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SecMOD: An Open-Source Modular Framework Combining Multi-Sector System Optimization and Life-Cycle Assessment

*Christiane Reinert[1], Lars Schellhas[1], Jacob Mannhardt[1], David Yang Shu[2], Andreas Kämper[1,2], Nils Baumgärtner[1], Sarah Deutz[1] and André Bardow[2,3]**

[1]Institute of Technical Thermodynamics, RWTH Aachen University, Aachen, Germany, [2]Energy & Process Systems Engineering, ETH Zurich, Zürich, Switzerland, [3]Institute of Energy and Climate Research - Energy Systems Engineering (IEK-10), Forschungszentrum Jülich GmbH, Jülich, Germany

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***Correspondence:**
André Bardow
abardow@ethz.ch

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Optimization models can support decision-makers in the synthesis and operation of multi-sector energy systems. To identify the optimal design and operation of a low-carbon system, we need to consider high temporal and spatial variability in the electricity supply, sector coupling, and environmental impacts over the whole life cycle. Incorporating such aspects in optimization models is demanding. To avoid redundant research efforts and enhance transparency, the developed models and used data sets should be shared openly. In this work, we present the SecMOD framework for multi-sector energy system optimization incorporating life-cycle assessment (LCA). The framework allows optimizing multiple sectors jointly, ranging from industrial production and their linked energy supply systems to sector-coupled national energy systems. The framework incorporates LCA to account for environmental impacts. We hence provide the first open-source framework to consistently include a holistic life-cycle perspective in multi-sector optimization by a full integration of LCA. We apply the framework to a case-study of the German sector-coupled energy system. Starting with few base technologies, we demonstrate the modular capabilities of SecMOD by the stepwise addition of technologies, sectors and existing infrastructure. Our modular open-source framework SecMOD aims to accelerate research for sustainable energy systems by combining multi-sector energy system optimization and life-cycle assessment.

Keywords: energy hub model, decarbonization, software, energy modeling, multi-objective optimization

1 INTRODUCTION

Energy systems are the backbone of our societies, providing a wide variety of energy services. It is now well recognized that energy systems need to reduce their environmental impacts. For this purpose, energy systems must integrate low-carbon electricity supply. Low-carbon electricity supply from wind and solar sources is highly weather-dependent. Hence, designing optimal multi-sector systems leads to the following challenges:

1) **Interconnected sectors**: Decarbonization of heating and industrial processes is often realized by sector coupling, e.g., by direct or indirect electrification (Ruhnau et al., 2019). Sector coupling, however, leads to dependencies between various products in a system, rendering synthesis more complex.
2) **Temporal and spatial limitations**: The availability of low-carbon electricity, such as wind or photovoltaics, is subject to high spatial and temporal variability (Ela et al., 2011). The resulting increasing dependence on temporal and spatial conditions must be taken into account in the synthesis of future systems.
3) **Environmental considerations**: Energy and process systems must comply with increasing environmental ambitions and regulations. Environmental impacts should thus be carefully monitored and fully considered in the synthesis (McDowall et al., 2018).
4) **Increased need for transparent models**: The transition to low-carbon energy systems can be planned and supported by energy models. The open provision of energy models can support the exchange of knowledge and methods to address mutual challenges.

To identify new energy system designs and operational strategies, mathematical optimization provides the most comprehensive approach (Andiappan et al., 2017). A prerequisite for optimization is a sufficiently accurate model. Guelpa et al. (2019) identify current trends in energy modeling: increasing connectivity, multiple interconnected sectors, and interaction of energy systems on multiple levels. These trends increase complexity. The trend of enhanced interconnection and interaction is complemented by environmental ambitions and regulations. Thus, energy models need to consider impacts on the environment, leading to further complexity. Holistic approaches assess environmental impacts by incorporating life-cycle assessment (LCA) to enable informed decision-making. As defined in ISO 14044 (2020), LCA targets the environmental assessment of a product or system over the whole life-cycle. Hence, LCA allows to systematically compare the environmental impact of different systems serving the same purpose. More than 1000 LCA studies of energy systems have been conducted, aiming at quantifying and reducing environmental impacts (Laurent et al., 2018). Conducting such LCA's is effortful, as they often require detailed data and models. In this work, we refer to a framework as a flexible software toolbox to construct models, as further discussed in Hilpert et al. (2018). A framework can comprise data processing, generalized equations, and optimization procedures. Frameworks can be used to develop and optimize specific energy models. As conceptualizing optimization models and frameworks and further performing system-level LCA is time-consuming, increasing reusability can significantly contribute to bundling and thus reducing research efforts. Ensuring reusability by flexible frameworks and publishing open-source software can help to design future energy and process systems more efficiently. Providing tools open-source is further crucial to validate and further develop models, thereby enhancing scientific understanding and progress. Overall, optimization models should meet the challenges of the energy transition by incorporating sector coupling, addressing spatiotemporal complexity, quantifying environmental impacts, and by pursuing transparency.

We use the term multi-sector energy model to describe models which have the functionality to provide more than one energy service (such as electricity, heat, or transport) or product (such as methane, steel). Multi-sector models, also called energy hubs, couple multiple sectors to increase overall system efficiency (Geidl, 2007). Mohammadi et al. (2017) reviewed energy hub models and concluded that they are particularly suited for modeling multi-energy systems because they enable a modular design and flexible coupling of different sectors using a matrix notation. Multi-sector system models support a wide range of planning areas from industrial (Sharif et al., 2014) and urban (Orehounig et al., 2015) to national (Krause et al., 2011) scale. The ability of energy models to support decision-makers in energy planning leads to a wide variety of available models: Chang et al. (2021) provide an overview over 54 energy modeling tools from local to global scope, categorizing their focus on relevance, suitability, and potential model linkage. Prina et al. (2020) review 22 energy models distinguished by geographical coverage, time resolution, methodology, programming technique, sectoral coverage and transparency. They find that the main challenge for current energy models, besides transparency, is achieving high detail, including the accuracy of the mathematical description resulting from the problem type (e.g., linear, nonlinear), or spatial, temporal, or sectorial resolution, referring to the number of nodes, time steps or sectors represented by the model. Fattahi et al. (2020) rank 20 integrated assessment models for the energy sector and emphasize the importance of adaptability to emerging technologies, sector-coupling and modeling non-monetary effects. On the large scale, further approaches are worth to be discussed: Inderwildi et al. (2020) review how the use of artificial intelligence via cyber-physical systems can support the energy transition. They stress that digitalization will improve environmental optimization and promote environmental advantages.

Multi-sector models are still typically based on an economic objective function. In addition to economic objectives, environmental aspects are becoming increasingly crucial in the synthesis of energy systems (Ringkjøb et al., 2018). The incorporation of environmental impacts into energy systems design requires their systematic evaluation by a system-level LCA and integration of LCA in the optimization on a process level. Moreno-Leiva et al. (2019) stress the need to consider both multi-sector systems and environmental impacts in the analysis of systems with rising shares of renewables.

In general, mathematical optimization can find designs and operation schedules that best satisfy any objective, not only minimal cost but also environmental impacts (Demirhan et al., 2019). Many recent multi-sector models consider greenhouse gas emissions as optimization constraint, limiting the overall system emissions. Often, only direct emissions are considered, neglecting upstream emissions from the production of supply technologies, such as energy converters

(McDowall et al., 2018). However, just as the overall cost-optimal system balances investment and operational costs, accounting for environmental impacts should include the whole life-cycle of a technology to identify environmental trade-offs. Hence, the assessment of environmental impacts should use life-cycle assessment, a standardized methodology to account for emissions over the whole life-cycle and assess a wide range of important environmental impacts (ISO 14044, 2020). Life-cycle assessment has been extended to life-cycle optimization using matrix notation (Suh, 2004; Saner et al., 2014; Kätelhön et al., 2016). The matrix notation in LCA can be regarded as a generalization of energy hubs in a sense that general processes convert and generate products and environmental flows. However, the above mentioned life-cycle optimization approaches are currently used only for systems with low spatiotemporal complexity.

