used as a primary energy carrier. Wind and solar power have to provide the major share of this, especially in countries such as Germany that have limited hydropower potential combined with high energy demands [7,8]. Irrespective of the strategy, the role of renewable energy as a primary energy carrier in transportation is expected to drastically increase, with well-known challenges.

The intermittent nature of wind and solar energy requires flexibility options to balance load and intermittent generation, and to ensure security of supply and system adequacy [9]. To assess intermittent RES integration into energy systems, both a high temporal resolution for short-term fluctuations and long horizons for seasonal effects must be considered [10]. Advanced energy system models need to be applied in order to analyze resulting systemic needs and implications along the chain of electricity supply, transmission, distribution, storage and consumption. It must be taken into account that the national electricity grids in Europe are intertwined which leads to spatial flexibility. Moreover there is both, scientific evidence [11] and political targets [12] that European electricity markets and infrastructure are becoming increasingly integrated.

The role of biogenic energy carriers in substituting fossil fuels and thus limiting electricity demand increase for electric fuels is still not well understood. This gains importance because increasing sector-coupling [13] of transport, heat and industry is expected to require fast expansions of intermittent RES capacities. However, sustainable biomass potentials for the energy sector are also limited [14] due to competing demands from food production [15], for basic chemical productions [16] and for heating purposes [17].

Nowadays, all European countries except Norway are net energy importers [18], especially of crude-oil for transport fuel demands and fossil gas. Because of the limited resource potential for intermittent RES, especially in densely populated countries such as Germany, imports of clean fuels from world regions with higher resources such as Australia, South America or North Africa are discussed [19]. As with biofuels, imported Renewable Fuels of Non-Biological Origin (RFNBO) can relieve countries of the challenge of rapidly expanding intermittent RES capacities in order to produce RFNBO themselves at higher cost. However, import dependence also has major challenges. First, the consequences of the Ukraine war has shown the disadvantages of European countries' energy import dependence, which pushed the European Union (EU) to introduce the REPowerEU plan [20], aiming at increasing Europe's energy sovereignty [21]. Secondly, importing from countries in the global south to the EU bears the risk of reproducing and strengthening postcolonial trade relations as described as barrier for renewable electricity trade between Europe and its southern neighbors [22]. It is therefore necessary to scrutinize the evidence base of trade-offs between domestic RFNBO, imported RFNBO and biofuels.

1.2. Literature review

From the vast body of literature on reaching energy system climate neutrality, we focus on studies that describe fully sector-coupled clean energy supply systems. From those, studies were selected that explicitly describe German transport sector fuel demands and their implications on energy supply infrastructure. Both, target year and transformation pathway studies are considered. To enrich the discussion by a broader perspective, we cite individual sources with a global scope.

Bu et al. propose two demand scenarios with one achieving net zero passenger transport for China in 2050 [23]. However, the supply of energy forms is not assessed. Combining top-down and bottom-up modeling, this shortcoming is addressed by [24] analyzing environmental and economic benefits. The authors' analysis focus on medium-term transformations with an energy system model setup that does not have sufficient temporal resolution for modeling fully sector-coupled energy systems beyond 80% intermittent RES.

Transport sector CO_2 emission reduction strategies are highly intertwined with socio-economic factors. Emodi et al. mention population growth, fewer government regulations, weak traffic demand management and low investment in public transport infrastructure among others as drivers of transport emissions [25] in countries of the global south. Although other mentioned factors, e.g. freight activities of fossil fuel vehicles and low penetration of zero-energy vehicles are shared globally, the before mentioned factors are not as relevant to most European countries.

1.2.1. Demands of clean transport scenarios

Fuel and electricity demands of a GHG neutral German transport sector have been reviewed by Wiese et al. [26] and Ruhnau et al. [6] and further detailed by Gnann et al. [27] and Sensfußet al. [28]. Fuel demands could imply electricity equivalents of 700–1000 TWh/a with liquid fuels for aviation and navigation contributing more than half of that primary energy demand across all scenarios [27]. In a global defossilization study, Teske et al. [29] show that following at least a 2 °C pathway requires an average share of 50% direct electrification of global transport demand.

1.2.2. The role of biomass for energy system GHG neutrality

Wiese et al. show that the use of biomass for energy supply – around 300 TWh in 2018 – is reduced only in 5 of 20 reviewed scenarios. In 8 scenarios, the consumption is comparable to today's consumption, while 7 scenarios require a biomass increase by 100–400 TWh/a for a climate neutral energy supply. The reciprocity of biomass supply and RFNBO imports is exemplified in a scenario without RFNBO that requires a doubling of biomass supply (650 TWh) [26]. Please see Appendix A for a critical reflection of clean fuel import potential quantification studies.

Incorporating feedbacks between biomass and electricity supply is demonstrated by Aliabadi et al. in a proof-of-concept [30]. The soft-coupling of the bioenergy model BENOPTex and energy system model REMix focuses on biofuels and alternative fuels. It is shown that the German transport sector requires imports for comprehensive defossilization under the EU Renewable Energy Directive (RED) policy framework. Two projects in Germany examined the relationship between biofuels and synthetic fuels, highlighting the significance of timing for biofuels as bridging technologies [31]. As the demand for biomass is anticipated to rise its availability [32] and the support for energetic use [33,34] remains uncertain.

1.2.3. The role of imports for energy system GHG neutrality

Wiese et al. show that imports of both RFNBO and electricity are among the largest uncertainties across the 20 reviewed scenarios with 0–140 TWh for electricity and 0–820 TWh for RFNBO [26]. Net electricity imports and exports are found from −9% (export of 102 TWh/a) to 13% (imports of 176 TWh) by Sensfußet al. [35]. Exports occur in the T45-PtG scenario that assume large amounts of imported RFNBO.

They show volumes of 800–1600 TWh/a of electricity equivalents, imported in the form of fuels across the scenarios with the electricity oriented scenario at the lower and the hydro-carbon oriented scenario at the upper bound. In total, import dependence is found to be reduced to 30%–40%. Of the 360–690 TWh/a of German H_2 demand, 190–270 TWh/a are domestically produced leading to an H_2 import share between 49 and 61% [28].

1.2.4. Infrastructure for GHG neutral energy supply

Focussing on energy supply infrastructure capacities in literature, Gong et al. find around 1000 GW of cumulative solar and wind power under "economic-wide carbon neutrality in 2045" (approximately 300 GW wind and 700 GW solar power) [36] compared to 290–770 GW under GHG neutrality found in a comprehensive review [26]. Sensfußet al. show fairly similar transformation pathways cumulating to 630–672 GW of solar and wind power capacity in 2045.

