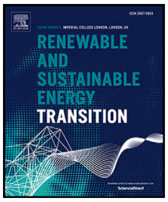
Renewable and Sustainable Energy Transition 6 (2025) 100094

Contents lists available at ScienceDirect

Renewable and Sustainable Energy Transition

journal homepage: www.journals.elsevier.com/renewable-and-sustainable-energy-transition



Full-length article

# Comprehensive and open model structure for the design of future energy systems with sector coupling

Beneharo Reveron Baecker [a,*], Thomas Hamacher [a], Viktor Slednev [b], Gian Müller [c,d], Vera Sehn [e], Jonas Winkler [e], Isela Bailey [e], Hedda Gardian [f], Hans Christian Gils [f], Christoph Muschner [g], Jann Michael Weinand [c], Ulrich Fahl [e]

[a] Technical University of Munich, School of Engineering and Design, Department of Energy and Process Engineering, Chair of Renewable and Sustainable Energy Systems, Lichtenbergstr. 4a, Munich, 85748, Bavaria, Germany
[b] Karlsruhe Institute of Technology (KIT), Institute for Industrial Production (IIP), Hertzstr. 16, Karlsruhe, 76187, Baden-Wuerttemberg, Germany
[c] Forschungszentrum Jülich GmbH, Institute of Climate and Energy Systems, Jülich Systems Analysis (ICE-2), Wilhelm-Johnen-Straße, Jülich, 52425, North Rhine-Westphalia, Germany
[d] RWTH Aachen University, Chair for Fuel Cells, Faculty of Mechanical Engineering, Eilfschornsteinstraße 18, Aachen, 52062, North Rhine-Westphalia, Germany
[e] Institute of Energy Economics and Rational Energy Use, Heßbrühlstraße 49a, Stuttgart, 70565, Baden-Wuerttemberg, Germany
[f] German Aerospace Center (DLR), Institute of Networked Energy Systems, Curiestraße 4, Stuttgart, 70563, Baden-Wuerttemberg, Germany
[g] Reiner Lemoine Institute, Rudower Ch 12, Berlin, 12489, Berlin, Germany

## ARTICLE INFO

Dataset link: OEP, DOI, documentation

*Keywords:*
Energy system modeling
Sector coupling
Renewable energy
Decarbonization
Model structure
Energy transition
Open source

## ABSTRACT

Energy system modeling supports the identification of the optimal technology mix to achieve decarbonization targets across multiple sectors. Especially when sector coupling is considered for future technology landscapes, the large solution space leads to a complex optimization problem in terms of computational feasibility and data requirements. The authors identify a research gap in developing an open-source model structure with consideration of the relevant future technologies of power, heat, other conversions, transport, and industry defined with a new level of detail in a sector-coupled energy world and in including detailed insights into the accompanying definition process. A strong focus is set on the transparency and reproducibility of the provided open-source structure and its flexible and consistent application to different framework families to foster the ease of applicability of this work. The paper first gives a detailed description of the model base, including an overview of the model frame definition process, the core adjustments to model sector coupling appropriately, and the measures to make the resulting problem computationally feasible. The core result of this work is the presentation of a detailed model structure to model sector coupling for a German energy system, yielding approximately 2000 processes that characterize the heterogeneous and technology-open landscape of existing and possible future technologies across relevant energy sectors. This supports energy system modelers in understanding and reproducing energy system models based on open-source data and thereby tries to accelerate the research on sector coupling and its role in the energy transition.

## 1. Introduction

Energy system modeling and its tools are strongly driven by the underlying research question. In the early years of modeling, the energy balance of a country or region was often the starting point in model generators such as MESSAGE [1] and MARKAL [2] and its successor, The Integrated MARKAL-EFOM System (TIMES) [3]. All final energy demand sectors were taken into account with a comprehensive collection of functions that enable the definition of models with rich technology detail. A central question was about the exploitation of fossil fuels and understanding the implications of a possible shortage. In the following decades, an additional key question had been the integration of Renewable Energy (RE) resources with their volatile temporal characteristics and their geographic heterogeneity. As a result, models with very high temporal and sometimes spatial resolution were created with model generators such as the Open Energy Modelling Framework (oemof) [4], often with a strong focus on the electricity sector instead of considering all final energy sectors consistently. In recent years, the combined consideration of all sectors and the special characteristics of renewables with possible direct and indirect applications has become particularly important for the achievement

---

[*] Corresponding author.
*E-mail address:* beneharo.reveron-baecker@outlook.com (B. Reveron Baecker).

https://doi.org/10.1016/j.rset.2024.100094
Received 14 March 2024; Received in revised form 26 August 2024; Accepted 28 August 2024

**Abbreviations**

| | |
|---|---|
| BEV | Battery Electric Vehicle |
| ICEV | Internal Combustion Engine Vehicle |
| RE | Renewable Energy |
| TCS | Trade, Commercial and Service |

of greenhouse gas neutrality. Only a combination of both aspects can adequately describe decarbonization strategies. Therefore, model generators such as the Framework for Integrated Energy System Assessment (ETHOS.FINE) [5] implemented additional aggregation methods to consider complex interactions through sector coupling.

It is important to consider these interactions as the ongoing energy transition and the related models are highly influenced by the diversity of future energy system components and their possible interactions through sector coupling. Consumers from different sectors and their related demands are merged together. First, their intersections increase through the conversion of electricity into additional secondary energy carriers that are exchanged through sectors. Second, they are actively involved within the constraints of the overall energy system through electricity or heating grid infrastructures as well as the technologies connected to them. Third, they can also act as prosumers or flexumers by decentrally feeding in their produced energy or providing flexibility services such as grid relief for the energy system by adjusting their demands, respectively. As a result, sector coupling is associated with a variety of possible multi-modal interfaces within the heterogeneous system and hence entails substantial challenges for modelers as the complexity increases significantly in terms of required knowledge, data, and computing power.

To deal with the latter, modelers have different possibilities: (a) implementing new framework features to describe both aspects in detail by applying well-known and promising decomposition approaches in optimization such as the alternating direction method of multipliers (ADMM) [6] or the Benders decomposition algorithm [7,8], and (b) the joint use of different modeling approaches, but based on a common database and reference energy system with a consistent model structure across all relevant energy sectors to create a common modeling environment, where the complexity can be regulated with individual aggregation measures for different modeling frameworks. To the best of the authors' knowledge, there is no such open and flexible model structure to define the related input data transparently.

As summarized in [9], there is a broad range of energy system optimization studies that focus on various research questions in different countries. Recent publications with German case studies have often focussed on the interdependencies from the power sector with chosen sectors such as heat [10–12] or transport [13–15] to analyze a specific research question. In comparison, in the present study, the sectors power, power-to-X & other conversion, heat, industry, and transport have been considered together in one harmonized model structure. Moreover, in the literature, a particular focus has been set on sector coupling and its influence on required network infrastructures considering spatial characteristics for the currently expected future technologies. For the German models [14,16] this has resulted in approximately up to 100 distinct processes or for the consulted European models [17–19] in up to 50 processes that have been defined for different spatial nodes each. In comparison, the present study focuses on the detailed technological characterization of possible future energy system landscapes resulting in 2000 parametrized processes for Germany. For instance, the model structure of the industry sector as described in Section 3.4 with approximately 500 processes to describe possible future production routes for energy-intensive industries offers a level of detail that, to the author's knowledge, has not been published and described open-source for energy system modeling tasks before. This increased level of detail results due to the following reasons. First, complex process chains consisting of multiple conversion steps have been considered instead of defining one aggregated process with various model-exogenous assumptions. This enables the investigation of critical sub-processes and the development of strategies for their decarbonization in a sector-coupled energy system. Although, some of the consulted studies considered all sectoral demands [16,19,20], different technological pathways with their associated technology landscape were generally determined by model-exogenous assumptions and scenarios, *e.g.*, regarding electrification rates in sectors. In contrast, there is a second difference and advantage of this approach, which is also responsible for the high number of processes. The reduction of exogenous assumptions by defining a technology-open model structure that does not only consider processes that are generally expected to prevail on the market under current assumptions on future developments but defines multiple parallel technologies that can also highly depend on the interactions between sectors. For instance, multiple furnace technologies have been defined for steel production in the industry sector, which depend on unforeseen gas price developments that would normally be ruled out in the optimization results and, as a result, have often been neglected. In comparison to the consulted literature, the introduced model structure is suitable to be used for different scenarios to get a more holistic view of possible energy system landscapes with special consideration of sector coupling and thereby enables analyzing tipping points for the selection between different substitutive technologies. This is described in more detail in Section 2.1.3.

Although a good representation of sector coupling requires good data, the reproduction of available models has been difficult due to little access to the model input data. Drawing clear conclusions only based on the results can be challenging as they are often dependent on the model generator that has been applied [21,22]. However, most publications focused on their model results instead of describing the model base, the model structure, and the underlying assumptions in detail. In comparison, in the present study, the focus lies on developing an open-source model structure and describing the methodology of the definition procedure in detail. Transparency and reproducibility, as well as the flexible and consistent application of the model structure to different framework families, are especially taken into account. Together with the data published on the Open Energy Platform, this article supports future modeling tasks that deal with holistic sector-coupled energy system models.

In summary, the scientific novelty of this work lies in the definition and comprehensive presentation of five harmonized energy sectors, with a particular focus on a diverse technological characterization. Furthermore, the model-exogenous selections are reduced in a technology-open definition approach. The resulting novel model structure is provided in an open-source format and is compatible with arbitrary model generators. In order to realize this, previous literature, models, and frameworks were analyzed, and the derived structure was refined in expert discussions within the project team, which has many years of modeling experience. Next, a common technology database is created to parametrize the introduced model structure. Therefore, a powerful model environment is developed that effectively incorporates the aspect of holistic modeling of the entire energy system with the specific description of renewable energies to depict sector coupling and its role in the energy transition. Taken together and as highlighted in Fig. 1, this yields a model structure that enables improved representation and understanding of sector coupling, and that is applicable across different model families. The usage of the model structure in the three different model generators TIMES [3], FINE [5], and oemof [4] demonstrates its flexible application. While other model generators such as PyPSA or Calliope would also be suitable for utilizing the developed model structure, TIMES, oemof and FINE were selected because the authors support their maintenance and also frequently use them for modeling tasks. Although it has been conceptualized for the German

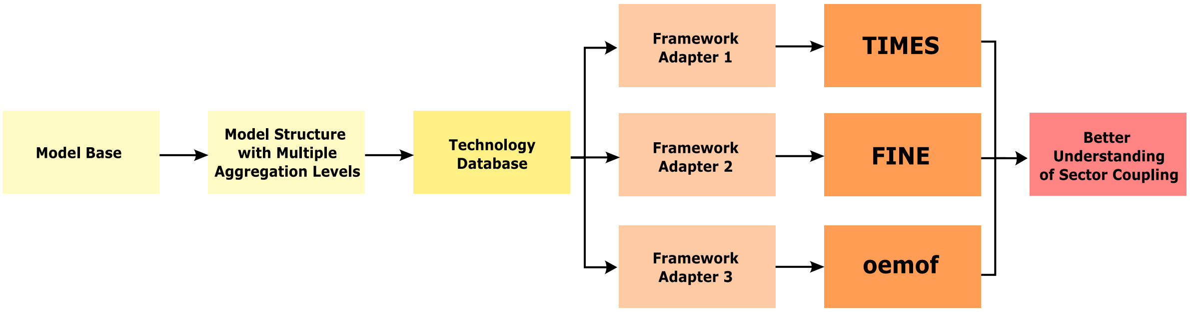


**Fig. 1.** Overview of the approach for developing an open and flexible model structure.

system, the technologies and their relation to the model structure can be transferred to other models of countries with similar energy system landscapes.