Optimizing multi-sector systems with high temporal and spatial resolution is especially important for energy systems, as many decarbonization strategies rely on fluctuating renewable electricity supply and sector-coupling (Brown et al., 2018). LCA is combined with large-scale energy system optimization in integrated assessment models, ranging from large-scale models of global or national energy systems to detailed models of individual processes. Integrated assessment models can predict and quantify environmental burden shifting (Hertwich et al., 2015). Currently, a soft link between optimization and LCA (as in García-Gusano et al. (2016) and Brinkerink et al. (2022)) is more common than a full integration between the optimization model and LCA (as in Volkart et al. (2018)). On a process design level, Helmdach et al. (2017) link LCA and process simulations using multi-objective optimization and demonstrate that such links contribute to identifying tradeoffs between costs and environmental impacts. The SESAME tool (Gençer et al., 2020) provides a soft link to assess the life-cycle of an energy system subsequent to the system design. However, a direct link between optimization and LCA is necessary to identify the overall most efficient carbon-mitigation strategies. Integrating LCA further aids to assess the overall impacts to address potential burden-shifting in an early stage of strategic planning. Hence, directly combining optimization and LCA in one tool is an important step to find optimal low-carbon energy system designs.

However, fully integrated models are often not published as open-source software and therefore not accessible. Pfenninger et al. (2018) discuss the importance of transparency and open availability in energy modeling to support decision-makers. Since the creation of optimization models incorporating LCA is demanding, a growing community is committed to this task. The LAEND model (Tietze et al., 2020) models a district energy system combining investment optimization and LCA. The LAEND model optimizes various environmental target functions and further meets high transparency standards by publishing their code. However, the LAEND model has been developed for design problems without spatial resolution and sector coupling. Vandepaer et al. (2020) couple energy system optimization and LCA to analyze environmental trade-offs in a model of the Swiss energy system, mostly using open-source software. They underline the need for transparent and reusable tools to integrate LCA in energy system modeling and decision-making. Still, although the linear design of energy hubs has strong parallels to LCA, a generalized, open-source framework for the full and consistent integration of life-cycle assessment into optimization problems is missing.

1.1 Contribution of the SecMOD Framework

This work provides the generalized open-source framework SecMOD for multi-sector system optimization incorporating LCA, enabling optimization and assessment of linear multi-sector systems at flexible spatial and temporal detail. In our framework, we optimize the synthesis and operation of multi-sector systems. SecMOD provides a flexible modeling framework applicable from decentralized to large-scale energy systems. The object-oriented framework allows easy process modeling and adaption and can thereby comprise multiple sectors and technologies by modifying the input data only. Further, we incorporate matrix-based LCA into the optimization framework. During the optimization, LCA can be used either in the objective function or in constraints. In result, a system-wide LCA of the considered multi-sector system is obtained.

In **Section 2**, we discuss the framework design, provide the mathematical formulation, discuss the optimization method, and result visualization in SecMOD. In **Section 3**, we demonstrate the modularity of SecMOD using the sector-coupled German energy system as an exemplary application. Finally, in **Section 4**, we provide the discussion and conclusions. The code and its full documentation is completely open-source and can be found here: https://git-ce.rwth-aachen.de/ltt/secmod.

2 THE SECMOD FRAMEWORK: OPTIMIZING AND ASSESSING LINEAR MULTI-SECTOR SYSTEMS

SecMOD is an object-oriented software framework to optimize multi-sector energy systems, accounting for environmental impacts by incorporating life-cycle assessment. The main feature of the framework is the flexible model generation, as it is possible to add sectors and processes that convert different forms of energy in a modular way, without adapting the code of the optimization framework. **Figure 1** shows the flowsheet to use SecMOD.

In this Section, we split the discussion how to use the framework and its features into three parts: First, we define the model types that can be handled by SecMOD (**Section 2.1**) and discuss the data structure used in SecMOD, defining necessary and optional input data both on a system and on a process level. Second, we discuss the problem formulation, solver options and numerical strategies applied in SecMOD (Section 2.2). Last, we discuss the result processing and outputs of the framework (Section 2.3) and its limitations (Section 2.4).

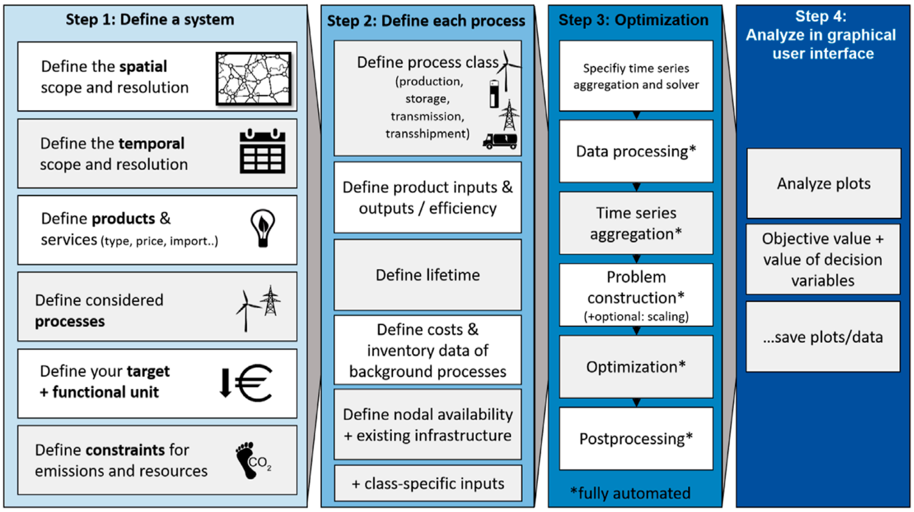

FIGURE 1 | Flowsheet of the SecMOD framework: First, the user needs to define a system. Second, the user needs to define processes used in the system. Third, the optimization is run. Last, the user can analyze the results in a graphical user interface.

2.1 Model Formulation

In general, an optimization problem can be formulated as minimization problem with equality constraints and inequality constraints (Nocedal and Wright, 1999). In this work, we present SecMOD for linear optimization (LP) problems. However, SecMOD can also be extended for mixed-integer linear programs (Reinert et al., 2022).

In our framework, the problem statement is as follows: Given

- a user-defined exogenous product demand (i.e., a predefined functionality which must be provided by the system, such as a specified amount of electricity, heat, and/or transport) that is spatially resolved in nodes $n \in N$ and temporally resolved to time steps $t \in T$ of length Δt_t in each year,
- a user-defined spatially and temporally resolved set of available processes $c \in C$ (e.g., wind turbines, heaters, and gas turbines) to convert ($C^{prod} \subset C$), store ($C^{sto} \subset C^{prod}$), and transport ($C^{grid} \subset C$) products $b \in B$,
- user-defined transport processes to deliver products between nodes via edges $l \in L$, of length Δl_l (e.g., electrical grids),
- and user-defined additional constraints,

we minimize the user-defined objective function (e.g., total annualized cost or total greenhouse gas emissions). The objective function consists of an annualized investment term (CAPEX$^{\text{prod}}$ and CAPEX$^{\text{grid}}$ for production and transport processes, respectively), and an operational term (OPEX). Costs $imp \in IMP$ may be of economic or environmental nature. In Eq. 2.1, we denoted the objective function for one optimization year, however, in general it is also possible to optimize a set of years to optimize a transition path with foresight (compare Baumgärtner et al. (2021)). The investment cost of all capacity installed in the current or previous years ($yex \in YEX$) consist of the specific investment costs $k^{\text{inv}}_{c,yex,imp}$ multiplied by the nominal capacity $p^{\text{nom}}_{c,n,yex}$ for production processes or by the product of nominal capacity and edge length $p^{\text{flow,nom}}_{c,l,yex} \Delta l_l$ for transport processes, respectively. The investment costs are further annualized using the net present value factor pvf_c, calculated according to Broverman (2017), with a user-defined interest rate. As time horizon to calculate the net present value factor, we use the minimum of the user-defined maximum discounting period and the actual component lifetime. The operational costs consist of the specific costs (e.g., maintenance) for operating a process $k^{op}_{c,imp}$ multiplied by the capacity that is used for product conversion $p_{c,n,t,yex}$ for each time step Δt_t and the import costs for a product $k^{op,import}_{b,t,imp}$ multiplied by the amount of product import $p^{import}_{b,t}$ for each time step. As decision variables, we consider capacity expansion of production and storage processes $p^{nom}_{c,n,yex}$, as well as the capacity expansion of transport processes $p^{flow,nom}_{c,l,yex}$ for the considered investment years, and the operation of processes $p_{c,n,t,yex}$, as well as product imports $p^{import}_{b,t}$.