Gong et al. find 37–45 GW of electrolysis and around 40 TWh of H_2 storage capacity under GHG neutrality [36]. Sensfußet al. on the other side show 58–77 GW of electrolysis and 244–413 TWh of H_2 storage capacity [35]. The authors call for electricity transmission grid expansion surpassing current planned capacities as per the German grid extension plan by 60%–100% with major shares before 2035.

Major uncertainties persist in the current body of literature on German transport emission reduction and respective energy system infrastructure transformation. Since subsector demand specifics are often neglected, the range of uncertainty of fuel demand is still found to be large and driven by authors' exogenous assumptions. The same holds true for the case of the role of biomass in transport emission reduction. Clean fuel imports are also mostly assumed as fix values before modeling, neglecting trade-offs between biofuel use, domestic production and imported hydro-carbons.

1.3. Research question and structure

On the background of the latest scientific literature reviewed, we arrive at the overarching research question: What are energy-system trade-offs between domestically produced RFNBO, imported RFNBO and biogenic fuels for transport sector defossilization in Germany? We will answer it, divided in three sub-questions:

- How large is the primary clean energy demand of a GHG neutral transport sector?
- How do the differences in conversion depth affect cost-optimal energy system compositions and build-up dynamics?
- To what degree alleviates biofuel availability sharp gradients in electricity and hydrogen supply infrastructure build-up?

The objective of the study is to show the impacts of policy driven fuel demand scenarios and biofuel availability on energy system transformation pathways up to greenhouse gas neutrality. In the following Section 2, we describe the research design, and data, while Section 3 describes, analyzes and discusses the results of eight scenarios. We conclude in Section 4 and identify the most relevant open questions.

2. Research design and data

One of the main uncertainties of future GHG neutral energy supply is the degree of direct and indirect electrification [6]. Mainly political decisions on infrastructure, climate ambition and energy independence will shape these futures which we consider via four scenarios in scope 1: A Reference scenario (REF) failing political targets on GHG reduction ambitions and three target scenarios focusing on direct electrification (Direct electrification scenario (DEL)), the use of H_2 as a final energy carrier (Hydrogen scenario (HYD)) and increased synthetic fuel demands (SYN). In scope 2, each of these four scenarios is complemented by a scenario allowing for biofuel supply of energy carriers, e.g. SYN_bio for SYN, resulting in a total of eight scenarios.

A scenario is a relevant possibility [37]. It constructs a set of coherent descriptions and parameters with the aim to operationalize an uncertain future that can never be known. For quantifying the above mentioned storylines, we leaned as much as possible on values from Senssfußet al. [35] The scenarios differ in political decisions taken (e.g. eligibility of drop-in fuels in fleet emission regimes), in techno-economic developments (costs of batteries, vehicles, fuel cells) and in infrastructure availability. For REMix specifically, the main differences between the scenarios are the shares of final energy forms of electricity, hydrogen and clean fuels as described in Appendix C.1.

We describe the results of transport sector demand modeling for road and aviation in Section 2.1 and for all other sectors in Section 2.2 for answering research question 1. Our assumptions on cost-potential of electricity-based fuel imports are described in Section 2.4. With the 3 demand models and REMix we answer research question 2 in scope 1. Assumptions on biofuel availability are described in Section 2.3. A bilateral model coupling between REMix and BENOPTex is then used in scope 2 to answer research question 3. A brief overview over the models REMix and BENOPTex, the data flow and the interfaces between the models are summarized in Section 2.5. Fig. 1 shows the data flow between the demand models and the bilateral model coupling of REMix and BENOPT. The model coupling was first introduced in [38].

We contribute to the body of scientific literature in three ways: We provide a set of four technology-driven scenarios of GHG-neutral transport in Germany with varying conversion depth. Secondly, we combine transport demand models with sector-coupled energy system models. Thirdly, we apply an iterative model coupling of two system models with two perspectives and analysis focus: The electricity system model REMix and the resource allocation model BENOPTex. This allows us to investigate feedback effects between optimal biofuel allocation and optimal energy supply infrastructure expansion and dispatch. All data described below except for the 33 national energy balances are published in a data appendix including all interface and plotting data routines.

2.1. Detailed sub-sector demand scenarios

From road, aviation and navigation sectors, the authors' demand models were used to create target-compliant energy demand paths for road and aviation modes as part of this analysis. Navigation was considered in the following via demand developments derived from other studies but is an interesting pursue for demand modeling in future research.

2.1.1. Road

Road passenger and freight vehicle energy demand is based on the scenario and market analysis software VECTOR21 [39]. The tool simulates the market development of vehicle technologies of newly registered cars and trucks until 2050, the stock development and the resulting energy demand.

The scenarios incorporate not only policy instruments such as passenger vehicle fleet quota or blends but also user-preferences in purchasing vehicles depending on price, infrastructure availability, acceleration, range and other factors. More details on the modeling logic, input assumptions and resulting final energy demands are given in Appendix B.4.

2.1.2. Aviation

The aviation energy demand estimation is based on DLR's traffic forecast, which includes passenger demand and aircraft movements up to 2050. The scenario is characterized by an increasing energy demand, as it assumes that traffic demand growth will outpace efficiency improvements in aircraft technology. In the scenarios REF and SYN, for geographical Europe, jet fuel demand is expected to grow from 66 Mt to 113 Mt between 2019 and 2050.

The actual demand for RFNBO will be determined by the blending quota from the RefuelEU Aviation initiative. According to the latest regulation of the European Commission, the blending quota will increase from 0.7% in 2030 to 35 % in 2050 [40]. In the scenarios DEL and HYD, a European-wide jet fuel demand of 65 Mt is expected in 2040, and 61 Mt in 2045, respectively. Jet fuel demand declines over time as the phase-in of hydrogen aircraft progresses.

Hydrogen accounts for 12.3% of energy consumption in aviation, as flights beyond 2780 km will still be operated with conventional aircraft. As electric flight will be limited to the segment of aircraft with a maximum of 19 seats, demand for electricity for direct use in aviation will be limited to about 600 MWh in Europe in 2050. Further details can be found in Appendix B.5.

2.2. National energy balances

The energy demand for other sectors has to be taken into account in order to capture systemic interactions and implications on energy supply and grid infrastructure in future system developments. For the transport sector, this includes shipping and rail energy demand. Furthermore, electricity and heat demands for industry and buildings (households and services/commercial sectors) are estimated in the holistic accounting framework LENS, complemented by the transport demand data described above in Section 2.1. As a result, we generate national energy balances for 33 countries for each scenario that are aggregated into annual final energy demand inputs to REMix model nodes as specified in Figure B.7. Integrating European energy demands, imports to Germany and exports from Germany is highly relevant as transmission expansion is among the cheapest flexibility options in electricity systems with high shares of intermittent RES [11].

