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A review of mixed-integer linear formulations for framework-based energy system models

Maximilian Hoffmann [a,*], Bruno U. Schyska [c], Julian Bartels [c], Tristan Pelser [a,b], Johannes Behrens [a,b], Manuel Wetzel [d], Hans Christian Gils [d], Chuen-Fung Tang [e], Marius Tillmanns [e], Jan Stock [f], André Xhonneux [f], Leander Kotzur [g], Aaron Praktiknjo [e], Thomas Vogt [c], Patrick Jochem [d], Jochen Linßen [a], Jann M. Weinand [a], Detlef Stolten [a,b]

[a] Forschungszentrum Jülich GmbH, Institute of Climate and Energy Systems – Jülich Systems Analysis (ICE-2), 52425 Jülich, Germany
[b] RWTH Aachen University, Chair for Fuel Cells, Faculty of Mechanical Engineering, 52062 Aachen, Germany
[c] German Aerospace Center (DLR), Institute of Networked Energy Systems, Carl-von-Ossietzky-Straße 15, 26129, Oldenburg, Germany
[d] German Aerospace Center (DLR), Institute of Networked Energy Systems, Curiestraße 4, 70563, Stuttgart, Germany
[e] RWTH Aachen University, Institute for Future Energy Consumer Needs and Behavior (FCN), Mathieustr. 10, 52074 Aachen, Germany
[f] Forschungszentrum Jülich GmbH, Institute of Climate and Energy Systems – Energy Systems Engineering (ICE-1), 52425 Jülich, Germany
[g] enerX GbR, Cologne, Germany, formerly Forschungszentrum Jülich GmbH, Institute of Climate and Energy Systems – Jülich Systems Analysis (ICE-2), 52425 Jülich, Germany

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ABSTRACT

Optimization-based frameworks for energy system modeling such as TIMES, ETHOS.FINE, or PyPSA have emerged as important tools to outline a cost-efficient energy transition. Consequently, numerous reviews have compared the capabilities and application cases of established energy system optimization frameworks with respect to their model features or adaptability but widely neglect the frameworks' underlying mathematical structure. This limits their added value for users who not only want to use models but also program them themselves.

To address this issue, we follow a hybrid approach by not only reviewing 63 optimization-based frameworks for energy system modeling with a focus on their mathematical implementation but also conducting a meta-review of 68 existing literature reviews.

Our work reveals that the basic concept of network-based energy flow optimization has remained the same since the earliest publications in the 1970s. Thereby, the number of open-source available optimization frameworks for energy system modeling has more than doubled in the last ten years, mainly driven by the uptake of energy transition and progress in computer-aided optimization.

To go beyond a qualitative discussion, we also define the mathematical formulation for a mixed-integer optimization model comprising all the model features discussed in this work. We thereby aim to facilitate the implementation of future object-oriented frameworks and to increase the comprehensibility of existing ones for energy system modelers.

1. Introduction

Energy system models are as diverse as their real-world counterparts, which is why dozens of reviews have been published over the last two decades in an attempt to categorize and compare them. Given the need for continuous adaptation of these models, the growing number of energy system models is accompanied by the development of object-oriented software tools that facilitate the setup of concrete model instances, so-called frameworks.

Frameworks for energy system modeling provide a mathematical structure that allows the quick creation of model instances by means of parameterization. In recent years, they have occasionally been subject to their own reviews (see, e.g., [1]), but hitherto none of these has provided information on their underlying mathematical formulations. Consequently, they do not provide answers on *how to set up* modeling frameworks and *how to model* their specific features.

* Corresponding author.
E-mail address: max.hoffmann@fz-juelich.de (M. Hoffmann).

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We address this shortcoming by reviewing 63 optimization-based frameworks for energy system modeling, defining common model dimensions, the concept of technological component classes, the provision of basic model features such as variables, constraints, and objective functions, and, among others, techniques to mitigate computational complexity issues. We focus on open-source linear and mixed-integer linear optimization frameworks in order to allow for comparability and the derivation of a basic mathematical model as the frameworks' largest common denominator. Thus, our work sets itself apart from previous work by not only comparing energy system modeling frameworks but also focusing on their mathematical foundations. While earlier reviews typically assessed frameworks based on their features and adaptability, this paper takes a step further by examining the mathematical structures, specifically mixed-integer linear programming formulations that drive these models. Additionally, by formulating a set of standardized mathematical formulations, we provide a practical tool for modelers looking to develop or refine their own frameworks. This combined approach offers a more in-depth and technically oriented perspective, making our study a valuable contribution for both users and developers of energy system models and potentially the first review to enable programmers to set up their own energy system optimizations.

The remainder of this work is structured as follows:

We first present the methodology of our review as well as the meta-data of the analyzed frameworks in Section 1.1, followed by a meta-review of works that have already reviewed a subset of these frameworks in Section 1.2.

In Section 2, we present the basic mathematical structure of energy system optimization models. This includes their dimensions, their component logic, and a basic set of equations to describe the fundamental capabilities of these technology networks.

Section 3 presents extended component formulations that account for more detailed financial or operational features, such as non-linear investment curves in Section 3.1.1 or technology dynamics in Section 3.1.2, as well as those features only associated with a certain component type, such as price-elastic demand from sinks in Section 3.2.1.

Section 4 sheds light on additional constraints that are imposed on energy systems, such as maximum technology potentials, regulations, or supply security requirements. The review of different methods to account for multiple system-related objectives in a single optimization program in Section 5 rounds off the formulation of optimization-based energy system models.

As the models can become computationally extremely demanding, Section 6 discusses methods to guarantee solvability by means of model aggregation or parallelization. Finally, Section 7 identifies current weak points of optimization-based energy system modeling, while Sections 8 and 9 discuss and conclude the findings of this work.

1.1. Framework review

The framework review relies on two databases for energy system modeling tools, the "Open Energy Platform" [2] and the "Open Energy Modelling Initiative" [3], containing 27 and 92 different energy system modeling tools, respectively. Of the 119 entries, 13 tools were listed in both databases, and three entries referred to different versions of the same tool, leaving 103 unique tools in both databases. Out of the 103 frameworks, we identified 63 frameworks based on linear or mixed-integer linear optimization by checking relevant publications, model reports (e.g., [4,5]), or model documentations on GitHub (e.g., [6]) and Read the Docs (e.g., [7–9]). The framework selection process is illustrated in Fig. 1 and the meta-data of these frameworks is listed in Table 12 in Appendix A.

Beyond the meta-data listed in both databases, we analyzed the country of origin of the respective framework as well as their earliest reported appearance in the literature. The latter aspect was identified via a year-based publication search using Google Scholar (including non-peer-reviewed documents such as conference proceedings), the

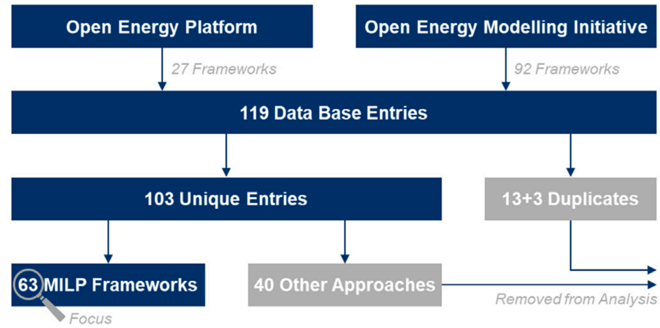

Fig. 1. Framework selection process based on the two online data bases "Open Energy Platform" [2] and the "Open Energy Modelling Initiative" [3].

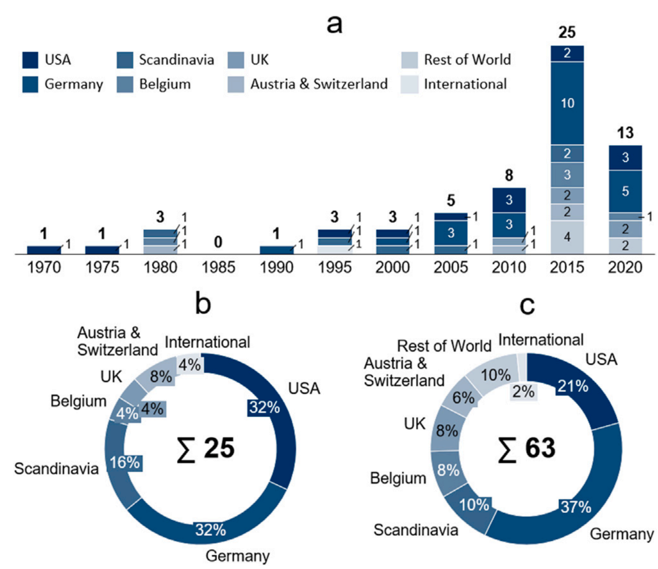

Fig. 2. Country of origin and start of development of the 63 reviewed frameworks. (a): number of frameworks by year of development in 5-year intervals; (b): frameworks by country 1970–2014; (c): frameworks by country 1970–2024.

license dates for the respective framework on GitHub, and data entries on the frameworks' webpages (if existent). The results are shown in Fig. 2.

From Fig. 2a, it is apparent that the number of framework developments per year has been continuously growing since 1990. Among the early frameworks before 1985, the predecessors of the TIMES (1998) modeling framework, MARKAL (1978), and EFOM (1982) can be found. The so-far strongest growth of open-source frameworks can be observed between 2015 and 2019. The period 2020–2024 is not yet completed and likely exhibits an additional time lag for two reasons: first, the databases may not be up-to-date, and second, the frameworks currently under development are not yet published. An additional time lag can be observed in the fifth column of Table 12, which shows that the latest frameworks have not yet been reviewed in literature, motivating our twofold approach of a direct framework review and a meta-review in order to be as up-to-date as possible.

Figs. 2b and c reveal that the number of frameworks has grown from 25 in 2014 to 63 in 2024 and thus almost tripled, indicating the increasing need for flexible and easy-to-parameterize software packages allowing rapid energy system modeling. It must be stated that the two databases exhibit a strong dominance of European or US developments, potentially indicating a bias towards Western publications. However, to the best of our knowledge, we are not aware of any comparable open-source energy system modeling community in other world regions.

Table 1
Categorization of procedural reviews.

Reference	Tools reviewed	Scope: Details	Focus: Models	Focus: Methodology	Type of models	Frame-works incl.	Description
				Approach #1: Procedural review of tools			
a. Scope: Geographically specific							
Jebaraj and Iniyan [10], 2006	–	Developing countries	✓	✗	sim, opt, other	✓	Various models used for developing countries
Foley et al. [11], 2010	7	USA, Europe	✓	✗	TD, BU, sim, gen, other	✗	Modeling response to renewable energy policies
Markovic et al. [12], 2011	24	Community	✓	✗	TD, BU, sim, gen, other	✓	Various tools used in community energy systems
b. Scope: Not specified/sector-specific							
Connolly et al. [13], 2010	37	n.a.	✓	✗	BU, sim, gen	✓	Tools for the integration of renewable energy into power systems
Mahmud and Town [14], 2016	67	Electric vehicles	✓	✗	sim	✓	Simulation tools for electric vehicle interactions with power networks
Müller et al. [15], 2018	47	Europe	✓	✗	TD, BU, sim, opt	✓	Development of an online platform regarding ESMs
				Approach #2: Procedural review of methodology			
a. Scope: Geographically specific							
Keirstead et al. [16], 2012	n.a.	Urban	✗	✓	sim, opt	✗	Approaches, challenges and opportunities in urban ESMs
DeCarolis et al. [17], 2017	n.a.	United Kingdom	✗	✓	n.a.	✓	Development of guiding principles for ESM modeling
Gardian et al. [18], 2022	40	n.a.	✓	✗	TD, BU, sim, opt	✓	Data harmonisation and transparency in the MODEX project
b. Scope: Not specified/sector-specific							
Baños et al. [19], 2011	n.a.	n.a.	✗	✓	opt	✗	Optimization methods for renewable energy
Pfenninger et al. [20], 2014	21	n.a.	✓	✓	sim, opt	✓	Approaches relevant to national and international energy policy
Lund et al. [21], 2017	n.a.	n.a.	✓	✓	opt, sim	✓	Comparison of methodology in simulation vs optimization tools
Mavromatidis et al. [22], 2018	n.a.	Distributed systems	✗	✓	other	✗	Review of approaches to characterize uncertainty
Morrison [23], 2018	n.a.	Open science	✗	✓	n.a.	✗	Reproducibility and open science in energy modeling
Priesmann et al. [24], 2019	n.a.	n.a.	✗	✓	opt	✗	Correlation between model complexity and accuracy of the results
Fridgen et al. [25], 2020	40	Sector coupling	✓	✓	n.a.	✗	Review of methodology for extending sector coupling
Hirt et al. [26], 2020	44	n.a.	✗	✓	n.a.	✗	Links between energy and climate models and socio-technical theories
Kotzur et al. [27], 2021	15	n.a.	✓	✓	BU, opt	✓	Various approaches to reducing complexity in ESMs
Blanco et al. [28], 2022	18	Hydrogen-based systems	✓	✓	opt, sim	✓	Taxonomies for energy models relating to hydrogen systems
Fodstad et al. [29], 2022	n.a.	n.a.	✓	✓	n.a.	✓	Key challenges in energy system modeling
Kriechbaum et al. [30], 2018	29	Multi-energy systems	✓	✓	opt	✓	Modelling grid-based Multi-Energy Systems
Mancarella et al. [31], 2016	4	Sector coupling	✓	✓	opt, sim	✓	Analysis of tools and methodologies for multi-energy systems