$$\min_{p^{nom}_{c,n,yex}, p^{flow,nom}_{c,l,yex}, p_{c,n,t,yex}, p^{import}_{b,t}} \underbrace{\sum_{c \in C^{prod}} \sum_{n \in N} \sum_{yex \in YEX} \frac{k^{inv}_{c,yex,imp}}{pvf_c} p^{nom}_{c,n,yex}}_{\text{CAPEX}^{\text{prod}}}$$
$$+ \underbrace{\sum_{c \in C^{grid}} \sum_{l \in L} \sum_{yex \in YEX} \frac{k^{inv}_{c,yex,imp}}{pvf_c} p^{flow,nom}_{c,l,yex} \Delta l_l}_{\text{CAPEX}^{\text{grid}}}$$
$$+ \underbrace{\sum_{c \in C} \sum_{n \in N} \sum_{t \in T} \sum_{yex \in YEX} k^{op}_{c,imp} p_{c,n,t,yex} \Delta t_t + \sum_{b \in B} \sum_{t \in T} k^{op,import}_{b,t,imp} p^{import}_{b,t} \Delta t_t}_{\text{OPEX}} \tag{2.1}$$

$$\textit{subject to } \mathbf{A}_1 \cdot \mathbf{p} = \mathbf{b}_1 \tag{2.2}$$

$$\mathbf{A}_2 \cdot \mathbf{p} \le \mathbf{b}_2 \tag{2.3}$$

The constraints for the decision variables **p** are given by the equalities and inequalities with the coefficient matrices $\mathbf{A}_1$, $\mathbf{A}_2$ and the vectors $\mathbf{b}_1$, $\mathbf{b}_2$. Our problem formulation comprises equality constraints (Eq. 2.2), such as product balances, and inequality constraints (Eq. 2.3), such as limitations for capacity, availability, and impacts. All constraints governing component and system behavior are documented in detail in the repository of the framework in git-ce. rwth-aachen.de/secmod/optimization.

We evaluate the system and its operation using life-cycle assessment, as standardized in ISO 14044 (2020). Our discussion of the modeling inputs in SecMOD is therefore structured according to the stages of an LCA. LCA is a methodology for the environmental assessment of processes or systems over the whole life-cycle. Through the life-cycle of a process or system, material and energy flows are exchanged with the environment. LCA quantifies and interprets the material and energy flows regarding their impacts on the environment.

We incorporate the four stages of LCA as follows:

1) Goal and Scope: The user must define a functional unit and the system boundary (see **Figure 2**). The functional unit quantifies the performance of a system, i.e., the desired output of the multi-sector system. The functional unit can be either a single product or a product system (example for energy systems: provision of electricity in Germany over 1 year). The system boundary defines the scope of the multi-sector system, specifying all processes within a topology that are considered to supply the functional unit. Within the system boundary, processes are either explicitly modeled in the so-called foreground system or implicitly modeled in the background system. The background system comprises the supply chains of construction and disposal processes and raw materials used in the system (**Figure 2**), as discussed in Saber et al. (2020).
2) Life Cycle Inventories (LCIs): In SecMOD, the user must model the life-cycle of each process according to the chosen system boundary. For example, a cradle-to-grave consideration throughout the whole life-cycle should contain the LCIs for construction, the use phase and dismantling of all processes. LCIs catalogue the mass and energy flows required for the LCA. We distinguish between infrastructural and operational LCIs. Infrastructural LCIs describe the supply chains of installing a process, for example, a gas power plant requires steel and concrete in the construction phase. We annualize the infrastructural LCIs over the minimum of lifetime and a user-defined maximal timespan to evenly distribute environmental impacts over the use phase. We assume that environmental damage is not discounted over time. Operational LCIs describe the requirements for operating a process. For example, a gas power plant requires natural gas, which is combusted during process operation, and maintenance.
3) Life Cycle Impact Assessment (LCIA): LCIA methods quantify the environmental impacts caused by the environmental flows of LCIs. The life-cycle impact

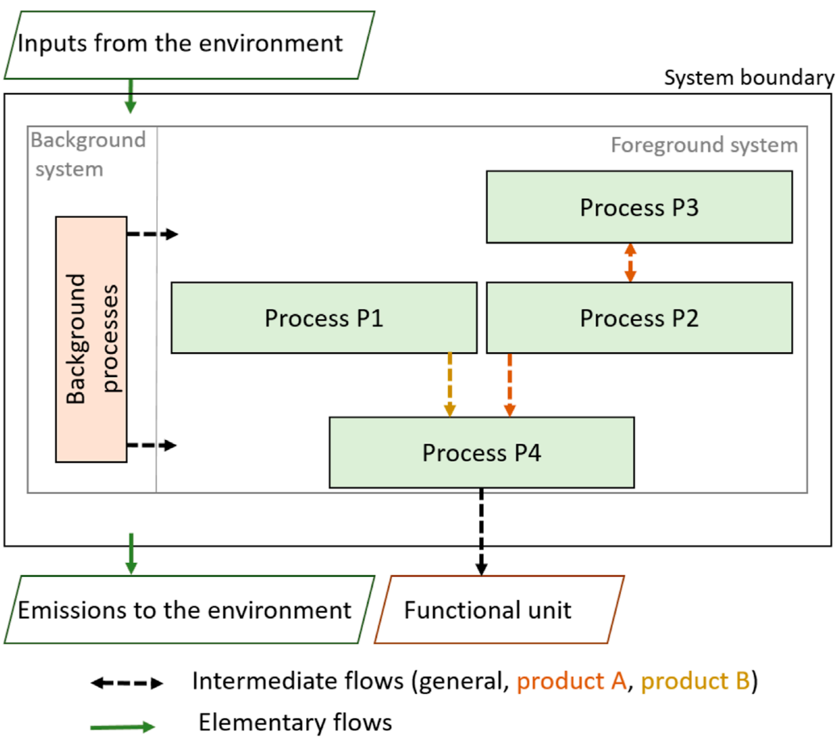

FIGURE 2 | Functional unit and system boundary of a generic multi-sector system.

assessment evaluates potential environmental impacts for a product system throughout the life-cycle of the product. In principle, SecMOD can assess systems using any impact assessment method. As default methods, we implemented environmental footprints, as recommended by the European Commission (Joint Research Center, 2010) and ReCiPe (Goedkoop et al., 2009). The impact assessment methods allow to quantify numerous environmental impact categories beyond climate change, for example the resource depletion of minerals and metals, land use changes or water scarcity.

4) Interpretation: The interpretation of an LCA involves a critical review, analysis of data sensitivity and the result presentation. SecMOD can support practitioners by showing the results in a graphical user interface, where a detailed analysis is possible.

In the SecMOD framework, environmental impacts can be integrated into the optimization problem in three distinct ways and in any of their combination:

1) By selecting environmental impacts as objective function: In addition to economic cost optimizations, the SecMOD framework allows minimizing the annualized impact of any impact category, e.g., the overall global warming impact.
2) By constraining environmental impacts: Any environmental impact category can be limited (globally or on a nodal level).
3) By assessing environmental impacts subsequent to the optimization: Environmental impact categories that are neither used as an objective function nor as constraint, can still be evaluated for the resulting system.