The REF scenario does not achieve GHG neutrality in 2050, but follows an 80% reduction of energy-related emissions in relation to 1990 emission levels. For EU-countries aside Germany, the national pathways for the REF scenario are based on the EU Reference Scenario 2018, which was adjusted in terms of target achievement, i.e. made more ambitious. The scenarios DEL, HYD and SYN achieve GHG neutrality

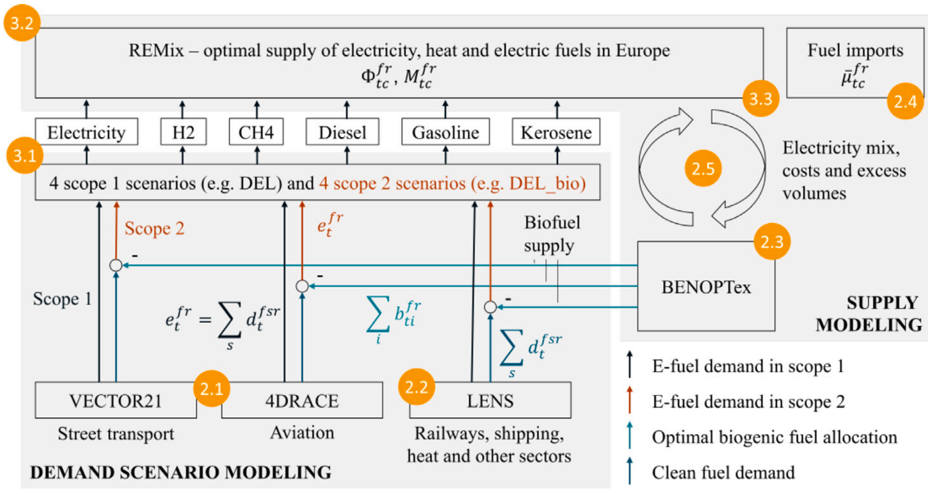

Fig. 1. Overview of the models used, the two modeling scopes and the model coupling logic. The other models shown contribute to the provision of solid scenario data for future transport sector demand (Section 2).

Table 1
Transport sector final energy demands in the four scenarios split into electricity, renewable gases and liquid renewable fuels. Liquid fuels contain jet fuel (e-kerosene), e-gasoline fuel and e-diesel fuel. All values given in TWh/a and rounded to 1 TWh/a.

			Target scenarios		
	2020	REF 2045	DEL 2045	HYD 2045	SYN 2045
Electricity	12	101	181	146	161
H_2 and methane (CH_4)	0	34	35	103	21
Liquid fuels	0	186	184	174	254

in 2045 by excessive expansion of renewable energy, electrification of end-use applications and through the complementary use of hydrogen and synthetic fuels. They are based on the EU long-term vision “A Clean Planet for All” [41] and the scenarios Electrification, Hydrogen (H_2) and Power-to-X (Power-to-X (PtX)) complemented by the 1.5TECH scenario for EU28.

In contrast to the European approach, the demand scenarios for Germany are based on the most recent German long-term scenarios developed for the German Federal Ministry for Economic Affairs and Climate Action [28], in order to better connect our work to the current discussions on the national energy transition. For both studies, we harmonized the scenario storylines on the demand side as far as possible and used system modeling to create new energy balances that are largely consistent between Germany and non-German countries. The resulting overarching demands for Germany are summarized in Table 1.

2.3. Biogenic resource potential and cost assumptions

In BENOPTex [42], ten energy crops and 13 groups of residues are modeled based on data provided in the “DE biomass monitor” [43]. The choice to cultivate various energy crops is an endogenous decision in the model based on the demand for fuel, heat, or electricity and respective costs. In Germany, wheat is considered the most common crop; hence, the final price of other energy crops is calculated such that their profit margins become on par with the wheat profit margin as the benchmark [44]. The production cost of energy crops consists of direct, labor, fuel, machine (fixed and variable), and service costs, which increase at a 4% rate until 2050. We incorporate energy consumption by agricultural and land machinery associated with biomass production for bioenergy, which includes consumed diesel (measured in liters per hectare) for various energy crop types [44,45]. The available land for planting energy crops is assumed to be 2.4 Mha in 2020, which will be reduced slightly in 2050 to 2.2 Mha in 2050 due to land competition among different sectors. Further information on biogenic feedstocks is given in Appendix B.3.

2.4. Fuel import cost-potential assumptions

Costs and maximum volumes of imports of renewable hydrogen and RFNBO are based on a global fuel market scenario analysis carried out in the MENA-Fuels project [46]. Global technical potentials for solar thermal, photovoltaic and wind power plants, taking into account exclusion areas, technical and economic assumptions for the production of hydrogen and synthetic crude oil, as well as assumptions on CO_2 supply costs from industry and Direct Air Capture (DAC), transport costs and import duties, represent the basis for bids on the global market [47].

These bids are combined into dynamic energy carrier-specific cost potential curves in 50 EUR/MWh-increments. In addition, further processing steps in the exporting countries are assumed, in order to estimate potentials for hydrogen, methane, synthetic gasoline, diesel and kerosene. In REMix, fossil fuel imports are only possible for gaseous CH_4. The transport sector is modeled as an increasing demand sector for electricity, clean gaseous and liquid fuels. More information is given in Appendix B.2.4.

2.5. Model coupling

The REMix-framework minimizes the costs of energy supply by varying the energy infrastructure capacities and their dispatch in high spatial and temporal detail. In this study, we employ a model with a 4h-resolution, 9 nodes in Germany and 13 European nodes outside of Germany (see Figure B.7). Each scenario is comprised of 4 base years — 2020, 2030, 2040 and 2045 that are myopically optimized. More technical details and assumptions can be found in Appendix B.2. The model was first introduced for the European electricity system modeling [48] and expanded to the heat sector [49], electric vehicles [50] and gas infrastructure [51].