The study first gives an overview of the overall model base (Section 2) where not only the outcome but also the decision process to yield this outcome is described. After careful assessments of all sectors with mutual evaluations within the project team, the important technologies of the future energy system landscape are presented with the resulting model structure in Sections 3.1–3.5. Section 3.6 introduces the possible usage of graphical representations to foster the understanding of the resulting sectoral interfaces and in 3.7 limitations of the results are discussed. Finally, Section 4 gives an outlook and concludes the study.

## 2. Model base

The following sections present relevant aspects to define the model scope in the form of a short guideline (Section 2.1), including the core measures to make endogenous modeling of sector coupling more effective and the steps to create a computationally feasible problem (Section 2.2).

### *2.1. Defining a suitable model frame*

The scope of problems that can be tackled with existing energy system modeling frameworks is broad. Many general model frame settings should be defined before diving deep into technological details from the sectors, as they can influence the model structure and the related required input data substantially. While this process is regularly conducted in the energy system modeling landscape, it has not been elaborated in more common result-oriented publications. Therefore, the next section highlights the steps to raise awareness of these considerations and could be used as a supporting checklist for new energy system modelers. It is divided into three model frame formulation categories: problem scope (Section 2.1.1), temporal scope (Section 2.1.2), and feature scope (Section 2.1.3) which are illustrated in Fig. 2.

#### *2.1.1. Problem scope*

Essentially, the task of a modeler is to create simplified representations of real entities and their relations to be able to understand and analyze complex systems and thus also estimate future developments. Often, mathematical models are the backbone for these representations. In the energy system modeling domain, this means that physical and economic models have to be simplified to yield feasible problems to solve. The conceptualization of the model determines the resulting problem formulation. Approaches such as partial differential equation (PDE)-constrained optimization are capable of depicting complex relations [23]. However, usually proven types of mathematical programming problems, such as Linear Programming (LP), Mixed Integer Linear Programming (MILP), or quadratic programming (QP), are applied for energy system analyses due to the availability of their efficient algorithms and solvers. In this case, due to the scope of the considered system and its expected mathematical complexity, only less computationally expensive LP and MILP solving approaches are taken into account. Therefore, this was the first conscious choice to take within the problem view formulation. Thanks to its well-established solving algorithms, convex problems can be efficiently assessed with LP approaches. Conversely, MILP offers a more detailed and realistic representation of single units by accommodating complexities like economies of scale in cost constraints and part-load behavior in operational constraints. However, MILP approaches significantly increase the computational requirements, especially for large systems, due to poor scalability. While mostly considering aggregated processes for Germany and focusing on the technological detail of sector-coupled systems, it has been decided to proceed with the more efficient LP formulations for all constraints.

Next, modeling can begin either as a greenfield from scratch or as a brownfield, taking into account existing stocks and infrastructures. Greenfield modeling can be interpreted as a proof of concept of a specific future system design. In contrast, brownfield modeling considers existing infrastructure, which can reduce initial costs but tends to lead to more gradual and realistic transition scenarios. The brownfield approach is chosen to set the focus on the gradual changes of the transition pathway from the current system and not only the resulting energy system.

Further, the solving perspective is essential. Its choice is related to the underlying market assumptions of the system. A central planner approach facilitates coordinated macroeconomic optimization, making it valuable for policy analysis to induce global pathways within perfect energy markets.

Alternatively, a decentralized and microeconomic approach better reflects real-world decision-making influenced by market distortions such as market regulations and behavioral incentives, which can have a high influence on market values. With the increasing importance of decentral decisions through the electrification in distribution systems, it might be of interest to consider more microeconomic aspects, such as profit-oriented prosumer's feed-in behavior in future work. Nevertheless, the focus is set on the central planner approach as it is (1) not fair to only consider chosen market distortions in a sector-coupled model and (2) not possible to predict and include all of them within the context of a long-term energy system transformation.

Furthermore, presupposing that future distribution functions could be estimated, the consideration of uncertainties for meteorological conditions or price developments can improve the robustness of the optimization results. This can be achieved by using stochastic optimization methods [24] instead of deterministic approaches. However, the estimation of future distribution functions is also a challenging task in long-term models and is, therefore, out of the scope of this work.

Lastly, it is important to define the spatial scope of the system and the resulting system boundaries. It should also be elaborated on how to consider important model drivers that lie outside the defined system boundary. For instance, the spatial scope of this work focuses on Germany, while the importance of the European electrical power system cannot be neglected. Therefore, scenario assumptions and interfaces are required. Within this spatial scope, the spatial resolution is also an

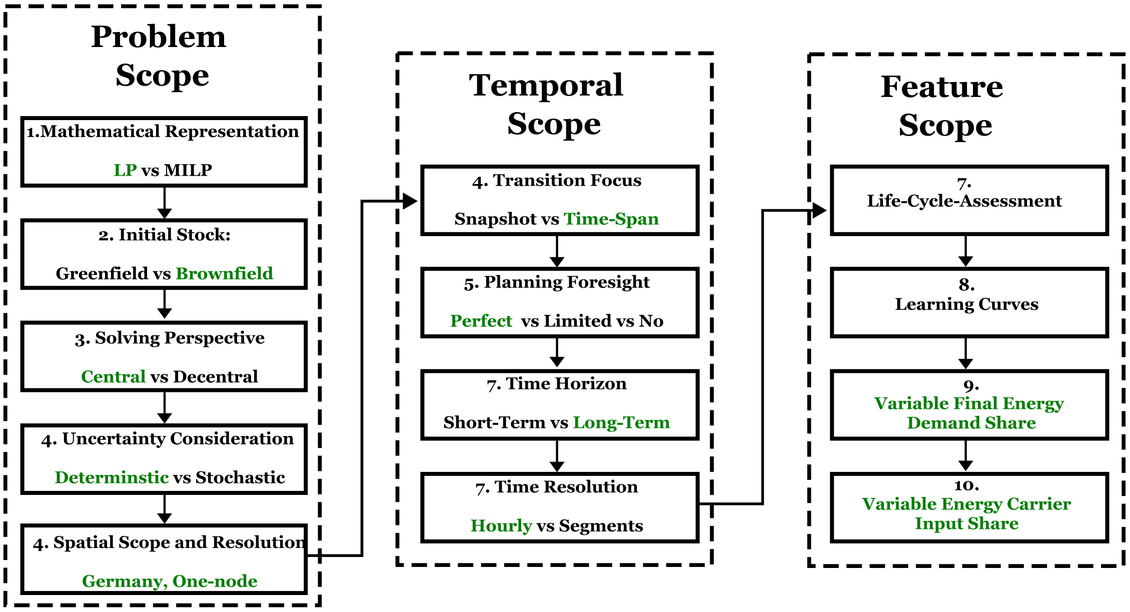


**Fig. 2.** Steps to define the model frame (green font indicates the choice within this work — other aspects have been discussed but not implemented for the model definition).

important factor that determines if and how to aggregate and model different elements within an energy system. These spatial aggregations are often also closely connected to technological aggregations that are elaborated in more detail in Section 2.2. While developing the model structure in this paper for Germany, it is generic and with a strong focus on future developments, and thus transferable to energy systems in other countries if the deviating parameters such as the installed capacities of existing technologies within a country can be adjusted.

### *2.1.2. Temporal scope*

For the temporal scope, the first choice to take is between a snapshot and a time-span view, which impacts the model's depth and accuracy. Snapshot modeling simplifies analysis and provides insights into radically altered systems, often projected far into the future where the current system configuration is assumed to have no direct influence due to the lifetime of the various components. Conversely, a time span perspective of multiple subsequent periods ensures a precise representation of transition pathways in evolving systems and thereby also indicates the order of the required steps to take. As the latter approach provides decision makers also with knowledge on optimal transition pathways, the time-span view has been selected for the model structure of this study.

For this time-span view, the chosen inter-yearly foresight horizon within the time range of the defined input data can profoundly affect the expansion planning of the modeled transition. Perfect foresight excels in long-term planning with complete information to find the intertemporal optimum over the whole time frame [25]. A rolling horizon is a myopic-limited foresight approach that includes medium-term planning, *e.g.*, until the next model year, to consider the evolutionary nature of market and technology developments and the related uncertainties. At the end of this spectrum, myopic no-foresight approaches determine optima for each model year and may yield more realistic but sub-optimal long-term outcomes. Generally speaking, the suitability of the inter-yearly perfect foresight assumption improves as long-term influence on decision-makers increases, for instance, through governing laws. In the domain of climate change mitigation, it can be observed that the importance of these long-term influences is rising. Therefore, this assumption might not always be accurate, but it is still acceptable. Moreover, the intra-yearly foresight horizon can also influence operational planning and could, therefore, be defined in a weekly rolling-horizon approach to consider that, *e.g.*, weather profiles for future months are difficult to anticipate. However, this has not been considered within the scope of this work.

In addition, a short time horizon of 1 to 3 years can yield rapid insights suitable for short-term decisions such as dispatch strategies in times of supply shortages. Conversely, a long time horizon supports robust long-term planning, and an appropriate consideration of investment decisions. Moreover, long-term horizons can prevent unrealistic effects that can arise when a critical milestone, such as a greenhouse gas-neutrality target, is at the end of the modeling timeline (*e.g.*, errors due to neglecting process lifetimes after the modeling period). To avoid this a time horizon of 50 years has been defined. This also allows to analyze investment decisions that can have a long-term benefit, such as deciding on an electrified production route for an industry branch, although it is not optimal in the first milestone years due to the available electricity mix.

However, non-equal intervals are defined to consider developments in the near future more accurately while having broader intervals for the more uncertain future at the end of the time horizon.

Finally, depending on the research question and the technologies to model, it can make sense to define larger time segments such as 4 h up to days or even weeks to reduce the model size to solve. However, in this approach an hourly resolution is defined while reducing the model size with additional aggregation measures that are described in Section 2.2.

### *2.1.3. Feature scope*

Additionally, the incorporation of further features has been discussed while defining the model base. One of these is model-endogenous learning curves to consider technology cost learning and thereby enable more realistic cost consideration for long-term models [26–28]. Another important feature to enhance the holistic view of the environmental impact on a system is the Life Cycle Assessment (LCA) [29–31]. However, the consideration of both introduced features is difficult within national energy system models as the system border is too limited to consider highly globalized relations and the resulting learning rates for learning curves or the production and recycling procedures for the LCA. Additionally, the incorporation of learning curves results in a non-linear mathematical program that complicates the problem-solving process. Therefore, both features are deemed to be out of the scope of this work. The features mentioned here are prominent examples but are not intended to be exhaustive. For an

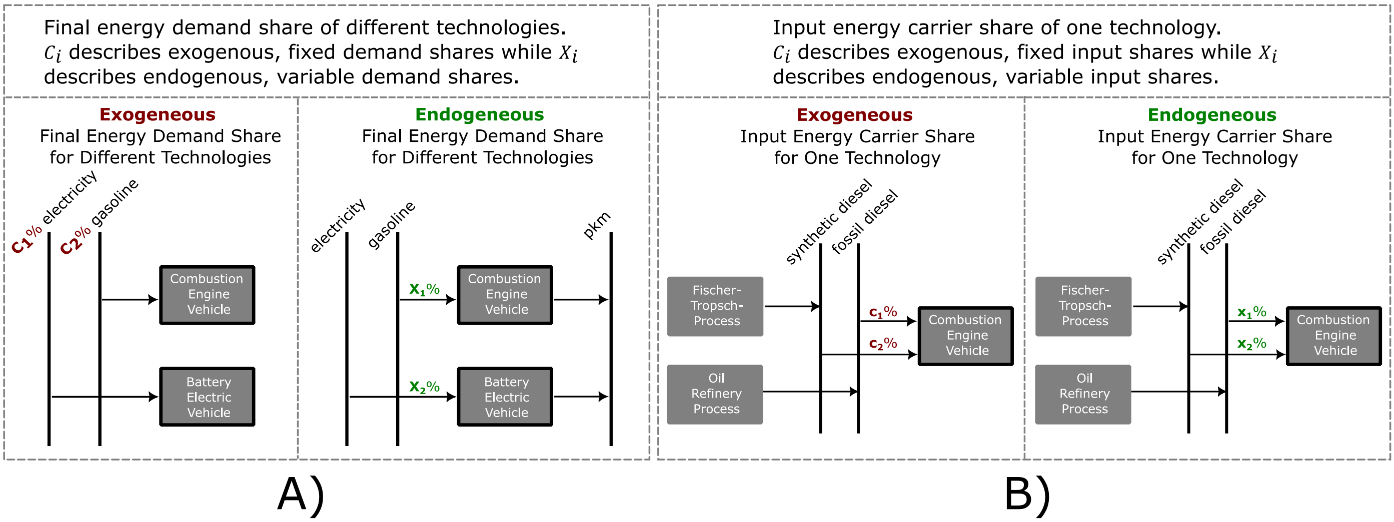


**Fig. 3.** Schematic overview of principles to model endogenous decisions for an effective representation of sector coupling.

effective representation of sector coupling, some other key features have been identified, which are described after defining what sector coupling means in the context of this study.