In the following, we first discuss the modeling on a system level (cf. **Figure 1**). Within each system, the demands can be met using a set of processes. In the process modeling, we define process classes that can be used in the system, and the required inputs for each process. Please note that in addition to the brief description of the SecMOD framework in this work, an implementation example is given in the git repository (see Supporting Information) and the code is documented extensively to provide a comprehensive introduction into the modeling. The SecMOD framework is independent from the investigated processes and systems: It is implemented such that new processes and systems can be investigated by the sole addition and modification of input data. Further, a detailed list of all *Python* packages we used in SecMOD is given in the setup and documentation of our code.

2.1.1 System Modeling

The system is characterized by a desired output (functional unit), modeled as exogenous product demand, an objective function and constraints (**Figure 1**). Optionally, constraints limiting costs or emissions can be violated at the cost of a penalty in the objective function, called overshoot.

SecMOD considers several sets: The topology is determined by a set of nodes and a set of connections. The temporal resolution is determined by a set of investment years, foresight, and time steps. Further, the set of products determines the available products and services, such as sectors and energy carriers. **Table 1** provides an overview and examples for each user-defined element.

TABLE 1 | Input data for system modeling in SecMOD.

System modeling	Input	Description
General	Objective function	At least one cost/impact category must be defined as objective function
	Impact categories and costs as additional constraints	All impact categories can be constrained in operation, in investment, or in total
	Overshoots	Slack variable penalized in the objective function to relax cost constraints
	LCIA database	LCIA database, must be integrated for environmental data, e.g. ecoinvent
	Product demands and costs	Each product can have temporally and spatially resolved product demands and temporally resolved costs
	Required secured capacity	User-defined minimal overall capacity that can provide a product
Sets	Topology	A set of connected nodes must be defined
	Investment horizon	Set of investment periods in which investment decisions can be made must be defined
	Time steps	Set of time steps within each investment year must be defined
	Products considered in the model	Products produced or consumed by the processes must be defined

Topology: The spatial resolution in SecMOD is flexible. Hence, SecMOD can model a wide range of energy systems: from industrial sites with a single node to highly interconnected multi-national energy systems. The set of nodes defines the location of each site or region modeled. At each node, the product balances need be closed, i.e., each product demand has to be met by either product conversion, storage discharge or by imports to the node. On a nodal level, limitations of environmental impacts may be defined. Connections allow transport of products between nodes. In the set of connections, the user defines the start- and end node of each connection. Transport processes can only be used or built on connections defined in the system model.

Temporal resolution: Next, the temporal scope of the system has to be defined: each system can be optimized for a single optimization period or a set of optimization periods which then form a transition pathway over the whole investment horizon. The user must define the functional unit and price developments for all years within the investment horizon.

When a transition pathway is optimized, the user can define the foresight of the optimizer: The periods can either be optimized with full knowledge in a perfect foresight optimization, individually per optimization period without any foresight or by employing a rolling horizon, where a subset of contiguous optimization periods is considered to optimize the current investment period (as described in Baumgärtner et al. (2021)). A rolling horizon hence optimizes the current optimization period under (limited) knowledge of the future and can therefore consider some future system conditions, such as higher restrictions on greenhouse gas emissions, in current investment decisions.

On a more granular level, within one optimization period, the considered time steps must be specified by the user. The TSAM package (Hoffmann et al., 2020) is embedded in SecMOD to use time series aggregation, clustering the full time series into typical periods. Each period consists of a specified set of connected time steps. If aggregation to typical periods is used, only short-term storage can be modeled. Therefore, seasonal storage is currently not in the scope of SecMOD.

Products: A product is any input or output of energy or mass. Typically, a product models a final energy sector (e.g., electricity or heat) or an energy carrier, which is converted to supply final energy products (e.g., hydrogen or natural gas). SecMOD is not limited to energy services: Generally, any physical output can be a product in the SecMOD framework, such as the production of an industrial product (e.g., a finite amount of steel or cement). Product demand can be user-defined exogenously, or arise endogenously as a result of conversion processes. The demands can be satisfied by conversion from other products or by import over the system boundary. Intermediate products can be produced and subsequently consumed within the system boundary. For each product, it is possible to specify whether it may be imported over the system boundary. For example, the user could specify that while fuels may be imported, electricity can only be produced within the system boundary to enforce local electricity generation. Import prices and nodal demand for each product may be defined as temporally resolved parameters.

Costs and Environmental Impacts: SecMOD supports the analysis of energy systems regarding their costs and impacts: Costs and impacts are employed in the objective function (Eq. 2.1) and in constraints (Eqs. 2.2 and 2.3). SecMOD requires an LCA impact database such as ecoinvent or a user-defined database provided as an impact matrix. The GitLab model already provides the functionality to include ecoinvent. As most impact matrices provide numerous LCIA methods, the user may specify the impacts considered in SecMOD, their global and nodal limitations, and their impact on the objective function.

2.1.2 Process Modeling

Processes produce, transport, or store products in the system. While the goal and scope are defined on the system level, the

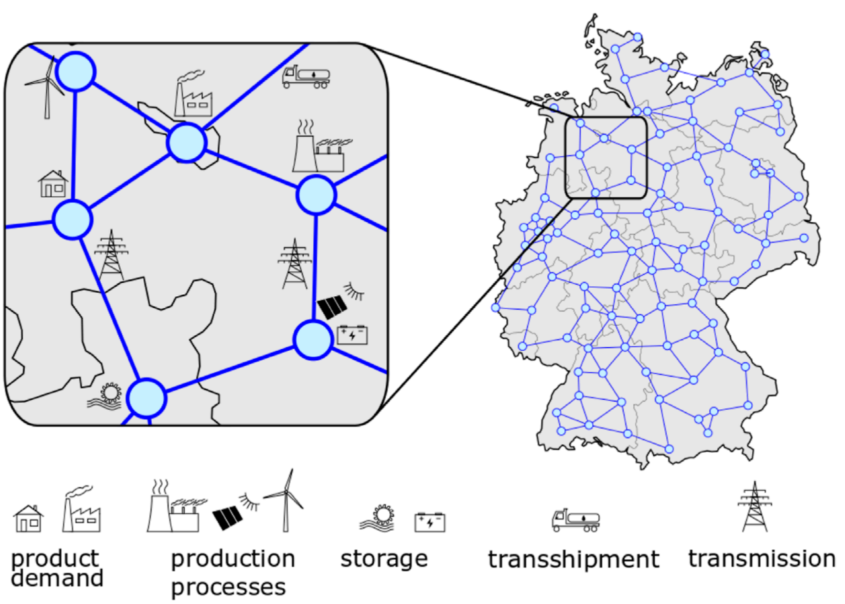

FIGURE 3 | Exemplary topology of a spatially resolved energy system with nodal energy demands. Production and storage processes are located at nodes and transport processes (transmission and transshipment) are located at edges.

user must define costs, impacts and technical specifications of the technologies employed to produce the required output on a process level. Processes are either related to converting/storing products and hence associated to nodes, or used to transport products between nodes and therefore associated with connections (**Figure 3**). Each process is modeled by the input data discussed in **Table 2**. The user needs to define costs, LCIs and technological specifications (such as the lifetime) for each process. All processes are part of one out of four process classes:

Production processes are processes at nodes, which produce and/or consume products, including the conversion of flows from a single product or a set of products to another single product or set of products (e.g., conversion of natural gas to electricity). The user needs to define the technology matrix, determining the ratio between the input and output products.

Storage processes are processes at nodes, which store a product over time (e.g., pumped-hydro storage). The user may define losses for storage and withdrawal.

Transshipment processes are processes at connections that transport a specific product between nodes with a transshipment approach (e.g., pipeline). Connections have no storage capacity for transshipment processes; hence, we assume no temporal delay in transportation. The user may define transshipment losses.

Transmission processes are processes at connections that transport electricity using the DC load flow approach (Van den Bergh et al., 2014). Transmission processes are assumed lossless. The user must define a safety margin for installed capacity, the voltage level, power limit and specific reactance and resistance, as additional process data.