The demand models VECTOR21, 4DRACE and LENS provide fuel demands d_t^{fsr} for fuel f in sector s and year t in region r. These demands are then added over all sectors per fuel to arrive at the fuel demand across sectors d_t^{fr}. In scope 1, these demands for renewable fuel are directly implemented as binding constraints in REMix' Linear Programming (LP) formulation as shown in Eq. (1). Here, biofuels are not assumed to supply the transportation sector, implying competition between domestic electricity-based fuel production and respective imports. In scope 2, the demands are reduced by the supply of biogenic

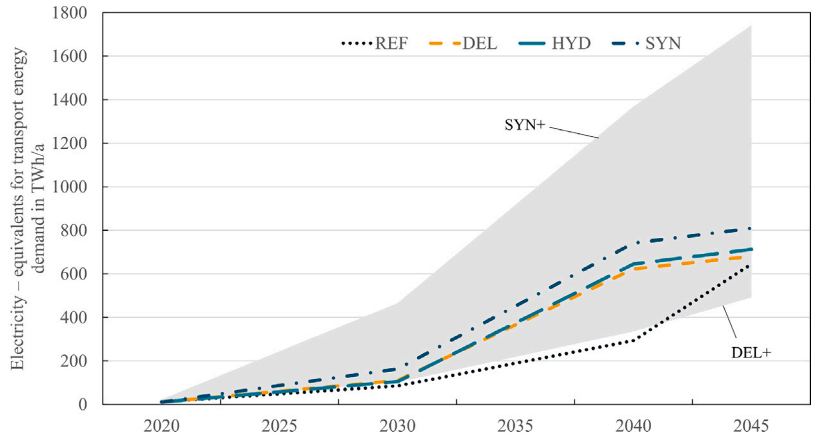

Fig. 2. Electricity equivalents of final energy demand in the transport sector in the four scenarios and two extremes of final energy use. All renewable energy demands are calculated to electricity equivalents to make them comparable. The REF scenario's GHG reduction ambition is lower especially in the years 2030 and 2040. Own depiction.

fuels b_{ti}^{fr} according to Eq. (2). for all mapped fuel supply technologies i.

$$\text{Scope 1: } e_t^{fr} = \sum_s d_t^{fsr} \tag{1}$$

$$\text{Scope 2: } e_t^{fr} = \sum_s d_t^{fsr} - \sum_i b_{ti}^{fr} \qquad ,\forall t \tag{2}$$

BENOPTex allocates the cheapest primary energy source – biofuel, synthetic fuel or fossil fuel – to the respective final energy demand harmonized with scope 1. The allocation builds on a broad set of 77 biomass residue streams, assumptions on agricultural land as well as efficiencies of conversion processes. For one transformation pathway, BENOPTex runs once relating to four REMix runs as BENOPTex includes interannual optimization along a pathway. The RFNBO demand (e_t^{fr}) comprises only electricity-based fuels and can be supplied by production facilities in Germany (Φ_{ti}^{fr}) or imported (M_{tc}^{fr}) drawing from discretized cost categories c (cf. Section 2.4) as described in Eq. (3).

$$\sum_i \Phi_{ti}^{fr} + \sum_c M_{tc}^{fr} = e_t^{fr} \qquad ,\forall t, f, r \tag{3}$$

Further formal description of REMix is given in Appendix B.7.

3. Results and discussion

We start by describing the differences of the transport sector's energy demands in different scenarios in Section 3.1. Then, we analyze the necessary energy system infrastructure build-up in Section 3.2. In Section 3.3, we show the effect of biofuel availability on energy supply infrastructure before we relate our results to earlier studies in Section 3.4.

3.1. The influence of conversion depth on transport sector energy demand

Fig. 2 shows transport sector final energy demand across the four scenarios . Results are shown against the background of two theoretical extreme cases: An almost complete switch to electricity as final energy (DEL+) and an almost complete switch to hydrocarbons (SYN+). While the impact of direct vs. indirect electrification is large in the thought experiment of lowest (DEL+) vs. highest (SYN+) conversion depth, scenarios incorporating sales preferences in road transport and technology shift details in aviation sectors show less divergence.

In 2045, transport sector final energy demands range from 680–810 TWh/a of electricity equivalents in the target scenarios (DEL, HYD and SYN) translating to an increase between 5%–25% compared to the reference case. All target scenarios exhibit stark gradients in the decade 2030–2040, mainly driven by a lack of drive-train shift in road transport, followed by a slower growth between 2040 and 2045, resulting in a S-shaped electricity demand.

The difference between DEL and HYD is small with 30 TWh/a difference in 2045, which can be explained by the fuel contributions shown in Figure C.16. In the HYD scenario, the road transport demand for both hydrocarbons and electricity is mainly replaced by hydrogen (see Figure C.16). While this implies less losses for the conversion step from H_2 to hydrocarbons, it implies more losses for the conversion from electricity to H_2. The aviation sector with its respective e-kerosene demand is the strongest driver of transport sector primary energy demand in 2045 across all three scenarios (between 39%–47% of electricity equivalents). All scenarios imply drastic changes in vehicle fleets, which are described and discussed in Appendix B.4.1. Transport sector contributions to overall transport energy demand for 2045 are depicted across the four scenarios in Figure C.14. Dynamic developments are shown in Figures C.13 and C.15.

The comparison of the two extreme cases with detailed subsector models for road and aviation demands show that incorporating technical detail and user preferences for vehicle purchases strongly reduces the uncertainty of future transport sector energy demand. This holds true when transport demand itself and modal choices remain similar to today's levels. The final energy demands we find are similar to the ones reported in Gnann et al. [27] with slightly higher electricity demands, slightly lower kerosene, more specific (i.e. narrower range) road sector demands and no CH_4 demands in transportation (see Appendix D.2 for a detailed comparison).

The most important limitation of our approach is that we did not explicitly model scenarios incorporating strong modal shifts and transport reduction policies as in Arnz et al. [52]. A combined approach of our detailed fleet modeling with their avoid and shift scenarios would provide an unprecedented transport sector modeling detail. Another limitation of our approach is that we do not consider spatially explicit fleet scenarios e.g. higher BEV developments in southern Germany from northern Germany. Incorporating navigation fuel demand scenarios similar to the ones for aviation is as well an interesting pursue for future research as demands for synthetic diesel and kerosene both imply demand for clean hydrogen.