The concept of sector coupling and its manifold meaning in relation to the perspective has been discussed in previous research [32–34]. Within the scope of this work regarding the transformation of the German energy system, the term sector coupling primarily refers to the ongoing process of substituting fossil fuels with renewable energy resources or other sustainable energy forms and the resulting cross-sectoral relations. Technology-wise, this can principally be established through:

1. the direct use of sustainable primary energy resources such as in biomass heat generators,
2. the direct use of green electricity based on RE resources such as in heat pumps or electric mobility,
3. the indirect approach with technologies that rely on the conversion of green electricity into hydrogen and its possible derived synthetic products such as synthetic fuels for aviation.
4. the increase of process efficiencies by including byproducts such as heat, *e.g.*, in combined heat and power plants or with the recovery of waste heat from industry.

Through all of these options, the interdependencies between sectors and the related technologies increase significantly, allowing many theoretical degrees of freedom to the model. To be activated, features are required to reduce the exogeneity of model decisions.

Many of the energy system models that describe sector coupling that have been mentioned in the introduction define the final energy demand exogenously as input to the model. This means that technological shares and, therefore, the final energy consumption in the demand sectors to supply the service energy requirements are anticipated by the modeler or taken from an upstream scenario. This may, for example, concern the future penetration of different drivetrain technologies in the transport sector (subgraph A) in Fig. 3). Consequently, the possible competitive interplay between technologies within a specific sector is reduced, which also influences technology choices in upstream sectors. This implies that the optimal sector-coupled result is biased by exogenous assumptions of sectoral developments.

Similarly, the model choice for the expansion of technologies from the supply sectors is also biased when technologies with multiple substitute inputs are defined with a fixed share of input energy carriers. For instance, assuming a real combustion engine can use both fossil gasoline and synthetic gasoline and if the model is not provided the option to endogenously choose between those, a fixed ratio must be assumed, whereas in a sector-coupled model, the market penetration of this vehicle class would always require supply processes for both energy carriers. This is illustrated in subgraph (B) in Fig. 3. To model sector coupling interactions effectively the focus has been set on model-endogeneity. Only the optimization result should decide on (A) the technology choice and (B) the input energy carrier and the related upstream technologies to meet the demand whenever possible. (A) is enabled by defining all demands as close to the service energy demand as possible. This means that the transport demand is defined in passenger- or tonne-kilometer, the residential energy demand in required space or water heat in terawatt hours, and the industry demand in million tonnes or other quantities of products. Thereby, technology competitions, *e.g.*, between the electrification of vehicles and the fuel switch in combustion engine vehicles to synthetic fuels, can be considered within the model. These demands are denoted as an exogenous commodity to distinctly indicate which model commodity values have to be given as model input. The other commodity classes are primary energy carriers, secondary energy carriers, and industrial intermediate products since industrial processes are complex to define and yield a high number of commodities that are only relevant in this sector (see Section 3.4). Fig. 4 shows the interdependencies between sectors for a sample reference energy subsystem for an arbitrary excerpt of processes from the model structure. This shows that the model endogenous decision, *e.g.*, between a BEV and an Internal Combustion Engine Vehicle (ICEV), influences the required upstream technologies in other sectors.

(B) is ensured by providing flexible shares of multiple input or output commodities, which can be included in the energy system modeling. Accordingly, to carry on with the previous example, if the least-cost system includes ICEVs, these could be supplied by a mix of fossil fuels based on refinery processes or by a synthetic fuel chain based on electrolyzers, which require additional electricity production facilities.

With this approach, sector coupling can be modeled endogenously with high degrees of freedom for the optimal solution. However, if too many components and their intercorrelations are considered, the model size and its computational requirements must be reduced. This work offers different aggregation steps, which are described in the next section.

### 2.2. *Model reduction by aggregation*

Focusing on the technical foundation of multiple sectors with a high degree of detail, aggregation methods can be helpful to reduce the computational complexity of the model and thereby yield a feasible model.

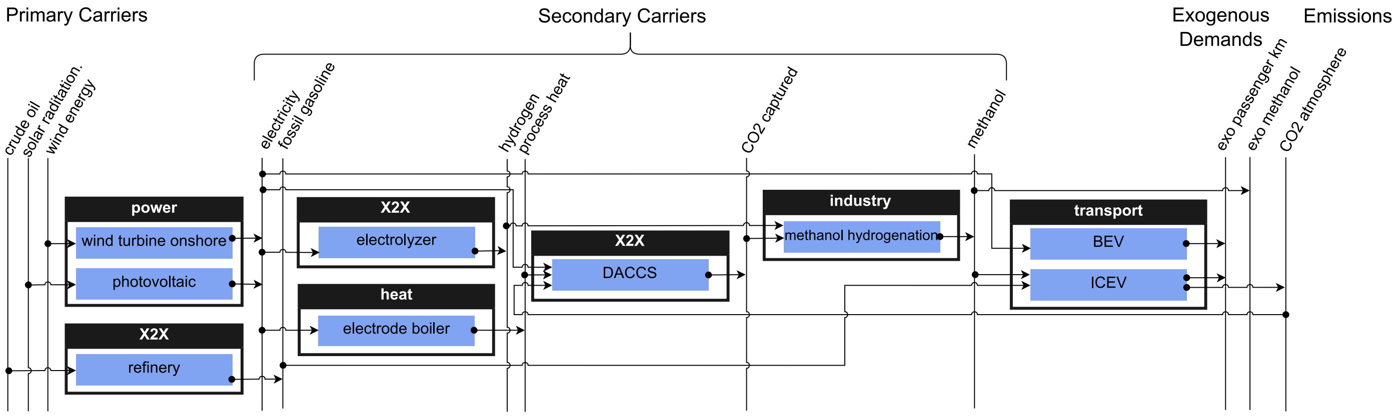


**Fig. 4.** Excerpt from the proposed model structure to illustrate the intercorrelations between the sectors.
Abbreviations: DACCS: Direct Air Carbon Capture and Storage; BEV: Battery Electric Vehicle; ICEV: Internal Combustion Engine Vehicle;.

There are various complexity[1] reduction methods that have been described in previous research [35,36]. In the present study, the complexity reduction is achieved on three levels: (1) spatial aggregation, (2) technological aggregation, and (3) temporal aggregation.

The spatial aggregation to one node is a crucial measure to dive deep into the vast sectoral diversity of technologies in the future energy system landscape. Due to this spatial aggregation, it is possible to define a highly complex sectoral structure where the most detailed level includes approximately 2000 processes that characterize the heterogeneous structure of existing and possible future technologies.

Additionally, technological aggregations are provided to enable a flexible composition of predefined aggregations from different sectors that also allow flexible adjustment with other model settings, such as the temporal resolution. For example, when specifically examining the industry, this sector can be considered at a detailed level, and the technologies from other sectors can be aggregated. In order to meet the specific requirements, aggregation levels and their order do not have to be uniform between the sectors. Moreover, one aggregation level does not have to consist exclusively of processes from the previous level as aggregation steps may only be applicable to a subset of processes as shown in Fig. 5, where, for instance, rail processes skip the blue aggregation step by vehicle size. Moreover, this figure highlights the complexity reduction of the transport sector by reducing it by one level of detail while incorporating different aggregation steps that depend on the length of the process branch. The logic and quantities of different aggregation levels for all sectors are shown in Table 1.

Temporal aggregation is accomplished using the Time Series Aggregation Module (tsam), which is a Python package that generates reduced time series based on a set of input time series, utilizing various heuristics and machine learning algorithms [37,38]. It strives to maximize the similarity of the produced time series consisting of typical periods to the underlying input time series. By only modeling and weighting the typical periods, the computational requirements can be reduced substantially while addressing the key characteristics of a model. The user should keep in mind that the optimal parameter selection for this tool is system-dependent and therefore also depends on the choice of the system components. With these three levers, the complexity of the model structure can be reduced substantially according to a specific research question.

## 3. Results

This section focuses on the description of the derived model structure results of this work and the considerations and key assumptions behind each sector. These are described starting with the sectors of power (Section 3.1), power-to-X & other conversion (Section 3.2) and heat (Section 3.3) followed by industry (Section 3.4) and transport (Section 3.5). In Section 3.6, network visualization approaches are discussed, and in 3.7 possible limitations to considering the interfaces are addressed.

The basic composition of the introduced sectors and their role are illustrated in Fig. 6. Apart from the previously described design criteria for sector coupling (Section 2.1.3) that highly influence the model structure of the sectors, there usually are additional shared assumptions across the sectors. Important drivers for exogenous model values across sectors can be harmonized by consulting the same projections. In the presented model structure projections for Germany from Ref. [39] have been consulted that include economic, demographic, and climatic developments as well as the progress of space requirements and transport volumes. Moreover, with the brownfield approach, processes are generally subdivided into existing and new technologies. Sector-specific considerations are elaborated in the following sections.

### 3.1. Model structure of the power sector

With the option to generate electricity from renewable and low-carbon primary and secondary energy carriers, the transformation of the power sector is a key element for the decarbonization of the whole energy system. However, adequate modeling of the various options for the decarbonization of the power system, such as the shift from a centralized and dispatchable fossil and nuclear-based conventional electricity generation toward a more decentralized wind and solar-based renewable electricity generation, is non-trivial within a detailed, sector-coupled national energy system model.

Considering the significant variance of the spatial and temporal resource availability of renewables in the coupled European power system and the large number of possible conversion processes, the challenge lies in the integration of an adequate modeling of the spatial and temporal balancing of various possible power supply and demand processes within a one-node modeling approach of the national energy system. In this context, the numerous technologies and resource classes are aggregated such that the merit order of the supply side is approximated sufficiently with a limited set of processes, and the consideration of transmission flows will be focused on an NTC (net-transfer capacities)-based modeling of cross-border flows with neighboring countries. On a country scale with a single-node modeling approach, the consideration of power transmission and distribution constraints remains a challenging task. The possibility of user-defined grid expansion expenses, which are coupled with the expansion of fluctuating renewables such as wind and solar energy, will be included but is not the focus of the presented approach.

---

[1] The word complex in this usage rather refers to extensive than to complex from the system theory domain.