At each node, processes can convert products into each other to fulfill the product demand specified in the functional unit. Process models are specified by mandatory and optional input data, as stated in **Table 2**. For the set of processes, the user may define existing capacities, availabilities, and limitations of capacities on a nodal level. For all transport processes, we allocate half of the impacts to each of the nodes that the process connects. However, the allocation principle does not impact the results since we minimize the total impacts of the system.

As an alternative to a manual definition of existing capacities of production processes in the electricity sector, it is possible

TABLE 2 | Mandatory and optional input data of processes in SecMOD.

Process modeling	Input	Function	Examples
Mandatory input data for each process	Technology matrix	Defines product inputs and outputs	Heat pump (production process): Consumes x kW electricity to produce y kW heat at low temperature ($<100°C$)
	Invest and operational costs	Fixed and variable cost parameters	
	LCIs for invest and operation	Life Cycle Inventories to consider environmental impacts of design and operation	Gas turbine: Construction of plant (e.g., cement), maintenance
	Lifetime duration	Lifespan of a process	
Optional input data for each process	Availability	Spatial and temporal availability of the process	Spatial and temporal limitation of wind power usage due to weather conditions
	Learning curves	Learning curves for costs, LCIs and efficiency development	Cost decrease and efficiency increase of photovoltaic cells due to expected technological developments
	Existing capacity	Capacity built before the optimization year	x MW wind turbines capacity at node n_1

to automatically integrate open-source data from the Open Power System Database for many countries (Wiese et al., 2019). In SecMOD, system models can be optimized using various topologies (e.g., local system and surrounding power system) based on the same process assumptions, thereby increasing consistency between different modeling scopes.

2.2 Optimization

The framework runs platform independent and was tested both on Windows and Linux. The creation and solution of the optimization problem are fully automated processes that run after the system and process modeling steps. However, the following optimization parameters need to be defined: the desired level of temporal aggregation (e.g., typical periods and time resolution within the period), scaling procedure, solver type, and settings (such as the number of optimization years).

First, the data processing module loads the input data into instances of the data classes. From the data classes, an input dictionary is created, which includes all information required to run the optimization. For the full description of the data processing module, please see the documentation of SecMOD in the git repository. The user needs to define the number of typical periods to aggregate the temporally-resolved input data, using the TSAM package for time series aggregation (Hoffmann et al., 2020). Furthermore, we use numerous python packages for scientific computing, handling physical units consistently, and for visualization. A full list of the packages we use is provided in the code documentation.

The optimization problem is built in Pyomo 5.7.1 (Hart et al., 2011; Bynum et al., 2021). The most important elements in pyomo are sets, parameters, variables, constraints and the objective function. Sets, for example the set of nodes, are used for indexing and are not changed during the optimization. Parameters, such as the costs of a technology, are static inputs that also do not change during the optimization. In the code, we defined default values for some parameters to reduce the amount of necessary input data. For example, if there is no existing capacity given in the input data for a certain process, the existing capacity is set to zero. Variables can change their value during the optimization. The decision variables used in SecMOD are discussed in **Section 2.1**. Constraints limit the solution space of the optimization problem and can be defined as both equality or inequality constraints. The objective function defines the goal of the optimization. The total investment and operational cost of the system are determined as the sum of the individual process impacts and can be used as objective function in the optimization (see **Section 2.1**). In SecMOD, the objective function contains many terms that can be activated or deactivated via the input data. Thereby, any environmental impact or economic cost can be optimized. Further, not only the overall costs or impacts can be set as objective function, but also the costs or impacts of the investment or operation only.

Before the optimization, SecMOD automatically iterates through the variables and fixes trivial variables to zero to reduce computational effort. To improve performance, we added an optional, automated scaling routine to reduce numerical problems when large-scale systems are optimized. Scaling can be applied to the constraints (i.e., rows of the optimization problem), variables (i.e., columns of the optimization problem), or both. When solving large-scale problems, both constraints and variables should be scaled.

The user needs to select a solver, e.g., Gurobi (Gurobi Optimization, LLC, 2021) or CPLEX (CPLEX, 2009).

The optimization problem can be solved for one single investment period. Alternatively, the problem can be solved for a transition pathway. If a rolling horizon with foresight is applied, each optimization optimizes several investment periods at once. When a transition pathway is optimized, the results of each investment period are used to update the existing infrastructure as input parameters for the next investment period. When the optimization is finished, the results are written back to the data classes and evaluated.

2.3 Visualization of Optimization Results

The results are the objective value and the values of the decision variables, typically the resulting capacity expansion and the optimized operational decisions (i.e., product flows) over the whole transition path. Further, we calculate a full LCA of the resulting system. Here, the impacts can be assessed either in total or distinguished by infrastructure-related and operation impacts. In SecMOD, we implemented an automized result assessment via a graphical user interface (see **Figure 4**). The user interface shows the capacity, product flows, and impacts for all products in three plot types (area plot, bar plot or line plot). By clicking on a process, the construction years of each process capacity are shown in a second layer. Further, all raw results are shown as a table next to the plot. Figures and numerical results can be exported in a variety of data formats: xlsx, tikz, png, pdf.

2.4 Limitations of SecMOD

SecMOD is currently formulated as a linear program. In an accompanying work, we extended SecMOD to MILP by allowing to consider part loads and component sizes (Reinert et al., 2022). However, modeling nonlinear effects, such as the dependency of LCIs on equipment scaling, is currently beyond the scope of SecMOD. In addition, enlarging the scope of energy system models can result in challenges arising from differences in nomenclature and definitions across fields covered by multi-sectoral models making integration challenging. Ontologies can aid in improving consistency between models and tools (Booshehri et al., 2021).

The user can define future trajectories for technologies costs and efficiency. The assumptions can heavily impact optimization results (Trutnevyte, 2016). Currently, the cost and efficiency assumptions are limited to parameter inputs for every investment horizon. The current version of SecMOD does not provide a feedback loop, where technology costs decrease upon higher market penetration and neglects technological breakthroughs.

In our framework, users often have to simplify spatial and temporal complexity and the system-wide interaction of energy systems to maintain computational tractability. Advances in methods for complexity management are

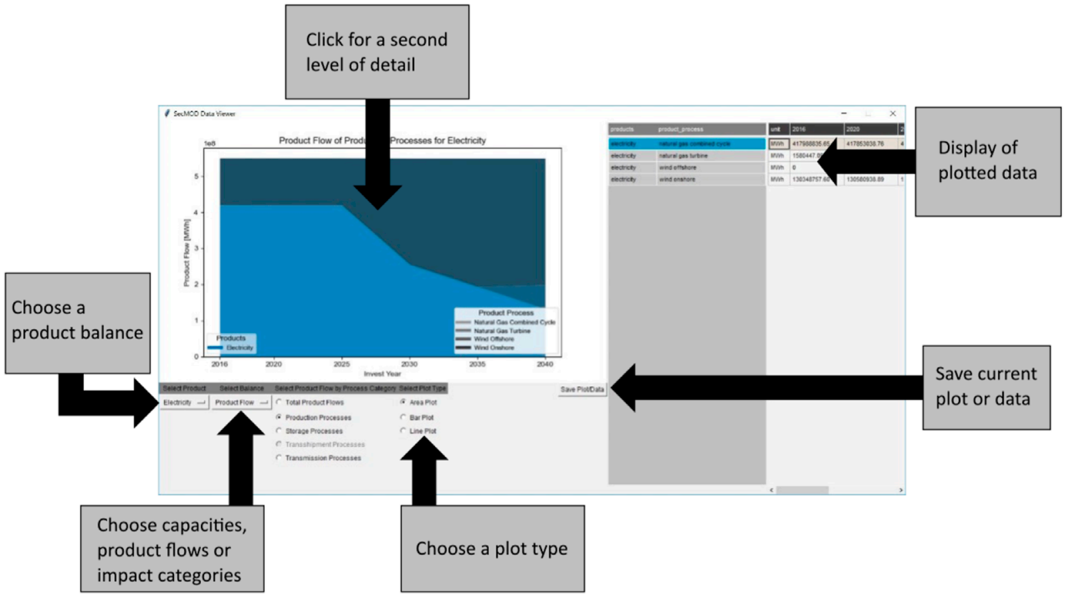

FIGURE 4 | Graphical user interface for the result assessment of SecMOD.

still needed to enhance the accuracy of energy models (Ridha et al., 2020). To reduce complexity, our optimizations are fully deterministic, as common for potentially large-scale energy system models (Ringkjøb et al., 2018). However, the framework could be extended to account for uncertainty, e.g., by using modeling to generate alternatives (DeCarolis et al., 2016), robust optimization (Majewski et al., 2017) or stochastic programming (Nolzen et al., 2021).