3.2. The influence of conversion depth on energy supply infrastructure extension and usage

As shown in the previous paragraph, conversion depth influences the demand for renewable fuels and, consequently, implicit electricity demand. We now turn to the second-order implications of these variations on energy supply infrastructure. Our primary interest lies in the differences across the three target scenarios: DEL, HYD, and SYN, with the lower-ambition REF scenario serving as a reference. The analysis in

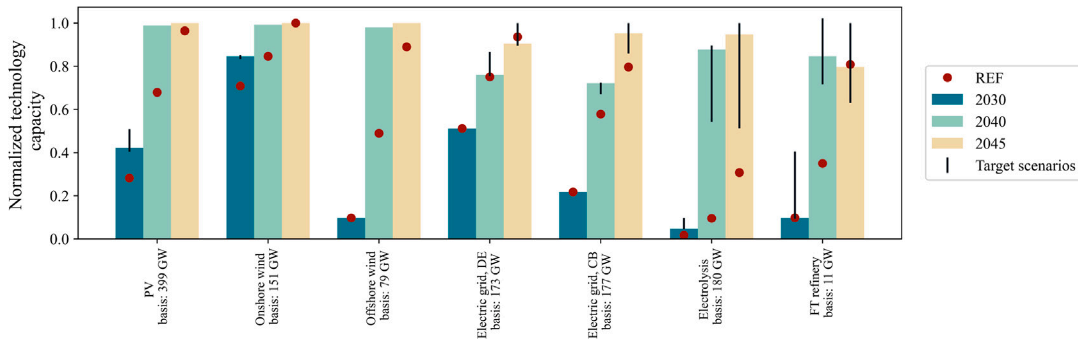

Fig. 3. Influence of conversion depth on cost-optimal technology capacity in Germany in 2030, 2040 and 2045. The red dots show the respective values from the reference scenario while the black lines show the variability of the respective technology capacity in the respective year for the three target scenarios. The bars show the middle value of the target scenarios. The normalization basis for all values in a group is the maximum value in 2045 across the scenarios. For intermittent RES – PV and wind power – the variability in the years 2040 and 2045 is negligible, thus no vertical lines exist.

this section is conducted within the scope of scope 1, meaning that no biofuel supply is available.

Fig. 3 illustrates the variability of cost-optimal technology expansion across the modeled scenarios and years. The power plant expansion depicted in the first three groups differs between the REF and target scenarios; however, it shows significant variability only for PV and onshore wind extensions in 2030. From 2040 onward, the variability between the target scenarios remains below 1% of the normalization basis. This supports previous findings that the expansion of intermittent RES is a no-regret option for GHG neutral energy supply systems. Under cost-optimal conditions, onshore wind capacity expands the earliest, continuing until 2030, accompanied by significant expansions of PV. In the decade from 2030 to 2040, all intermittent RES options are rapidly expanded, reaching their exogenously defined maximum potential.

Wind and solar power curtailment occurs only in 2030, ranging between 15–20 TWh/a, with the lowest value found in the SYN scenario. Due to early diesel and gasoline demands in 2030, demand-driven electrolysis capacities are expanded, which can help balance intermittent RES feed-in to some extent, thereby reducing curtailment compared to the DEL and HYD scenarios.

The following groups illustrate the expansion of inner-German power lines and cross-border interconnectors within the electricity grid. The inner-German electric grid expansion shows some variability beyond 2030 across all scenarios, including REF. The variabilities in 2040 and 2045 are attributed to increased inner-German Direct Current (DC) grid expansions (approximately 10 GW more in 2040) in the DEL scenario compared to HYD and SYN. The inner-German Alternating Current (AC) grid is expanded in all scenarios by 43–60 GW by 2040, with further expansions of 23–32 GW in the years leading up to 2045. The results indicate that inner-German grid expansion is cost-optimal, regardless of the degree of GHG reduction ambition. Achieving primarily direct electrification necessitates increased inner-German grid expansion.

Increased CO_2 reduction ambition requires higher cross-border grid capacities between Germany and its neighbors. Increasing conversion depth affects DC grid expansion in 2040 (15, 25 and 26 GW) and AC grid expansion in 2045 (35, 40 and 50 GW). In total capacities, around 100 GW is the minimal cross-border capacity in REF with 120–130 GW in the target scenarios in 2040. In 2045, capacities are expanded to 150–180 GW for the target scenarios. For comparison, the German grid development plan foresees aggregated interconnector capacities of around 40 GW with Germany's electrical neighbors. This fourfold increase transfers findings by Sensfußet al. calling for increased inner-German transmission grid expansion compared to the grid development plan to crossborder interconnectors [35].

H_2 production capacity is affected the strongest by conversion depth. It strongly varies across DEL, HYD and SYN. Conversion depth influences both, electrolysis capacity and H_2 production very similarly. In 2030, DEL and HYD require 7–8 GW while SYN requires more than twice the capacity mainly driven by increased e-diesel and e-gasoline demands from private vehicles. While the 20 TWh/a of H_2 produced in DEL and HYD mainly supply industry and early stage kerosene and diesel demands, the H_2 production of 50 TWh/a in SYN supplies significant domestic synfuel production of over 40 TWh/a of synthetic fuels.

In the following decade, H_2 production is vastly expanded in the three target scenarios, however with around 75 GW in DEL only half of the 150 and 145 GW in HYD and SYN respectively. Strongly increased e-kerosene demands and stable e-diesel demands between 2040 and 2045 are compensated by imports of RFNBO.

In 2040, all target scenarios reach above 300 TWh/a of domestic H_2 production with slightly below 400 TWh/a in DEL at the lower limit and slightly above 630–650 TWh/a in HYD and SYN, respectively. The split between DEL on the one hand and HYD and SYN intensifies in 2045 where H_2 production is around 350 TWh/a in the former and ranges from 700–750 TWh/a for the latter two, complemented by additional H_2 imports of 50, 190 and 340 TWh/a in DEL, HYD and SYN, respectively. This strong dynamic is not only driven by transport sector defossilization but even stronger by drastically increased H_2 and synthetic CH_4 usage in Combined Heat and Power (CHP) power plants in HYD and SYN. From 2040 onwards, more H_2 is used for methanation (160–300 TWh/a) for heat provision than for Fischer–Tropsch refineries (around 100 TWh/a) for transport final energy demands in all scenarios. Of the 175–250 TWh/a final energy demand for liquid hydro-carbons between 52%–57% are produced in Germany while the rest is imported.

Looking at the spatial distribution of H_2 production within Germany, deeper pathways increase the variability of H_2 production volumes across nodes as shown in the turquoise bars of Fig. 4. While they lie between 20–60 TWh/a for most nodes with the northern node Bremen, Lower-Saxony (BLS) at 120 TWh/a in DEL, this range increases to 10–100 TWh/a with BLS at 190 TWh/a in HYD and SYN.

Calculatory electrolysis full load hours increase from below 3000 in 2030 to around 4000 in 2040 and 3900–4200 in 2045 increasing with conversion depth. This demonstrates the challenge of profitable electrolysis operation especially in the medium term where H_2 demands are still comparably low. We identify this as a field of further research.