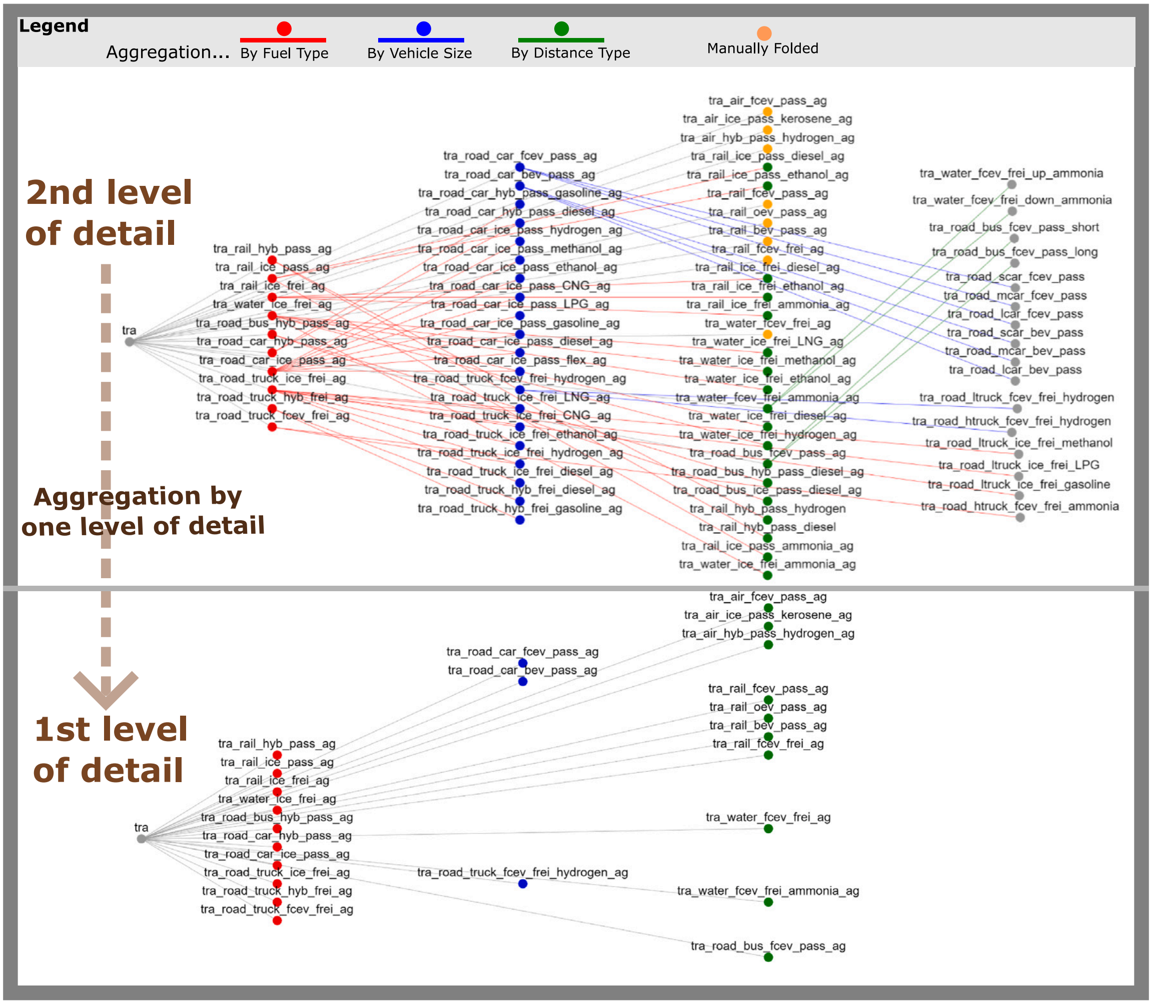


**Fig. 5.** Aggregation from second to first level of detail for the transport sector. There are two more detailed levels that are not shown here due to the size of the graph. Orange points are manually folded leaves within a level of detail. This possibility fosters the flexible selection by the user.

**Table 1**
Approximate number of processes per sector and aggregation step. Note: The minimal number of processes is not the sum of the lowest row of each sector, as aggregation steps do not apply to all processes of higher levels.

| | Power | X2X | Heat | Industry | Transport |
|---|---|---|---|---|---|
| Detailed data | 300 | 80 | 650 | 480 | 330 |
| Aggregation step 1 | technology type: 55 | technology type: 3 | building types: 124 | process route: 60 | distance types: 33 |
| Aggregation step 2 | renewable type: 2 | | fuel types: 33 | - | vehicle sizes: 82 |
| Aggregation step 3 | – | | – | – | fuel types: 21 |

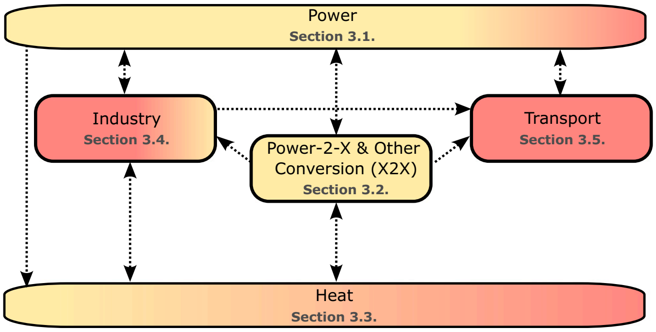


**Fig. 6.** General overview of the considered sectors and their basic interfaces that are described in Section 3 (yellow indicates a supply role and red a demand role).

With increasing sector coupling and flexibilization of the demand side, the power sector is more and more driven by the availability of low-carbon energy sources. Consequently, the processes of the power sector are structured with respect to the conversion input commodities in the first place. This includes renewable primal energy conversion processes from wind, solar, hydro, and geothermal, the nuclear fission and fusion processes, and finally, the broad class of combustion processes of solid, liquid, and gaseous as well as fossil, biogenic, and synthetic energy carriers.

Besides the supply side, the power sector also comprises the final electricity demand of processes that are not explicitly modeled in the industry, transport, and heat sector, such as the final demand of electrical appliances from residential and Trade, Commercial and Service (TCS) sector (*e.g.*, lightning, cooking, etc.).

Storage processes, which are both, producer and consumer of electricity, are allocated between the demand and supply side of the power sector. In this context, pure reservoir storages and pondage processes

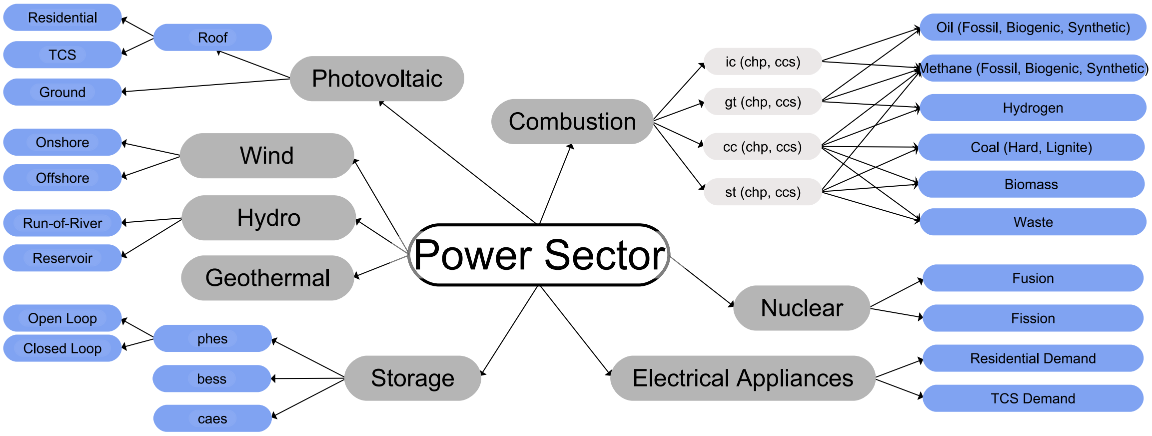


**Fig. 7.** Categorization of the power sector.
Abbreviations: ic: internal combustion; gt: gas turbine; cc: combined cycle; st: steam turbine; chp: combined heat and power; ccs: carbon capture and storage; phes: pumped hydroelectric energy storage; bess: battery energy storage systems; caes: compressed air energy storage;.

are classified as hydro generation processes in the first place, as a pumping process, like in the case of open-loop pumped hydroelectricity storages (PHES), is missing. Besides closed-loop and open-loop PHES, battery electric storage systems (BESS) and compressed air energy storages (CAES) are considered for the electricity storage, while hydrogen storages are regarded as part of the X2X sector (Section 3.2) and are therefore not included in the modeling of the power sector. As illustrated in Fig. 7, the structure of the power sector is thus dominated by processes that generate electricity as their main output.

Besides combustion processes, which also result in emissions ($CO_2$, $CH_4$, $N_2O$) and/or combined heat production, electricity is the only considered output commodity of all other generation processes of this sector. Multiple process configurations with varying power, heat, and emission output levels can be differentiated according to different characteristics. First, the combustion technology, which may be an internal combustion engine (IC), a gas turbine (GT), a steam turbine (ST), or a combined cycle (CC). Second, the fuel type (oil, methane, hydrogen, coal, biomass, or waste). And third, the specification of the emission and combined heat handling. In this context, different process configurations are defined for combined heat and power (CHP) process configurations that depend on a potential grid-based supply of heat, as well as carbon capture and storage (CCS) or carbon capture and utilization (CCU). Similar to the modeling in other sectors, a differentiation between existing and new processes is considered in the power sector. In order to capture the characteristics of regionally varying resource potentials for the conversion of onshore and offshore wind energy conversion systems and ground-mounted or rooftop photovoltaic (PV) systems with respect to generation capacities and profiles, multiple processes per national node are defined. The goal is to approximate the merit-order regarding the levelized cost of electricity (LCOE) of potential repowered or greenfield wind and PV units within a country with a reduced set of processes, considering the trade-off between model complexity and accuracy. In a pre-processing step, the corresponding generation profiles of existing and potential units are therefore modeled with a high spatial and temporal resolution, sorted depending on the average LCOE in multiple weather years, and aggregated accordingly for a limited set of processes depending on the potential. For non-weather dependent electricity generation processes, including hydro, a further differentiation besides existing processes and investment processes is omitted. This results in a single investment option per year and technology and a representative existing process per technology class with averaged techno-economic parameters (*e.g.*, one existing natural gas turbine process per country).

The produced electricity from this sector can be used directly or converted to various other secondary energy carriers to cover the demands of other sectors. The main technologies responsible for these intermediate conversions are part of the X2X sector, which is described in the next section.

### 3.2. Model structure of the X2X sector

The majority of the conversion technologies that make up the X2X sector are novel technologies with a low technology readiness level but can have a high value in future energy systems with sector coupling due to their role as connecting elements. The processes here summarized as X2X sector entail both typical Power-to-X processes (water electrolyzers, Fischer–Tropsch process, etc., see Fig. 8) as well as conventional conversion processes that are not suitable to be modeled in other sectors, such as refinery processes or steam-methane reforming. Conversely to other sectors, the X2X sector is a pure conversion sector without final demands. This unique property leads to a high number of intersections with and an extended connectivity to the other sectors. Furthermore, these numerous intersections result in a complex definition of the system boundaries for the X2X sector particularly.

While most of the processes defined in the X2X sector are modeled on a technology level, certain assumptions have been made to reduce the complexity of the system and to delimit the X2X sector from other sectors. To this end, processes providing the transport sector with biogenous fuels are not modeled on a technology level but are introduced through source components satisfying the exogenous demand of the transport sector. Furthermore, the transport of all fuels to the refueling station is subject to a cost component, which adds a markup per liter of transported fuel to the total cost of fuel. The markup depends on the transported fuel but not on the means of production. Therefore, no difference between the transportation of *e.g.*, conventional diesel, biodiesel, or synthetic diesel is assumed.