In addition, the level of spatial and temporal detail depends also on data availability. The data availability can be different across technologies and sectors, but also between the modeling and its underlying LCA data. Differing levels of detail lead to inconsistencies: For example, LCIs are often available only at a country level, whereas energy models usually rely on a much more granular spatial resolution.

Despite our efforts to provide a comprehensive open-source tool, LCA databases, such as ecoinvent, are often not openly available. Furthermore, LCA databases rely on models that introduce modeling errors themselves. In this sense, we emphasize the need for openly available and transparent LCA data, such as the European Platform on Life Cycle Assessment is aiming for (Fazio et al., 2016). Further improvements, such as improvements in regionalization, will improve consistency between LCIs and energy system model and LCA results.

Last, users should be aware that assumptions in the input data can significantly impact optimization results: Practitioners should be aware that any large-scale multi-sector energy system model can only represent a simplified version of reality (Sgouridis et al., 2022). Tools like SecMOD can find the mathematically best solution of a given problem, however, they show only one out of many possible future scenarios. Hence, the resulting transition pathways must be understood as decision support based on current information, but not as a definite prediction of the future.

3 CASE STUDY

3.1 Problem Definition

As an exemplary application, we economically optimize the German energy system, gradually adding technologies and sectors by solely modifying the input data. In the first part, we optimize the German electricity system with only few processes (Case 1: greenfield simple), then add further processes (Case 2: greenfield extended). In the next step, we add existing infrastructure to the extended model (Case 3: brownfield extended), demonstrating the flexible process model generation in SecMOD. We optimize the extended brownfield case by an economic and an environmental objective, by again modifying the input data only. Here, we compare the economic objective of cost minimization to minimizing the greenhouse gas emissions. Last, we focus on sectoral interactions: we jointly optimize the electricity, heating and transport sectors in Germany, first, without any sector-coupling processes (Case 4: parallel sectors) and then with the option of sector-coupling (Case 5: sector-coupling). Here, we demonstrate how SecMOD can be used to analyze the impact of emerging processes in energy systems.

An overview of products and processes used in each case study is given in **Table 3**. The system and process parameters of our case studies are largely based on Baumgärtner et al. (2021), as they discuss the optimization and life-cycle assessment of the German energy system in detail. However, for demonstration,

TABLE 3 | List of case studies considered to demonstrate the modular setup of SecMOD. All cases built up on the previous cases. Extensions of previous case settings are indicated by a '+'. For each case study, we highlighted the most important extension, compared to the respective previous case, in bold.

	Case 1	Case 2	Case 3	Case 4	Case 5
	greenfield simple	greenfield extended	brownfield extended	parallel sectors	sector-coupling
Sectors	Electricity	Electricity	Electricity	Electricity, heat, transport	Electricity, heat, transport
Products	Natural gas, electricity	+ **lignite, coal, oil, biogas, nuclear**		+ **heat at 3 levels, mobility,** fuels	
Processes	Wind turbine, natural gas turbine, battery storage, grid	+ electricity production processes		+ heat /transport processes	+ **sector-coupling** production processes
Optimization years	2016–2040	2016–2040	2016–2040	2016–2030	2016–2030
Approach	Greenfield	Greenfield	**Brownfield**	Brownfield	Brownfield

we consider a simplified system, as the purpose of our case studies is to illustrate the modular setup of SecMOD. Products and processes can be added to modify the case study by changing the input data only. To add a product or process, the user can simply copy an existing product or process folder and modify its parameters (stored in . csv files) as desired. To delete a process, the respective folder can just be deleted. The modified input data will automatically be considered during the next optimization run.

The case studies consider a national energy system - a topic which is currently highly discussed in the literature (Naegler et al., 2021). Additionally, our framework is suitable for modeling many other use cases, such as the optimization of industrial utility systems (Reinert et al., 2022), and we are excited to see what use cases will emerge in the future.

Functional Unit and System Boundaries: The functional unit is the provision of the overall electricity (Case 1–3) and, where applicable, heating and mobility (Case 4–5) demands in Germany for the respective year in the transition pathway until the year 2030 (Case 4–5) or 2040 (Case 1–3) (optimization in 5 years steps). As processes, we consider different energy converters and an electricity grid (see **Table 3**).

System modeling: The model of the German energy system is aggregated to 18 nodes, using the topology and product demands from Baumgärtner et al. (2021). The time-dependent parameters, such as the demand, have an hourly temporal resolution. As objective function, we minimize the total annualized costs for the considered investment period without foresight. An exception is **Figure 7**, where we minimize the greenhouse gas emissions. We constrain the energy system according to the current climate targets in Germany: As environmental constraint, the operational greenhouse gas emissions until year 2030 (2040) must be reduced by 65% (88%), compared to the year 1990. The allowed greenhouse gas emissions are stepwise lowered over the investment horizon.

Process modeling: We model the processes according to Baumgärtner et al. (2021), and use the same set of processes. In cases where we consider pre-existing infrastructure, we included infrastructure for the base year 2016 as parameters in the process models but permitted further expansion of capacities as design variables of the optimization problem.

LCIA: For consistency, we apply the same LCIA database ecoinvent 3.5 APOS (Wernet et al., 2016) as in Baumgärtner et al. (2021), with a dynamization to account for long-term changes in the supply chains of products (Reinert et al., 2021). As impact assessment method, we use Environmental Footpoints 2.0, as it is available in ecoinvent 3.5 and recommended by the European Union. However, the database can easily be updated to more current versions.

Optimization: For numerical stability, we apply scaling to the constraints and variables. As a solver, we used Gurobi (Gurobi Optimization, LLC, 2021). In the time series aggregation, we aggregate the time steps to 10 typical periods, each consisting of 24 hourly time steps.

Figure 5 compares two greenfield and one brownfield optimizations with different varieties of available processes (Cases 1–3 in **Table 3**). Please note that we scale the resulting capacity of each case study by the same reference. As a reference, we use the brownfield optimization (case study 3, as defined in **Table 3**). Thus, the capacity in the first year of the brownfield optimization (Case 3) is used to normalize all results. Hence, a capacity of 200% in 2016 indicates that the overall infrastructure is twice as high as in the reference case study 3. In the simple