Turning to liquid hydrocarbons, domestic synthetic diesel, gasoline and kerosene supply shows some variation, especially in the short term, and interesting dynamics due to changing import shares. While road sector fuel demands peak in 2040 before declining until 2045, the demand for electric kerosene and diesel in aviation and shipping increases steadily. Fischer Tropsch fuel production facility (FT) refineries are expanded to around 10 GW of H_2 input with no further additions in 2045 due to increasing import volumes at low prices and limited intermittent RES production potential. Fuel production itself peaks in

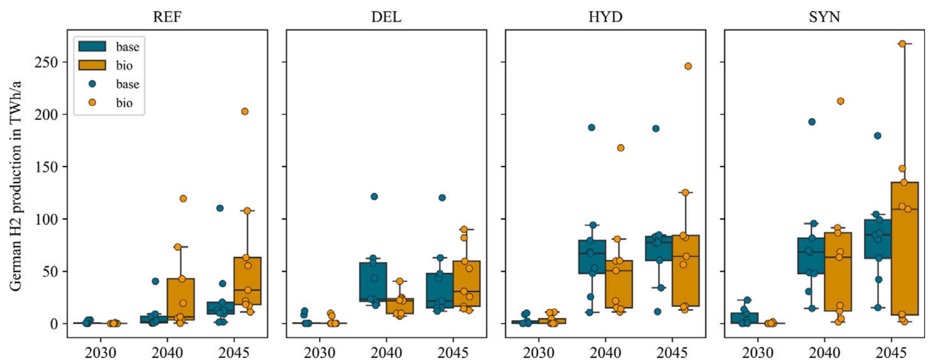

Fig. 4. Absolute H_2 production distribution across the nine German nodes in the four scenarios for scope 1 (base) and 2 (bio).

2040 with 60–90 TWh/a and is reduced towards 2045 to 30–70 TWh/a.

Refineries' production ratio of the three products is fixed, whereas final energy demand shares of the respective fuels develop dynamically towards dominant diesel shares in 2040 and balanced diesel and kerosene shares in 2045. This effect can be illustrated using the example of the model node Saarland, Rhineland-Palatinate, Hesse (SRH), where Germany's airport with the highest kerosene demand (Frankfurt am Main) is located. Across the target scenarios, below 5 TWh/a gasoline, 5–10 TWh/a diesel and 45–50 TWh/a kerosene are demanded in 2045, showing the discrepancy to the balanced production output. This discrepancy is compensated by imports, as can be seen in Figure C.23. Future research should give (potentially fixed but various) output shares for refineries to account for chemical plant heterogeneity.

Increased conversion depth leads to higher final energy demands for renewable fuels. This can be exemplified in the cases of gasoline and diesel demand. While domestic gasoline production shows no strong dependence on conversion depth, higher final energy demand in 2040 is compensated mostly by imports. In 2045, the SYN scenario shows an increase of domestic production to around 50% of final demand (27 TWh/a vs. 6 TWh/a in DEL). This dynamic is also observed for diesel and kerosene demand from 2040 onwards with decreasing or stable domestic production shares and growing imports supplying increasing kerosene and diesel final demand in 2045. For a discussion of our methods as well as a comparison of our scenario results with previous studies see Appendix D.3.

Our energy system modeling is limited since we do not explicitly model European fuel imports and exports between countries (only transmission grids). Gaseous and liquid fuel transport infrastructure modeling can yield interesting insights into European energy sovereignty and how it can be affected by European biofuel policies.

To our knowledge, we here for the first time combine results of a detailed modeling of transport subsector fuel demands with a fully sector-coupled energy system modeling in both high detail and transformation dynamic. Because our intermittent RES expansion potential assumptions are comparably low, we may overestimate power and fuel imports. However, we found very little H_2 imports only under GHG neutrality (in 2045) and resulting imports of diesel, gasoline and kerosene seem in line with or even below today's volumes.

3.3. The effect of biofuels on electricity supply infrastructure expansion

Biofuel availability may reduce the demand for electricity-based fuels as illustrated for the scenarios SYN and SYN_bio in Fig. 5. Various biomass streams lead to the reduction of e-fuels demands shown in Fig. 5. In all scenarios, there is a discernible decline in the consumption of rapeseed and sugar beet, which are traditionally used for biodiesel and bioethanol production. This decrease can be attributed to the assumed phased-out policies on conventional biofuels by policymakers under the EU regulation REDII. On the other hand, the combined consumption of maize silage and poplar exhibits an upward trajectory, indicating an increasing utilization of these feedstocks in the future. Poplar is mostly allocated to biomass-to-liquid processes to produce biodiesel and Sustainable Aviation Fuel (SAF) for road and aviation sectors. Also, paludiculture usage grows in all scenarios.

In the following, we assess how decreased e-fuels demands affect energy supply infrastructure expansion and usage. Liquid synthetic fuels are required at a level of 260 TWh/a in SYN vs. 110 TWh/a in SYNbio in 2045. As shown in Fig. 5, the difference mainly stems from a substitution of both, e-diesel and e-kerosene demand by biodiesel and biokerosene. Road sector synthetic fuel demand plays a larger role only in 2040. However, due to technical differences between Otto and Diesel engines, e-gasoline can only substitute up to 10%, thus only in early years when significant fossil gasoline is used. This is shown in Fig. 5 where gasoline substitution in 2030 is significant, because still large fossil gasoline demand exists, but this potential is diminished with reduced fossil gasoline demand in the consecutive years.

Fig. 6 shows the fuel origins in the SYN and SYN_bio scenarios for e-diesel, e-gasoline and e-kerosene. Biofuel availability drastically reduced efuel demand, especially for kerosene and Diesel, also reducing absolute domestic efuel production in 2045 and limiting necessary imports. Domestic efuel production is especially high in 2040 when still some emissions from heating and power are allowed for and strongly reduced in 2045.

Intermittent RES expansion is only slightly affected in 2030 and not from 2040 onwards, due to large electricity demands from other sectors. The reduced demand for electricity-based liquid hydrocarbons has strong implications on H_2 and refinery production capacities. This is especially true for the year 2040 as can be seen in Fig. 4 showing lower and less variable H_2 production across the nine German nodes in all three target scenarios DEL with biofuel availability (DEL_bio), HYD with biofuel availability (HYD_bio) and SYN_bio. See Figure C.21 for a direct comparison of the German electrolysis capacity in all 8 scenarios.

We now look at the effect of an optimal biofuel supply for transport on the necessary expansion of energy supply infrastructure in the two synthetic fuel scenarios SYN and SYN_bio. This is done for the technologies with the highest gradients shown in Table C.12.