As a brownfield approach is used in the context of this work, the portfolio of existing plants has a particular importance to the energy system. However, the majority of the novel X2X technologies are often not yet available on a commercial scale. Consequently, the number of existing plants and the corresponding data set is relatively small compared to other sectors. Despite the low number of existing plants, the potential of newly built plants, which are needed for sector coupling in the future energy system, is immense. This adds the challenge of modeling the market entry and ramp-up of many X2X technologies with limited techno-economic information due to their novelty. Not only the novelty of the processes but also their design may add challenges in modeling the processes of the X2X sector. Owed to its function as a conversion sector, there exists a set of processes with variable outputs. One process can produce a set number of different proportions between

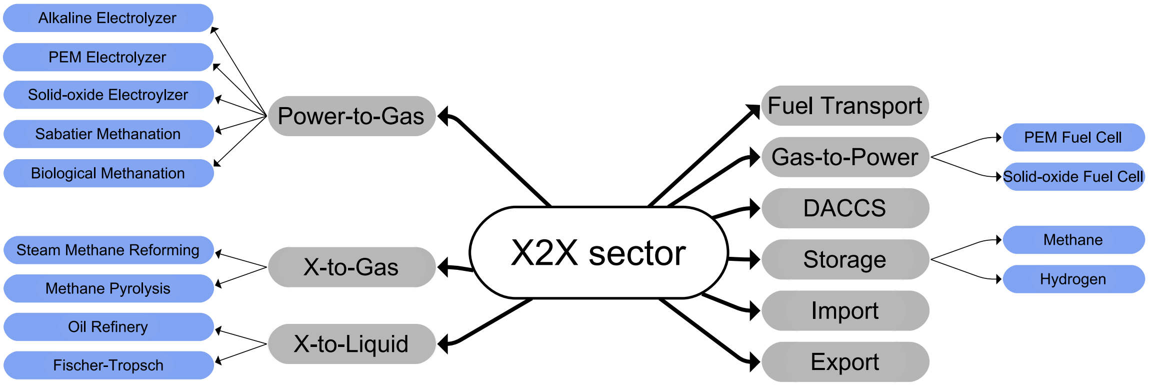


**Fig. 8.** Categorization of the X2X sector. Abbreviations: PEM: Proton exchange membrane; DACCS: Direct Air Carbon Capture and Storage.

the commodities it produces based on the physical process conditions. Examples of these processes in the X2X sector include refinery processes as well as Fischer–Tropsch processes. Note that flexible shares (as described in Section 2.1.3) would be possible, but not required for these processes.

The processes are structured with respect to the commodity types which are converted. This implies that processes that convert power into a gas (*e.g.*, hydrogen or methane), so-called Power-to-Gas processes, are part of the same category on the lowest level of detail. A representation with a higher degree of detail differentiates between the educts or products of a process. In this representation, processes producing hydrogen from power would be separated from processes producing methane. The highest level of detail entails a differentiation of the processes that are able to perform a certain conversion, *e.g.*, PEM, alkaline, and solid-oxide electrolysis. Different processes for the same commodity conversion are implemented in order to depict a more realistic competition between different processes. For example, solid-oxide electrolysis can exhibit higher efficiencies as waste heat potentials can be utilized by the system, and conversely, PEM electrolysis exhibits a higher technology readiness level and, hence lower investment costs, making it potentially more suitable for near-future investments.

Another conversion category that is not considered in this sector is the conversion into heat. The required technologies based on electricity or other input energy carriers from the X2X sector are elaborated in the next section.

### 3.3. Model structure of the heat sector

Decarbonizing the heat supply sector has been hindered by a historical reliance on fossil fuels, compounded by the challenge of retrofitting an aging building stock. The heat market and its interdependencies between sectors are defined according to [40] for public and industrial heat production, households, agriculture, industry and TCS. Its processes are primarily divided into the district heating supply and the building sector (see Fig. 9).

For the district heating supply, centralized heating generation consists of a variety of different generation technologies based on fossil and RE sources. In addition to the existing fossil and waste heating plants, heating plants based on hydrogen, biogas, biomass, solar thermal energy as well as large electric heat pumps are taken into account. Surplus heat can be stored in a water tank-based heat storage system. The waste heat of industry processes (Section 3.4) or X2X (Section 3.2) processes is considered as a potential for future district heating generation if the waste heat cannot be used locally.

With regard to grid-based heat supply, the model structure distinguishes between two independent heating networks (district heating and local heating), which are mapped as successive parallel chains of processes according to the different functional subtasks (transport, main distribution, medium, and fine distribution). The two district heating networks differ in terms of the flow temperature. Local heating networks are operated with flow temperatures below 95 °C while district heating networks are operated up to 120 °C. Within the model, the existing networks are depicted as stocks that can be expanded accordingly in the event of an increase in district/local heating supply, taking into account the costs incurred and the associated supply potential. The district heat can be delivered to consumers from household, TCS, and industry sectors. Heat exchangers are used to connect either to the higher-temperature district heat or to the lower-temperature local heating grid.

In the household sector, the heat market is represented by the demand categories space heating, space cooling, and hot water as well as their differentiation by building type and age. Single- and multi-family homes in urban and rural areas are additionally divided into three existing building categories based on the building age and new buildings. The aggregated data for the base year of residential buildings is based on Tabula [41] and the statistical data of the German Census [42]. Depending on population development, the specific demand for living space, the assumed demolition rate, and the changing climate conditions, the demand for space heat in residential buildings is updated.

In addition to the various decentral or central heating options, energy-efficient refurbishment options for the different building types are considered in terms of costs and savings potentials. This means, that the demand could also be reduced by replacing the windows or through thermal insulation compared to the renovation standard. The structure of the building types allows the modeling of specific local conditions, *e.g.* in the rural building types, access to the natural gas grid is not possible everywhere. Furthermore, each building type is characterized by a typical thermal power class for the heater, which results in different investment costs for the different sizes of the same heating technology. To provide investment costs for different heater sizes, a regression analysis of several actual heaters was collected from catalogs of companies providing heating systems. With several data points for investment costs and the corresponding thermal power size of the heating system, a regression curve was calculated, which is used to determine specific investment costs for each thermal power class associated with each building type. A distinction is also made between heat generators that only produce space heat or domestic hot water and heat generators that can provide both.

The TCS sector is represented by a similarly structured reference energy system and includes the heat demand categories of space heating, hot water, process heat, and space cooling. In order to account for the different heating supply costs and the possible options for decentralized heating generation a distinction is made between the function of office or service buildings and production or transport buildings of non-residential buildings. The underlying building typology and thus the energy-related characterization of the building envelope is based on an aggregation of the ENOB:dataNWG [43] database. Depending on

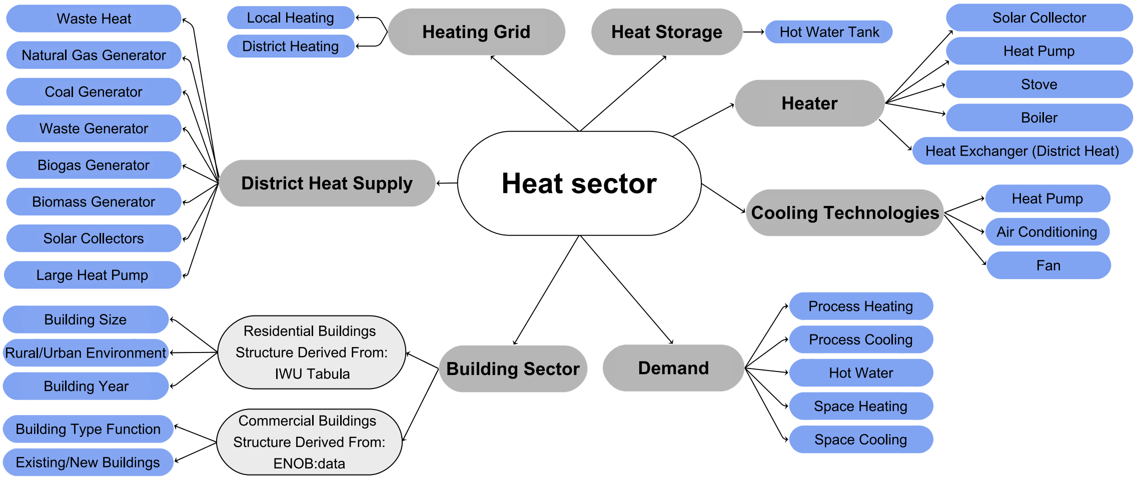


**Fig. 9.** Categorization of the heat sector model structure.

population development, climate conditions, gross domestic product (GDP) development, and a demolition rate, the demand for space heating in non-residential buildings is updated.

For the consideration of sector coupling, synergies to other sectors are of specific interest. For instance, depending on the industrial sector, the waste heat of industry processes could be integrated into the heat supply of future district heating networks. The details of the industry sector are described in the next section.

### *3.4. Model structure of the industry sector*

In the past century, industrialized countries have scaled up production capacities that have been mainly dependent on fossil resources. The transition in this sector is challenging as it requires a turnaround that considers the balance of a sustainable and competitive supply of goods. Therefore, the detailed representation of its model structure is essential.

The industry sector has been classified into 11 major branches, with detailed modeling applied to seven of them, including automotive, cement, chemicals, glass and ceramics, iron and steel, non-ferrous metals, and paper. The remaining four branches food and tobacco, rubber and plastic, metalworking, and machinery equipment are included in the model structure in a simplified manner. Fig. 10 depicts a comprehensive overview of the representation of the industrial sector, including the 11 branches, their main exogenous demand products, and the considered existing and relevant novel production routes for each of those demands. The inclusion of self-generation technologies, particularly for electricity, is a key component of the industry model structure. This model differentiates between externally supplied electricity (Section 3.1) and self-generation within the industry, providing insight into energy generation-related investments and potential grid infrastructure needs. Self-generation technologies are used across the entire industrial sector, with no regard for industry branch specificity.

For each industrial demand, the overarching modeling concept entails identifying key production steps across diverse production routes (see Fig. 11). Energy, material flows, and production steps are identified, and the model structure is built to model the current state of production. In a following step, investment options for the best available technologies are introduced for each process. Furthermore, fuel switch, carbon capture technologies and novel process routes investment options are considered at the relevant production technologies.

The production in the various branches of the industrial sector involves a complex production chain consisting of multiple production steps. Therefore, a key aspect of this sector is the use of intermediate material commodity flows. Such commodities are needed to connect process steps and create the basis for the energy flows required throughout the production line, leading to a demand commodity. Fig. 11 shows multiple intermediate commodities in the iron and steel industry (sinter, raw iron, and crude steel) which provide the linkage between production steps. For example, raw iron is the main output of the blast furnace processes while simultaneously being an input of the oxygen furnace processes.

Lastly, synergies with other sectors in the energy system are modeled. For example, as a result of the modeling of electricity self-generation, the option to feed electricity back into the grid is incorporated. In the same manner, the modeling structure allows for industrial waste heat to be fed into the district heating network. Moreover, the model structure requires the industrial sector to provide products such as ammonia and methanol not only for the supply of exogenous demands but also to be used as fuel in the transport sector, which is described in the next section.

### *3.5. Model structure of the transport sector*

As the transport sector relies largely on fossil fuels, emissions have not been significantly reduced within the last decades. Structural changes in upstream sectors that have been elaborated in previous sections are required to decarbonize this sector. However, there are many potential decarbonization pathways within the various categories of its subsectors. To analyze these in the transport sector, it is therefore not only necessary to consider new types of powertrains and fuels but also to precisely allocate emissions to the individual categories of transport. Thus, the transport sector is finely subdivided in terms of technologies in order to be able to represent the current fleet and its emissions on the one hand and future fleets with new technologies on the other hand.