The share of US developments has decreased, whereas the share of German developments has increased. In the period from 2015 to 2019 alone, 10 out of 25 frameworks, or 40%, were of German origin. The reasons are manifold. On the one hand, Germany, together with other European countries, takes over a leading role in decarbonization among industrialized countries. On the other hand, the publication of source codes was supported by different German research associations, such as the Helmholtz Association, in an endeavor to increase result transparency and reproducibility. However, many of these frameworks are still solely used by their home institutions, raising the question of redundancy and the necessity of joining research efforts in order to avoid redundancies. Notably, this question is not a particularly German one given the overall increasing number of yearly developments.

Furthermore, Table 12 in Appendix A reveals that only a minor share of new developments is driven by new software architectures or programming languages such as R or Julia since 2017. The prevalent modeling languages are GAMS and Python, with GAMS being consistently used at least since the 1990s, whereas Python has seen an uptake since the 2010s with its optimization language package Pyomo. The most popular solvers are CPLEX and Gurobi. These findings support the hypothesis that the development of new frameworks is not so much driven by new and potentially more powerful programming languages or solvers, but rather by either the neglect of existing frameworks or know-how barriers that make it difficult to enter an existing framework, despite being open-source available, and to develop it further.

Against this backdrop, it is first questionable whether open-source development alone suffices to reduce rival and potentially redundant developments or whether documentation needs to be equally improved to allow modelers to build upon each other's preliminary work. Second, it is a strong motivation for this work to demonstrate the basic concepts of mixed-integer linear energy system optimization shared by the reviewed frameworks to allow for easy entry into existing codes.

1.2. Meta-review and original contribution

Tables 1 and 2 as well as Table 13 in Appendix B present an additional meta-review on existing reviews on energy system modeling. In contrast to the framework review, it is based on a backward reference search, i.e., based on the reference lists of most current publications, prior reviews were identified. This approach was chosen because it successfully identified those reviews on energy system models with a special focus on frameworks, as the sixth column in Tables 1, 2, and 13 illustrate. Notably, this approach can be prone to bias, among others, a time lag with respect to the latest relevant reviews or regarding citation clusters. Despite its shortcomings, it proved more practical than a keyword search for multiple reasons:

- The words "review" and "survey" were found to be used interchangeably or not at all in the title, abstract, or keywords of relevant reviews.

Table 2
Categorization of feature-based reviews.

Reference	Tools reviewed	Scope: Details	Focus: Models	Focus: Methodology	Type of models	Frameworks incl.	Description
Approach #3: Define features/types and then sort tools to draw conclusions							
a. Scope: Geographically specific							
Van Beeck [32], 1999	10	Developing countries	✓	✓	TD, BU, sim, opt	✓	Modeling approaches applicable to small-scale settings
Bhattacharyya and Timilsina [33], 2010	10	Developing countries	✓	✓	TD, BU, sim, gen, other	✓	Various ESMs for developing countries
Mundaca et al. [34], 2010	12	Household	✓	✓	BU, sim, opt, acc	✓	Decision frameworks for energy economy models
Manfren et al. [35], 2011	14	Urban	✓	✓	sim, opt, acc, other	✓	Selection of models for distributed energy planning
Mendes et al. [36], 2011	6	Community	✓	✓	BU, sim, opt	✓	Selection of models used for integrated energy systems
Mirakyan and De Guio [37], 2013	12	Urban	✓	✓	sim, opt, acc, other	✓	Tools and methods for integrated energy planning in cities
Allegrini et al. [38], 2015	24	District	✓	✓	sim	✗	Modeling approaches and tools for district-level systems
Huang et al. [39], 2015	(?)	Community	✓	✓	TD, BU, sim	✓	Methods and tools for community energy planning
van Beuzekom et al. [40], 2015	12	Urban	✓	✓	opt	✓	Multi-energy system tools for urban development
Olsthoorn et al. [41], 2016	14	District heating	✓	✓	sim, opt	✓	Integration of renewable energy and storage into district heating
Lyden et al. [42], 2018	13	Community	✓	✓	sim, opt	✓	Tool selection process for community systems
Abbasabadi and Ashayeri [43], 2019	13	Urban	✓	✓	BU, sim	✓	Review of models for urban energy systems
Oberle and Elsland [44], 2019	40	Germany	✓	✓	TD, BU, sim, opt, acc	✓	Focus on open access and accessibility in long-term models
Scheller and Bruckner [45], 2019	8	Municipal	✓	✓	BU, opt	✓	Optimization-based decision support tools for municipal planning
Ridha et al. [46], 2020	145	n.a.	✓	✓	TD, BU, sim, opt	✗	Focus on complexity of tools in temporal, spatial, mathematical, and modeling content
Klemm and Vennemann [47], 2021	145	District	✓	✓	opt, BU	✓	Focus on optimization tools for multi-energy systems in urban districts
b. Scope: Not specified/sector-specific							
Li et al. [48], 2015	14	n.a.	✓	✓	other	✗	Socio-technical energy transition (STET) models
Crespo del Granado et al. [49], 2018	7	n.a.	✓	✓	TD, BU, opt	✓	Review of intersection between energy and economic models
Lopion et al. [50], 2018	24	n.a.	✓	✓	BU, sim, opt	✓	National-scale ESMs that incorporate all energy sectors
Ringkjøb et al. [1], 2018	75	n.a.	✓	✓	sim, opt, TD, BU, other	✓	General overview of various energy system models
Groissböck [51], 2019	31	n.a.	✓	✓	sim, opt	✓	Evaluates maturity of open source ESMs vs proprietary models
Fattahi et al. [52], 2020	19	n.a.	✓	✓	opt, sim	✓	Identify modeling gaps and suggestion of two conceptual modeling suites.
Prina et al. [53], 2020	24	n.a.	✓	✓	BU	✓	Resolution in time, space, techno-economic detail, and sector coupling
Weinand et al. [54], 2020	359	Decentralized systems	✓	✓	TD, BU, sim, opt	✓	Focus on off-grid decentralized systems
Approach #4: Describe/categorize tools and then draw conclusions							
a. Scope: Geographically specific							
Hall and Buckley [55], 2016	22	United Kingdom	✓	✓	TD, BU, sim, opt, acc, other	✓	Prevalent ESM tools used in the UK: approaches and methods
Ferrari et al. [56], 2019	17	Urban	✓	✓	sim, opt	✓	User-friendliness in tools for urban energy planning
Musonye et al. [57], 2020	30	Sub-Saharan Africa	✓	✓	TD, BU, sim, opt,	✓	Scoping review of integrated energy system models
Kumar et al. [58], 2022	16	District	✓	✓	opt, BU	✓	Development of decision support tree for optimization tool selection
b. Scope: Not specified/sector-specific							
Savvidis et al. [59], 2019	40	n.a.	✓	✓	TD, BU, sim, opt	✓	Attempts to bridge gap between energy system models and policy
Chang et al. [60], 2021	54	n.a.	✓	✓	sim, opt, other	✓	Reviews tool features, linkages, accessibility, and policy relevance
Riera et al. [61], 2022	99	Hydrogen production	✓	✓	opt	✓	Comparison of hydrogen supply chain and process design models
Misconel et al. [62], 2022,	4	Electricity system	✓	✓	opt	✗	High-resolution electricity system modeling

- The words "energy", "system", and "model", as well as, in the case of electricity system models, "power" or "electricity" in place of "energy", appear in arbitrary order.
- Relevant reviews either speak of "models", "frameworks", or "tools", partly with the same and partly with a varying meaning.
- A keyword search yielded either far too many irrelevant publications or missed a notable share of the reviews found by a citation search.

The tables delineate two fundamental and one additional type of review of energy system models, which are illustrated in Fig. 3. Procedural reviews listed in Table 1 enumerate either tools (Approach 1) or methodologies (Approach 2) in a procedural manner, i.e., they focus on tools or aspects separately and take a bird's eye view. The feature-based reviews presented in Table 2 focus on a comparison of tools and models by means of their features, i.e., their capability to model certain aspects. Their focus is either centered on the features, and different models are categorized according to them (Approach 3) or vice versa (Approach 4). These reviews provide good guidance for modelers searching for the right tools to address the problem at hand, but they likewise do not provide exact mathematical formulations. Recently, an additional approach for comparing energy system frameworks has been developed within the MODEX project (MODel EXperiments for the energy transition). As some of the authors of this publication have been part of this project and we want to avoid bias, the corresponding review is listed in Table 13 in Appendix B. The approach can be considered a fifth type of review that plugs identical input data into different models and compares them by analyzing the different results they yield.

Tables 1 and 2 reveal that the overall number of reviewed models or frameworks has steadily increased over the years in accordance with the growing number of modeling tools. However, the demand for both a bird's-eye view of modeling and detailed feature comparisons has grown equally over the years, indicating that there is no trend in favor of comprehensibility or level of detail. MODEX reviews, on average, compare fewer models and frameworks with each other, given the fact that for result comparisons, these reviews run different models, making the analyses far more complex than those based on fact sheets.

With respect to the scope of the reviews, the largest groups are spatially defined scopes, e.g., regional, national, or continental systems, or a non-specified one, i.e., general reviews of tools for modeling. With respect to Approach 2 in Table 1, a stronger focus on certain sectors or

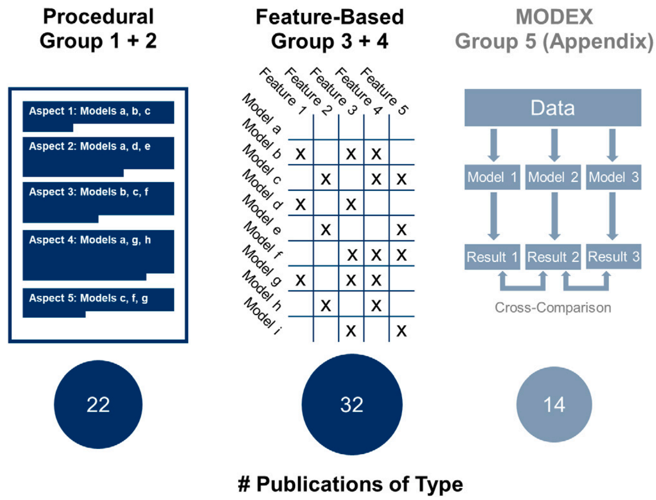

Fig. 3. Classification of review types of energy system modeling. The numbers beneath the three types correspond to the respective number of reviews analyzed as part of the present study.

system aspects such as distribution [22] or hydrogen systems [28] can be observed.

While Approach 1 heavily focuses on existing models and Approach 2 on modeling approaches rather than existing models, approaches 3 and 4, listed in Table 2, treat models and their feature-based capabilities equally, i.e., we recommend these publications when searching for the right model for a certain application case. Most notably, Ringkjøb et al. [1] and Groissböck [51] conduct highly detailed matrix comparisons.

