Interaction of hydrogen infrastructures with other sector coupling options towards a zero-emission energy system in Germany

Hans-Christian Gils[a,*], Hedda Gardian[a], Jens Schmugge[a]

[a]*Department of Energy Systems Analysis, Institute of Networked Energy Systems, German Aerospace Center (DLR), Curiestr. 4, 70563 Stuttgart, Germany*

Abstract

The flexible coupling of sectors in the energy system, for example via battery electric vehicles, electric heating or electric fuel production, can contribute significantly to the integration of variable renewable electricity generation. For the implementation of the energy system transformation, however, there are numerous options for the design of sector coupling, each of which is accompanied by different infrastructure requirements. This paper presents the extension of the REMix energy system model to include the gas sector and its application for investigating the cost-optimal design of sector coupling in Germany's energy system. Considering a co-optimisation of all relevant technologies in their capacities and hourly use, a path to a climate-neutral system in 2050 is analysed. We show that the different options for flexible sector coupling are all needed and perform different functions. Even though flexible electrolytic production of hydrogen takes on a very dominant role in 2050, it does not displace other technologies. Hydrogen also plays a central role in the seasonal balancing of generation and demand. Thus, large-scale underground storage is part of the optimal system in addition to a hydrogen transport network. These results provide valuable guidance for the implementation of the energy system transformation in Germany.

Word count: 5735 (+1340 words Appendix)

Keywords: energy system modelling, sector coupling, integrated energy systems, optimisation, hydrogen, REMix

---

*Corresponding author
Email address: hans-christian.gils@dlr.de (Hans-Christian Gils)

Highlights

- Combination of all options for flexible sector coupling has high synergy potential
- Flexible hydrogen production is a key enabler of renewable energy system integration
- Hydrogen storage and transport networks are important future energy infrastructures
- Climate targets require a timely acceleration of sector coupling implementation

List of abbreviations

BEV	battery electric vehicle
CHP	combined heat and power
CH_4	methane
CO_2	carbon dioxide
DH	district heating
DR	demand response
EU	European Union
FLH	full load hour
GAMS	General Algebraic Modeling System
H_2	hydrogen
HP	heat pump
HVAC	high-voltage alternating current
HVDC	high-voltage direct current
MILP	mixed-integer linear programming
O&M	operation and maintenance
PEM	proton-exchange membrane
PV	photovoltaic
RE	renewable energy
REMix	Renewable Energy Mix
SOEC	solid oxide electrolyser cell
TES	thermal energy storage
TYNDP	Ten Year Network Development Plan
V2G	vehicle-to-grid
VRE	variable renewable energy

1. Introduction

1.1. Background and motivation

The transformation towards a climate-neutral European energy system requires the installation of very large capacities for power generation from variable renewable energy (VRE) sources such as wind and photovoltaic (PV) [1]. This results in particular from the fact that the transformation of industry and the transport sector can only be achieved through electrification and the use of synthetic fuels generated from renewable electricity [2]. The significant increase in wind and PV capacity is accompanied by large fluctuations in the daily and seasonal generation of electricity. These fluctuations can be balanced by a wide range of load balancing technologies, each with different functionalities and costs [3]. In this context, the closer interconnection of the different parts of the energy system, for example via electric heat generation, battery electric vehicles (BEVs), or electricity-based generation of fuels, commonly referred to as sector integration or sector coupling, can provide flexibility for the power system [4]. Especially the flexible production of hydrogen (H_2) by electrolysis can contribute substantially to this, as large amounts of gaseous and liquid fossil fuels need to be substituted. Furthermore, gas networks can play an important role, as they are capable of transporting large amounts of energy.

1.2. State of research

The role of sector coupling and hydrogen in future energy systems is an active field of research in energy systems analysis. In an earlier study of Samsatli et al. [5], a mixed-integer linear programming (MILP) approach is utilised to investigate the production of hydrogen from onshore wind power to decarbonise the transport sector in Great Britain. Other sectors are not addressed, and the temporal resolution is limited to representative days. These limitations are tackled in a later work [6], which focuses on the utilisation of renewable hydrogen in space and water heating and therefore introduces a hydrogen supply chain covering production, storage, transport and use. The sectoral scope is still limited, though. Fu et al. developed a multi-energy systems model that investigates the impact of different hydrogen production technologies on an economic and environmental level and for each considered energy sector (electricity, heat, transport) [7]. The energy transport infrastructures in their study are modelled in low spatial resolution and the two investigated scenarios do not lead to a zero-emission energy system. This applies also to Ameli et al., who investigated the costs of different flexibility options for the power and natural gas system with the target year 2030 [8]. Given this short time horizon, hydrogen was not considered. In [1], the feasibility to transform the European energy system to carbon neutrality by 2050 mainly exploiting VRE resources is investigated. The endogenous optimisation is, however, restricted to the electricity and heat sectors and lacks sub-national resolution.

The future implementation of sector coupling in Germany has been addressed in earlier works. A temporally and spatially resolved energy system of Germany is investigated in [9], including the usage of hydrogen in the transport sector and industry. Furthermore, the impact of salt caverns for hydrogen storage on overall system costs is quantified. Since the study is based on representative days and only considers onshore wind as a power generation technology, it still has a limited scope. In [10], different transport options for hydrogen to serve the demand of the German transport sector are evaluated. To do so, a simulation model previously presented in [11] is increased in spatial resolution to calculate more realistic hydrogen transport costs. A temporal resolution is not considered nor are further sectors. Cerniauskas et al. assess the natural gas pipeline reassignment potential for future hydrogen utilisation in Germany [12]. They find a potential of more than 80 % for the German pipeline network with deduced cost reductions of more than 60 % for hydrogen transmission pipelines compared to a newly-built dedicated hydrogen grid until 2050. An investigation of the entire energy system with regard to decarbonisation is not conducted. Finally, [13] modelled the infrastructures needs for the transport and storage of hydrogen, gas and electricity as well as the conversion between those energy carriers along three transformation scenarios with a carbon dioxide (CO_2) emission reduction of 95 % until 2050. In its focus area, Germany and the Netherlands, the model features a high spatial detail of 39 regions, while the technological granularity is comparatively limited and other sector coupling is neglected. Results show a high potential for the reassignment of natural gas pipelines for hydrogen transport. Depending on the hydrogen demand scenario, the installed electrolyser capacity in Germany reaches between 8 GW and 91 GW in 2050. In contrast, methanation is almost not used as the remaining gas power plants can still rely on natural gas.

Despite the wide range of preliminary work, it remains unclear how the various options for flexible sector coupling interact with each other in a spatially and temporally resolved energy system. Similarly, the least-cost combination of the various load balancing technologies along the transformation to a climate-neutral energy system in Germany has not yet been investigated.

1.3. Contribution of this paper

This paper closes the identified research gap by providing a co-optimisation of all sector coupling options along the pathway to a zero-emission power, heat and ground-transport energy system in Germany in the year 2050. To this end, we apply a regionally and hourly resolved optimisation model with high technological granularity for an integrated evaluation of the capacities and operation of the required infrastructures for energy conversion, storage and transport of power, heat, hydrogen, and methane (CH_4)[1]. This allows for a comprehensive evaluation of the operation and interaction of different sector coupling technologies as well as electricity storage and transmission. We focus in particular on the evaluation of the expansion of large-scale hydrogen infrastructures and their interaction with the energy system. Additionally, we study the robustness of

[1] Here and in the following, methane (CH_4) refers to natural gas, bio-methane, synthetic methane and any mixture of these.

the results against powerful input assumptions, such as the limitation of power grid expansion. Following an introduction of the methodology and data used (Section 2), we present the results of the model application (Section 3). These are then discussed and related to previous research (Section 4). Finally, the key conclusions of our work are presented (Section 5).

2. Materials and Methods

2.1. Modelling approach

The case study presented here relies on the application of a model derived from the Renewable Energy Mix (REMix) energy system modelling framework (Figure 1). REMix provides the basis for analysing energy system transformation scenarios in spatial and temporal resolution. Originally limited to the power sector [14], the framework has been continuously enhanced to include the flexible coupling to the heating and transport sectors. The models built from REMix were initially used primarily to analyse the European electricity system [15]. Building on this, other countries and sectors were then brought into focus [16, 17]. The framework provides a multi-node approach, where the nodes can be connected by different types of transport infrastructure. Within the regions, all units of one technology are aggregated and treated as one single unit.

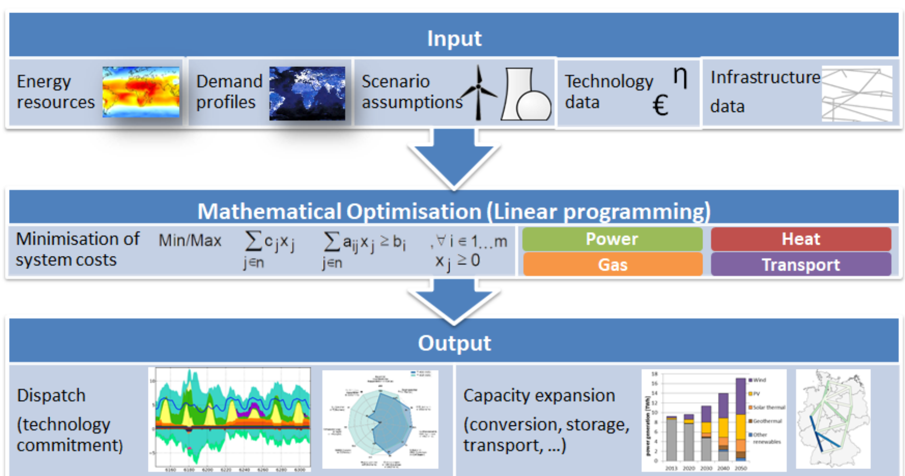

Figure 1: Set-up of the REMix modelling framework.

REMix relies on a linear cost minimisation approach, with its objective function containing the annuities C_{invest} and fixed operation and maintenance (O&M) costs C_{OMFix} of endogenously added capacities, variable O&M costs C_{OMVar} of all assets, fuel costs C_{fuel}, optional emission costs C_{emission}, and penalty costs for unsupplied energy demand $C_{\text{unsupplLoad}}$ (Eq. (1)).

$$\min \left\{ \boldsymbol{C}_{\text{OMFix}} + \boldsymbol{C}_{\text{OMVar}} + \boldsymbol{C}_{\text{fuel}} + \boldsymbol{C}_{\text{emission}} + \boldsymbol{C}_{\text{unsupplLoad}} + \boldsymbol{C}_{\text{invest}} \right\} \tag{1}$$

The REMix framework is implemented in the General Algebraic Modeling System (GAMS) and solved using CPLEX. The construction of energy system infrastructures and their hourly operation over the course of a year are optimised integrally in one model run and with perfect foresight. Detailed model descriptions can be found in [15] for the power sector, in [18] for the heating sector, and in [19] for BEVs.

For the preparation of this case study, the framework has been further extended to include a simplified representation of the gas sector. This essentially comprises the production, import, storage and transport of gas, as well as its use in the electricity, heat and transport system. This refers to any type of gas, including hydrogen or chemically produced methane. A detailed introduction of the framework enhancement is provided in Appendix A.