In addition, the high technological resolution of the transport sector enables a precise analysis of the interaction with other sectors (power sector — electricity for BEVs; industry sector — fuels for ICEVs; X2X sector — hydrogen for Fuel Cell Electric Vehicles (FCEVs)), to identify possible flexibilities of the future transport sector resulting from sector coupling.

The model structure distinguishes freight transport via ship, rail, and truck as well as passenger transport by air, rail, and road, with the latter being divided into public and private transport. In addition, the transport services of the construction sector are reflected in the model structure. Fig. 12 provides an overview of which characteristics are used to differentiate the processes in the transport sector, with a color code allowing the transport type to be assigned to the categories. A distinction is made between the size classes light car, mid-size car,

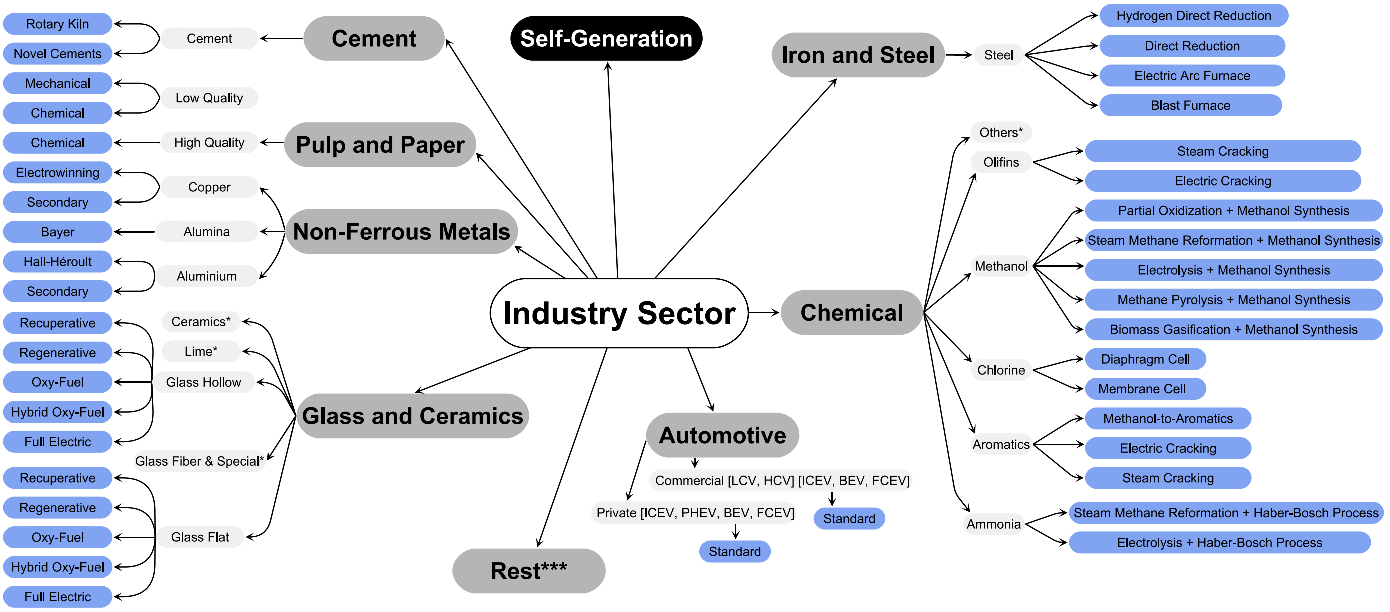


**Fig. 10.** Categorization of the industry subsectors (dark gray), its products (light gray) and the possible production routes (blue). *are modeled in an aggregated manner. **Food and tobacco, rubber and plastic, metalworking and machinery equipment industries are modeled individually yet in a simplified manner.
Abbreviations: LCV: Light Commercial Vehicle; HCV: Heavy Commercial Vehicle; ICEV: Internal Combustion Engine Vehicle; PHEV: Plug-in Hybrid Electric Vehicle; BEV: Battery Electric Vehicle; FCEV: Fuel Cell Electric Vehicle.

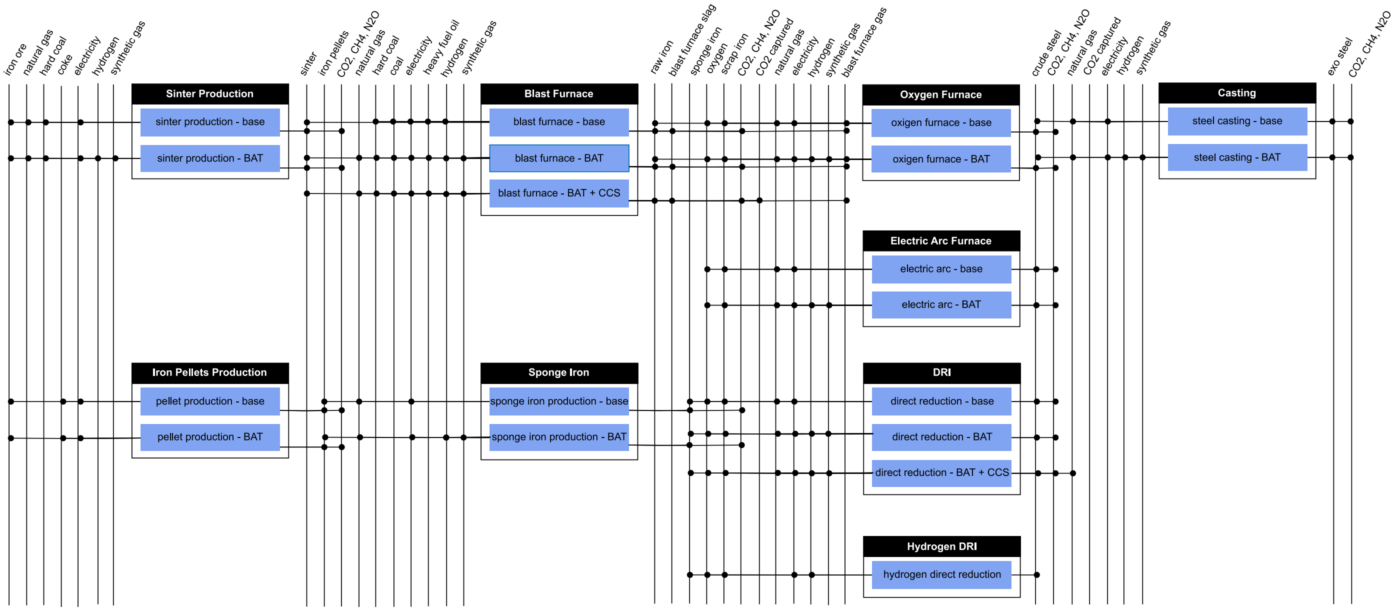


**Fig. 11.** Part of the reference energy system for the example iron and steel industry. Processes ending with '- base' represent the current installed capacities. Processes containing '- BAT' are new investment options based on best available technologies. Multiple BAT investment options can be available according to the specific process. For some processes, suitable investment options for carbon capture have been identified and provided in the model structure; such processes contain 'CCS' in their name. DRI stands for direct reduced iron.

and heavy car for individual road passenger transport, or the distance types local (streetcar/subway) and intercity (passenger train) for rail transport. Since the techno-economic data for the current stock differs from that of the vehicles available in the future, an additional two subprocesses are created for each process type in the model, namely the existing stock and the fleet expansion.

One of the main focal points of the process selection was a technology-open approach in order to avoid pre-selection, especially when combining vehicle types with powertrain types and fuels. The aim of this approach is to ensure that the models are able to generate an optimized fleet based on the available investment options. This means that a wide range of fuel types for combustion engines is available for every mode of transportation (air, rail, road, water), as well as electric and fuel cell powertrains. There is no competition in the transport sector between the individual vehicle categories (*e.g.*, the distribution of vehicle size classes or the share of public transport in the exogenously defined demand), but only in terms of the powertrain and fuel type. The demand for passenger- and tonne-kilometer is specified exogenously for each category. This ensures that the optimization models can only choose within the vehicle categories themselves when expanding, as otherwise, the real conditions (*e.g.*, the distribution of vehicle size classes) would be distorted.

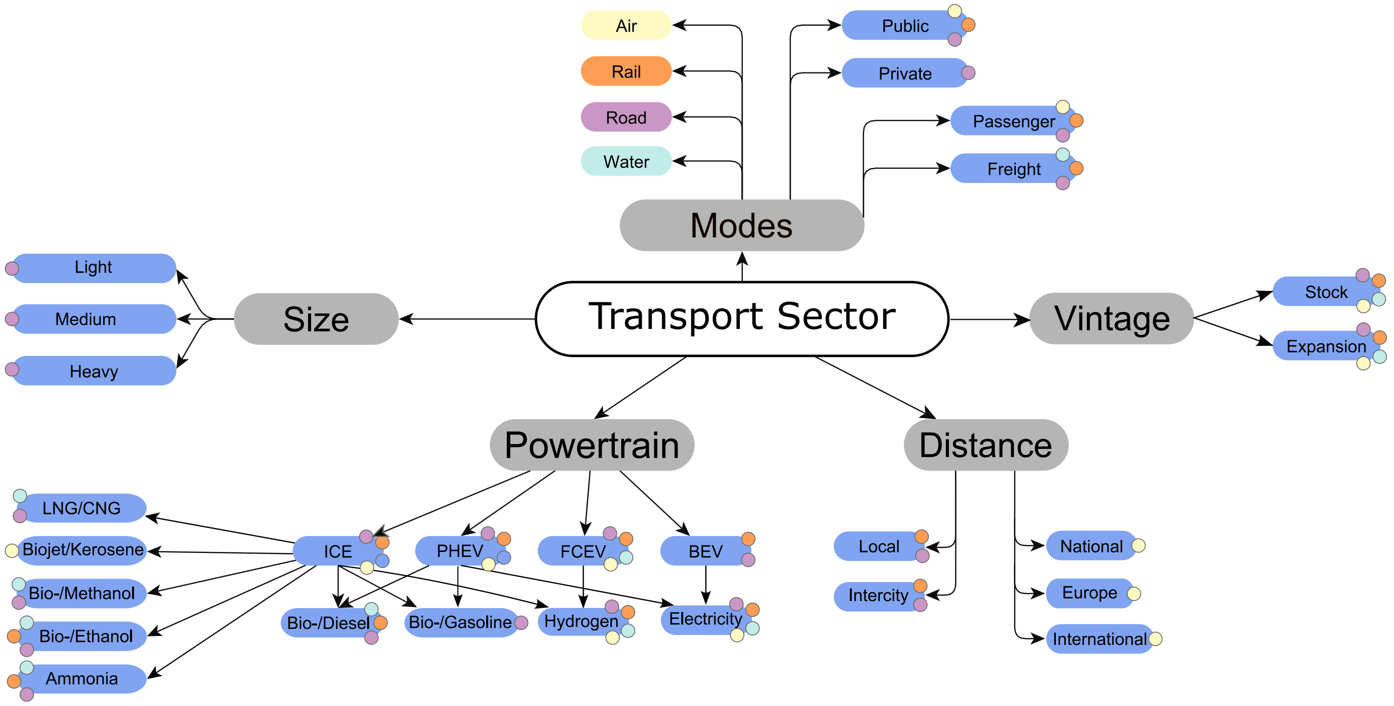


**Fig. 12.** Categorization of the transport sector. The subdivision and differentiation of the modes air (yellow), rail (orange), road (violet), and water (turquoise) is indicated by the correspondingly colored dots.
Abbreviations: LNG: Liquified Natural Gas; CNG: Compressed Natural Gas; ICEV: Internal Combustion Engine Vehicle; FCEV: Fuel Cell Electric Vehicle; BEV: Battery Electric Vehicle.