Furthermore, Tables 1 and 2 show that tools or models are consistently distinguished by their techno-economic perspective, namely top-down (TD) vs. bottom-up (BU), or by their modeling technique, e.g., optimization vs. simulation. The separation into TD and BU was already defined by Van Beeck [32], with TD models focusing on economic laws and treating technical aspects in a less detailed manner, whereas BU models consider differentiated energy systems and network topologies and pay less attention to market mechanisms. In contrast, modeling techniques have become less diverse over time, or the terminology for approaches has become more unified. While early reviews differentiated between optimization, simulation, generation, accounting, and other models, modern ones use either simulation or optimization, with a tendency towards optimization. This trend benefits from the significant progress of mixed-integer linear optimization solvers, so that simulation approaches continuously transition from large-scale models to small-scale algorithmic operational modeling, covering topics such as model predictive control.

As mentioned above, the majority of identified reviews consider frameworks as part of their analyses. Over the years, a shift in terminology can be observed: while the term "framework" was originally used for programs consisting of a multitude of loosely connected (soft-coupled) sub-models, tool chains, or "accounting frameworks", the modern definition of framework refers to a modular, object-oriented definition of non-parameterized component classes that can be freely connected to each other and turned into various system components by means of appropriate parameterization [2,3,23]. As frameworks can be turned into any model with appropriate parameterization, they have become an indispensable tool for energy software development. In the following, we focus on the semantic and mathematical description of optimization-based mixed-integer linear programming frameworks, given their dominance in recent years.

2. Model dimensions and basic model

2.1. Model dimensions

Energy system models can consist of a multitude of dimensions, among which are commodities, spatial and temporal resolutions, in some cases stochastic scenarios and transformation pathways, and, most importantly, components. In bottom-up models relying on single optimization problems with single objectives, as well as associated frameworks, these dimensions roughly correspond to the indices of the model.

Commodities

Sector-coupled [63,64] energy systems often comprise a multitude of **commodities**, be it energy forms, energy carriers, or even raw materials, as part of life-cycle assessments (LCA). Power systems focusing on electricity are an example of systems with few commodities, whereas models with integrated LCA and a detailed representation of chemical transformation processes are models with numerous different commodities. Commodities constitute the medium that "flows" between components that consume and/or produce commodities.

Space

Another dimension covered by many models, especially those focusing on infrastructure-related questions, is the spatial one, also referred to as **regions**, **locations**, or **nodes**. Single-nodal systems only consider a single location, known as the "copper plate assumption", i.e., congestion-free commodity flows between demand and supply, whereas multi-nodal systems explicitly consider the capacity-related transport restrictions of commodities between different locations. Note that transmission losses can be considered in both single- and multi-nodal models, though in a simplified manner in single-nodal ones (see, e.g., [65–67]).

Time

The variability of demand and intermittency of renewable energy sources have led to the need to consider different demand and supply situations using discrete **time steps**. The components must handle changing commodity supplies and demands, i.e., the operational variables are defined for each time step and must stay within the capacity limits. This dimension is also crucial for storage modeling, as energy storage levels depend on transient energy supply and demand cycles over time.

A smaller number of models and frameworks have options for handling uncertainty and transformation processes in the system, i.e., transient system designs over time. These model dimensions are of particular interest for models in which operational reliability is a priority (e.g., if the system has to cope with various extreme scenarios) or for long-term planning models in which a status quo system is gradually replaced by newer systems.

Stochastic scenarios

Some energy system models consider uncertainty by adding a fourth dimension to represent a set of discrete **scenarios** with predefined probabilities of occurrence. With this dimension, uncertainties in model parameters, such as the weather determining the availability of wind and solar resources or diverging demand projections, can be considered simultaneously. It also allows the modeling of a multitude of potentially system-critical events, such as unexpected transmission line or power plant outages. Technically, this approach adds an additional stage to optimization models, turning them into two- or multi-stage stochastic programs, also referred to as deterministic equivalent programs (DEPs). Despite their similarity to time steps likewise representing discrete load and supply situations, stochastic scenarios do not imply a chronological order, i.e., each scenario has its own chance of occurrence and no preceding or succeeding scenario. Thus, this dimension can be used for creating robust system designs but not for modeling energy storage.

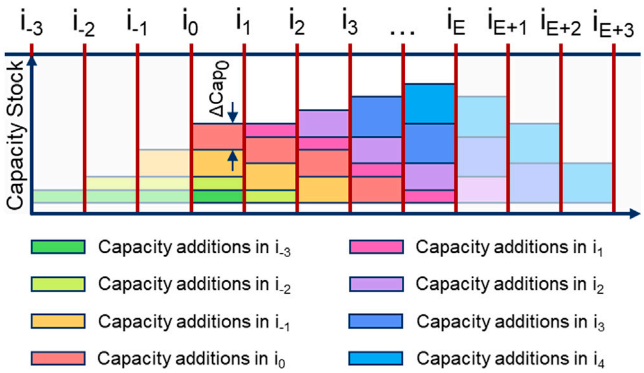

Fig. 4. (De-)commissioning and investment stock. In an optimization with a transformation pathway between the investment periods i_0 and i_E, each component has a total capacity in each investment period, which is given by the sum of commissioned capacities from prior and current investment periods that are still within their lifetime, e.g., in i_2 orange, red, magenta, and purple. Capacities are decommissioned as soon as they reach their lifetime limit, in this case, after four investment periods.

Transformation pathway

Energy system models and frameworks designed to cover multiple decades face the challenge of projecting the transformation of the system over time, starting with an already existing system (brownfield analysis as opposed to designing from scratch in greenfield analyses). To capture the stepwise transformation of the system in a more realistic manner, these models often comprise multiple **investment periods**, along which the capacities of the energy technologies gradually change.

As system components normally have a predefined lifetime, the capacities of a technology being commissioned at a certain point in time must be decommissioned at the latest at the end of their respective lifetimes. This leads to a transient capacity stock, as illustrated in Fig. 4. Many contemporary frameworks incorporate this index given the importance of long-term system planning to reach climate neutrality, among which are, e.g., the frameworks ETHOS.FINE [68,69], OSeMOSYS [70], REMix [71] and TIMES [4,5,72–74].

Components

Finally and most importantly, all modern optimization-based frameworks for bottom-up energy system modeling explicitly consider energy technologies, that is, **components** with a size and functionality that are part of a larger energy network. In general, these components comprise capacities and operational variables. The capacities are variable in capacity expansion models (CEPs), which aim at finding cost-minimal energy system designs, whereas they are fixed in dispatch- or unit commitment (UC) models, which only minimize the operation costs of an existing system and therefore parameters. In any case, the operational variables must not surpass the installed capacity of the respective component.

These components are core to bottom-up modeling frameworks as they form system networks in which commodities flow from supply to demand sites. These networks can be modeled as undirected graphs with nodes representing either energy system components or hubs (see Fig. 5a). The edges connect these components to each other. Each component comprises the basic set of capacity and operational variables but also belongs to a certain component type that has specialized roles in the energy system. In many frameworks, the basic component types are sinks and sources, converters, storage, and transmission lines.

Sources and sinks can feed commodities into or withdraw them from the system; e.g., photovoltaic panels provide the system with electricity, whereas households withdraw it. **Converters** convert two or more commodities into one another, e.g., fuel cells turn hydrogen into water and electricity. The commodity flows are linked with each other at any point in time via conversion rates that define how much of one or more commodities is turned into one or more other commodities.

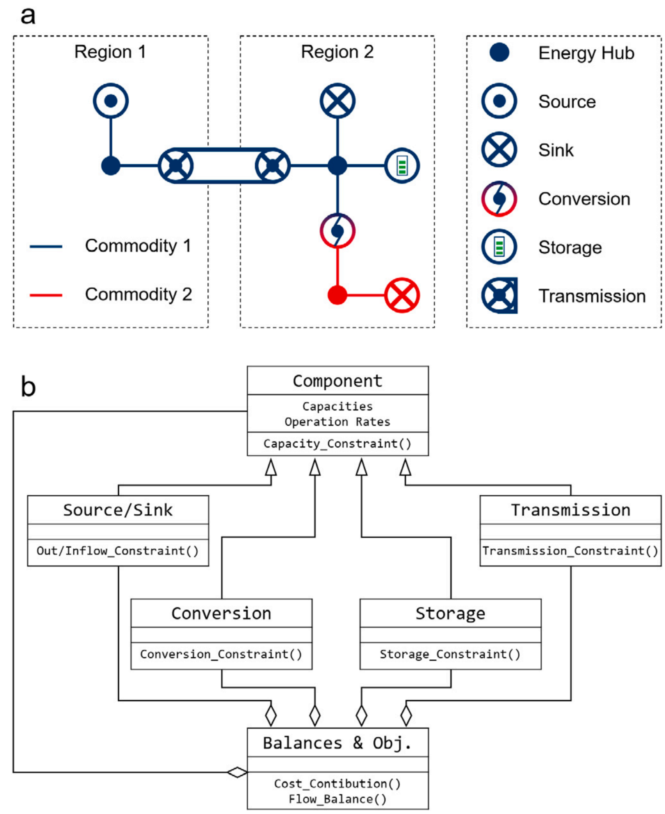

Fig. 5. (a): a demonstrative multi-nodal energy system model with basic components for supply, demand, conversion, storage, and transmission between regions; (b): a typical framework architecture in which specialized components inherit from a general component class and whose costs and inputs or outputs contribute to the objective function and energy balances, respectively.

Storage, such as hydrogen storage, consumes commodities at one point in time to release them at a later point. The sum of charges and withdrawals over time defines the state of charge (SOC) of the respective storage. **Transmission** units connect different regions with each other; that is, they simultaneously serve as a source in one region and a sink in another region, and they are linked by capacity and operation. For instance, these transmissions can be, e.g., direct current lines or hydrogen pipelines.

Most components contribute to the overall costs of the energy system via their net capacity and operation costs, with their maximum input or output being capped by their respective net capacities. However, some components, such as demand sinks, do not necessarily have a variable net capacity but a fixed demand for commodities that must be satisfied at any point in time.

Hubs within a spatial region serve to maintain the flow conservation of each commodity in each spatial region but generally do not represent cost-driving network components. This implies that each spatial region is regarded as a separate copper plate.

Although the components are named differently in the frameworks examined, they share many basic properties, in particular a capacity variable and several operational variables, one for each time step. Therefore, basic common functionalities are often defined in a general component class, from which subordinate classes for the respective component types inherit and to which they add component type-specific functionalities. Fig. 5b visualizes how specialized components in optimization frameworks such as ETHOS.FINE [69] inherit from a general component class and contribute to total system costs and energy balances.

Table 3
Abbreviations and symbols.