2.2. Case study design

The focus of the case study is to investigate the contribution of flexible sector coupling to the implementation of energy system transformation in Germany. However, to adequately model the contribution of the international electricity grid and large-scale hydro power plants to the integration of VRE power generation, the modelling also includes the European neighbouring countries as well as Italy, Norway and Sweden (Figure 2). While these are each represented as a model node, i. e. any domestic restrictions on electricity transport are neglected, Germany is divided into ten model regions. These result from a partial aggregation of the federal states, which considers bottlenecks in electricity and gas transport.

The case study relies on a transformation scenario to a climate-neutral supply of the considered part of the energy system. This includes all demands except for air flight and shipping. Essential assumptions regarding the development of energy demand and the technology paths in the industry, heating and transport sectors are made exogenously. They include a strong decline in the use of fossil fuels, which is compensated by electrification and hydrogen use. While the exogenous methane demand falls to 15 % of the 2020 value by 2050, the electricity demand doubles in the same period due to exogenous demand for hydrogen, electric heat generation and electric mobility. A detailed description of the scenario is provided in [20]. The modelling covers the scenario years 2020, 2030, 2040 and 2050, which are considered in myopic model application. This implies that the plants endogenously added in the previous years will remain in the system until the end of their technical lifetime.

The transformation is driven by an increasing CO_2 price of 25 €/t in 2020, 94 €/t in 2030, 154 €/t in 2040, and 216 €/t in 2050. In 2050, the CO_2 emissions are additionally capped to zero.

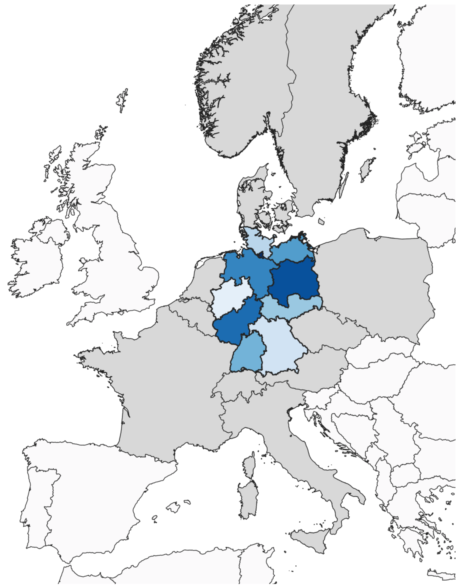

Figure 2: Model regions considered in the analysis in blue (German regions) and grey (neighbouring countries).

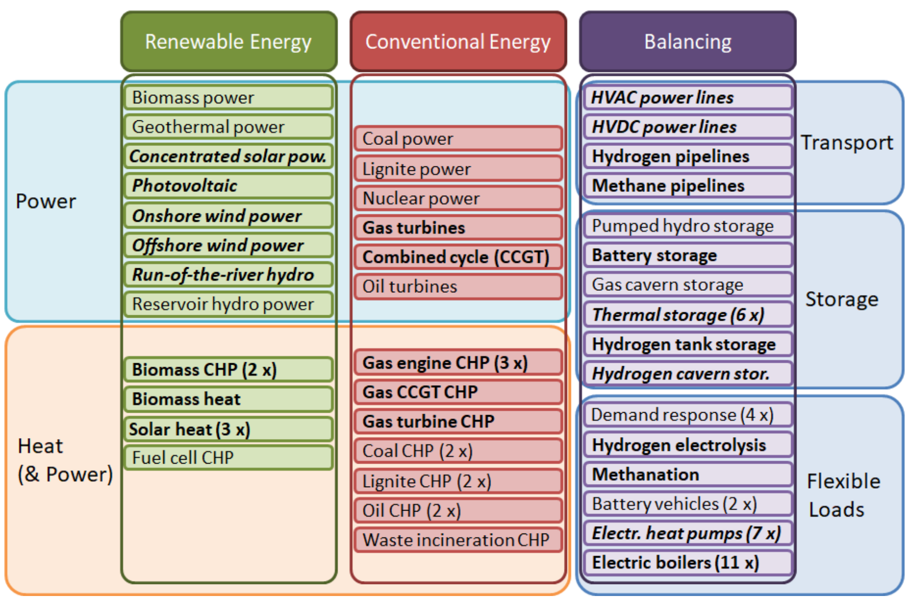

Figure 3: Technologies considered in the analysis. For the technologies highlighted in bold not only the hourly operation is optimised but also the installed capacity. The technologies in italics have an upper limit in their capacity. Biomass heat and power production is indirectly limited through the available fuel. The number in brackets indicates the consideration of different sub-technologies, e. g. combined heat and power (CHP) in district heating (DH) and industry, or thermal energy storage (TES) in DH and buildings.

The model applied here covers a broad spectrum of conversion, storage and transport technologies in the electricity, heat and gas sectors (Figure 3). The techno-economic assumptions for these technologies are provided in [20] [2].

Not only the spatial, but also the technological detail considered in the model differs between Germany and the other countries. A full consideration of the heat supply is only realised for Germany, whereas in the other countries only the decentralised electrical heat production is modelled. A flexibilisation of electric heat generation and BEV charging is also only considered in Germany as well as the modelling of large-scale infrastructures for the storage and transport of hydrogen and methane. For the modelled European neighbouring countries, only the hydrogen demand for transport and industry as well as its decentralised and partly flexible production is considered. Flexibility is provided by a tank sized to store the amount of hydrogen produced by the electrolyser in six hours, which allows to avoid large load peaks [21].

By considering a set of scenario variants, the robustness of the model results regarding flexible sector coupling is examined. To this end, deviating paths of technology implementation are considered, and central technology and scenrio assumptions are changed. The scenario variants focus on diverging import options for electricity and green hydrogen, the consideration of a more continuous operation of gas production, as well as the variation of the techno-economic parameters of the technologies in the gas system (Table 1).

Table 1: Considered scenario variants.

Label	**Properties**
PowGrid+	Unlimited endogenous expansion of power grid capacities in 2040 and 2050.
PowGrid-	No endogenous expansion of power transmission capacities.
LowH2Import	Green H_2 can be imported at the North Sea coast at 28 €/MWh(H_2).
HighH2Import	Import H_2 price is reduced to 20 €/MWh (H_2).
MedH2FLH	Electrolysis must be operated with at least 6500 FLHs per year.
HighH2FLH	Electrolysis must be operated with at least 8000 FLHs per year.
HighCH4FLH	Methanation must be operated with at least 8000 FLHs per year.
CO_2Cost	The CO_2 required for methanation has a cost of 50 €/MWh(CH_4).
H2CompEn+	Compression energy for H_2 pipeline transport is increased by a factor of five, corresponding to a higher pressure level.
SOEC	In 2040 and 2050, SOEC are considered to be available at the same costs. Assumed efficiencies increase from 77 % and 80 % to 88 % and 93 %, respectively.

2.3. Input data for the power, heat and transport sector

For the year 2020, the current stock of power plants, networks and storage facilities is included in REMix. Due to changes in demand and the decommissioning of old plants, the power plant park will change over the course of the scenario years. This change is essentially part of the modelling results, but is limited by some exogenous specifications. For example, hydro, wind and PV power plants are assumed to have constant capacities until 2050, which implies a

[2] For review purposes, a detailed input data file is provided as additional material. Upon acceptance, it will be made available online and the link included here.

Table 2: Spatial and temporal distribution of the demand data.

Parameter	**Spatial distribution**	**Time series**
Renewable energy production	Technical potentials [14]	Weather year 2006
Residential/commercial heat demand	Population, commercial areas [18]	Air temperature [18]
Industrial heat demand	Industrial value added [18]	Industrial activity [18]
Transport H_2 demand	Number of registered vehicles [25]	Fuelling profiles [25]
Industrial H_2 demand	Industrial value added [18]	Industrial activity [18]
BEV power demand	Number of registered vehicles [25]	Charging profiles [26]
Other electricity demand	Population [27]	Grid load in 2006 [28]

replacement at the end of their lifetime. Upper limits for the use of VRE sources are given by the available potentials [20]. For the existing conventional power plants and CHP plants, simplified mortality lines are assumed according to [20]. Contrary to that, for pumped storage a small expansion from 6.5 GW today to 7.6 GW in 2050 is considered. For electricity demand in the transport sector, it is assumed that only fully electric and hybrid electric cars are eligible for controlled charging. Furthermore, the share of flexible charging is limited to 60 % of the vehicles, and that of feeding back into the power grid (vehicle-to-grid (V2G)) to 20 %. For the electricity transmission grid, the existing high-voltage alternating current (HVAC) and high-voltage direct current (HVDC) line capacities are taken into account as well as the expansion planned within the framework of the German grid development plan [22] and the Ten Year Network Development Plan (TYNDP) [23]. In the scenario years 2040 and 2050, 5 GW per interconnection and decade can be endogenously added. This restriction avoids a sudden increase in capacity. The potentials for demand response (DR) in industry and commerce are considered according to [18, 24]. The implementation of flexible sector coupling is a key result of this analysis. Consequently, the capacities of hydrogen and thermal storage systems, heat generators, electrolysers and hydrogen transport pipelines are determined endogenously (Figure 3).

The overall heat demand is subdivided to different technologies including CHP in DH, buildings and industry, fossil- or biomass-fuelled boilers, or electric heat pumps (HPs) in buildings (Figure 3). These main suppliers can be supplemented by other heat generators including electric boilers, HPs, solar thermal systems, conventional peak boilers, and TES systems. Considering restrictions on the availability of space, TES facilities are limited in the permitted expansion. The expansion of HPs in DH is also partly limited due to the required development of heat sources as specified in [20]. The spatial and temporal downscaling of the demands is specified in Table 2.

A construction period for plants is not taken into account; if the model makes an investment decision, the corresponding plant is available from the first day of the year under consideration.

2.4. Representation of the gas system in Germany

To ensure manageable model solution times, a detailed examination of the gas system is only carried out for Germany. Transit flows and the origin of the fuel for the supply of gas power plants outside Germany are not modelled explicitly. Figure 4 gives an overview of the consideration of the German gas system in REMix and shows how the different gases can flow between the system components.

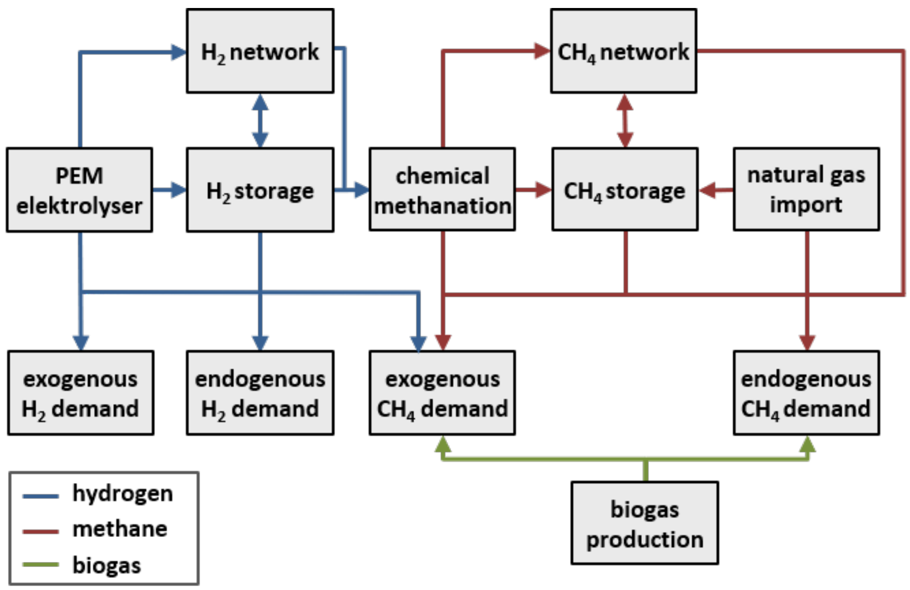

Figure 4: Configuration and interconnection of the gas system in the model. Boxes mark individually modelled components (converters, gas sources and gas sinks), while arrows indicate gas flows.