In the SYN scenario, biofuels can reduce necessary intermittent RES capacity expansions in 2030. Needed PV power plant capacity could be reduced from over 200 GW in 2030 by more than 40 GW to 160 GW. Onshore wind power plant capacity expansion could be reduced by 13 GW from 129 to 116 GW. Germany-internal grids can be slightly reduced, while cross-border capacities can be significantly reduced from 2040 onwards from 130 and 180 to 120 and 160 GW in 2040 and 2045 respectively. In the DEL scenario, this effect cannot be observed. Here, a decrease in expanded offshore wind power capacity from 80 to 70 GW can be observed. Germany-internal grid extension is higher by 15 and 29 GW while cross-border capacities are slightly lower by around 12 and 18 GW in 2040 and 2045 respectively.

Electricity imports are high in the four high conversion depth scenarios HYD, SYN, HYD_bio and SYN_bio with biofuel availability

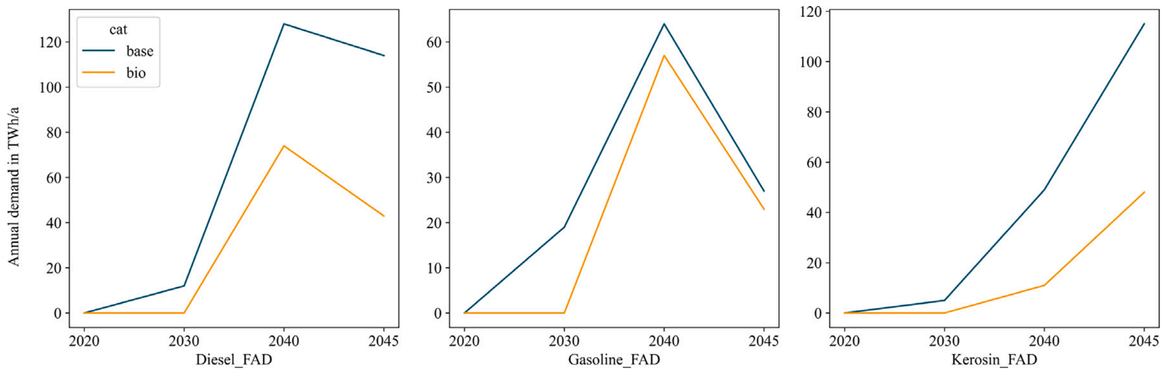

Fig. 5. Influence of biofuel supply availability on transport sector final energy demand exemplified for Diesel, Gasoline and Kerosene for the scenarios SYN (turquoise) and SYNbio (orange). See C.22 for all fuels and scenarios.

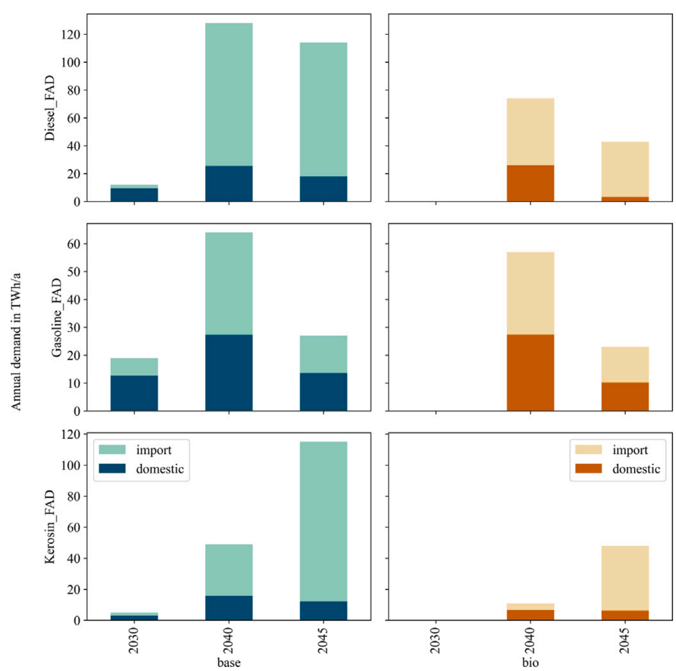

Fig. 6. Demand for electricity based fuels in scenarios SYN and SYN_bio differentiated in imported and domestic supply. Imports from non-EU countries. Domestic: Fuel production in Germany by Fischer Tropsch and refinement with fixed production ratio of products.

slightly reducing imports in 2040. However, in DEL_bio electricity imports can be kept to today's levels in 2040, halved compared to DEL and significantly reduced by a factor of 4 compared to the above mentioned scenarios. This shows, that biofuel availability may reduce electricity import dependence.

The two models are bilaterally soft-coupled, i.e. results of REMix are fed into BENOPTex and vice-versa until convergence is reached [30]. However, this approach implies that the competition between biofuels and RFNBO imports is not assessed in high spatial detail. This might be an interesting pursue for future research.

To our knowledge, the impact of biofuel availability on energy system transformation scenarios has never been assessed in the presented detail for Germany. The only study that assesses the implication of a biofuel shortage is [53]. However, their focus is on all three demand sectors: Heat, industry and transport with a coarser detail in transport and specifically road and aviation subsector demand modeling. Their central finding – that the transport sector is only slightly affected from a biofuel shortage – only holds true when clean fuels contribute little to the energy system demand. See Appendix D.4 for a more detailed discussion.

3.4. Overarching discussion

Here, we discuss the main results on the background of previous findings. For a more comprehensive description of limitations, see Appendix D.1.

Penny-switching effects occur in linear optimization models such as the one used here. The starkest example of this is the offshore wind expansion as can be observed in Figure C.17. In 2030, offshore wind is still more expensive than PV and onshore wind combined with remaining gas power plants for periods of low wind and solar feed-in. This contradicts current policy targets of 30 GW installed capacity of offshore wind in 2030. The near-optimal feasible solution space may vary despite only small differences in objective function [54]. Thus, the precise supply capacity mix before 2040 should be interpreted carefully. Beyond 2040, this effect does not occur, since solar and wind power capacity is expanded to its maximum potential.

H_2 production in Germany in 2045 is found to be very high between 400–650 TWh/a. This is in line with H_2 demands of 360–690 TWh/a reported in [28]. While they assume a European H_2 grid and find H_2 imports of 180–420 TWh/a, we assume transmission only in Germany.

This results in higher shares of domestic H_2 production in our scenarios of 70%–90%. Thus, our scenarios can be read as scenarios where European electricity markets are integrated but H_2 and clean fuel supply are managed nationally.