Symbol	Description
Sets	
$\mathbb{M}^{source,}$	subset of components representing sources
$\mathbb{M}^{sink}$	subset of components representing sinks
$\mathbb{M}^{conv}$	subset of components representing conversion units
$\mathbb{M}^{store}$	subset of components representing storage units
$\mathbb{M}^{trans}$	subset of components representing transmission units
$\mathbb{M}^{g}$	components associated with a commodity (a good) in g
$\mathbb{G}$	commodities
$\mathbb{I}$	investment periods
$\mathbb{R}$	regions
$\mathbb{S}$	scenarios
$\mathbb{T}$	time steps
$\mathbb{P}$	(typical) periods (e.g., typical days)
Variables	
C^{CAPEX}	capital expenditures of commissioned capacities
f	commodity flow variable
x^{op}	operation-rate variable
$x^{op,bin}$	binary variable indicating whether a component is active (1) or not (0)
$x^{op,bin,sd}$	binary variable indicating whether a component is deactivated (1) or not (0)
$x^{op,bin,su}$	binary variable indicating whether a component is activated (1) or not (0)
$x^{op,ch}$	operation-rate variable representing charging
$x^{op,dis}$	operation-rate variable representing discharging
$x^{op,net}$	net operation-rate (mass-flow) variable
x^{SOC}	variable representing the state of charge of a storage
x^{cap}	installed capacity variable
x^{commis}	commissioned capacity
Parameters	
c^{cap}	annualized net capacity cost
c^{op}	operation cost
d	discount factor
lt	lifetime
MDT	minimal down-time
MUT	minimal up-time
r_c^{down}	maximum down-ramping rate
r_c^{up}	maximum up-ramping rate
Δt	time-step length
γ	conversion factor for conversion of one commodity into another
λ	dimensionless weighting factor with values between 0 and 1
η^{ch}	charging efficiency of a storage
η^{dis}	discharging efficiency of a storage
η^{sd}	self-discharge rate
θ	net capacity factor
Abbreviations	
$CAPEX$	capital expenditures
$LODF$	line outage distribution factor
$PTDF$	power transfer distribution factor
$PVIFA$	present value interest factor of annuity

2.2. Basic model

The basic set of equations that most multi-regional bottom-up energy system models have in common is given by Eqs. (1a)–(1r) using the notation from Table 3. This illustrative formulation forms a linear minimization problem. Similar descriptions can be found in both journal articles [68,75–79], framework descriptions [73,74,80–82], and online framework documentations [6–9]. Here, $\mathbb{M}^{source}$, $\mathbb{M}^{sink}$, $\mathbb{M}^{conv}$, $\mathbb{M}^{store}$, and $\mathbb{M}^{trans}$ denote the set of components representing sources, sinks, conversion, storage, and transmission units. $\mathbb{M}^{g}$ represents those components that produce, consume, convert, store, or transmit a commodity, that is, a good $g \in \mathbb{G}$.

$$\min \quad \left(\sum_c \sum_i \sum_r \left(C^{capex}_{c,r,i} + \sum_s \sum_t p_s c^{op}_{c,i,r,s,t} x^{op}_{c,i,r,s,t} \right) \right) \tag{1a}$$

$s.t. \quad \forall c \in \mathbb{M}, i \in \mathbb{I}, r \in \mathbb{R}:$

$$C^{capex}_{c,r,i} = \sum_{i'=i-lt_c/|i|+1}^{i} c^{cap}_{c,r,i'} \cdot x^{commis}_{c,r,i'} \cdot \frac{PVIFA(d,|i|)}{PVIFA(d,lt_c)} \cdot \frac{1}{(1+d)^{i'\cdot|i|}} \tag{1b}$$

$$x^{cap}_{c,r,i} = \sum_{i'=i-lt_c/|i|+1}^{i} x^{commis}_{c,r,i'} \tag{1c}$$

$s.t. \quad \forall g \in \mathbb{G}, \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T}:$

$$\sum_{c \in \mathbb{M}^g} f_{c,g,i,r,s,t} = 0 \tag{1d}$$

$$f_{c,g,i,r,s,t} = x^{op}_{c,i,r,s,t} \qquad \forall \quad c \in \mathbb{M}^{source} \cap \mathbb{M}^g \tag{1e}$$

$$f_{c,g,i,r,s,t} = -x^{op}_{c,i,r,s,t} \qquad \forall \quad c \in \mathbb{M}^{sink} \cap \mathbb{M}^g \tag{1f}$$

$$f_{c,g,i,r,s,t} = \gamma_{c,g,i,r,s,t} x^{op}_{c,i,r,s,t} \qquad \forall \quad c \in \mathbb{M}^{conv} \cap \mathbb{M}^g \tag{1g}$$

$$f_{c,g,i,r,s,t} = x^{op,dis}_{c,i,r,s,t} - x^{op,ch}_{c,i,r,s,t} \qquad \forall \quad c \in \mathbb{M}^{store} \cap \mathbb{M}^g \tag{1h}$$

$$f_{c,g,i,r,s,t} = x^{op}_{c,i,(r',r),s,t} - x^{op}_{c,i,(r,r'),s,t} \qquad \forall \quad c \in \mathbb{M}^{trans} \cap \mathbb{M}^g \tag{1i}$$

$s.t. \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T}:$

$$x^{op}_{c,i,r,s,t} \geq 0 \qquad \forall \quad c \in \mathbb{M}^{source,sink,conv,store} \tag{1j}$$

$$x^{op}_{c,i,(r,r'),s,t} \geq 0 \qquad \forall \quad c \in \mathbb{M}^{trans}, r' \in \mathcal{R} \setminus \{r\} \tag{1k}$$

$$x^{op}_{c,i,r,s,t} \leq \theta_{c,i,r,s,t} x^{cap}_{c,i,r} \Delta t \qquad \forall \quad c \in \mathbb{M}^{source,sink,conv} \tag{1l}$$

$$x^{SOC}_{c,i,r,s,t+1} = x^{SOC}_{c,i,r,s,t} + \eta^{ch}_{c,i,r,s,t} x^{op,ch}_{c,i,r,s,t} - \frac{x^{op,dis}_{c,i,r,s,t}}{\eta^{dis}_{c,i,r,s,t}} \qquad \forall \quad c \in \mathbb{M}^{store} \tag{1m}$$

$$x^{SOC}_{c,i,r,s,t} \geq 0 \qquad \forall \quad c \in \mathbb{M}^{store} \tag{1n}$$

$$x^{SOC}_{c,i,r,s,t} \leq x^{cap}_{c,i,r} \qquad \forall \quad c \in \mathbb{M}^{store} \tag{1o}$$

$$-x^{cap}_{c,i,r,s,t} \Delta t \leq x^{op}_{c,i,(r',r),s,t} - x^{op}_{c,i,(r,r'),s,t} \qquad \forall \quad c \in \mathbb{M}^{trans}, r' \in \mathcal{R} \setminus \{r\} \tag{1p}$$

$$x^{cap}_{c,i,r,s,t} \Delta t \geq x^{op}_{c,i,(r',r),s,t} - x^{op}_{c,i,(r,r'),s,t} \qquad \forall \quad c \in \mathbb{M}^{trans}, r' \in \mathcal{R} \setminus \{r\} \tag{1q}$$

$$x^{cap}_{c,i,r,s,t} \Delta t \geq x^{op}_{c,i,(r',r),s,t} + x^{op}_{c,i,(r,r'),s,t} \qquad \forall \quad c \in \mathbb{M}^{trans}, r' \in \mathcal{R} \setminus \{r\} \tag{1r}$$

Eq. (1a) is the objective function, minimizing the net present value of the capacity and operation costs of all components, all investment periods, all spatial regions, and for all load scenarios, as well as every time step. The capacity-related net present value of capacity expenditures (CAPEX) of the capacity stock of a component throughout an investment period and its capacity in that investment period are defined by Eqs. (1b) and (1c). Here, Eq. (1b) uses the present value interest factor of annuity[1] (PVIFA) to first transform the commissioning costs of a component into annuity costs and to subsequently transform them into costs per investment period. Eq. (1d) maintains the flow conservation for all commodities entering and leaving a hub, which is defined for each commodity, time step, region, investment period, and scenario of the model.

Eqs. (1e) and (1f) link the operation of sources and sinks to the respective flows of commodities produced or consumed by the respective sources and sinks. Eq. (1g) links the operation of conversion units to the production or consumption of commodities. As conversion units link multiple commodities to each other, e.g., fuel cells link water, hydrogen, electricity, and oxygen with one another, their operation is linked to each involved commodity with an individual conversion factor γ. Eqs. (1h) and (1i) refer to the flow of storage and transmission components. These components operate in two directions, i.e., charge and discharge in the case of storage components and transmitting energy either from region r to region r' or r' to r in the case of transmission components. Therefore, these components have two operational variables for the commodity the respective component operates with, defined for each time step, region, investment period, and scenario.

[1] Defined as $PVIFA(d,lt) = \frac{(1+d)^{lt}-1}{(1+d)^{lt}\cdot d}$.

Eqs. (1j) and (1l) guarantee the non-negativity of the components' variable operation, as well as that none of the operations surpasses the components' net capacity. Depending on the type of component, the maximum power output can deviate from the nominal net capacity; e.g., photovoltaic panels are limited by their respective net capacity factor, denoted as θ in Eq. (1l). The amount of produced, consumed, converted, stored, or transmitted commodities further depends on the length of the discrete time steps Δt. Eq. (1m) links the states of charge between subsequent time steps for storage components. Similar to the operational variables for source, sink, and conversion units, the state of charge variables are constrained to be non-negative and must not surpass the storage net capacity, which is guaranteed by Eqs. (1n) and (1o).

Eqs. (1p) and (1q) ensure that the net flow of commodities along a transmission line never exceeds the transmission line's net capacity in any direction. As consideration of the net flow can lead to poor scaling behavior and unnecessary flows in opposite directions within a single transmission line, Eq. (1r) limits the flow of commodities in each direction to be at most as big as the built transmission line net capacity multiplied by the time step duration. This constraint reduces the model's numeric stability and convergence behavior by limiting its indifference regarding gross flows in opposite directions. Alternatively, the problem of indifference can be circumvented by imposing operational penalty costs in either direction, which, however, distorts the total system costs.

3. Component extensions

The following section provides extended model formulations to account for real system behavior that cannot be adequately captured by the model in Eqs. (1a)–(1r).

3.1. General component extensions

First, we review the model extensions that can be applied to all component types.

3.1.1. Non-linear capacity expenditures

Capital expenditures (CAPEX) usually grow non-linearly with capacity because of effects such as technological learning or (dis-)economies of scale. In the case of technological learning and economies of scale, marginal costs reduce with output or size. Degressive CAPEX curves lead to non-convex optimization problems, i.e., the model can have multiple local minima. This is illustrated by the simple model in Eqs. (2a)–(2c) with a degressive CAPEX function, in which two rival technologies with the same initial costs must meet a cumulative demand of 1 MW:

$$\min \quad c\sqrt{x_1} + c\sqrt{x_2} \tag{2a}$$

$$\text{s.t.} \quad x_1 + x_2 \geq 1 \tag{2b}$$

$$x_1, x_2 \geq 0 \tag{2c}$$

The model is solved graphically in Fig. 6a and shows two local optima: either completely in favor of one or the other technology. This non-convexity significantly drives model complexity. In contrast, models with convex CAPEX functions, as in the case of the simplified example in Eqs. (3a)–(3c) and in Fig. 6b, remain convex with a single minimum. For these models with convex cost functions, by contrast, efficient solvers for mixed-integer quadratic programs (MIQPs) exist that rely on quadratic approximations [83] of the cost functions.

$$\min \quad cx_1^2 + cx_2^2 \tag{3a}$$

$$\text{s.t.} \quad x_1 + x_2 \geq 1 \tag{3b}$$

$$x_1, x_2 \geq 0 \tag{3c}$$

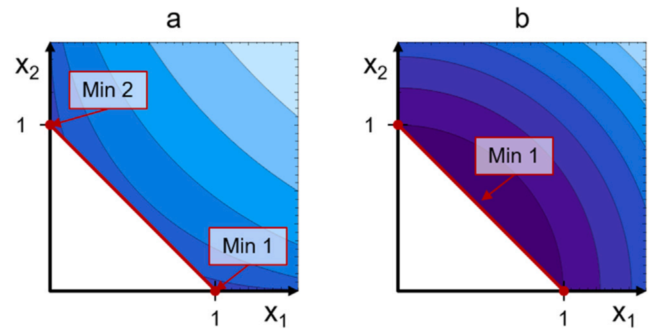

Fig. 6. Graphical solution of a simple optimization problem (a): with a concave CAPEX curve and (b): with a convex CAPEX curve. The diagram (a) is adapted from Behrens et al. [84] and illustrates the non-convexity of this problem type, i.e., the existence of multiple local minima.