Electrolysis and methanation. Being the most developed technologies, proton-exchange membrane (PEM) electrolysis and chemical methanation are considered in REMix. Given their development potential for higher efficiencies, high-temperature SOECs are considered in one scenario variant.

Gas compression. Compression for transport and storage can be realised using electric compressors for hydrogen and electric or gas-driven compressors for methane. Both can be endogenously optimised in their capacity, currently existing compressors are considered.

Gas storage. A distinction is made between methane and hydrogen caverns and cylinder bundle storage for decentralised hydrogen storage. The existing storage volume of natural gas caverns is considered for methane. An endogenous installation of cavern storage is allowed only for hydrogen. It is limited to the regions with existing cavern storage and an energy capacity exceeding today's methane storage capacity by a factor of six. The installation of hydrogen tank storage is not limited.

Import and transport of gas. Gas transport networks are only considered between the model regions in Germany. Existing pipeline capacities are included both within the country and for the import of fossil natural gas. The volume of imported natural gas is limited by the existing pipeline capacities and related to the same cost and emissions regardless of its origin. The model can install hydrogen transport pipelines between neighbouring regions. The lengths of the pipelines refer to the distance between the corresponding region centres. A design for bidirectional flows is assumed for all transport pipelines.

Admixture of hydrogen and biogas. Hydrogen and biogas can be injected into the methane network. The admixture of hydrogen is only considered at the distribution network level, and is approximated by the regional demand. Its proportion is limited to 10 vol% in 2020, 15 vol% in 2030, 20 vol% in 2040 and 25 vol% in 2050. Biogas is modelled under the premise that the fuel quality has been brought into line with that of natural gas through prior treatment. There is no limit to biogas admixture, but a maximum potential specified.

The techno-economic assumptions and considered capacities are provided in [20].

3. Results

The presentation of the model results is divided into five parts. Firstly, the transformation of the power system in the overall area and in Germany is addressed (Section 3.1). Based on this, a detailed analysis of the design and operation of the German system is carried out, focusing on the interaction between different sector coupling options (Section 3.2), the installation of large-scale hydrogen infrastructures (Section 3.3), and the hourly system operation (Section 3.4). Finally, the scenario variants are examined (Section 3.5).

3.1. Power system development

Driven by the increasing CO_2 price, the model results show a steep increase in the VRE power generation across the European study area (Figure 5a). Wind and PV become the most important electricity generation technologies from 2030 onward. Inversely, the power generation from conventional technologies decreases with only nuclear and gas power plants remaining after 2040. Substantial emission reductions are already achieved until 2030, finally reaching zero emissions in 2050.

On a national level, the power system transformation in Germany is realised even faster. Driven by the phase-out of coal and nuclear power even higher VRE shares are reached (Figure 5b). Due to the cheaper VRE power generation abroad (e. g. by means of PV in Italy and France, wind power in Denmark or hydro power in Norway), the exogenous electricity import limit of 20 % of the demand is reached from 2040 on.

The transformation of the power generation is realised by a significant increase in the installed VRE capacities. In Germany, this is particularly pronounced between 2020 and 2030, with an increase from 54 GW to 132 GW for

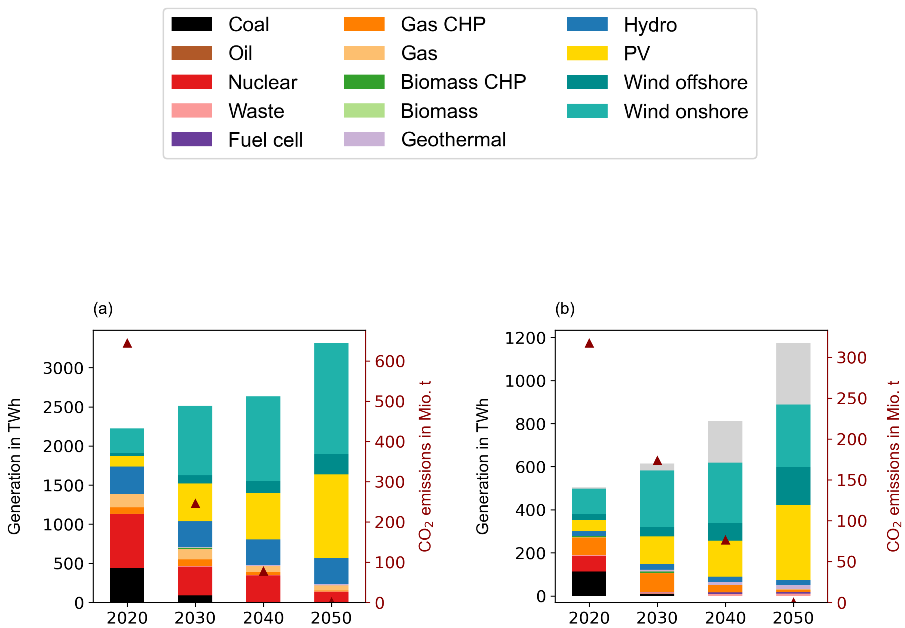

Figure 5: Power generation (left axis) and CO_2 emissions (right axis) in the overall assessment area (a) and in Germany (b) along the transformation pathway.

PV and from 48 GW to 106 GW for onshore wind. In contrast, the following decade shows a significantly lower increase, since rising demand is preferably covered by imports, which are made possible by the model-endogenous electricity grid expansion. However, since both imports and grid expansion are capped, there is again a very strong increase in VRE capacities between 2040 and 2050. Since the potential for onshore wind energy is already almost exhausted by 2040, this is realised by a further doubling of the installed capacities of PV and offshore wind energy. This corresponds to a net increase in PV systems with a total capacity of over 170 GW. The annual increase required would thus be twice the highest value ever achieved (a good 8 GW in 2012 [29]). For offshore wind energy plants, the maximum annual capacity increase reaches 2.3 GW between 2040 and 2050, corresponding to the value realised in 2015 [29]. VRE capacities are regionally concentrated according to their resource potential, i. e. PV in southern Germany and wind energy plants mainly in northern Germany.

The VRE plants are supplemented by a stock of predominantly gas-fired CHP plants that remains almost constant in terms of total capacity between 2030 and 2050. Their total capacity of about 40 GW is used to generate electricity during periods of low VRE generation.

3.2. Interaction of sector coupling in Germany

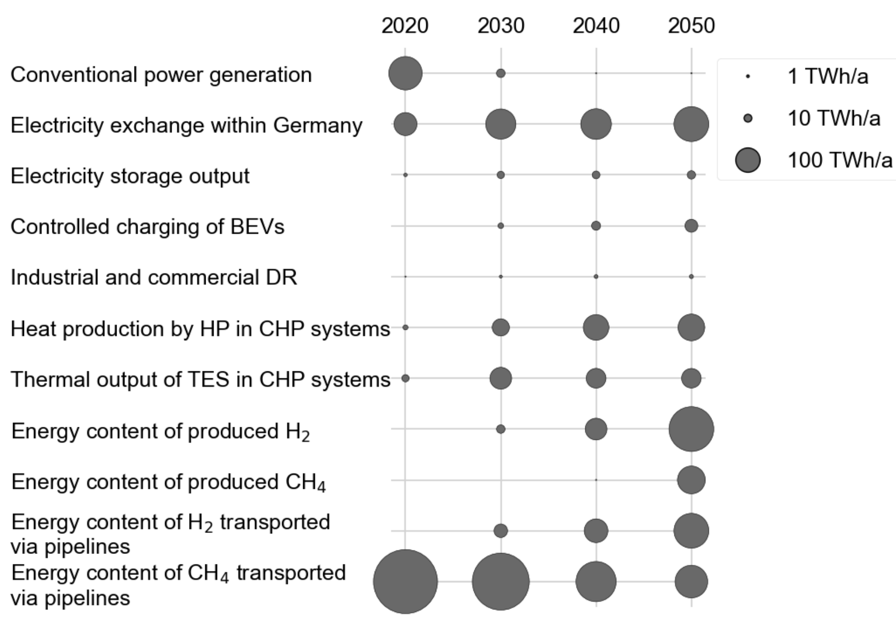

Figure 6: Usage of different balancing options in Germany during the system transformation. The size of the bubbles indicates the annual flexibility provided.

According to Figure 6, there are significant differences in the contribution of the different load balancing options. While controllable power generation dominates there at first, flexibility in heat generation comes to play an important role in the course of the transformation. In DH, this includes supplementing CHP with HP, electric boilers and TES. This allows for an increasing electrification of heat generation. However, since CHP will be needed until 2050 for power generation during periods of low VRE availability, it will remain part of the system but switch to fully electricity-oriented operation. The use of TES is not limited to heating networks, but also includes heat supply for buildings and process heat production. In the final year 2050, the flexibility of hydrogen supply is the most important balancing option. To enable electrolysis to be geared to electricity generation, large hydrogen cavern storage facilities are being built (Section 3.3). Due to the assumed decrease in the gas demand, the gas transport across region borders is significantly reduced. This opens up the possibility of reassigning parts of the existing infrastructure to hydrogen. It is important to note that the identified gas transport does not include international transit. Electricity storage, controlled charging of BEVs, and DR are also part of the cost-optimal system, but remain at a lower level.

In Germany, the maximum annual VRE curtailment reaches 3 TWh/a in 2030, corresponding to 0.7 % of the potential production. This implies that almost all generation can be used by exploiting the various load balancing options. At 1.5 %, the VRE curtailment in the overall study area is only marginally higher.

Figure 7 shows in detail how the utilisation of balancing options develops over time. We observe an increase in the use of all flexibility options except for those in the heating sector. The picture there is heterogeneous, with a continuous decline in CHP heat generation, a steady increase in HP use, and intermediate maxima in TES and electric boiler usage. In 2050, the overall capacities reach 22.5 $\mathrm{GW_{th}}$ for HP in DH systems, 390 $\mathrm{GWh_{th}}$ for TES, of which 80 % are in DH and 20 % in buildings and 27 $\mathrm{GW_{th}}$ for electric boilers, of which 80 % are in DH and 20 % in industry.

The significant increase in energy transmitted via the power grid is made possible by a strong expansion of transmission capacities. Despite the restriction to 5 GW per line and decade, it reaches a value of 120 TWkm by 2050, corresponding to a tripling compared to the exogenous value for 2030. While the transmission capacity within Germany increases only by about 70 %, the lion's share of the grid expansion is realised to and between the European neighbouring countries under consideration.