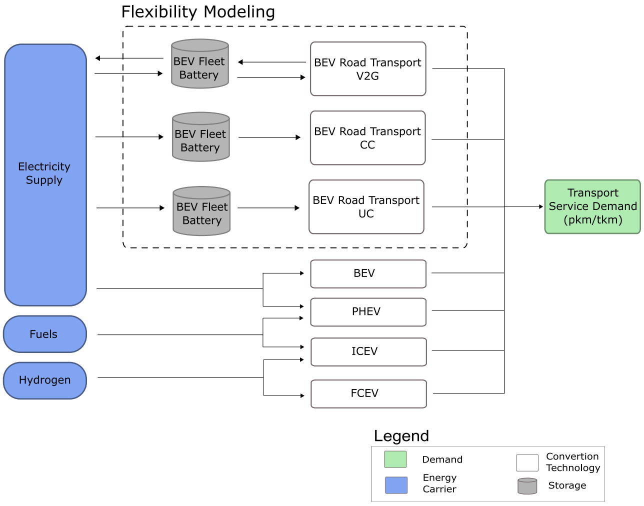


**Fig. 13.** Overview of the modeling concept applied to the transport sector.
Abbreviations: V2G: Vehicle-To-Grid; CC: Controlled Charging; UC: Uncontrolled Charging; BEV: Battery Electric Vehicle; PHEV: Plug-in Hybrid Electric Vehicle; FCEV: Fuel Cell Electric Vehicle; ICEV: Internal Combustion Engine Vehicle.
*Source:* Adapted from Ref. [44].

The main difference in the modeling of transport processes lies in a flexible vs. an inflexible approach, which has a strong influence on the parameter requirements and complexity. As shown in Fig. 13, all vehicles apart from road BEVs are characterized in particular by their specific fuel consumption to transform a fuel into transport services. The vehicle's internal tanks are not taken into account; instead, it is assumed that fuel is provided directly by the fuel production plant during the conversion into transport service in pkm or tkm. The fixed transport service demand is, therefore, inflexibly linked to the fuel demand.

The representation of BEVs in the model structure differs fundamentally from that of other vehicles (upper part of Fig. 13), as the storage capacity and direct link to the electricity grid require precise time-dependent modeling of the electricity demand. For this reason, the timing and flexibility of BEV charging processes are explicitly represented in the model structure to allow the consideration of a decoupling of demand for transport services from the electricity supply. As the charging flexibility is closely linked to the charging strategy, a distinction between three charging categories is made: Uncontrolled Charging (UC), unidirectional controlled Charging (CC), and bidirectional charging or Vehicle-To-Grid (V2G). The share of vehicles following each of these strategies can be specified exogenously based on the proportion of drivers who are willing to offer their storage for grid balancing in return for remuneration. Time series to model these three BEV charging strategies, which include the transport service demand, the fleet maximum and minimum battery levels, and the available charging power, can, for example, be generated using the open source tool venco.py [45].

### *3.6. Sectoral interfaces*

As previously elaborated, sector coupling is naturally related to a large number of interfaces. This must be considered while defining the system, as one sector might supply inputs for another sector. Graphical representations can help the modeler to support the understanding of this kind of complex system. With the very high number of processes included in the presented model structure, automatized network plotting based on graph algorithms is favorable (see Fig. 14). Here, the modeler is able to explore the energy system and particularly its sectoral interfaces by selecting sectors and aggregation levels while getting information and accessing the related data of the components by hovering over them. Apart from the system perspective (B) in Fig. 14 with all interconnections, selected commodities (A) can be assessed regarding their connected processes as well as selected processes (C) regarding their input and outputs. These interactive visualizations may

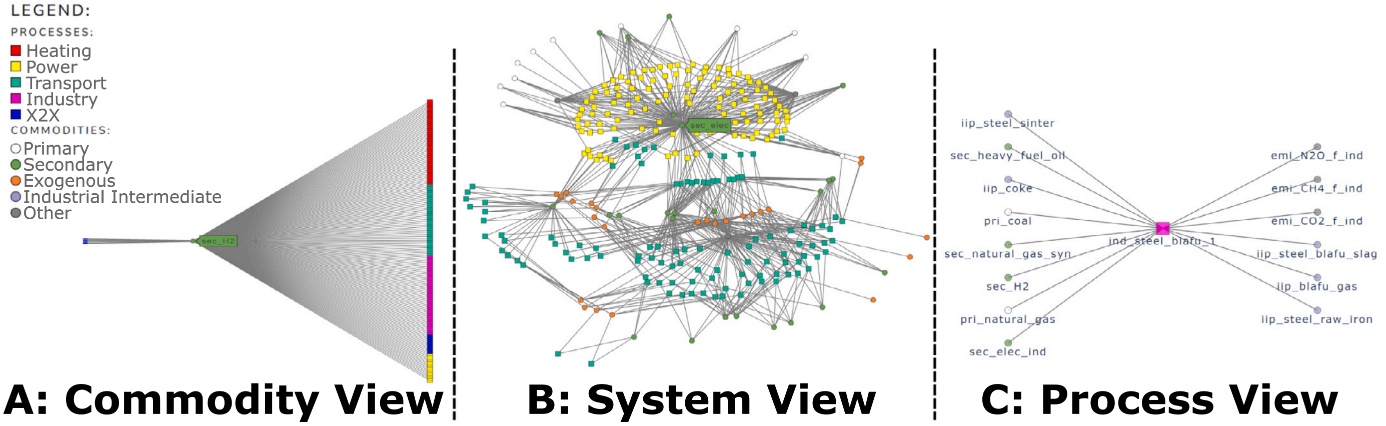


**Fig. 14.** Sample Network graph visualization use cases to explore the model structure qualitatively. Case (A): Related supply and consumption processes for hydrogen. For instance an electrolyzer and a blast furnace that is shown in Case (C). Case (B): Interfaces between power and transport sector — the main intersections can be identified at the adjacent sector boundaries. In this case, electricity generation technologies and the BEVs from the transport sector. Case (C): Possible inputs and outputs of a future blast furnace for steel.

be integrated into a graphical user interface to allow the modeler to walk through the system and thereby gain an understanding of the intersections of the provided large data set.

### 3.7. Discussion of the results

The system view on Fig. 14 highlights that the complexity of system interfaces increases with interconnected components from various sectors. Not all interfaces can be considered without a detailed analysis of spatial potentials and limitations of sector coupling, where available infrastructures play an important role. Therefore, a better understanding of these constraints requires a more detailed view of patterns of regional characteristics and interconnections. However, this enables a very high level of detail of the presented model structure with a focus on the technological characterization and thereby allows a holistic view of potential energy system configurations with special consideration of sector coupling. Another aspect that must be mentioned is that the long-term horizon also comes with increasing uncertainty for data points. This is mitigated by defining value ranges for especially uncertain parameters such as the costs of novel technologies where consulted literature values differ greatly.

Moreover, as indicated in Section 1, the presented model structure has been conceptualized for the German system as an example, but the future technologies and their relations within the model structure can be transferred to other country models and thereby reduce the required research work substantially. The feasibility of this transfer depends on the similarity of the country's energy system landscape. For instance, adaptation might be easier for developed countries than for emerging or developing ones. Regardless, brownfield parameters such as the installed capacities of existing technologies or potential national energy resources must always be adjusted in this process and hence require additional data.

Last but not least, it turned out that the direct comparison to the data of the existing literature is often difficult due to a lack of metadata and comprehensive descriptions of the model structure and its underlying assumptions. This article additionally concentrates on these factors to improve its ease of applicability for future studies.

## 4. Outlook and conclusion

The presented work enables modelers to analyze Germany's future technological pathways across the relevant energy sectors. The next planned step with the presented model structure is to run model scenarios and compare them to existing model results in the literature. Here, the comprehensive description of the novel model structure from this study facilitates the interpretation and comparison of its model results. Although the focus is on the specifics of sector-coupled energy systems, the model structure remains modular to allow users to work on their research questions with different foci. Depending on the research focus, due to the detailed process definition, it can also bring substantial added value to focus only on one chosen demand sector combined with aggregated supply sectors or to choose a subset of the provided milestone years according to the research question. Furthermore, as framework-specific adaptors are provided open-source on github, it is also easy to adjust the approach to other frameworks. Further, this is a suitable modeling base to perform sensitivity analyses based on the sectors' different available technological aggregation levels to investigate which technological aggregations significantly impact the results. As elaborated in Section 3.7, future research is also needed to enhance the representation of local characteristics by identifying typical structures in energy systems. This can be conducted based on the proposed model structure from the present study that lays the technological foundation for modeling energy systems across multiple sectors.

The presented article elaborated on the definition procedure of the model base with key principles, such as reducing exogenous assumptions with a technology-open approach and focusing on sector coupling. Moreover, each sector's resulting extensive model structure has been presented transparently to enable modelers to understand Germany's possible future technological pathways of relevant energy sectors. A reference data set with all relevant information to set up energy system optimization models based on the introduced model structure of this work, including extensive metadata with all consulted sources, is published on the Open Energy Platform (OEP) and registered on the energy databus which is linked in the data availability section below — free to share and adapt and to create novel research based on it. The energy data are annotated with available concepts from the Open Energy Ontology (OEO) [46] to foster clarity and transparency in data interpretation.

In summary, this paper contributes to the energy system modeling community by describing a comprehensive open-source model structure while elaborating basic background modeling assumptions. This transparent structure allows a smooth reproduction of energy system models with different modeling frameworks under special consideration of sector coupling.

## CRediT authorship contribution statement

**Beneharo Reveron Baecker:** Writing – original draft, Visualization, Supervision, Conceptualization. **Thomas Hamacher:** Writing – original draft, Conceptualization. **Viktor Slednev:** Writing – original draft, Visualization, Data curation. **Gian Müller:** Writing – original draft, Visualization, Data curation. **Vera Sehn:** Writing – original draft, Visualization, Data curation. **Jonas Winkler:** Writing – original draft, Visualization, Data curation. **Isela Bailey:** Writing – original draft, Visualization, Data curation. **Hedda Gardian:** Writing – original draft, Visualization, Data curation. **Hans Christian Gils:** Writing – review & editing. **Christoph Muschner:** Writing – review & editing. **Jann Michael Weinand:** Writing – review & editing. **Ulrich Fahl:** Writing – review & editing.

## 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.

## Data availability

The underlying open dataset for the model structure is uploaded on the OEP and the collection is registered on the energy databus (DOI). More extensive data-specific information can be accessed in the documentation.

## Acknowledgments

This work was supported by the Federal Ministry for Economic Affairs and Climate Action of Germany (BMWK) [project SEDOS, grant number 03EI1040A-F]. All figures and tables used in this manuscript were created by the authors themselves and are subject to the CCBY4.0 license unless otherwise declared. You are free to share and adapt the figures and tables. The authors thank Audrey Dobbins for proofreading the manuscript.

## References

[1] L. Schrattenholzer, The energy supply model MESSAGE, IIASA Research Report, 1981.

[2] L.G. Fishbone, H. Abilock, Markal, a linear-programming model for energy systems analysis: Technical description of the bnl version, Int. J. Energy Res. 5 (4) (1981) 353–375, http://dx.doi.org/10.1002/er.4440050406.

[3] R. Loulou, G. Goldstein, A. Kanudia, A. Letilla, U. Rmme, Documentation for the TIMES Model, IEA, 2016, URL https://github.com/etsap-TIMES/TIMES_Documentation/tree/master.

[4] U. Krien, P. Schönfeldt, J. Launer, S. Hilpert, C. Kaldemeyer, G. Pleßmann, Oemof. solph—A model generator for linear and mixed-integer linear optimisation of energy systems, Softw. Impacts 6 (2020) 100028, http://dx.doi.org/10.1016/j.simpa.2020.100028.