Technological learning

Technological learning describes the tendency of a technology to become more mature over time. Hence, its capacity-specific costs decrease with its total installed capacity [85]. This effect can also affect aspects such as efficiencies [86,87], which, however, will be neglected in the following. In the simplest case, technological learning can be described as a power function of a technology and its capacity-specific costs, i.e., with c_0 and x_0 the initial cost and capacity, respectively, and $c(x)$ being the cost after having built a cumulative capacity x [88]:

$$c(x) = c_0 \left(\frac{x}{x_0}\right)^{\log_2(1-LR)} \tag{4}$$

The learning rate $LR \in (0,1)$ denotes the relative cost reduction after doubling the cumulative capacity and yields a degressively growing total cost (TC) function. For a learning rate of 30%, we obtain the same degressive total cost growth for a technology as stated in the example in Eq. (2a):

$$TC(x) = c(x)x = c_0 \left(\frac{x}{x_0}\right)^{\log_2(1-0.3)} x \approx c_0\sqrt{x_0} \cdot \sqrt{x} \tag{5}$$

The resulting non-convexity imposes challenging requirements on solving algorithms and generally leads to significant runtime increases [89]. In the literature, listed in Table 4, three different approaches are used to find (local) optima of these problems, which are schematically shown in Fig. 7. Problems can be solved directly with an appropriate solver, but despite this method's exactness, finding a global optimum may take an unacceptable amount of time [90].

Alternatively, an iterative linearization of the learning curve to find a local optimum starts with an initial assumption regarding the slope of the cost curve [91]. The optimization model is solved, yielding a capacity for which the cost gradient varies from the initial assumption. This gradient is then taken for the next iteration, which is repeated until convergence is achieved. However, the solution depends on the initial assumption regarding the cost gradients and likely only yields a local optimum due to the non-convexity of the problem. Improvements in these local optima can be achieved via multiple initializations with different starting conditions.

The last approach is a piecewise linearization of the learning curves and requires the introduction of binary variables and so-called *special ordered sets of type 2* (SOS2) constraints defining the linear segment to be chosen depending on the capacity of the technology [88]. This method is computationally less expensive than non-linear optimization but normally more complex than the iterative linear approach. Furthermore, despite not being numerically exact, as the accuracy depends on the number of linearized segments, the method is capable of finding the global optimum, which, e.g., can be found using the branch-and-bound algorithm.

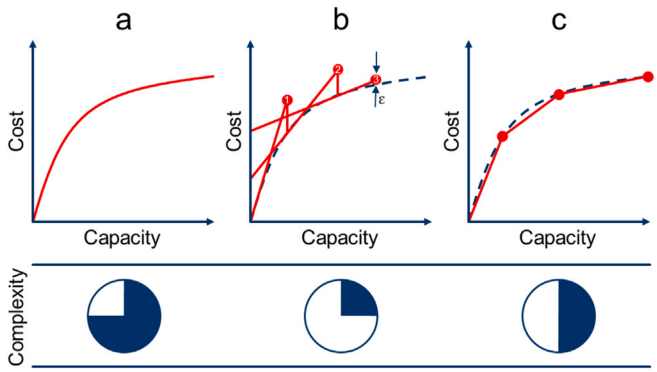

Fig. 7. Different options to optimize technologies with degressive technological learning curves and their computational complexity adapted from Behrens et al. [84]; (a): direct solution of a non-linear program (NLP); (b): iterative solutions with multiple linear programs (LPs); (c): solution with a piecewise linear approximation using a mixed-integer linear program (MILP).

Economies of scale

Economies of scale are a basic principle frequently observed in microeconomics, whereby output-specific costs decrease with total output [128,129]. One reason for this phenomenon is fixed cost degression, i.e., the product-specific fixed cost contribution of a machine decreases with its total output, and running it at full capacity is incentivized [130].

Economies of scale are a plant-specific phenomenon and therefore only applicable to models considering individual plants, i.e., those with a narrow spatial focus. Unlike technological learning, economies of scale only focus on individual capacity investments. Previously installed capacities at other sites do not influence the investment costs.

In energy system models, economies of scale are typically applied to large power plants, such as nuclear power plants [131] or power transmission systems [132]. Newer energy system models focusing on renewable energy technologies also apply it to technologies such as on- and offshore wind turbines [133,134], or electrolysis [135].

There are different options for implementing economies of scale in energy system models or frameworks. One of these is to use the previously presented piecewise linearization and map a non-linear cost function with SOS2 constraints [136–139]. The cost curve can thereby have any shape and does not necessarily need to be an exponential function. The number of necessary binary variables rises as the number of segments used to approximate the cost curve increases, thereby increasing the model's complexity.

Additionally, discrete combinations of capacities and costs can map economies of scale using different investment options [140,141]. The number of necessary binary variables depends on the available investment options. SOS1 constraints can guarantee the use of only one investment decision. Finally, the representation of economies of scale can also be achieved through the use of an intercept-slope formulation [142–144]. This method allows for the representation of the fixed cost of a component while increasing model complexity only moderately. For this approach, heuristics based on temporal resolution [145] and budget-cut algorithms for the early removal of non-financially viable system setups [146] have also been proposed to decrease the comparably small additional computational complexity even further.

3.1.2. Technology dynamics

The operation of system components is usually constrained by more technical limitations than installed capacities alone. In the following, a non-exhaustive list of dynamic constraints is presented.

Ramping

Ramping refers to the gradient by which a component's operation can change over time and is thus a measure of inertia. It is frequently used in large-scale system models, including inert baseload plants such

Table 4
Technological learning in energy system optimizations. The table is adapted from the review of Behrens et al. [84].

Authors	Year	Scope	Foresight	Modeling
Mattsson [92]	1997	Global electricity	PF	MILP
Mattsson and Wene [90]	1997	Global electricity	PF	NLP
Messner [93]	1997	Global energy	PF	MILP
Barreto and Kypreos [94]	2000	Global electricity	PF	MILP
Gritsevskyi and Nakićenovi [95]	2000	Global energy	RH	MILP
Seebregts et al. [96]	2000	W. European energy	PF	MILP
Barreto and Kypreos [97]	2002	Global electricity	PF	MILP
Mattsson [98]	2002	Global electricity	PF	MILP
De Feber et al. [99]	2003	W. European energy	PF	MILP
Barreto and Klaassen [100]	2004	Global electricity and fuel production	PF	MILP
Barreto and Kypreos [101]	2004	Global electricity and fuel production	PF	MILP
Barreto and Kypreos [102]	2004	Global electricity	PF	NLP
Miketa and Schratten-holzer [103]	2004	Global electricity	PF	NLP
Riahi et al. [104]	2004	Global electricity	PF	MILP
Hedenus et al. [105]	2006	Global electricity, heat and transport	lim. F	LP
Rafaj et al. [106]	2005	Global energy, six sectors and multiple commodities	PF	dyn. LP
Rafaj and Kypreos [107]	2007	Global energy, six sectors and multiple commodities	PF	dyn. LP
Turton and Barreto [108]	2007	Global energy	PF	MILP
Rout et al. [109]	2009	Global energy	PF	MILP
Rout et al. [110]	2010	Global electricity and transport	PF	MILP
Hayward et al. [111]	2011	Global electricity	PF	MILP
Kim et al. [112]	2012	South Korea electricity, four demand sectors	PF	NLP
Anandarajah et al. [113]	2013	Global energy, focus on transport	PF	MILP
Wu and Huang [114]	2014	Taiwan electricity	PF	NLP
Choi et al. [115]	2016	South Korea energy	PF	MILP & NLP
Hayward et al. [116]	2017	Global electricity	PF	MILP
Heuberger et al. [89]	2017	UK electricity	PF	MILP
Huang et al. [117]	2017	Global electricity	PF	LP & MILP
Karali et al. [118]	2017	USA industry	PF	LP

(*continued on next page*)

Table 4 (*continued*).

Authors	Year	Scope	Foresight	Modeling
Handayani et al. [119]	2019	Java–Bali electricity	PF	LP
Chapman et al. [120]	2020	Global energy	PF	LP
Kim et al. [91]	2020	South Korea energy	MF & PF	LP & MILP
Xu et al. [121]	2020	PV in China	PF	dyn. NLP
Straus et al. [122]	2021	Europe electricity	PF	MILP
Tibebu et al. [123]	2021	USA electricity	PF	MILP
Felling et al. [124]	2022	German electricity	PF	LP, MILP & Benders
Lee et al. [125]	2022	South Korea industry	MF	PMP
Rathi and Zhang [126]	2022	UK electricity	PF	MILP
Seck et al. [127]	2022	Europe energy	PF	MILP & dyn.
Zeyen et al. [88]	2023	Europe energy	PF	MILP

as coal-fired ones. In the linear case, up- and down-ramping constraints can be defined as follows, with r_c^{up} and r_c^{down} being the maximum admissible ramping rates of component c in $\%/h$ [147–149]:

$$x^{op}_{c,i,r,s,t1} - x^{op}_{c,i,r,s,t-1} \leq r^{up}_c x^{cap}_{c,i,r} \Delta t \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{6a}$$

$$x^{op}_{c,i,r,s,t-1} - x^{op}_{c,i,r,s,t} \leq r^{down}_c x^{cap}_{c,i,r} \Delta t \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{6b}$$

Note that, in contrast to the cited sources, we ignore spinning reserves and startup or shutdown rates in Eqs. (6a) and (6b).

Minimum part load

In contrast to ramping, many other operational model features rely on binary variables and therefore greatly increase computational complexity. The minimum part load is an example of this. Given the fact that an operation must be either zero or above the minimum part load θ_c^{pl} (in %), a big-M formulation [150,151] can be applied using the operational binary variable $x^{op,bin}_{c,i,r,s,t} \in \{0,1\}$, indicating whether component c is running or not:

$$x^{op}_{c,i,r,s,t} \geq \theta^{pl}_c x^{cap}_{c,i,r} \Delta t - M(1 - x^{op,bin}_{c,i,r,s,t}) \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{7a}$$

$$x^{op}_{c,i,r,s,t} \leq M x^{op,bin}_{c,i,r,s,t} \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{7b}$$

Eq. (7a) states that the operation is larger than the minimum part load if the component is running because, in that case, the second term on the right-hand side is zero. If the component is not in operation, the second term is subtracted from the first one and turns the right-hand side into a negative expression, which makes the constraint non-binding. Eq. (7b), by contrast, is only binding if the component is not running and thereby forces the operation rate to be zero in the respective time step. Note that the smaller the big-M parameter is, the tighter and thus less computationally expensive the resulting model is [152].

Minimum up- and down-times

Minimum up- and down-times require components to remain active or inactive for a minimum amount of time before they can change their operational status, which is, like ramping, particularly relevant for baseload plants. To limit the number of start-ups and shut-downs, additional binary variables $x^{op,bin,su}_{c,i,r,s,t} \in \{0,1\}$ and $x^{op,bin,sd}_{c,i,r,s,t} \in \{0,1\}$ are needed, as presented by Van den Bergh et al. [148]:

$$x^{op,bin}_{c,i,r,s,t} - x^{op,bin}_{c,i,r,s,t-1} - x^{op,bin,su}_{c,i,r,s,t} + x^{op,bin,sd}_{c,i,r,s,t} = 0 \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{8a}$$

$$x^{op,bin}_{c,i,r,s,t} \geq \sum_{t'=t+1-MUT_c/\Delta t}^{t} x^{op,bin,su}_{c,i,r,s,t'} \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{8b}$$

$$1 - x^{op,bin}_{c,i,r,s,t} \geq \sum_{t'=t+1-MDT_c/\Delta t}^{t} x^{op,bin,sd}_{c,i,r,s,t'} \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{8c}$$

Eq. (8a) specifies that either $x^{op,bin,su}_{c,i,r,s,t}$ or $x^{op,bin,sd}_{c,i,r,s,t}$ become 1 if the activation status of component c changes between $t-1$ and t. Eq. (8b) states that component c can be deactivated as soon as the start-up time MUT_c has passed. Eq. (8c) states that component c can be activated as soon as the shut-down time MDT_c has passed.

3.2. Sources and sinks

Sources and sinks are not only affected by economic principles such as price elasticity but also by modern consumption concepts such as demand response, which will be described in the following.

3.2.1. Price elasticity

For most goods other than luxury articles, known as Veblen goods [153], the demand increases with decreasing prices [154]. This especially holds true for mass-produced goods and commodities such as energy resources [155,156]. This principle is defined by the (inverse) demand curve shown in Fig. 8a.