In contrast to the expansion of the electricity grid, decentralised battery storage systems play only a very minor role in the model results for Germany. Their storage and discharge capacity reaches only about one third of the values of pumped storage. Since flexible sector coupling is not available in other European countries, a much more extensive expansion of battery storage is taking place there, especially in countries with a high PV share.

3.3. Hydrogen infrastructure in Germany

The model results show an extensive expansion of infrastructure for the production, storage and transport of hydrogen (Figure 8). In the year 2050, the

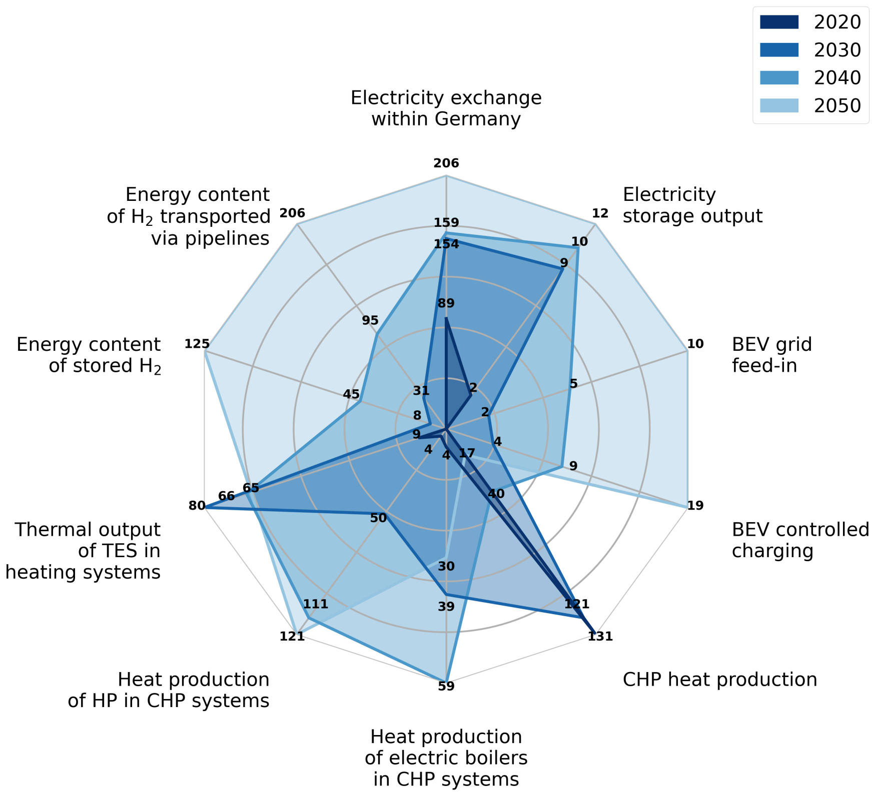

Figure 7: Technology-specific development of load balancing along the system transformation. All values in TWh/a.

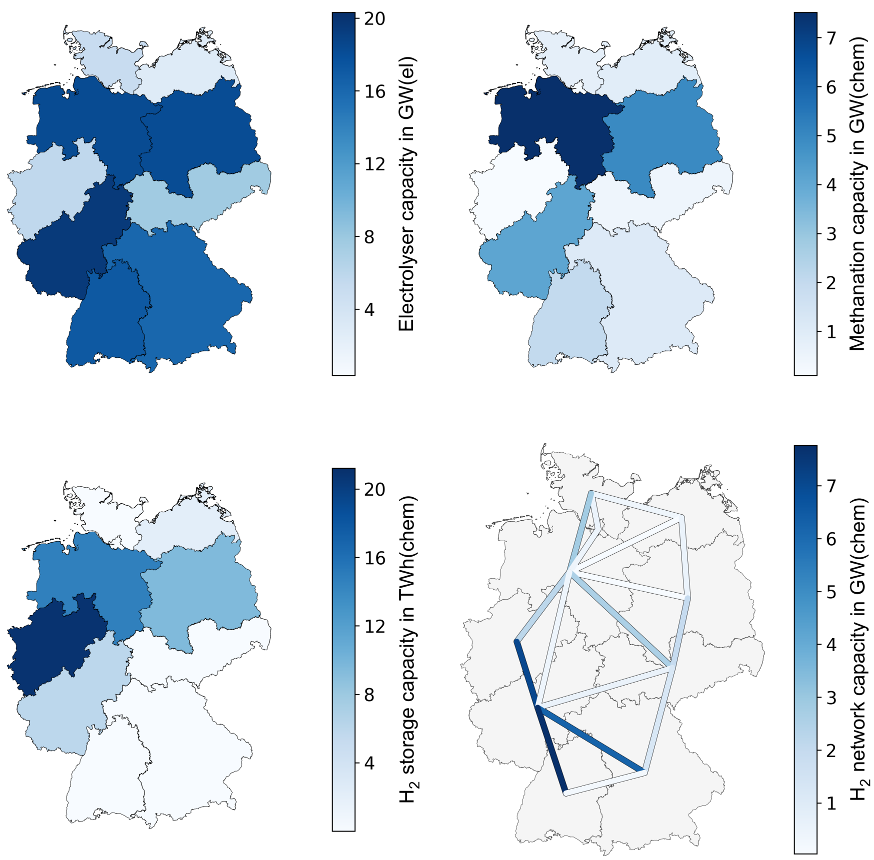

Figure 8: Regional distribution of hydrogen infrastructure in the scenario year 2050.

electrolyser capacity reaches a total of 111 GW, corresponding to more than the current electricity generation capacity of all thermal power plants in Germany [30]. For the seasonal storage of hydrogen, underground storage facilities with a capacity of 53 TWh are required, amounting to about a quarter of today's existing natural gas storage capacities [31]. An essential element of the hydrogen infrastructures is the construction of a transport network between the model regions in Germany. This enables regional decoupling of the production, storage, methanation and demand for hydrogen. Their overall capacity reaches 35 GW, which is only a fraction of today's existing natural gas transport capacities. This suggests that a partial reassignment of the existing stock could be an attractive option to reduce costs. Pipelines are built to connect the large electrolyser capacities in the southwest of the country to the demand centres in the west and south as well as to the hydrogen cavern storage facilities in the north (Figure 8). The aggregated methanation capacity in 2050 reaches about 22 GW(H_2).

3.4. Operation of flexible sector coupling

The time series of the plant operation offer additional insights into the balancing of the fluctuating VRE feed-in (Figure 9). The operation of the electrolysers shows a very strong correlation with VRE power generation (Figure 9a, 9b). Periods of high wind and PV electricity generation are clearly visible. Very little hydrogen is produced in winter, which is related to the higher demand for heat. With the exception of some lull periods, HP in DH run almost continuously during the heating period, in summer they use parts of the midday sun to produce hot water for the evening and night (Figure 9c). Very high generation peaks are absorbed by the electric boilers in DH and industry, which reach about 1100 annual FLHs. The high PV electricity production during the midday hours is still used for the charging of BEVs (Figure 9d) and stationary electricity storage. These storage facilities are then preferably discharged in the morning and evening hours (Figure 9e). In contrast to the electrolysers, the methanation plants only show a seasonal characteristic (Figure 9f). This operating behaviour is also reflected in the storage level of the hydrogen and methane storages, which exhibit a seasonal pattern with maximum filling levels in December (Figure 10).

3.5. Scenario variants

The analysis of the scenario variants (Table 1) focuses on changes in the power generation structure, system costs and the capacities of load balancing options. It is limited to the year 2050, where the greatest effects can be observed.

Structural changes in the power supply structure are only triggered by an import of green hydrogen and the inhibition of power grid expansion (Figure 11). With lower grid capacities, power imports are significantly reduced, which requires a higher domestic generation from both VRE and controllable power plants. In contrast to that, domestic PV and wind offshore power generation is substantially reduced by hydrogen imports. All other scenario variants exhibit

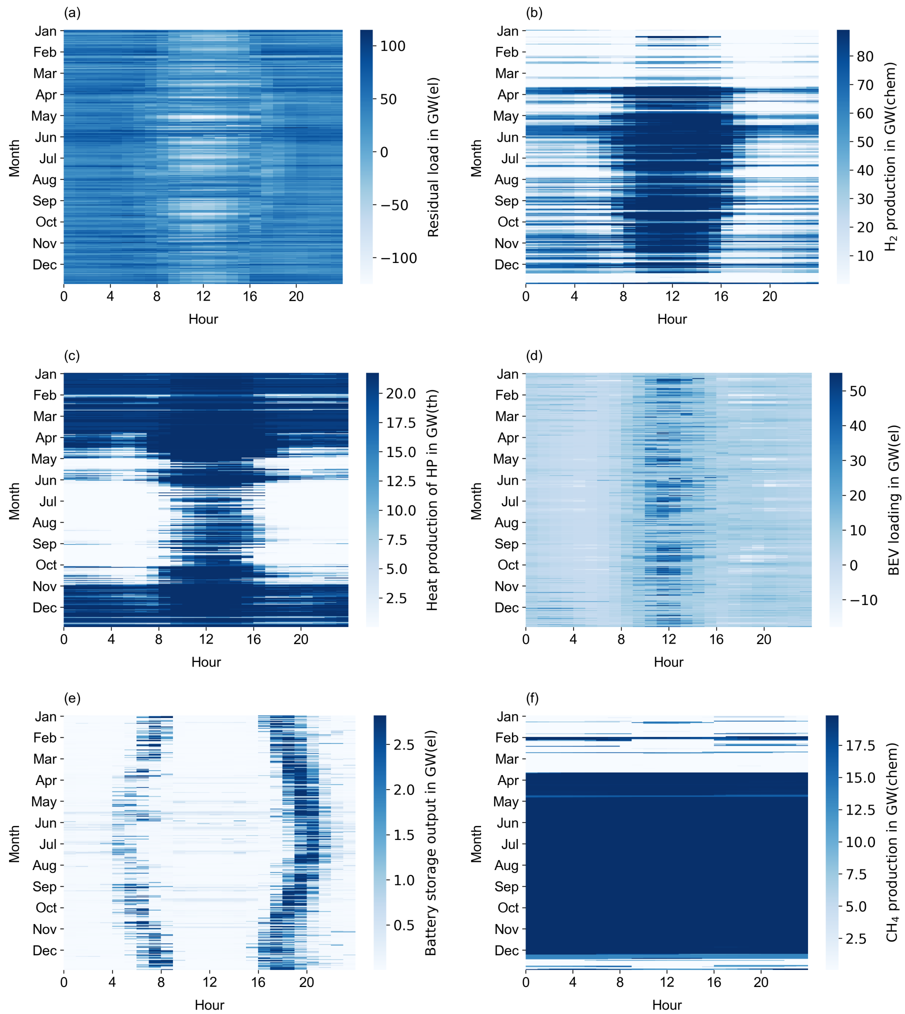

Figure 9: Hourly residual load (a), operation of hydrogen electrolysers (b), electric HPs in DH (c), BEVs (d), stationary battery storage (e), and methanation (f) in the scenario year 2050.