[5] T. Groß, K. Knosala, M. Hoffmann, N. Pflugradt, D. Stolten, ETHOS. FINE: A framework for integrated energy system assessment, 2023, arXiv preprint arXiv:2311.05930.

[6] S. Boyd, N. Parikh, E. Chu, B. Peleato, J. Eckstein, Distributed optimization and statistical learning via the alternating direction method of multipliers, Found. Trends® Mach. Learn. 3 (1) (2011) 1–122, http://dx.doi.org/10.1561/2200000016.

[7] J.F. Benders, Partitioning procedures for solving mixed-variables programming problems, Comput. Manag. Sci. 2 (1) (2005) 3–19, http://dx.doi.org/10.1007/s10287-004-0020-y.

[8] R. Rahmaniani, T.G. Crainic, M. Gendreau, W. Rei, The benders decomposition algorithm: A literature review, European J. Oper. Res. 259 (3) (2017) 801–817, http://dx.doi.org/10.1016/j.ejor.2016.12.005.

[9] F.A. Plazas-Niño, N.R. Ortiz-Pimiento, E.G. Montes-Páez, National energy system optimization modelling for decarbonization pathways analysis: A systematic literature review, Renew. Sustain. Energy Rev. 162 (2022) http://dx.doi.org/10.1016/j.rser.2022.112406.

[10] H.-M. Henning, A. Palzer, A comprehensive model for the german electricity and heat sector in a future energy system with a dominant contribution from renewable energy technologies—Part I: Methodology, Renew. Sustain. Energy Rev. 30 (2014) 1003–1018, http://dx.doi.org/10.1016/j.rser.2013.09.012.

[11] M.N.I. Maruf, Open model-based analysis of a 100% renewable and sector-coupled energy system–the case of Germany in 2050, Appl. Energy 288 (2021) http://dx.doi.org/10.1016/j.apenergy.2021.116618.

[12] M. Metzger, M. Duckheim, M. Franken, H.J. Heger, M. Huber, M. Knittel, T. Kolster, M. Kueppers, C. Meier, D. Most, S. Paulus, L. Wyrwoll, A. Moser, S. Niessen, Pathways toward a decarbonized future—Impact on security of supply and system stability in a sustainable german energy system, Energies 14 (3) (2021) http://dx.doi.org/10.3390/en14030560.

[13] M. Robinius, A. Otto, K. Syranidis, D.S. Ryberg, P. Heuser, L. Welder, T. Grube, P. Markewitz, V. Tietze, D. Stolten, Linking the power and transport sectors—Part 2: Modelling a sector coupling scenario for Germany, Energies 10 (7) (2017) http://dx.doi.org/10.3390/en10070957.

[14] H.C. Gils, H. Gardian, J. Schmugge, Interaction of hydrogen infrastructures with other sector coupling options towards a zero-emission energy system in Germany, Renew. Energy 180 (2021) 140–156, http://dx.doi.org/10.1016/j.renene.2021.08.016.

[15] Z. Wang, P. Jochem, H.U. Yilmaz, L. Xu, Integrating vehicle-to-grid technology into energy system models: Novel methods and their impact on greenhouse gas emissions, J. Ind. Ecol. 26 (2) (2022) 392–405, http://dx.doi.org/10.1111/jiec.13200.

[16] C. Müller, A. Hoffrichter, L. Wyrwoll, C. Schmitt, M. Trageser, T. Kulms, D. Beulertz, M. Metzger, M. Duckheim, M. Huber, M. Küppers, D. Most, S. Paulus, H.J. Heger, A. Schnettler, Modeling framework for planning and operation of multi-modal energy systems in the case of Germany, Appl. Energy 250 (2019) 1132–1146, http://dx.doi.org/10.1016/j.apenergy.2019.05.094.

[17] J. Gawlick, T. Hamacher, Impact of coupling the electricity and hydrogen sector in a zero-emission European energy system in 2050, Energy Policy 180 (2023) http://dx.doi.org/10.1016/j.enpol.2023.113646.

[18] F. Neumann, E. Zeyen, M. Victoria, T. Brown, The potential role of a hydrogen network in europe, Joule 7 (8) (2023) 1793–1817, http://dx.doi.org/10.1016/j.joule.2023.06.016.

[19] 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, http://dx.doi.org/10.1016/j.energy.2018.06.222.

[20] B. Reveron Baecker, S. Candas, Co-optimizing transmission and active distribution grids to assess demand-side flexibilities of a carbon-neutral german energy system, Renew. Sustain. Energy Rev. 163 (2022) 112422, http://dx.doi.org/10.1016/j.rser.2022.112422.

[21] M.M. Dekker, V. Daioglou, R. Pietzcker, R. Rodrigues, H.-S. de Boer, F. Dalla Longa, L. Drouet, J. Emmerling, A. Fattahi, T. Fotiou, P. Fragkos, O. Fricko, E. Gusheva, M. Harmsen, D. Huppmann, M. Kannavou, V. Krey, F. Lombardi, G. Luderer, S. Pfenninger, I. Tsiropoulos, B. Zakeri, B. van der Zwaan, W. Usher, D. van Vuuren, Identifying energy model fingerprints in mitigation scenarios, Nat. Energy 8 (12) (2023) 1395–1404, http://dx.doi.org/10.1038/s41560-023-01399-1.

[22] S. Candas, C. Muschner, S. Buchholz, R. Bramstoft, J. van Ouwerkerk, K. Hainsch, K. Löffler, S. Günther, S. Berendes, S. Nguyen, A. Justin, Code exposed: Review of five open-source frameworks for modeling renewable energy systems, Renew. Sustain. Energy Rev. 161 (2022) http://dx.doi.org/10.1016/j.rser.2022.112272.

[23] S. Halilovic, F. Böttcher, K. Zosseder, T. Hamacher, Optimization approaches for the design and operation of open-loop shallow geothermal systems, Adv. Geosci. (2023) http://dx.doi.org/10.5194/adgeo-62-57-2023.

[24] J.R. Birge, F. Louveaux, Introduction to Stochastic Programming, Springer Science and Business Media, 2011.

[25] S. Babrowski, T. Heffels, P. Jochem, W. Fichtner, Reducing computing time of energy system models by a myopic approach: A case study based on the PERSEUS-NET model, Energy Syst. 5 (1) (2014) 65–83, http://dx.doi.org/10.1007/s12667-013-0085-1.

[26] L. Barreto, Technological learning in energy optimisation models and deployment of emerging technologies, Journal article, Swiss federal institute of technology Zurich, 2001.

[27] U.K. Rout, U. Fahl, U. Remme, M. Blesl, A. Voß, Endogenous implementation of technology gap in energy optimization models—a systematic analysis within TIMES G5 model, Energy Policy 37 (7) (2009) 2814–2830, http://dx.doi.org/10.1016/j.enpol.2009.03.034.

[28] E. Zeyen, M. Victoria, T. Brown, Endogenous learning for green hydrogen in a sector-coupled energy model for Europe, Nature Commun. 14 (1) (2023) 3743, http://dx.doi.org/10.1038/s41467-023-39397-2.

[29] K. Volkart, C.L. Mutel, E. Panos, Integrating life cycle assessment and energy system modelling: Methodology and application to the world energy scenarios, Sustain. Prod. Consum. 16 (2018) 121–133, http://dx.doi.org/10.1016/j.spc.2018.07.001.

[30] C. Reinert, S. Deutz, H. Minten, L. Dörpinghaus, S. von Pfingsten, N. Baumgärtner, A. Bardow, Environmental impacts of the future german energy system from integrated energy systems optimization and dynamic life cycle assessment, Comput. Chem. Eng. 153 (2021) 107406, http://dx.doi.org/10.1016/j.compchemeng.2021.107406.

[31] T. Addanki, A. Cadavid Isaza, C. de la Rúa, L. Odersky, T. Hamacher, Impulsurbs: Integration of life cycle assessment into energy system models, Renew. Sustain. Energy Rev. 198 (2024) http://dx.doi.org/10.1016/j.rser.2024.114422.

[32] M. Wietschel, Sektorkopplung-Definition, Chancen und Herausforderungen, econstor, 2018, http://dx.doi.org/10.24406/publica-fhg-298838.

[33] J. Ramsebner, R. Haas, A. Ajanovic, M. Wietschel, The sector coupling concept: A critical review, WIREs Energy Environ. 10 (4) (2021) e396, http://dx.doi.org/10.1002/wene.396.

[34] G. Fridgen, R. Keller, M.-F. Körner, M. Schöpf, A holistic view on sector coupling, Energy Policy 147 (2020) http://dx.doi.org/10.1016/j.enpol.2020.111913.

[35] Y. Scholz, Speeding up Energy System Models a Best Practice Guide, beam-me, 2020.

[36] L. Kotzur, L. Nolting, M. Hoffmann, T. Groß, A. Smolenko, J. Priesmann, H. Büsing, R. Beer, F. Kullmann, B. Singh, A. Praktiknjo, D. Stolten, M. Robinius, A modeler's guide to handle complexity in energy systems optimization, Adv. Appl. Energy 4 (July) (2021) 100063, http://dx.doi.org/10.1016/j.adapen.2021.100063.

[37] L. Kotzur, P. Markewitz, M. Robinius, D. Stolten, Impact of different time series aggregation methods on optimal energy system design, Renew. Energy 117 (2018) 474–487, http://dx.doi.org/10.1016/j.renene.2017.10.017.

[38] L. Kotzur, P. Markewitz, M. Robinius, D. Stolten, Time series aggregation for energy system design : Modeling seasonal storage, Appl. Energy 213 (January) (2018) 123–135, http://dx.doi.org/10.1016/j.apenergy.2018.01.023.

[39] R. O. Harthan, H. Förster, K. Borkowski, H. Böttcher, Projektionsbericht 2023 für Deutschland, Umweltbundesamt, 2023.

[40] M. Blesl, Kraft-Waerme-Kopplung im Waermemarkt Deutschlands und Europas - eine Energiesystem- und Technikanalyse, Institute of Energy Economics and Rational Energy Use, 2014, http://dx.doi.org/10.18419/opus-2342.

[41] Institut Wohnen und Umwelt, TABULA, 2012, URL https://www.iwu.de/index.php?id=205.

[42] Statistisches Bundesamt, Zensus 2011, 2018, URL https://www.zensus2011.de/DE/Home/Aktuelles/DemografischeGrunddaten.html?nn=559100.

[43] H. Cischinsky, N. Diefenbach, ENOB:dataNWG: Forschungsdatenbank Nichtwohngebäude, 2021, URL https://www.datanwg.de/forschungsdatenbank/.

[44] German Aerospace Center (DLR), REMix [online], 2023, URL https://gitlab.com/dlr-ve/esy/vencopy/vencopy_015 [accessed 2023-11-28].

[45] F. Miorelli, N. Wulff, B. Fuchs, H.C. Gils, P. Jochem, An open-source python-based model to represent the charging flexibility and vehicle-to-grid potential of electric vehicles in energy systems models: venco.py, Preprint (2024).

[46] M. Booshehri, L. Emele, S. Flügel, H. Förster, J. Frey, U. Frey, M. Glauer, J. Hastings, C. Hofmann, C. Hoyer-Klick, L. Hülk, A. Kleinau, K. Knosala, L. Kotzur, P. Kuckertz, T. Mossakowski, C. Muschner, F. Neuhaus, M. Pehl, M. Robinius, V. Sehn, M. Stappel, Introducing the open energy ontology: Enhancing data interpretation and interfacing in energy systems analysis, Energy and AI 5 (April) (2021) 100074, http://dx.doi.org/10.1016/j.egyai.2021.100074.