In a perfectly competitive market, supply is increased up to a point at which the marginal cost of one additional commodity unit equals the price that can be obtained for it on the market, i.e., the intersection of the supply and demand curves. This price, represented by the dashed line in Fig. 8a, is defined as the market-clearing price. When energy demand is imposed as a fixed constraint, the market-clearing price equals the dual variable of the "supply-equals-demand" constraint. This well-known fact is often used in dispatch models [157]. The demand curve can be imagined as an infinite group of customers, only a few of whom are willing to pay a lot for their energy. The lower the price, however, the more of them are willing to buy energy, increasing the overall demand. Then, the area between the dashed line and demand curve is the customer's welfare, i.e., every customer on the demand curve above the market-clearing price is willing to pay more for the energy than the market-clearing price. Similarly, the energy provider makes a profit on every unit of energy as long as the marginal cost of that specific unit is lower than the market-clearing price.

This welfare-optimal market clearing only occurs if perfect competition with an infinite number of energy providers and complete market information are assumed. A monopolist, however, could increase prices in order to increase its profits. In Fig. 8a, the profit of the (single) energy provider is represented by the green area, whereas the welfare of the consumers is given by the red one. The gray area is the so-called deadweight loss – a loss in total welfare that occurs if the monopolist maximizes its profit, i.e., the green area in Fig. 8a. Thereby, the violet rectangle between the abscissa, ordinate, and demand curve stands for the revenues of the energy provider.

The difference between welfare and profit optimization is an important aspect with respect to modeling. Welfare optimization can occasionally be found in energy system frameworks such as TIMES [4,5,72,73], as well as DER-CAM and REMIND, according to Ringkjøb et al. [1]. It can be easily implemented by discretizing the demand curve using a series of energy sinks. As the energy sinks yield revenues in a decreasing order, the most profitable one, i.e., the one generating the highest revenue per energy unit, is supplied first, followed by the one with the second-highest revenue, etc., as illustrated in Fig. 8b. This means that the order of price segments is automatically kept by the energy system model, and it does not require additional binary variables or SOS2 constraints. The energy supply is increased up to a point at which the additional system costs equal the revenues generated

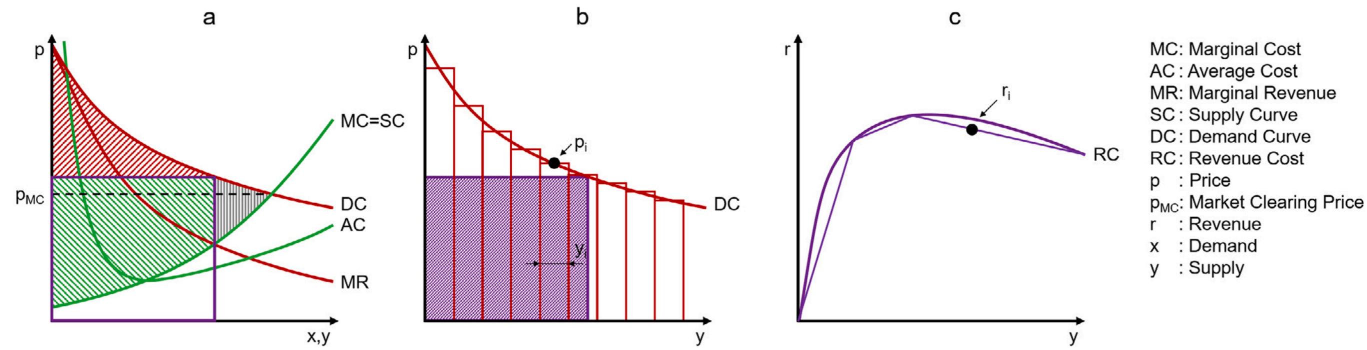

Fig. 8. (a): supply, demand, market clearing, consumer surplus (red), and supplier profit (green); (b): discretization of the demand curve for welfare maximization; (c): discretization of the revenue curve.

from the elastic energy sink and, more precisely, the market-clearing price under perfect competition.

In contrast, a micro-economic point of view would focus on the revenues generated by an energy provider, defined by the area of the violet rectangle. As it is a non-linear concave function with a maximum at the supply level that maximizes the rectangular area, its discretization requires piecewise linear approximations, as shown in Fig. 8c. However, to the best of the authors' knowledge, this approach has not been used by any of the reviewed frameworks.

3.2.2. Demand response

Demand response, or demand-side management, makes power demand more flexible, which is advantageous for systems with intermittent renewable energy sources. Some demand response measures can even provide their services with no additional investment and with low system costs, whereas others might be more costly but are associated with significant potential, such as battery electric vehicles [158].

Demand response is commonly understood as controlled load shedding, which is not designed for permanent demand reduction or the temporal shifting of electricity demand within a predefined time window. According to the overview by Morales-España et al. [159], demand response can be further categorized into self- and third-party-dispatched load changes. Self-controlled load changes are implemented by the user and stimulated by time-variable electricity tariffs, so-called time of use (TOU) tariffs. In contrast, externally controlled load changes are automated and serve to either reduce supply costs by reacting to day-ahead and real-time markets or stabilize the system within the balancing energy market. For instance, Germany has passed a law making direct load control compulsory for heat pumps, non-publicly accessible charging points for electric vehicles, systems for generating cooling or storing electrical energy, and storage heaters as of January 1, 2024 (§14a EnWG).

According to Morales-España et al. [159], two main types of demand response measures can be defined, which are depicted in Fig. 9a and 9b, namely curtailment and load shifting.

Curtailment

Curtailment or load shedding focus on the reduction of load peaks. This could be due to pure energy savings, grid bottlenecks, or a shortage of backup capacity. It is assumed that the reduced load does not lead to an increased load during the other time steps, as shown in Fig. 9a. These processes occur, for example, if demand can be met by a perfect substitute. While the option for supply curtailment is already given by Inequality (1l), load shedding with a fixed sink operation $\bar{x}^{op}_{c,i,r,s,t}$ can be realized by adding an auxiliary energy source for shed energy to Eq. (1f) (see [159] for a similar formulation):

$$f_{c,g,i,r,s,t} = -\bar{x}^{op}_{c,i,r,s,t} + x^{op,ls}_{c,i,r,s,t} \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{9a}$$

$$0 \leq x^{op,ls}_{c,i,r,s,t} \leq \bar{x}^{op}_{c,i,r,s,t} \quad \forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T} \tag{9b}$$

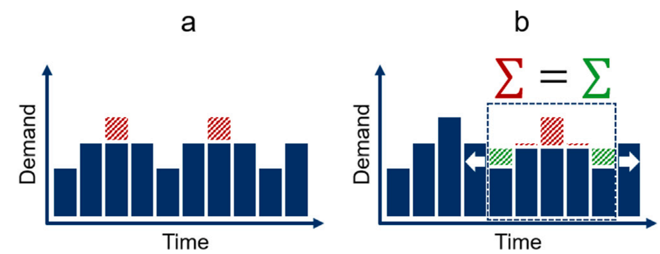

Fig. 9. (a): Curtailment or load shedding, which both limit the supply (curtailment) or demand (load shedding) without replacement; (b): load shifting, which compensates a reduced energy supply at one point in time with an increased supply at earlier or later times while keeping the cumulative amount of supplied energy constant.

Note that load shedding usually causes additional costs that must be added to the objective function:

$$obj^{ls} = obj + \sum_c \sum_i \sum_r \sum_s \sum_t p_s c^{op,ls}_{c,i,r,s,t} x^{op,ls}_{c,i,r,s,t} \tag{10}$$

Load shifting

Load shifting can avoid load peaks as well, but this load decrease leads to an advanced or postponed load catch-up during another point in time, e.g., when sufficient amounts of electricity from renewables are available, as shown in Fig. 9b. The net sum might be null or positive. Examples are manifold, especially in heavy industry, where some production processes are flexible over time (see, e.g., Gils [160]). There are various approaches for modeling demand response. Simplified models incorporate load shifting in a similar way to energy storage [161], while more complex approaches explicitly consider shifting durations, rest periods, and maximum energy volumes [162]. Due to the interaction of charging and driving processes, different approaches are used for battery electric vehicles, in which, for example, maximum and minimum battery levels can be incorporated [163]. Load shifting can be modeled using additional variables for increases in demand $x^{op,ls+}_{c,i,r,s,t}$ and decreases $x^{op,ls-}_{c,i,r,s,t}$ $\forall i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T}$ (see [159] for a similar formulation):

$$f_{c,g,i,r,s,t} = -\left(\bar{x}^{op}_{c,i,r,s,t} + x^{op,ls+}_{c,i,r,s,t} - x^{op,ls-}_{c,i,r,s,t}\right) \tag{11a}$$

$$\sum_{t}^{t+LSTW-\Delta t} x^{op,ls+}_{c,i,r,s,t} = \sum_{t}^{t+LSW-\Delta t} x^{op,ls-}_{c,i,r,s,t} \tag{11b}$$

$$\bar{x}^{op,min}_{c,i,r,s,t} \leq \bar{x}^{op}_{c,i,r,s,t} - x^{op,ls-}_{c,i,r,s,t} \leq \bar{x}^{op}_{c,i,r,s,t} \leq \bar{x}^{op}_{c,i,r,s,t} + x^{op,ls+}_{c,i,r,s,t} \leq \bar{x}^{op,max}_{c,i,r,s,t} \tag{11c}$$

Eq. (11a) allows for an increase and a decrease in demand, and Eq. (11b) ensures that the increased and reduced demands balance each other within the load shift time window (LSTW). Inequality (11c) limits the maximum shifted energy within each time step and maintains the positivity of $x^{op,ls+}_{c,i,r,s,t}$ and $x^{op,ls-}_{c,i,r,s,t}$, respectively. Note that different definitions for the load shift time window can be found in the literature [164–

167], many of which focus on a shift into the future only [164,167]. Furthermore, additional costs may arise for the shifted load.

3.3. Converters

Converters link different energy carriers and commodities, making them especially crucial for sector-coupled models and those dispatch models that explicitly consider fossil fuel consumption. Although the conversion factor $\gamma_{c,g,i,r,s,t}$ in Eq. (1g) was assumed to be constant, real converters can exhibit significantly non-linear part load efficiencies. These can be modeled by piecewise linear functions that couple the operation rate of one commodity with those of the others [168–172]. The approach is analogous to the piecewise linear modeling of CAPEX presented in Section 3.1.1. It must be noted that efficiencies can depend on various parameters and that they are not necessarily defined by the specific partload rates alone (see, e.g., [173]).

3.4. Storage

Storage is pivotal for the future energy system, given the rising share of intermittent renewable energy sources. In the modeling context, it is represented by a certain maximum power level and energy level, as well as losses. Apart from the basic formulation in Eq. (1m) with constant charge and discharge efficiencies, the power constraint of the storage might depend on its filling level, i.e., its state of charge (SOC). This is, for instance, the case for lithium-ion batteries, which cannot easily cope with high charging rates at high or low SOC levels [174].

Typically, losses are categorized into charging losses, discharging losses, and self-discharge losses. Together with the power- and energy-related capacity-specific costs of storage components, these losses are crucial parameters for deciding whether a storage technology should be operated in a dynamic daily or preferably static seasonal manner [175,176].

Charging and discharging losses

Most storage devices have losses due to charging or discharging; e.g., the efficiency of water storage is mainly determined by the efficiency of the pump, but also batteries generate heat during charging or discharging processes – especially at high charging rates [174]. Considering this in energy system models is important because their usage is strongly overestimated otherwise [177].

Self-discharge

Apart from losses that occur during storage usage, self-discharge is another severe issue for most storage systems. This rate is comparatively low for some technologies, such as hydrogen storage, whereas it might be significant for others, such as flywheels. This can be considered by equipping Eq. (1m) with a self-discharge rate η^{sd} in $1/\Delta t$ and $\forall\ i \in \mathbb{I}, r \in \mathbb{R}, s \in \mathbb{S}, t \in \mathbb{T}$, which leads to an exponential decay function [178]:

$$x^{SOC}_{c,i,r,s,t+1} = \left(1 - \eta^{sd}\right) x^{SOC}_{c,i,r,s,t} + \eta^{ch}_{c,i,r,s,t} x^{op,ch}_{c,i,r,s,t} - \frac{x^{op,dis}_{c,i,r,s,t}}{\eta^{dis}_{c,i,r,s,t}} \tag{12}$$

3.5. Transmission and distribution

Depending on the carrier, energy transport is subject to significant physical constraints. Some of the most commonly used ones are phase angles in alternating current (AC) networks, as well as temperature and mass flow dependence in heating networks. We will review the mathematical formulations for these in the next two Sections 3.5.1 and 3.5.2.