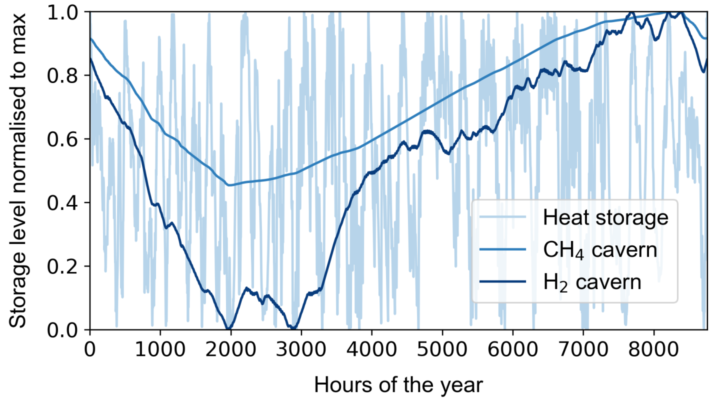

Figure 10: Storage filling levels over the course of the year normalised to their maximum value.

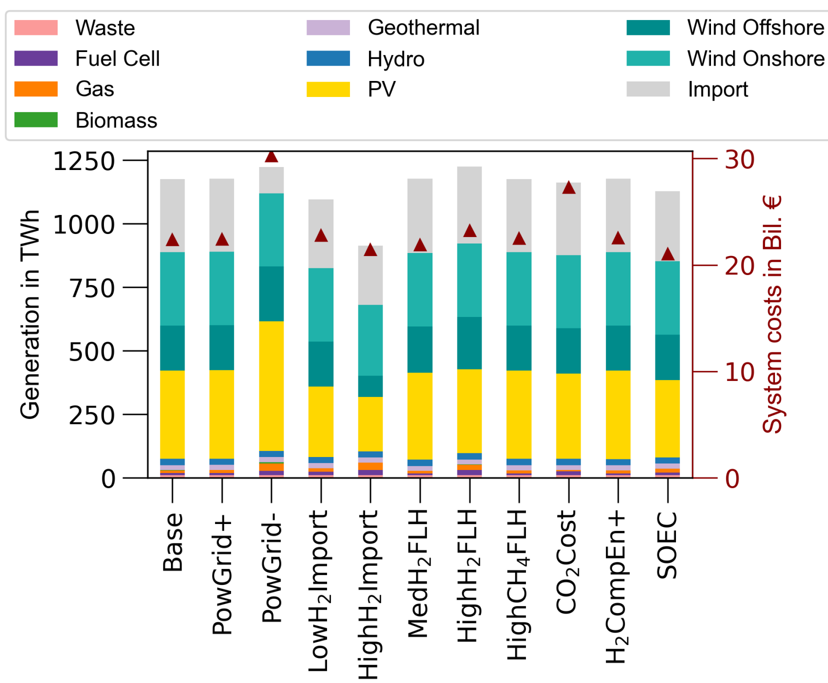

Figure 11: Electricity generation (left axis) and system costs (right axis) in the scenario variants. These are defined in Table 1. All values for Germany and the scenario year 2050.

only minor changes in both overall amount and structure of power generation in Germany. A significant increase in supply costs is observed for the limited grid expansion (+35 %), which requires the usage of more expensive balancing technologies, and consideration of CO_2 costs (+22 %). The highest reduction is achieved by the usage of more efficient electrolysers (−6 %), while all other variants change the system costs by less than 5 %.

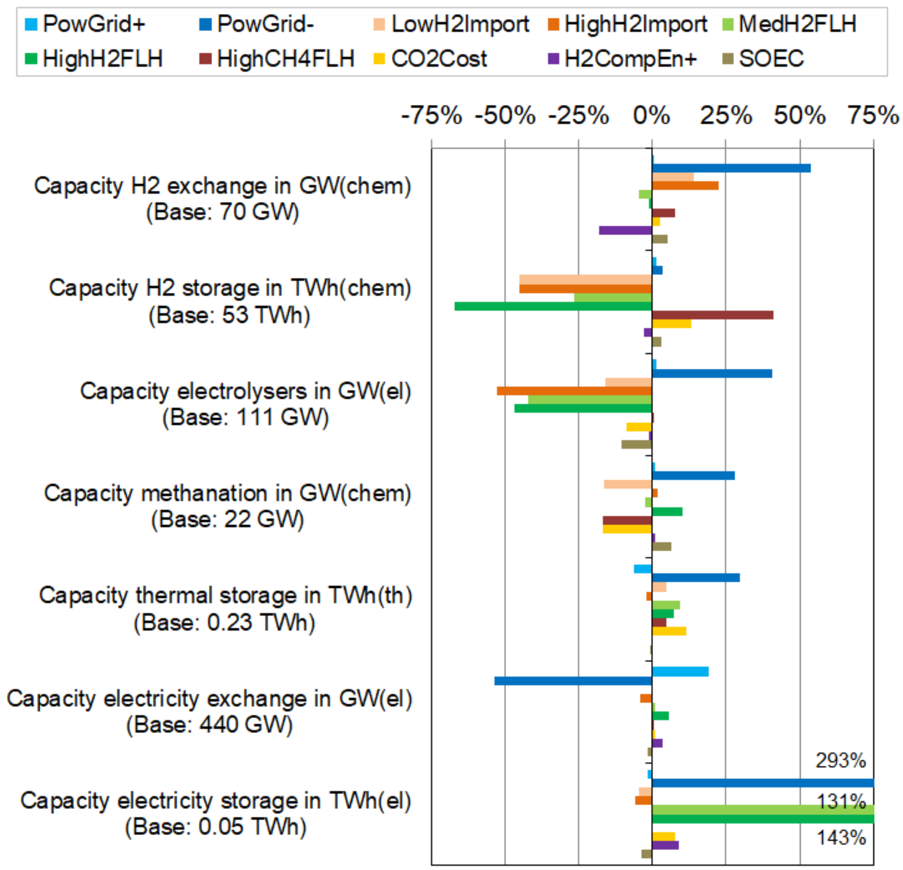

Figure 12: Deviations in the capacities of balancing technologies in the scenario variants compared to the base scenario. The scenario variants are defined in Table 1. All values for Germany and the scenario year 2050.

The effect of the scenario variants on the capacities of the balancing technologies is more diverse (Figure 12). Nevertheless, the construction of large-scale hydrogen infrastructures and the minor use of renewable fuels for electricity and heat supply proves to be robust against the various and diverse additional boundary conditions. This also applies to the positive interaction of a model-endogenous exploitation of all available load balancing options.

Limited power grid expansion is compensated by an increase in the capacities of almost all other balancing technologies. To bridge periods of low VRE availability, much higher amounts of methane are needed, which is reflected in higher electrolyser and methanation capacities. Their flexible operation contributes to the balancing, such as additional electric and thermal storage systems. Additional spatial balancing is realised through a steep increase in hydrogen pipeline capacity.

If hydrogen is imported or produced more continuously, electrolyser and hydrogen storage capacities can be reduced notably. Ship-based hydrogen imports reduce the production especially in the coastal regions and require the installation of additional pipelines, while other balancing technologies are almost not affected. In contrast, enforced higher annual FLHs of electrolysers require additional thermal and especially electric storage capacities. The consideration of CO_2 costs and minimum FLHs for methanation plants have an almost identical effect on the methanation capacity. Nonetheless, their impact on the system operation is very different. The CO_2 costs significantly reduce the production and usage of methane, which is compensated by all available storage technologies. Contrary to that, the minimum FLHs require additional flexibility almost exclusively in the hydrogen system.

An unlimited expansion of power lines increases their capacity notably, while not significantly affecting any of the other technologies. This implies that the applied limit of 5 GW per connection and decade does not pose a major constraint. Similarly, the consideration of higher compression energy demands notably reduces the hydrogen transfer capacities, but does not affect the other balancing technologies. The implementation of balancing technologies is furthermore robust against the availability of more efficient electrolysers.

4. Discussion

Our results offer a broad spectrum of findings on the transformation of the German energy system in general, and on the design and use of flexible sector coupling in particular. By additionally considering the gas sector in an energy system model, we are able to analyse the interactions between different options for flexible sector coupling much more comprehensively than before. This can provide a more informed basis for decisions on policy strategies and targets, but also for the definition of incentive mechanisms. By simultaneously optimising the different load balancing options, their least-cost combined design can be evaluated more comprehensively than was the case in previous work, which mostly focused on individual areas of sector coupling. A comparison with the similar study [13] shows the additional challenges of a completely climate-neutral energy supply. This includes, for example, the even higher electrolysis capacities required and the complete replacement of fossil natural gas. The results of [12] indicate that the reassignment of natural gas pipelines to hydrogen enables cost reductions compared to the construction of new pipelines. This suggests that hydrogen pipelines could have an even more important role in the system than in our case study, which only allows for new construction.

The analysis is subject to various limitations resulting from the modelling approach. For example, infrastructures are aggregated to the model regions considered, which means that effects on smaller spatial scales and line-specific grid bottlenecks are not visible. This can have relevant effects on the plant distribution, for example of the electrolysers. Furthermore, despite the comparatively high technological resolution of the analysis, technologies have to be partially aggregated or neglected, which concerns, for example, the consideration of different wind turbine types or power plant size classes. Furthermore, the abstraction of technology use to a system of linear equations with a manageable number of input parameters can in part only approximate reality. The necessity of these aggregations and simplifications results from the challenge of keeping the size of the system of equations to be optimised within the limits of what can be solved with the available computing resources. These model-related limitations imply that conclusions about the operation of individual plants can only be drawn to a limited extent. These require detailed technological modelling, which can be based on our results with regard to the interaction with the surrounding energy system.

A certain distortion in the results can arise due to the fact that the use of flexible sector coupling is only considered in Germany. This implies the assumption that the operation of decentralised flexibility options abroad is not geared to the needs in Germany and can therefore be neglected. As a consequence, the flexibility demand in the other countries has to be covered by a reduced range of technologies and at higher costs. This is reflected in a much greater expansion of battery storage and power grid capacity than in Germany.

In addition, the modelled system does not include the entire transport sector, as the fuel quantities required for air and shipping traffic are not considered. To provide these in a climate-neutral way, significant additional VRE capacities are required, or an import would have to be realised.

With regard to the capacities shown, it should be noted that, with the exception of DH, backup capacities were not taken into account. Additional capacities to the extent of the desired backup would therefore be necessary to protect against the failure of individual system components.

It is inherent in the consideration of future scenarios that they are based on uncertain assumptions regarding the development of energy demand and technology development in particular, but also user behaviour. Thus, the results are subject to these assumptions. The effects of some of the crucial assumptions are examined more closely via the scenario variants; others were addressed in earlier work with the REMix model [21, 32, 33]. Further scenario variants with a similar model setup show that the restrictions applied to TES and HPs in DH have only limited effect on the model results, that decentralised battery storage can partially substitute flexible sector coupling at the expense of higher costs, and that a limited potential of PV can be compensated by biomass and solar thermal heating [20].