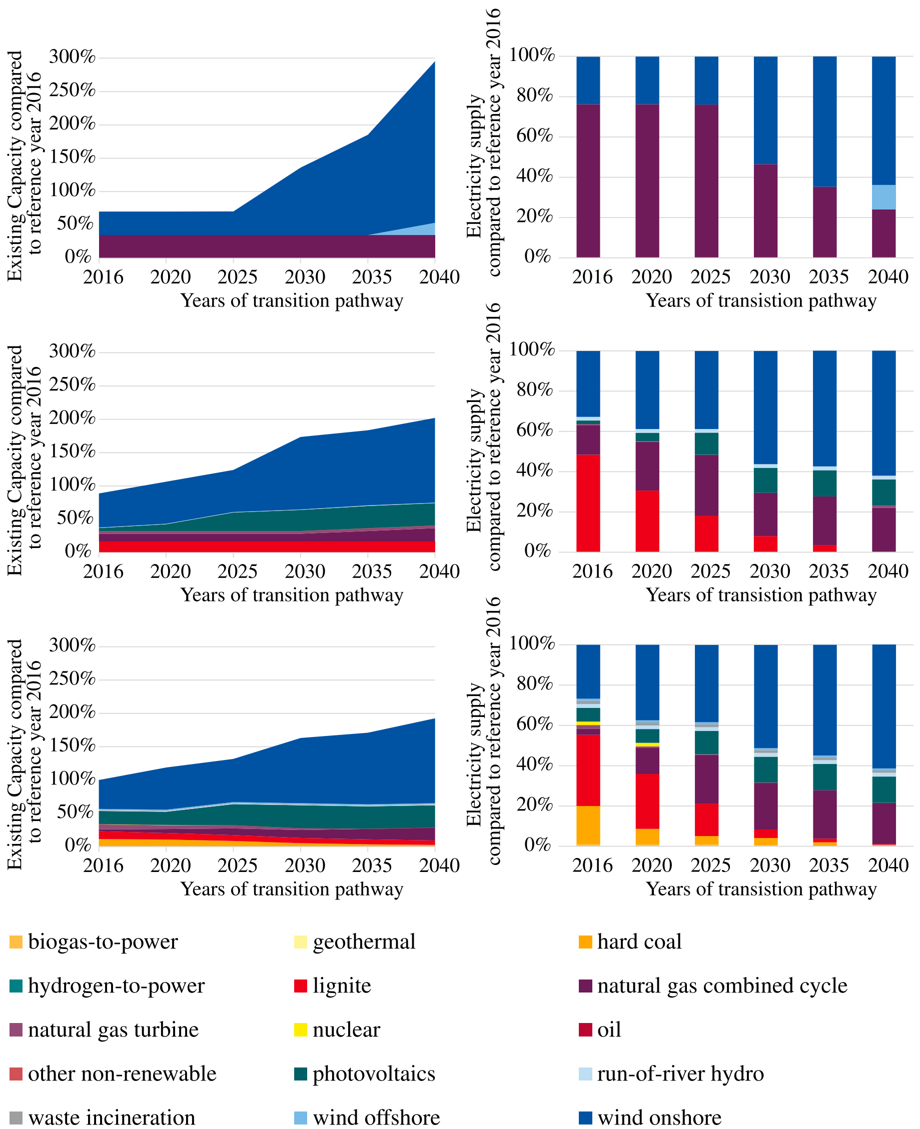

FIGURE 5 | Transition pathway of the German electricity sector until the year 2040 for three cases (Cases 1–3 in **Table 3** from top to bottom). The left column shows the optimized production process capacity for electricity generation compared to the overall production process capacity in the reference case (Case 3, year 2016, as defined in **Table 3**). The right column shows the electricity production shares of the different production processes.

greenfield case, the overall production process capacity is lowest in the reference year 2016. Please note that for brevity, we show only production processes and do not include storage and transport processes in the figures. As electricity generation by natural gas has relatively low greenhouse gas emissions compared to other fossil energy conversion, smaller amounts of renewable energy are necessary, compared to the other systems. Therefore, in the simple greenfield case, the constraints in greenhouse gas emissions only restrict the system starting in year 2025, leading to a change in operational strategy. In the extended greenfield and brownfield cases (Cases 2 and 3), the restriction on greenhouse gas emissions leads to an immediate transition.

We assess the environmental impacts of the production processes for case study 3, following the Environmental Footprints 2.0 method (**Figure 6**, left). We observe numerous co-benefits of the transition to low-carbon electricity supply with 13 out of 15 impacts reducing from 2016 to 2040. However, the depletion of minerals and metals and ozone depletion are substantially higher. These findings are in line with other LCAs of the German electricity sector (e.g., Rauner and Budzinski (2017)). For an in-depth LCA of the full sector-coupled German energy system, please also refer to Baumgärtner et al. (2021) who discuss these environmental trade-offs building upon the same data set.

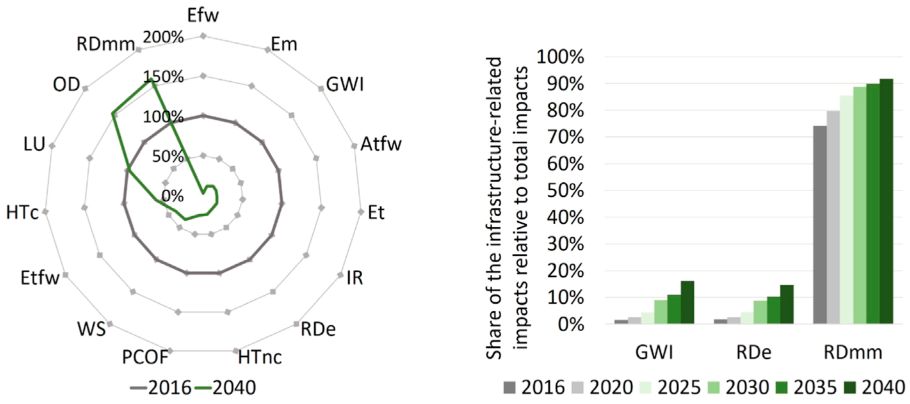

FIGURE 6 | Environmental impacts of the production processes in case study 3 for year 2040, relative to the base year 2016 (left). Share of infrastructure-related impacts on the total impacts for selected impact categories (right). Shown impact categories: freshwater eutrophication (Efw), marine eutrophication (Em), global warming impact (GWI), freshwater and terrestrial acidification (Atfw), terrestrial eutrophication (Et), ionizing radiation (IR), resource depletion, energy (RDe), human toxicity, non-carcinogenic (HTnc), photochemical ozone formation (PCOF), water scarcity (WS), freshwater ecotoxicity (Etfw), human toxicity, carcinogenic (HTc), land use (LU), ozone depletion (OD), resource depletion, mineral and metal (RDmm).

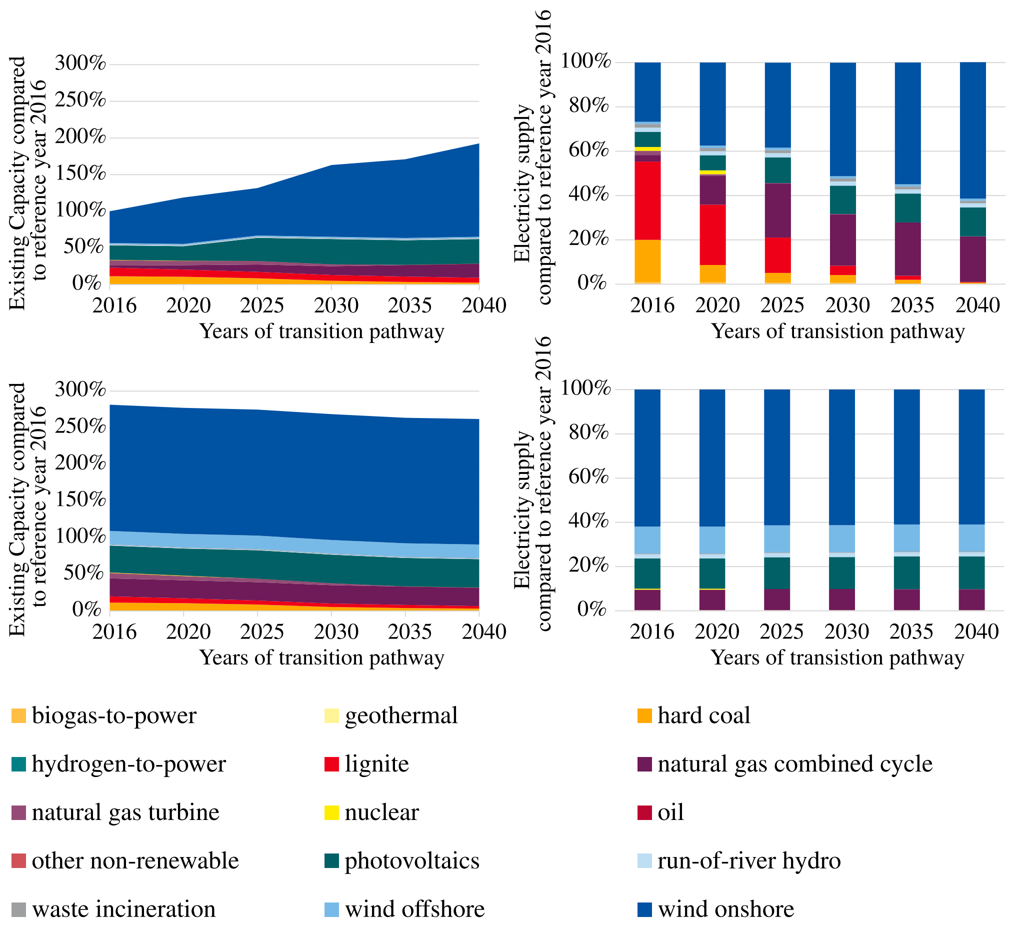

FIGURE 7 | Extended brownfield case with different objective functions: The upper figures show the cost minimal case, whereas the figures on the bottom show an environmental objective, where the global warming impact (GWI) of the system is minimized. The left column shows the optimized production processes for electricity generation compared to the reference year of 2016 in case study 3 (**Table 3**). The right column shows the electricity production shares of the different production processes.