3.5.1. AC power grid

In an alternating current (AC) network, the starting point of the theoretical derivation of power flows is the line equation for the active power Φ_l and reactive power Q_l over a transmission line $l \in \mathbb{M}^{trans}$ connecting a bus/region/node $r \in \mathcal{R}$ with another bus/region/node $r' \in \mathcal{R}\backslash\{r\}$ [179]:

$$\Phi_l = \Phi_l(\delta_{r,r'}, V_{r,r'}) = |V_r|^2 g_l + |V_r||V_{r'}| \left(g_l \cos(\delta_r - \delta_{r'}) + b_l \sin(\delta_r - \delta_{r'})\right) \tag{13}$$

$$Q_l = Q_l(\delta_{r,r'}, V_{r,r'}) = |V_r|^2 b_l + |V_r||V_{r'}| \left(g_l \sin(\delta_r - \delta_{r'}) - b_l \cos(\delta_r - \delta_{r'})\right) \tag{14}$$

with $V_{r,r'}$ being the voltage magnitudes at buses/regions/nodes r and r', $\delta_{r,r'}$ being the voltage angles, and b_l, g_l being the susceptance and conductance of the transmission line. Below, this section follows the derivations of Kies [180] on the nodal injection pattern. It introduces the so-called *DC-approximation* for load flows in AC networks, which can also be found in textbooks.

The aim of the DC approximation is the linearization of the above-mentioned non-linear equations in order to be able to include the load flows, i.e., the active power, in a linear optimization problem. It is based on the following four assumptions:

1. The reactive power in an AC network is small and can consequently be neglected.
2. Voltage angle differences are also small, hence $\sin(\delta_r - \delta_{r'}) \approx \delta_r - \delta_{r'}\ \ ,\forall r, r' \in \mathcal{R}$
3. The conductance is much smaller than the susceptance, such that the corresponding term can be neglected.
4. Voltage magnitudes are approximately one.

When these assumptions hold, Eq. (13) can finally be simplified to:

$$\Phi_l = b_l(\delta_r - \delta_{r'}) = f_l \tag{15}$$

This equation expresses the load flow along a transmission line l as a function of the voltage angles at the end regions r and r'. Due to its similarity to the load flow in DC networks, where the voltage angles are replaced by the voltage magnitudes, this equation is called the DC approximation [180].

The physicality of the flows f_l is ensured by invoking Kirchhoff's current (KCL) and voltage law (KVL), which state that:

1. The power reaching each region must equal the power withdrawn from it, either via attached lines or by consumption, and
2. All partial voltages, i.e., differences in the electrical potential, along a closed cycle sum up to zero.

For the subsequent derivations, we must define the following three matrices:

1. The incidence matrix $\mathbf{K}$ with:
$$k_{rl} = \begin{cases} 1 & \text{if line l begins at region r} \\ -1 & \text{if line l ends at region r} \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$
2. The diagonal susceptance matrix $\mathbf{X}$ with $x_{ll} = b_l$ and
3. The network Laplacian $\boldsymbol{\Lambda} = \mathbf{KXK}^T$

With the incidence matrix, the flows can be expressed as:

$$f_l = b_l \sum_r k_{rl}\delta_r\ \ ,\forall l \in \mathbb{M}^{trans} \tag{17}$$

and KCL reads:

$$p_r = \sum_l k_{rl} f_l \tag{18}$$

$$= \sum_{r'} \lambda_{rr'}\delta_{r'}\ \ ,\forall r \in \mathcal{R} \tag{19}$$

where p_r is the net active power at bus/region/node r, i.e., the difference between consumption and generation, and $\lambda_{rr'}$ is the element of the network Laplacian $\boldsymbol{\Lambda}$ [180].

From these considerations, several different methods to determine the flow of electricity in the framework of a power system model can be derived, for instance the well-known power transfer distribution factors (PTDF; see Section 4.3). Here, the formulation used by Hörsch et al. [181] will be introduced first: In order to determine the active power flow, the voltage angles are set as auxiliary variables to the linear program, and the following corresponding constraints are invoked:

$$\left| \sum_r \left(XK^T\right)_{lr} \delta_r \right| \leq f_l \qquad ,\forall l \in \mathbb{M}^{trans} \tag{20}$$

$$p_n = \sum_{r'} \lambda_{rr'} \delta_{r'} \qquad ,\forall r \in \mathcal{R} \tag{21}$$

$$\delta_0 = 0 \tag{22}$$

Here, Eq. (20) prohibits line overloading, Eq. (21) ensures the fulfillment of KCL, and Eq. (22) fixes the voltage angle at a reference bus (the slack) because Eq. (21) is under-determined. Compared to the PTDF approach, this formulation increases the number of decision variables and equality constraints. However, the PTDF approach leads to a significant increase in the solution time for a number of different test cases caused by dense matrices in the PTDF formulation and the corresponding large sizes of the linear programming files [181].

In a more simplified setup, the transmission lines can be replaced by simplified high-voltage direct current (HVDC) links. In this case, the load flows along these links are introduced as additional decision variables, and the only constraint ensures that these flows do not exceed the net transfer capacity of the respective link [182].

3.5.2. Heat grid

Heat grids are usually organized as two-pipe systems with one flow line (fl) and one return line (re). The flow line transports the warm fluid from the source to the sink. After heat has been extracted from the fluid at the sink, the fluid flows back to the source via the return line at a lower temperature. The energy balance in a heat grid is calculated according to [183]:

$$\dot{Q}_s = \sum_c \dot{Q}_{d,c} + \dot{Q}_{loss,fl} + \dot{Q}_{loss,re} \tag{23}$$

with $\dot{Q}_s$ being the supplied heat at source s, $\dot{Q}_{d,c}$ being the heat demand of consumer c, and $\dot{Q}_{loss}$ being the thermal losses occurring in the flow and return line [183].

The transmission line in a heat grid is defined as the heat transported along a pair of flow and return lines. The sink symbolizes all connected consumers $\sum_c \dot{Q}_{d,c}$, which can be buildings or the adjacent transmission lines. Therefore, the flow of a transmission line in a heat grid is formed according to:

$$f_l = \sum_c \dot{Q}_{d,c} = \dot{Q}_s - \dot{Q}_{loss,fl} - \dot{Q}_{loss,re} \;,\forall l \in \mathbb{M}^{trans}. \tag{24}$$

The thermal losses in the flow and return lines can be calculated using the temperature difference between the fluid and ground temperature ΔT_{ground}, as well as the heat transfer coefficient UA of the grid:

$$\dot{Q}_{loss} = \Delta T_{ground} \cdot UA. \tag{25}$$

The optimization of heat grids usually focuses on the energy balance using linear formulations [184]. Therefore, the temperature dependency of the heat flow is neglected, and constant temperature values must be assumed to avoid non-linearities. An alternative approach is provided by Schönfeldt et al. [185], where several discrete temperature levels are defined. In this way, the non-linearities are avoided, but the temperature dependency can only be modeled to a limited extent. For linear heat grid flows, i.e., assuming constant or discrete temperature levels, Eq. (24) can be expressed as follows:

$$f_l = \sum_c \dot{Q}_{d,c} = \dot{Q}_s - UA \cdot (\Delta T_{ground,fl} + \Delta T_{ground,re}) \;,\forall l \in \mathbb{M}^{trans}. \tag{26}$$

If the temperature dependency is not neglected, the calculation of the heat flow:

$$\dot{Q} = \dot{m} \cdot c_p \cdot (T_{fl} - T_{re}) \tag{27}$$

becomes non-linear because the mass flow $\dot{m}$ and fluid temperature T are operational variables. As the specific heat capacity c_p of the fluid is constant, the non-linear formulation constitutes a quadratic problem. To ensure a correct heat flow, the following temperature constraints between the source and sink are required:

$$T_{fl,source} \geq T_{fl,sink} \tag{28}$$

$$T_{re,source} \leq T_{re,sink} \tag{29}$$

Hering et al. [186] present a simplified formulation for non-linear heat grid models by neglecting the spatial distribution of consumers and assuming the grid as a water reservoir. To reduce the computational complexity of the problem, the temperature difference between the flow and return lines at the sinks in the grid can be set to a constant value [187].

The temperature difference between the fluid and ground ΔT_{ground} can be calculated for a fixed ground temperature T_{ground} for both heat grid lines in a simplified manner according to [187] as follows:

$$\Delta T_{ground} = \frac{T_{source} + T_{sink}}{2} - T_{ground}. \tag{30}$$

Considering the temperature dependency of the heat flow in a heat grid, the flow is formulated as follows:

$$\begin{aligned} f_l = \sum_c \dot{Q}_{d,c} &= \dot{m} \cdot c_p \cdot (T_{fl,source} - T_{re,source}) - UA \cdot \\ &\left(\frac{T_{fl,source} + T_{fl,sink}}{2} + \frac{T_{re,sink} + T_{re,source}}{2} - 2 \cdot T_{ground} \right) \;,\forall l \in \mathbb{M}^{trans}. \end{aligned} \tag{31}$$

The storage effects in the heat grid can be considered by defining the corresponding temperature in the flow and return line as state variables, so $x^{SOC}_{fl,grid,t} = T_{fl,grid,t}$ and $x^{SOC}_{re,grid,t} = T_{re,grid,t}$ describe the current SOC in the corresponding line of the heat grid. Thus, the time derivatives of the flow and return line temperature describe the changing rate of the SOC [186]. The derivative for the flow line temperature is calculated according to [186]:

$$\frac{\Delta T_{fl,grid,t}}{\Delta t} = \frac{\dot{m}_{source} \cdot (T_{fl,source,t} - T_{fl,grid,t})}{m_{grid}} - \frac{UA \cdot (T_{fl,grid,t} - T_{ground})}{c_p \cdot m_{grid}} \tag{32}$$

with $T_{fl,source,t}$ being the flow temperature at the heat source and $T_{fl,grid,t}$ being the actual grid temperature in the flow line. Furthermore, $\dot{m}_{source}$ describes the mass flow at the heat source and m_{grid} the total fluid mass in the grid.

Similarly, the storage effects in the return line are calculated as follows [186]:

$$\frac{\Delta T_{re,grid,t}}{\Delta t} = \frac{\dot{m}_{source} \cdot (T_{re,sink,t} - T_{re,grid,t})}{m_{grid}} - \frac{UA \cdot (T_{re,grid,t} - T_{ground})}{c_p \cdot m_{grid}} \tag{33}$$

with $T_{re,grid,t}$ being the return line temperature and $T_{re,sink,t}$ being the temperature at the sink.

4. Boundary conditions

Apart from purely technical component constraints, energy systems face additional constraints such as geological, geographical, or social limitations, also referred to as technology potentials, and regulatory frameworks.

4.1. Potentials

Potentials are simple constraints that limit the maximum installable capacity of a technology in a region and investment period:

$$x^{cap}_{c,i,r} \leq x^{cap,pot}_{c,i,r} \qquad \forall i \in \mathbb{I}, r \in \mathbb{R} \tag{34a}$$

The potential of a technology is defined by geographical factors such as the total available land defined by distance restrictions to inhabited areas or surface slopes [188], but also technical ones such as the technology-specific space consumption per capacity in an eligible area [189]. These potentials also depend on the concrete component types of a technology, e.g., wind turbine types, leading to standalone potential analyses such as, e.g., conducted by Ryberg et al. [190], Caglayan et al. [191], and reviewed by Pelser et al. [192] for wind power, conducted by Risch et al. [193] for wind power and photovoltaic, as well as by Maier et al. [194] for photovoltaic.

Similar to price elasticity, regions can contain a distribution of more and less profitable sites, which can be modeled as a discrete set of separate technology potentials with distinct capacity factor characteristics. For instance, Caglayan et al. [195] proposed a discretized set of wind potentials sorted by levelized cost of electricity (LCOE) based on status quo price structures. Especially in electricity-centered systems, the LCOE is the only metric that has become an omnipresent standard for all kinds of systems, be it for plant siting or microgrid assessments [196]. In this way, a supply elasticity similar to the price elasticity of energy demands can be realized by first expanding the most profitable generation sites.