5. Conclusions

This work underlines that a complete avoidance of emissions in the German energy system is accompanied by a significant increase in the demand for new infrastructures, including a tripling of the installed power plant capacity compared to today. The integrated capacity and operation optimisation of all options for flexible sector coupling reveals that these are all needed, fulfil different functions and partly benefit from each other. Although flexible hydrogen generation is a key contributor to VRE integration in 2050, it does not replace other sector coupling options. Thus, the design of sector coupling must be geared to the use of all available flexibility. In the heat supply, this concerns the usage of thermal storage and hybridisation of generation, for BEVs controlled and bidirectional charging.

Furthermore, the results show that the construction of large-scale infrastructures for hydrogen production, transport and storage can help to reduce supply costs. Despite the possibility of transport, we find no strong geographical concentration of hydrogen production and storage. On the way to climate neutrality in 2050, the construction of hydrogen infrastructures must begin as early as this decade. This includes both the deployment of large cavern storage and a Germany-wide hydrogen transport network. Our results suggest that reassignment of existing natural gas infrastructure may be an attractive option in this regard. Relying on these infrastructures, hydrogen is a key element for providing seasonal balancing. This indicates that the use of hydrogen in transport and industry increases the attractiveness of its use in other areas and should be accompanied by the development of seasonal storage capacities. These are supplemented by electrical and thermal energy storage systems that compensate for fluctuations on a daily and weekly level respectively.

Despite the massive increase in wind and PV capacities, virtually no VRE generation needs to be curtailed. In winter, generation peaks are absorbed by electric boilers in heating networks and during the rest of the year by electrolysers for hydrogen production. The model results show that power system benefits justify large-scale domestic hydrogen production despite higher costs.

According to the model results, the power grid also plays a central role in load balancing. If further expansion of the grid is not possible, the balancing must and can be provided by greater use of sector coupling and stationary battery storage. However, this is accompanied by a substantial increase in system costs.

Against the background of our results, the focus of further research and development should not be limited to individual sector coupling options but should rather encompass their full range. This includes modelling which must consider the interplay of technologies in even greater spatial, temporal and technological detail, and be based on a wider range of scenarios. In addition, aspects of resilience and security of supply of highly coupled energy systems deserve complementary attention. Additionally, the European interactions in the gas system, the production and use of synthetic fuels, and the conversion of infrastructures, for example from natural gas to hydrogen must be further examined in future work. Furthermore, the interaction of a domestic hydrogen supply with possible imports must be analysed in detail, as well as the availability and cost of CO_2 for the production of methane and other hydrocarbons.

Acknowledgements

The research for this paper was performed within the projects 'MuSeKo' and 'Fahrplan Gaswende' supported by the German Federal Ministry of Economic Affairs and Energy under grant numbers 03ET4038B and 03EI1030B. The authors thank Thomas Pregger, Max Fette, Johannes Schaffert, Christine Brandstädt, Eren Tali, and all current and former members of the EnSyM group of DLR for their contribution to the input data provision and continuous discussion about the model results. Furthermore, the authors acknowledge the contribution of Felix Cebulla, Manuel Wetzel and Eileen Meyer to the development and testing of the gas sector enhancement of REMix.

Author contribution

Hans-Christian Gils: Conceptualisation, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing - Original draft preparation, Writing - Review & Editing, Visualisation, Supervision, Project administration, Funding acquisition

Hedda Gardian: Software, Validation, Formal analysis, Investigation, Data curation, Writing - Original draft preparation, Visualisation, Supervision

Jens Schmugge: Writing - Original draft preparation

Data Availability

The technology and capacity data used in the model are available in [DataFile][3]. All other raw data supporting the conclusions of this manuscript will be made available by the authors to any qualified researcher.

Conflicts of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

[3]For review purposes, a detailed input data file is provided as additional material. Upon acceptance, it will be made available online and the link included here.

Appendix A. Gas system representation in REMix

Nomenclature

Table A.3: Variables used in the model description.

Symbol	Unit	Variable
$\boldsymbol{C}_{\text{emission}}$	k€/a	Emission certificate costs
$\boldsymbol{C}_{\text{fuel}}$	k€/a	Fuel costs
$\boldsymbol{C}_{\text{invest}}$	k€/a	Proportionate investment costs
$\boldsymbol{C}_{\text{OMFix}}$	k€/a	Fixed operation and maintenance costs
$\boldsymbol{C}_{\text{OMVar}}$	k€/a	Variable operation and maintenance costs
$\boldsymbol{C}_{\text{unsupplLoad}}$	k€/a	Penalty costs for not supplied demand
$\boldsymbol{C}_{\text{WaT}}$	k€/a	Wear and tear costs
$\boldsymbol{P}_{\text{addedCap}}$	$\text{GW}_{\text{el/chem}}$	Capacity of additional units
$\boldsymbol{P}_{\text{charge}}(t)$	GW_{chem}	Gas storage energy input
$\boldsymbol{P}_{\text{compGasDem}}(t)$	GW_{chem}	Gas demand of compressors
$\boldsymbol{P}_{\text{compGridLoad}}(t)$	GW_{el}	Grid power demand of compressors
$\boldsymbol{P}_{\text{compPow}}(t)$	GW_{comp}	Compaction power provided
$\boldsymbol{P}_{\text{discharge}}(t)$	GW_{chem}	Gas storage energy output
$\boldsymbol{P}_{\text{elLoad}}(t)$	GW_{el}	Electrolyser power demand
$\boldsymbol{P}_{\text{endDem}}(t)$	GW_{chem}	Endogenous gas demand, e. g. of power plants
$\boldsymbol{P}_{\text{flowIn}}(t)$	GW_{chem}	Gas import flow over pipelines
$\boldsymbol{P}_{\text{flowOut}}(t)$	GW_{chem}	Gas export flow over pipelines
$\boldsymbol{P}_{\text{fuelIn}}(t)$	GW_{chem}	Fuel input to the converter
$\boldsymbol{P}_{\text{fuelOut}}(t)$	GW_{chem}	Fuel output of the converter
$\boldsymbol{P}_{\text{gasTransp}}(t)$	GW_{chem} km	Potential energy for gas transport
$\boldsymbol{P}_{\text{H2Prod}}(t)$	GW_{chem}	Hydrogen production
$\boldsymbol{P}_{\text{import}}(t)$	GW_{chem}	Gas imported from outside the modelled regions
$\boldsymbol{P}_{\text{negPowCh}}(t)$	GW_{chem}	Negative load change of fuel conversion
$\boldsymbol{P}_{\text{posPowCh}}(t)$	GW_{chem}	Positive load change of fuel conversion
$\boldsymbol{P}_{\text{unsupplLoad}}(t)$	GW_{chem}	Not supplied gas demand
$\boldsymbol{W}_{\text{addCapSt}}$	GWh_{chem}	Capacity of additional storage reservoir units
$\boldsymbol{W}_{\text{level}}(t)$	GWh_{chem}	Gas storage filling level

Table A.4: Parameters used in the model description.

$P_{\mathrm{exDem}}(t)$	$\mathrm{GW_{chem}}$	Exogenously defined gas demand
P_{existCap}	$\mathrm{GW_{el/chem}}$	Installed capacity of a technology
$W_{\mathrm{existCapSt}}$	$\mathrm{GWh_{chem}}$	Installed storage reservoir capacity
W_{maxCapSt}	$\mathrm{GWh_{chem}}$	Maximum storage reservoir capacity
c_{OMFix}	%/a	Operation and maintenance fix costs per year
c_{OMVar}	k€/MWh	Operation and maintenance variable costs
c_{WaT}	k€/MW	Wear and tear costs
c_{specInv}	k€/MW	Specific investment cost
$c_{\mathrm{unsupplLoad}}$	k€/$\mathrm{MWh_{chem}}$	Specific penalty cost for not supplied gas demand
f_{annuity}	-	Annuity factor
i	%	Interest rate
l_{landLine}	km	Length of power lines at land
l_{seaLine}	km	Length of power lines at sea
$r_{\mathrm{gasTransp}}$	$\frac{\mathrm{GW_{comp}}}{\mathrm{GW_{chem}km}}$	Gas transport energy demand
$r_{\mathrm{storInject}}$	$\frac{\mathrm{GW_{comp}}}{\mathrm{GW_{chem}}}$	Compression energy demand for storage injection
s_{maxPow}	$\frac{1}{100}$	Maximum hourly charging/discharging relative to storage capacity
t_{a}	a	Amortisation time
Δt	h	Calculation time interval
η_{charge}	$\frac{1}{100}$	Storage charging efficiency
η_{compEl}	$\frac{1}{100}$	Electrical compressor efficiency
η_{compGas}	$\frac{1}{100}$	Gas compressor efficiency
$\eta_{\mathrm{discharge}}$	$\frac{1}{100}$	Storage discharging efficiency
η_{el2fuel}	$\frac{1}{100}$	Electrolyser efficiency
$\eta_{\mathrm{fuel2fuel}}$	$\frac{1}{100}$	Fuel conversion efficiency
η_{inject}	$\frac{1}{100}$	Fuel injection efficiency
η_{self}	$\frac{1}{100}$	Storage self-discharging rate

To facilitate the analysis of comprehensive sector coupling and the impact of large-scale hydrogen infrastructures, the REMix model is extended to include the production, import, storage, transport, and usage of gas. Due to the large technological scope and the spatial resolution of the model, any extension must be based on substantial simplifications, which are described in the following.

Key requirement is a fully linearised representation of the gas sector. Furthermore, the use of integer variables has to be avoided to limit the model solution time. In line with the model's focus on energy quantities, neither pressures nor temperatures are explicit variables of the model. Rather, the chemical energy of the gas serves as the central model variable. The fact that REMix does not reflect any information about system operation within the model regions, implies that gas transport within regions is possible without restriction.

To model the different components of the gas system in REMix, different modules with specific functionalities of individual system elements are implemented. The modules can be flexibly networked with one another by means of energy flows as for example shown in Figure 4.

REMix input generally consists of sets and parameters. Parameters provide the technology and scenario input data for the optimisation, whereas sets are the indices that specify the domains of parameters, variables and equations. For better readability of the model equations, parameters and variables are displayed differently: variables are always written in bold font and parameters in normal font. Furthermore, all variables, parameters and equations are shown in a reduced denotation here. This concerns the boundary conditions of all variables only allowed to have positive values on the one hand, and the waiver of the sets indicating that all equations are applied to each model node and year on the other.

Gas demand

The model considers endogenous $\boldsymbol{P}_{\mathrm{endDem}}(t)$ and exogenous $P_{\mathrm{exDem}}(t)$ gas consumption. For the exogenous demand, which is separate for different gases, a standardised profile or the maximum withdrawal rate per time unit can be specified.