Biofuels have been controversially discussed due to competition with agriculture, and, in the future, bio-based chemical industries [55]. Biofuel policies have also been shown to increase land-use change effects in a US policy analysis [56]. However, we considered biomass only from waste biomass (see Table B.9) or sustainable agricultural potential by assuming the available land for conventional energy crops to decrease compared to the status quo and by limiting the use of conventional biofuels according to RED II (see [30], Table 1).

Within the scope of our model setup, investment and import decisions are taken from a central European planner perspective which is a significant simplification. Especially the trade of clean fuels depends on a multitude of external individual, social, environmental, technical and economic factors and path-dependencies.

Furthermore, the modeling is based on exemplary demand scenarios from a holistic projection of future economic activities and demand drivers as well as different narratives of the technological development of the demand sectors, which cannot be evaluated here in terms of robustness and evidence. Optimistic assumptions are usually made regarding the development of efficiency in all sectors; in reality, however, long-term energy demand and its spatial distribution may develop significantly differently. Since both, very progressive road sector policies, ambitious CO_2 pricing regimes as well as efficiency gains are assumed, fuel demands may be higher than reported here. Under the given constraint of GHG neutrality in 2045, this implies higher clean-fuel imports, higher electricity imports from neighboring countries or structural changes to transport demands e.g. through fundamental behavioral changes in travel patterns [52].

Our findings from answering research question 1 for Germany can be translated to other regions and countries to some extent. They hold true only if ambitious transport sector CO_2 emission reduction policies are implemented and no significant lifestyle changes occur. Incorporating purchase preferences into vehicle demand modeling narrows down demand uncertainty. Our quantification can act as a first-guess for other regions with similar sub-sectoral composition as Germany. While the answer to research questions 2 and 3 are highly specific to the German energy system with its specific resource availability, demand characteristic, positioning in the European grid etc. some qualitative insights may be transferred. Increased demand for clean fuels (higher conversion depth) leads to higher electricity imports, lower internal transmission needs, larger hydrogen infrastructure, and higher H_2 imports in the long-term compared to a largely electrified scenario. Biofuels may reduce high gradients of H_2 production and crossborder interconnection capacity in the medium term, reduce transport sector import-dependence and act as a bridge to infrastructure-heavy electricity-based energy systems.

4. Conclusion

This paper sheds light on the implications of different transport sector defossilization pathways on cost-optimal energy system infrastructure build-up. We focus on two factors that are especially unknown, the impact of conversion depth and biofuel availability on energy supply infrastructure transformation.

We propose a methodology that introduces three important innovations to the field of research: First, a combination of transport demand modeling in the key transport demand sectors of aviation and road transport with energy system optimization at high temporal and spatial resolution. Secondly, the integration of detailed potentials and costs for the import of green energy carriers to Germany. And thirdly, the optimization of fuel allocation to meet demand in the transport sector, taking into account a wide range of biogenic feedstocks. To account for the most important policy uncertainties, we consider four demand-scenarios each without and with biofuel availability.

We find that considering user behavior and technical specifics of airplane fleet planning strongly limits the realistic range of assumptions on transport final energy demand development. All scenarios show the strongest increase in final energy demands for renewable fuel between 2030 and 2040. Road sector contribution to final energy demand peaks in 2040 and decreases beyond that while synthetic kerosene demand for aviation and synthetic diesel demand for shipping gain increasing importance. German transport energy demand in electricity equivalents of a synthetic fuel oriented scenario is more than 100 TWh/a higher than in lower conversion-depth scenarios.

Our results for the target scenarios support German intermittent RES expansions as no-regret option in all scenarios and underpin their outstanding importance for transport sector defossilization. Conversion depth affects cost-optimal energy transmission networks. Electricity grids in Germany are expanded slightly more in a low conversion-depth scenario while cross border grid expansion capacity increases with higher conversion depth, especially in later years. This supports previous findings that the current grid extensions planned in the German grid development plan are insufficient and extends them to interconnectors between Germany and its neighboring countries.

Hydrogen production capacity is strongly expanded in all scenarios between 2030 and 2040 under the assumption of domestic hydrogen supply strategies. Fischer–Tropsch refinery capacity is only slightly expanded in 2030 except for the high conversion depth scenario where 5 GW are needed. This capacity is approximately doubled in the following decade up to 2040 in all scenarios but not further expanded afterwards. From thereon, increasing final energy demands are supplied by imports due to limited intermittent RES and increased low-price volumes.

Lastly, we show that biofuel substitution in transport sector demands can have an influence on energy supply infrastructure dynamic, especially in high fuel demand scenarios. Cross-border electric grid expansion can be reduced by around 10 GW and 15–20 GW in the years 2040 and 2045 through biofuel availability. Under direct electrification, biofuel availability leads to electricity import reductions to 50% (around 100 TWh/a). Electrolysis capacity expansion before 2040 can be reduced and shifted to consecutive periods by biofuel availability. Import dependence of clean Diesel is around 70-80 % and kerosene beyond 80% with biofuel availability mainly reducing 2030 and 2040 import dependence. Biofuel availability may thus reduce import dependence of fuels and electricity in the medium term.

Further research questions remain. We assume a fair-share for Germany accessing clean fuel imports corresponding to the German share of global population. Relaxing this constraint and incorporating trade-mechanisms similar to how we incorporated biofuel demands is an interesting pursue. Integrating liquid fuel transport between model nodes and gaseous fuel infrastructure expansion across Europe may yield further insights. The model instances were solved using a time resolution of 4 h. Increasing this resolution may further increase the need especially for short-term flexibility but is not expected to drastically change the effects described here. In order to scrutinize the results, multiple weather years for the electricity demand and intermittent RES feed-in should be used for calculation.

CRediT authorship contribution statement

Niklas Wulff: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Writing – original draft, Writing – review & editing, Visualization, Project administration. **Danial Esmaeili Aliabadi:** Conceptualization, Methodology, Software, Writing – original draft, Writing – review & editing, Visualization. **Samuel Hasselwander:** Software, Data curation, Writing – original draft. **Thomas Pregger:** Data curation, Writing – original draft, Writing – review & editing. **Hans Christian Gils:** Resources, Writing – review & editing, Supervision. **Stefan Kronshage:** Data curation. **Wolfgang Grimme:** Software, Data curation, Writing – original draft. **Juri Horst:** Writing – original draft. **Carsten Hoyer-Klick:** Resources, Project administration. **Patrick Jochem:** Writing – review & editing, Supervision.

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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All authors have read and agreed to the published version of the manuscript.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.esr.2024.101606.

Data availability

All result data used for creating the Figures of this document is available in a Zenodo repository https://doi.org/10.5281/zenodo.14203522. Raw model output data is made available upon request.

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