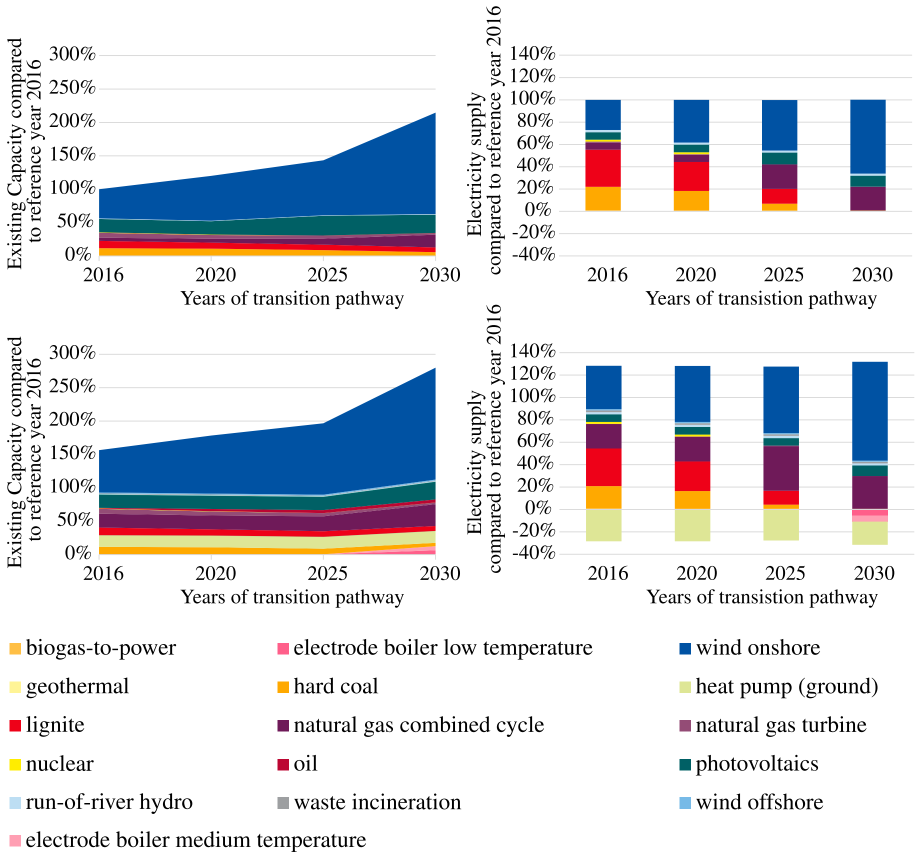

FIGURE 8 | Case studies considering the electricity, heat and transport sector without sector-coupling (top) and with sector-coupling (bottom). The left column shows the optimized production processes for electricity generation compared to the reference year of 2016 without sector coupling (Case 4). The right column shows the electricity production shares of the different production processes.

In addition, we assess the share of infrastructure-related impacts for three exemplary impact categories, which are often discussed for electricity systems: climate change, fossil depletion, and mineral and metal depletion (**Figure 6**). We find an increasing relevance of infrastructure in all impact categories, which further underlines the importance of a full life-cycle perspective when low-carbon energy systems are analyzed.

We further demonstrate the flexible objective function in SecMOD (**Figure 7**): In the extended brownfield case (Case 3), the cost optimal case (top) is compared to the case with minimal greenhouse gas emissions (bottom). The transition to high shares of renewable energy happens almost immediately, when the global warming impact is optimized, as cost-efficiency is not a criterion and the low operational emissions of renewable energy converters outweigh the environmental cost of the additional infrastructure.

The German multi-sector energy system (**Figure 8**) comprises the sectors electricity, heat and transport (Cases 4 and 5) and an overall GHG emission limit for all sectors. In Case 4, no sector-coupling processes are available. In case study 5, we allow sector-coupling by electricity-based heating (heat pumps and electrode boilers) and electrified transport. In the system without sector-coupling, the operation of electricity-producing processes changes earlier than in the sector-coupled system, as only few decarbonization options exist in the other sectors, when electrification is prohibited. Sector-coupling increases the electricity demand and hence the necessary process capacity for electricity production. In our case, until year 2030, sector coupling is only employed to decarbonize the heating sector. Hence, we do not observe any transport electrification.

Please note that the primary goal of all case studies shown is to demonstrate the functionalities of the SecMOD framework. Therefore, we decided to keep the discussion of all numerical results very brief. For a detailed discussion regarding the LCA of the sector-coupled German energy system, please refer to Baumgärtner et al. (2021), which served as our data source.

Overall, we demonstrate how SecMOD can be used to stepwise extend a system by products and processes to analyze the role of specific processes and sectoral interactions. Further, SecMOD can consider for pre-existing infrastructure, enabling its use for both greenfield and brownfield optimizations. In addition, different objectives can be chosen and compared.

4 CONCLUSION

In this work, SecMOD is presented: an open-source framework to consistently include a holistic life-cycle perspective in multi-sector energy system optimization by the full integration of life-cycle assessment in the objective function and constraints.

Being an object-oriented framework, the range of considered products and processes in SecMOD can be flexibly adapted by modifying the input data only. We demonstrate the modularity of SecMOD in a case study of the German energy system, comprising the sectors electricity, heating and private mobility. We gradually add products, sectors, and pre-existing infrastructure. Further, we modify the objective function from an economic optimization to a minimization of greenhouse gas emissions. SecMOD's modular design also enables the use on multiple scales: from optimizing and assessing a single industrial site to national and international energy system optimizations.

Furthermore, SecMOD enables modeling sector-coupled energy systems with flexible spatial and temporal resolution and comparing different system designs. SecMOD allows considering numerous environmental criteria and objectives, thereby facilitating life-cycle assessments of energy systems.

As an open-source framework, SecMOD is meeting transparency standards and can be used and further-developed by practitioners. Thereby, SecMOD enables a broader consideration of LCA in the design optimization of low-carbon energy systems on any scale.

DATA AVAILABILITY STATEMENT

The data analyzed in this study is subject to the following licenses/restrictions: The framework code itself is published in a Git repository: https://git-ce.rwth-aachen.de/ltt/secmod. While our code is available under a MIT license, the datasets we used as case studies partly require a seperate license. Therefore, all proprietary data was replaced in the examplary case study (case study 1) provided with our framework. Further inquiries can be directed to the corresponding author. Please note that the Gurobi solver and the ecoinvent data used in our case study require a separate license. Requests to access the ecoinvent database should be directed to Ecoinvent, https://ecoinvent.org/.

AUTHOR CONTRIBUTIONS

CR: Writing - Original Draft, Conceptualization, Methodology, Software, Investigation, Visualization, Data Curation, Project administration. LS: Software, Methodology, Investigation. JM: Software, Visualization. DS: Writing - Review & Editing, Data Curation. AK: Writing - Review & Editing, Supervision. NB: Writing - Review & Editing, Conceptualization, Methodology, Supervision. SD: Writing - Review & Editing, Conceptualization, Methodology, Supervision. AB: Writing - Review & Editing, Conceptualization, Methodology, Supervision, Resources, Funding acquisition.

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