Hydrogen electrolysis

The electrolyser module considers the energetic flows of electricity as input $\boldsymbol{P}_{\mathrm{elLoad}}$ and hydrogen as output $\boldsymbol{P}_{\mathrm{H2Prod}}$, which can be converted into each other by a conversion factor η_{el2fuel} according to Eq. (A.1).

$$\boldsymbol{P}_{\mathrm{H2Prod}}(t) = \boldsymbol{P}_{\mathrm{elLoad}}(t) \cdot \eta_{\mathrm{el2fuel}} \qquad \forall\ t \tag{A.1}$$

The maximum fuel production is limited by the exogenously defined P_{existCap} and endogenously added capacity $\boldsymbol{P}_{\mathrm{addedCap}}$ according to Eq. (A.2).

$$\boldsymbol{P}_{\mathrm{H2Prod}}(t) \overset{!}{\leq} (\boldsymbol{P}_{\mathrm{addedCap}} + P_{\mathrm{existCap}}) \qquad \forall\ t \tag{A.2}$$

The cost evaluation considers capital costs and operational costs. Capital costs $\boldsymbol{C}_{\mathrm{invest}}$ are considered for all endogenously added capacities $\boldsymbol{P}_{\mathrm{addedCap}}$ and calculated from the specific costs c_{specInv}, interest rate i and amortisation time t_{a} of the investment (Eq. (A.3) and Eq. (A.4)). Annual operational costs are composed of a fixed $\boldsymbol{C}_{\mathrm{OMFix}}$ and a variable $\boldsymbol{C}_{\mathrm{OMVar}}$ element: the previous scales with the capacity of newly installed units, the latter with the annual utilisation according to Eq. (A.5) and Eq. (A.6), respectively.

$$
\begin{aligned}
f_{\text{annuity}} &= \frac{i \cdot (1+i)^{t_{\text{a}}}}{(1+i)^{t_{\text{a}}} - 1} && \text{(A.3)} \\
\boldsymbol{C}_{\text{invest}} &= \boldsymbol{P}_{\text{addedCap}} \cdot c_{\text{specInv}} \cdot f_{\text{annuity}} && \text{(A.4)} \\
\boldsymbol{C}_{\text{OMFix}} &= \boldsymbol{P}_{\text{addedCap}} \cdot c_{\text{specInv}} \cdot c_{\text{OMFix}} && \text{(A.5)} \\
\boldsymbol{C}_{\text{OMVar}} &= \sum_{t} \boldsymbol{P}_{\text{H2Prod}}(t) \cdot c_{\text{OMVar}} \cdot \Delta t && \text{(A.6)}
\end{aligned}
$$

The module allows hydrogen to be fed into the natural gas system. A limitation of the hydrogen feed-in is done on an hourly basis and relative to the exogenous demand.

Methanation

This module considers the conversion of one fuel ($\boldsymbol{P}_{\text{fuelIn}}$) into another ($\boldsymbol{P}_{\text{fuelOut}}$). This conversion can go along with losses in the chemical energy caused by the conversion $\eta_{\text{fuel2fuel}}$ and subsequent compression, e g. for injection into a gas network η_{inject} according to Eq. (A.7). Additionally, an electricity demand of the conversion can be considered.

$$
(\boldsymbol{P}_{\text{fuelOut}} - \boldsymbol{P}_{\text{fuelIn}}) \cdot \eta_{\text{fuel2fuel}} \cdot \eta_{\text{inject}} = 0 \qquad \text{(A.7)}
$$

The hourly fuel input is limited according to Eq. (A.2), investment and fixed and variable operation costs according to Eq. (A.4), Eq. (A.5), and Eq. (A.6), respectively. For the methanation, an additional cost component arising from the consideration of simplified ramping costs can be considered. These are calculated according to Eq. (A.8), (A.9) and (A.10).

$$
\begin{aligned}
\boldsymbol{P}_{\text{posPowCh}}(t) &\geq \boldsymbol{P}_{\text{fuelIn}}(t) - \boldsymbol{P}_{\text{fuelIn}}(t-1) \qquad \forall\, t && \text{(A.8)} \\
\boldsymbol{P}_{\text{negPowCh}}(t) &\geq -\boldsymbol{P}_{\text{fuelIn}}(t) - \boldsymbol{P}_{\text{fuelIn}}(t-1) \qquad \forall\, t && \text{(A.9)} \\
\boldsymbol{C}_{\text{WaT}} &= \sum_{t} (\boldsymbol{P}_{\text{posPowCh}}(t) + \boldsymbol{P}_{\text{negPowCh}}(t)) \cdot c_{\text{WaT}} \cdot \Delta t && \text{(A.10)}
\end{aligned}
$$

Gas storage

This module is designed to represent storage technologies with gaseous input and output. Gas storage unit and converter unit are modelled separately. Central equation is the storage balance (Eq. (A.11)), which reflects all variations in the filling level. It assures that in every time step the change in storage level $\boldsymbol{W}_{\text{level}}$ equals the sum of storage input $\boldsymbol{P}_{\text{charge}}$, output $\boldsymbol{P}_{\text{discharge}}$, self discharge η_{self} and gas demand for compression $\boldsymbol{P}_{\text{compGasDem}}$. Losses arising at charging (η_{charge}) or discharging ($\eta_{\text{discharge}}$) are considered in the balance equation.

$$
\begin{aligned}
\boldsymbol{W}_{\text{level}}(t) = {} & \boldsymbol{W}_{\text{level}}(t-1) + \boldsymbol{P}_{\text{charge}}(t) \cdot \eta_{\text{charge}} - \frac{\boldsymbol{P}_{\text{discharge}}(t)}{\eta_{\text{discharge}}} \\
& - \frac{\boldsymbol{W}_{\text{level}}(t) + \boldsymbol{W}_{\text{level}}(t-1)}{2} \cdot \eta_{\text{self}} - \boldsymbol{P}_{\text{compGasDem}}(t) \qquad \forall\, t \quad \text{(A.11)}
\end{aligned}
$$

The hourly storage level is limited to the overall storage capacity in line with Eq. (A.2). To consider capacity restrictions, e. g. due to cavern availability, an upper limit to storage expansion W_{maxCap} can be defined according to Eq. (A.12).

$$\boldsymbol{W}_{\text{addCapSt}} + W_{\text{existCapSt}} \overset{!}{\leq} W_{\text{maxCapSt}} \tag{A.12}$$

Furthermore, charging (Eq. (A.13)) and discharging (Eq. (A.14)) can be limited to a certain share s_{maxPow} of the available storage capacity per hour.

$$\boldsymbol{P}_{\text{charge}}(t) \leq s_{\text{maxPow}} \cdot (W_{\text{existCapSt}} + \boldsymbol{W}_{\text{addStorCap}}) \qquad \forall\ t \tag{A.13}$$

$$\frac{\boldsymbol{P}_{\text{discharge}}(t)}{\eta_{\text{discharge}}} \leq s_{\text{maxPow}} \cdot (W_{\text{existCapSt}} + \boldsymbol{W}_{\text{addStorCap}}) \qquad \forall\ t \tag{A.14}$$

The module provides the possibility of a storage bypass to use the gas directly. As it is not entering the storage, no losses occur.

Storage charging requires the provision of compaction power $\boldsymbol{P}_{\text{compPow}}$, which can be provided using electric $\boldsymbol{P}_{\text{compGridLoad}}$ or gas compressors $\boldsymbol{P}_{\text{compGasDem}}$ according to Eq. (A.15), where η_{compGas} and η_{compEl} are the corresponding compression efficiencies.

$$\begin{aligned} \boldsymbol{P}_{\text{compPow}}(t) =& \boldsymbol{P}_{\text{compGridLoad}}(t) \cdot \eta_{\text{compEl}} \\ &+ \boldsymbol{P}_{\text{compGasDem}}(t) \cdot \eta_{\text{compGas}} \qquad \forall\ t \end{aligned} \tag{A.15}$$

Compression is in each case limited by the available capacities in accordance with Eq. (A.2). The amount of gas that can be injected into the storage with the provided compaction power is calculated considering an injection efficiency according to Eq. (A.16).

$$\boldsymbol{P}_{\text{charge}}(t) \leq \frac{\boldsymbol{P}_{\text{compPow}}(t)}{r_{\text{storInject}}} \qquad \forall\ t \tag{A.16}$$

Costs are calculated using Eq. (A.4), Eq. (A.5) and Eq. (A.6) considering investment and operational costs of the storage and compressors.

Gas transport

The gas transport between the model regions is considered in a simplified way. Gas pipelines are defined by a chemical energy transfer capacity. They are fully available for gas export $\boldsymbol{P}_{\text{flowOut}}$ or import $\boldsymbol{P}_{\text{flowIn}}$ at any time, independent of pipelines to other regions. The energy flow along the lines is limited by the exogenous and endogenous line capacity according to with Eq. (A.2). The overall line capacity can be limited to an exogenous value similar to Eq. (A.12). Since the central variables are not pressures but capacities and energy quantities, the pressure loss during gas transport cannot be explicitly modelled. Rather, it is implicitly taken into account via the energy requirement of a pressure increase required for the gas transport over a certain distance. This gas transport energy demand $\boldsymbol{P}_{\text{gasTransp}}$ scales with the pipeline length (l_{landLine}, l_{seaLine}) and the volume of gas transported $\boldsymbol{P}_{\text{flowOut}}$.

$$\boldsymbol{P}_{\text{gasTransp}}(t) = \boldsymbol{P}_{\text{flowOut}}(t) \cdot (l_{\text{landLine}} + l_{\text{seaLine}}) \qquad \forall\ t \tag{A.17}$$

The gas transport energy $\boldsymbol{P}_{\text{gasTransp}}$ is calculated from the overall compressor output $\boldsymbol{P}_{\text{compPow}}$ and the gas transport efficiency $\eta_{\text{gasTransport}}$ according to Eq. (A.18).

$$\boldsymbol{P}_{\text{gasTransp}}(t) \leq \frac{\boldsymbol{P}_{\text{compPow}}(t)}{r_{\text{gasTransp}}} \qquad \forall\ t \tag{A.18}$$

The overall compaction power $\boldsymbol{P}_{\text{compPow}}$ again depends on the operation and efficiencies of the compressors according to Eq. (A.15). As for the compressors in gas storage, compaction is furthermore limited by the available compressor capacity (Eq. (A.12)). Consequently, the amount of gas that can be transferred depends on the energy consumption of electric or gas compressors. The energy demand for gas transport is considered for individual pipelines and not for the nodes. This means that a pressure increase for the transport of gas from node A to node B has no effect on any pipelines to other nodes. Furthermore, it is assumed that compression power available in a region can be used completely for each of the pipelines. This implies that Eq. (A.17) is applied to the sum of all outgoing pipelines of each node. A restriction of the transport over individual lines results on the one hand from their capacity and on the other hand from the available compression power that is not used for transport through other lines. It is further assumed that the chemical energy of the transported gas remains constant, unless gas is used to operate the compressors.

The costs of gas transport are calculated from the investment in gas pipelines and compressors according to Eq. (A.4) as well as their operational costs (Eq. (A.5) and (A.6)).

Gas import

To consider gas imports from outside the modelled regions, import flows $\boldsymbol{P}_{\text{import}}$ of different gases can be assigned to individual regions. Thereby, a limitation of the annual energy quantity and the hourly output can be specified. To differentiate between the different import gases, emission factors and specific costs can be assigned to the imports.

Gas balance

The gas balance (Eq. (A.19)) assures that the inflow and outflow equals each other for each model node and gas type considered.

$$
\begin{aligned}
&\boldsymbol{P}_{\text{fuelOut}}(t) + \boldsymbol{P}_{\text{H2Prod}}(t) + \boldsymbol{P}_{\text{unsupplLoad}}(t) + \boldsymbol{P}_{\text{import}}(t) \\
&\qquad + \boldsymbol{P}_{\text{discharge}}(t) + \boldsymbol{P}_{\text{flowIn}} = \\
&\boldsymbol{P}_{\text{fuelIn}}(t) + \boldsymbol{P}_{\text{endDem}}(t) + P_{\text{exDem}}(t) + \boldsymbol{P}_{\text{charge}}(t) + \boldsymbol{P}_{\text{flowOut}} \qquad \forall\ t
\end{aligned} \tag{A.19}
$$

The term $\boldsymbol{P}_{\text{unsupplLoad}}$ allows the model to leave some of the gas demand unsupplied. However, this is related to additional costs $\boldsymbol{C}_{\text{unsupplLoad}}$, which are calculated considering penalty costs $c_{\text{unsupplLoad}}$ according to Eq. (A.20).

$$
\boldsymbol{C}_{\text{unsupplLoad}} = \sum_t \boldsymbol{P}_{\text{unsupplLoad}}(t) \cdot c_{\text{unsupplLoad}} \cdot \Delta t \tag{A.20}
$$

References

[1] M. Victoria, K. Zhu, T. Brown, G. B. Andresen, M. Greiner, Early decarbonisation of the European energy system pays off, Nature Communications 11 (1) (2020) 6223. doi:10.1038/s41467-020-20015-4.

[2] G. Luderer, Z. Vrontisi, C. Bertram, O. Y. Edelenbosch, R. C. Pietzcker, J. Rogelj, H. S. de Boer, L. Drouet, J. Emmerling, O. Fricko, S. Fujimori, P. Havlík, G. Iyer, K. Keramidas, A. Kitous, M. Pehl, V. Krey, K. Riahi, B. Saveyn, M. Tavoni, D. P. van Vuuren, E. Kriegler, Residual fossil CO_2 emissions in 1.5–2°C pathways, Nature Climate Change 8 (7) (2018) 626–633. doi:10.1038/s41558-018-0198-6.

[3] P. J. Heptonstall, R. J. K. Gross, A systematic review of the costs and impacts of integrating variable renewables into power grids, Nature Energy 6 (1) (2021) 72–83. doi:10.1038/s41560-020-00695-4.

[4] T. Brown, D. Schlachtberger, A. Kies, S. Schramm, M. Greiner, Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system, Energy 160 (2018) 720–739. doi:10.1016/j.energy.2018.06.222.

[5] S. Samsatli, I. Staffell, N. J. Samsatli, Optimal design and operation of integrated wind-hydrogen-electricity networks for decarbonising the domestic transport sector in Great Britain, International Journal of Hydrogen Energy 41 (1) (2016) 447–475. doi:10.1016/j.ijhydene.2015.10.032.

[6] S. Samsatli, N. J. Samsatli, The role of renewable hydrogen and interseasonal storage in decarbonising heat – Comprehensive optimisation of future renewable energy value chains, Applied Energy 233-234 (2019) 854–893. doi:10.1016/j.apenergy.2018.09.159.

[7] P. Fu, D. Pudjianto, X. Zhang, G. Strbac, Integration of hydrogen into multi-energy systems optimisation, Energies 13 (7) (2020) 1606. doi:10.3390/en13071606.

[8] H. Ameli, M. Qadrdan, G. Strbac, M. T. Ameli, Investing in flexibility in an integrated planning of natural gas and power systems, IET Energy Systems Integration 2 (2) (2020) 101–111. doi:10.1049/iet-esi.2019.0065.

[9] L. Welder, D. Ryberg, L. Kotzur, T. Grube, M. Robinius, D. Stolten, Spatio-temporal optimization of a future energy system for power-to-hydrogen applications in Germany, Energy 158 (2018) 1130–1149. doi:10.1016/j.energy.2018.05.059.

[10] M. Reuß, T. Grube, M. Robinius, D. Stolten, A hydrogen supply chain with spatial resolution: Comparative analysis of infrastructure technologies in Germany, Applied Energy 247 (2019) 438–453. doi:10.1016/j.apenergy.2019.04.064.

[11] M. Reuß, T. Grube, M. Robinius, P. Preuster, P. Wasserscheid, D. Stolten, Seasonal storage and alternative carriers: A flexible hydrogen supply chain model, Applied Energy 200 (2017) 290–302. doi:10.1016/j.apenergy.2017.05.050.

[12] S. Cerniauskas, A. Jose Chavez Junco, T. Grube, M. Robinius, D. Stolten, Options of natural gas pipeline reassignment for hydrogen: Cost assessment for a Germany case study, International Journal of Hydrogen Energy 45 (21) (2020) 12095–12107. doi:10.1016/j.ijhydene.2020.02.121.

[13] DBI Gas- und Umwelttechnik GmbH, Institute of Energy and Climate Research (IEK), IAEW at RWTH Aachen University, Gasunie, TenneT, Phase II – Pathways to 2050. A joint follow-up study by Gasunie and TenneT of the Infrastructure Outlook 2050, Tech. rep., Gasunie and TenneT (2020). URL https://www.tennet.eu/fileadmin/user_upload/Company/News/German/Hoerchens/2020/200204_Phase_II_Project_report.pdf

[14] Y. Scholz, Renewable energy based electricity supply at low costs. Development of the REMix model and application for Europe, Dissertation, Universität Stuttgart, Stuttgart (2012). doi:10.18419/opus-2015.

[15] H. C. Gils, Y. Scholz, T. Pregger, D. Luca de Tena, D. Heide, Integrated modelling of variable renewable energy-based power supply in Europe, Energy 123 (2017) 173–188. doi:10.1016/j.energy.2017.01.115.

[16] H. C. Gils, S. Simon, Carbon neutral archipelago – 100% renewable energy supply for the Canary Islands, Applied Energy 188 (2017) 342–355. doi:10.1016/j.apenergy.2016.12.023.

[17] H. Gils, S. Simon, R. Soria, 100% renewable energy supply for Brazil—The role of sector coupling and regional development, Energies 10 (11) (2017) 1859. doi:10.3390/en10111859.

[18] H. C. Gils, Balancing of intermittent renewable power generation by demand response and thermal energy storage, Dissertation, Universität Stuttgart, Stuttgart (2015). doi:10.18419/opus-6888.

[19] D. Luca de Tena, T. Pregger, Impact of electric vehicles on a future renewable energy-based power system in Europe with a focus on Germany, International Journal of Energy Research 42 (8) (2018) 2670–2685. doi:10.1002/er.4056.

[20] M. Fette, C. Brandstätt, H. Gardian, T. Pregger, J. Schaffert, E. Tali, N. Brücken, Multi-Sektor-Kopplung (MuSeKo): Modellbasierte Analyse der Integration Erneuerbarer Stromerzeugung durch die Kopplung der Stromversorgung mit dem Wärme-, Gas- und Verkehrssektor. Endbericht, Tech. rep., Fraunhofer-Institut für Fertigungstechnik und Angewandte Materialforschung IFAM, Energiesystemanalyse and Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Institut für Technische Thermodynamik and Gas-und Wärme-Institut Essen e.V., Brennstoff- und Gerätetechnik (2020-08-31).
URL https://elib.dlr.de/135971/1/MuSeKo-Endbericht-2020-08-31.pdf#page=1&zoom=auto,-274,848

[21] H. C. Gils, T. Pregger, F. Flachsbarth, M. Jentsch, C. Dierstein, Comparison of spatially and temporally resolved energy system models with a focus on Germany's future power supply, Applied Energy 255 (2019) 113889. doi:10.1016/j.apenergy.2019.113889.

[22] K. M. Rippel, A. Preuß, M. Meinecke, R. König, Netzentwicklungsplan Strom 2030. Offshore-Netzentwicklungsplan 2030. Zahlen, Daten, Fakten, Tech. rep., 50 Hertz Transmission GmbH and Amprion GmbH and TenneT TSO GmbH and TransnetBW GmbH (2017).
URL https://www.netzentwicklungsplan.de/sites/default/files/paragraphs-files/NEP_2030_2_Entwurf_Zahlen-Daten-Fakten_online.pdf

[23] ENTSO-E, TYNDP 2016. Scenario Development Report. - Final after public consultation -, Tech. rep., ENTSO-E (2015).
URL https://www.entsoe.eu/Documents/TYNDP%20documents/TYNDP%202016/rgips/TYNDP2016%20Scenario%20Development%20Report%20-%20Final.pdf

[24] H. C. Gils, Economic potential for future demand response in Germany – Modeling approach and case study, Applied Energy 162 (2016) 401–415. doi:10.1016/j.apenergy.2015.10.083.

[25] Statistische Ämter des Bundes und der Länder, Regionaldatenbank Deutschland. 46251-01-02-4: Kraftfahrzeugbestand nach Kraftfahrzeugarten - Stichtag 01.01. - regionale Tiefe: Kreise und krfr. Städte. Stichtag: 01.01.2015 (2021).
URL https://www.regionalstatistik.de/genesis//online?operation=table&code=46251-01-02-4&bypass=true&levelindex=0&levelid=1619512343317

[26] H. C. Gils, Y. Scholz, F. Cebulla, K.-K. Cao, D. Luca de Tena, T. Pregger, Data input for the RegMex model experiment on the power system and flexible sector coupling (2019).
URL https://www.dlr.de/tt/en/Portaldata/41/Resources/dokumente/st/Model_Input_RegMex_ME2_final_corrected.xlsx

[27] ArcGis Resources. Europe NUTS 3 Demographics (2018).
URL https://resources.arcgis.com/de/help/main/10.1/index.html#/na/001z0000006q000000/

[28] ENTSO-E, Power Statistics (Archive) (2019).
URL https://www.entsoe.eu/data/power-stats/

[29] BMWi, Renewable energy sources in figures. National and international development, 2018, Tech. rep., Federal Ministry for Economics Affairs and Energy (2019-10).
URL https://www.bmwi.de/Redaktion/EN/Publikationen/renewable-energy-sources-in-figures-2018.html

[30] Bundesnetzagentur, List of power plants (2021).
URL https://www.bundesnetzagentur.de/EN/Areas/Energy/Companies/SecurityOfSupply/GeneratingCapacity/PowerPlantList/PubliPowerPlantList_node.html

[31] ENTSOG, GIE, System Development Map 2019/2020 (2020).
URL https://entsog.eu/sites/default/files/2021-01/ENTSOG_GIE_SYSDEV_2019-2020_1600x1200_FULL_047.pdf

[32] K.-K. Cao, T. Pregger, Grid expansion, power-to-gas and solar power imports - Multi-scenario analysis of large infrastructure options for the decarbonization of the European energy system, in: C. Rehtanz (Ed.), Internationaler ETG-Kongress 2019, ETG-Fachbericht, VDE Verlag GmbH, Berlin and Offenbach, 2019, pp. 16–21.

[33] M. Moser, H.-C. Gils, G. Pivaro, A sensitivity analysis on large-scale electrical energy storage requirements in Europe under consideration of innovative storage technologies, Journal of Cleaner Production 269 (2020) 122261. doi:10.1016/j.jclepro.2020.122261.