4.2. Regulations

Particularly with regard to the legal framework, contemporary optimization-based frameworks for energy system modeling only reflect interactions with other economic sectors to a limited extent but respect externally defined economic and ecological constraints. Still, it is vital that regulations align the incentives of all stakeholders and allow for efficiently designed and operated energy systems [197].

Regulations and subsidy mechanisms can be almost freely designed, address arbitrary components, and refer to installed capacities, cumulative operating hours, component-specific emissions, cross-combinations of entire system setups, etc. These factors make it difficult to formulate generally applicable modeling approaches and frameworks but remain an important source of uncertainty when modeling energy systems (see Table 5). Therefore, the following section refrains from providing mathematical formulations for the far too diverse field of regulations. Instead, we provide an aspect-oriented and non-exhaustive overview of occasionally integrated regulatory constraints and incentives. For a more methodological approach to embedding these regulatory mechanisms into optimization problems with single objective functions, we refer the reader to Section 5, which provides general concepts to integrate aspects such as CO_2 restrictions into energy system models.

4.2.1. Volume-related restrictions

Volume-related restrictions are those in which model components, i.e., sources, sinks, converters, storage systems, or transmission units, are restricted in their design and/or operation without a direct impact on cash flows. The regulatory implications are not implemented via price mechanisms but via explicit restrictions on commodities or components. Therefore, implementation in energy system models is carried out via the formulation of constraints for the respective commodities or components, as well as the parameterization of the components, whereas the objective function remains unaffected. Volume-related restrictions that are depicted in energy system models in the literature include, among others, the limitation or ban of CO_2 emissions, minimum renewable energy utilization shares [198,199], or limitations in feed-in and minimum self-consumption rates for prosumers [171,200], e.g., electricity generated from CHP units [200]. Notably, almost every contemporary framework for energy system modeling reviewed in Table 12 is capable of modeling emissions explicitly, a trend that has already been demonstrated by Ringkjøb et al. [1] in 2018, making them the most frequently employed subject to regulatory restrictions in frameworks. By contrast, other regulatory restrictions are far less frequently integrated into frameworks, given that they are highly dependent on national law and frameworks are usually not designed to optimally represent a single nation's energy-related regulations. This finding is supported by the fact that those publications considering nation-specific regulations have conducted their analyses with custom-made energy system models instead of framework instances.

4.2.2. Price-related restrictions, subsidies, and market characteristics

Price-related restrictions, subsidies, and market characteristics are regulations with an influence on prices, costs, and revenues. They work via price mechanisms and monetary cash flows and must therefore be implemented by means of corresponding terms in the objective function. These can be mapped as constant or variable values and affect capital and/or operating costs. As these regulations are usually complex, are subject to additional conditions regarding the model components and commodities, and depend on binary variables (e.g., subsidies), they often require a set of additional constraints besides their representation in the objective function. This, in turn, impedes the above-mentioned integration into generic frameworks for energy system modeling. Price-related restrictions, subsidies, and market characteristics that are depicted in energy system models in the literature include CO_2 pricing schemes and taxes [201,202], modalities for power exchange with the grid [199], surcharges on resource prices, as well as subsidies for investments in renewable power generation units and electricity-based consumer appliances such as heat pumps or electric vehicles [171,198,199,203–206]. Others are pricing schemes for consumed electricity based on certain end-use technologies [171,207], as well as time-of-use tariffs [208,209]. For a renewable energy system with PV, micro-wind turbine installations, battery storage [171,209–211], special above-market feed-in remuneration [171, 209,210,212] was studied. Furthermore, levies on self-consumed electricity [171,206], and tax exemptions [171,207,213] were investigated. While pricing schemes for commodities and feed-in tariffs usually influence operating costs, subsidies can affect both capital and operating costs. In addition to their representation in objective functions and constraints, pricing schemes for commodities and feed-in tariffs can also be implemented via scenario and sensitivity analyses.

4.2.3. Risks and risk management

Regulations regarding risk management in energy systems include, amongst others, n-1 criteria, reserve margins, firm capacities to ensure the security of supply in energy systems, and the stability of network operations. In the literature, energy system models are used for scheduling reserves, for instance, by means of security-constrained unit commitment, accounting for n-1 criteria, and forecasting uncertain generation from renewable energy sources, as well as load. Reserves are typically modeled as constraints on the hourly generation capacity, with stochastic modeling representing risks and uncertainties [214].

4.3. System security and resource adequacy

System cost minimization alone does not account for the need to ensure the security of supply in the event of forced outages of system components. To ensure this, different approaches exist, ranging from system monitoring over contingency analysis to security-constrained optimal power flow [179]. For the latter, the resilience of the system to a series of contingencies is tested and integrated into how the system is operated. To derive a complete picture of the system's resilience, one would, in principle, need to consider the failure of any of the system's components. As this might lead to several thousand power flow calculations, so-called *linear sensitivity factors* are used. Two types can be distinguished [179]:

1. Power transfer distribution factors (PTDFs)
2. Line outage distribution factors (LODFs)

These factors estimate the average change in line flow for any change in generation (in the case of PTDFs) or any potential outage of transmission lines (in the case of LODFs), respectively. They are defined as:

$$\mathrm{PTDF}_{r,r',l} = \frac{\Delta f_l}{\Delta P_{rr'}} \tag{35}$$

$$\mathrm{LODF}_{l,k} = \frac{\Delta f_l}{f_k^0} \tag{36}$$

Table 5
Studies on regulation in energy system optimization models.

Authors	Year	Scope	Type
Lozano et al. [212]	2009	Electricity feed-in remuneration	MILP
Lozano et al. [200]	2010	Maximum power, minimum efficiency, and self consumption quota for cogeneration systems	MILP
Mehleri et al. [201]	2012	Carbon emission tax	MILP
Akbari et al. [202]	2014	Carbon emission tax	MILP
Piacentino et al. [213]	2015	Tax exemption for efficient cogeneration systems	MILP
Steinbach [198]	2016	Minimum utilization shares for RE in new buildings and alternative measures according to EEWärmeG, Investment grants and subsidized loans for renewable heat generators, large heat storage systems, heating networks and biogas upgrading systems	Agent-based investment decision-making model
Harb et al. [207]	2016	CHP tax exemptions, HP electricity tariffs	MILP
Klein and Deissenroth [210]	2017	PV remuneration tariffs, feed-in tariffs	NPV, MCS, Prospect utility model
Renaldi et al. [203]	2017	Electricity tariffs, subsidy for non-fossil fuel domestic heating systems	MILP
Schütz et al. [171]	2017	Prosumer regulations: EEG feed-in limit, EEG levy on self-consumed electricity, EEG feed-in remuneration, payment for self-consumption and feed-in from CHPs, financial support for battery assisted PV systems, fuel tax exemption/refund for CHP units, cheaper electricity tariff for HPs, Multiple electricity and gas tariffs with different fixed and variable costs and different emission factors	MILP
Antenucci and Sansavini [214]	2018	Electricity reserves, reserve margins, n-1 security	MILP
González-Mahecha et al. [211]	2018	Utility and feed-in electricity tariff schemes, bi-hourly tariffs	MILP
Luo et al. [204]	2019	Subsidies for a standalone multi-generation energy system	Bi-level optimization
Benalcazar et al. [205]	2020	Capital subsidies across all distributed generation technologies, capital subsidies for renewable technologies, capital subsidies for PV technologies, capital subsidies for wind technologies, diesel price subsidies	LP
Pinto et al. [206]	2020	Self-consumption subsidy and tax	MILP
Pina et al. [199]	2021	Power exchange modalities, subsidies and surcharges on energy prices and CAPEX, ban on fossil fuels	MILP
Marocco et al. [208]	2021	Time-of-use tariffs	MILP
Sarfarazi et al. [209]	2023	PV self-consumption, Prosumer regulations, Real-time pricing, variable feed-in tariff, dynamic EEG levy	MILP, ABM

with $r \in \mathcal{R}$ being the index of the bus/region/node where power is injected, $r' \in \mathcal{R}\backslash\{r\}$ the index of the bus/region/node where power is withdrawn, $\Delta P_{rr'}$ being the power transferred from bus/region/node r to r', and Δf_l being the change in power flow on line $l \in \mathbb{M}^{trans}$ connected to $\Delta P_{rr'}$ [179].

Assuming that a generator must reduce its power generation by $\Delta P_{rr'} = -P_r^0$ and that a reference generator is able to compensate for this loss in power by ramping its own generation up, the resulting new flow f_l' on line l can be computed via:

$$f_l' = f_l^0 + \mathrm{PTDF}_{r,ref,l}\,\Delta P_{rr'} \tag{37}$$

Similarly, the impact of losing (opening) a transmission line on the flow of the remaining lines can be estimated from:

$$f_l' = f_l^0 + \mathrm{LODF}_{l,k}\,f_k^0 \tag{38}$$

Here, f_l^0 and f_k^0 denote the original flow on these lines ($l, k \in \mathbb{M}^{trans}$) prior to a loss in capacity [179].

Hence, $\mathrm{PTDF}_{r,r',l}$ and $\mathrm{LODF}_{l,k}$ provide the sensitivity of the flow on line l regarding a potential loss of power transferred from a generator at bus r to a generator at bus r' or an opening of line k, respectively. It can be shown that both PTDF and LODF only depend on system parameters and not on actual voltages and/or loads [179]. This means they can be precalculated without performing any power flow calculations. Using these factors, a contingency analysis can be performed, and the power flow can be adjusted to avoid the largest risks of system failure. This procedure is commonly referred to as security-constrained optimal power flow [179].

In the process of planning power systems, the aspect of system security is addressed by applying the so-called n-1 rule, stating that the system must stay in a safe mode of operation when any of the system components are taken out of service. This can, for instance, be done by limiting the flow on the lines to a certain percentage of the installed capacity or by invoking additional constraints, which ensures that the operation of the system always plans for sufficient reserves (see, e.g., [215]). Power systems planned in such a way are considered adequate, i.e., they are able to ensure the security of supply with reasonable probability. As part of their policy mandates, transmission system operators must regularly prove this adequacy. This process is called resource adequacy assessment.[2]

5. (Multi-criteria) objectives

The planning and operation of energy systems often involves multiple and sometimes opposing objectives, such as low costs and low emissions. The most common concepts to address multiple objectives in energy system modeling are illustrated in Fig. 10 and reviewed in the following.

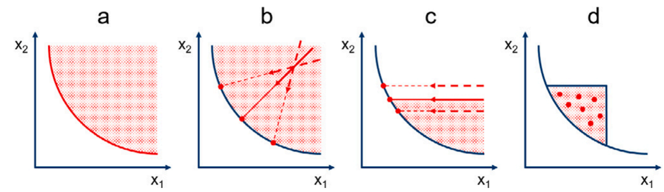

Fig. 10. Multi-objective optimization concepts. (a): Pareto front; (b): weighted sum method; (c): ε-constraint method; (d): modeling to generate alternatives.

5.1. Pareto-optimal fronts

Pareto-optimal fronts are a basic concept of multi-criteria optimization, which is shown in Fig. 10a. The concept states that value tuples along two or multiple dimensions of objectives are considered Pareto-efficient if there is no solution, which is at least as good with respect

[2] For the European Resource Adequacy Assessment (ERAA) implemented by ENTSO-E, see https://www.entsoe.eu/outlooks/eraa/.

to all objectives and better with respect to at least one [216,217]. Assuming x_1 and x_2 are to be minimized, all values along the solid red line are Pareto-efficient because for each point on the line, it holds that there exists no configuration of x_1 and x_2 that is at least as good with respect to one of the objectives and strictly better with respect to the other one.

5.2. Weighted sum method

As optimization models normally search for a single optimal solution, Pareto fronts are not directly accessible. Instead, a number of different methods exist to determine single Pareto-efficient solutions. The method of weighted sums is illustrated in Fig. 10b and combines different objectives by assigning individual costs to each criterion and summing them up. The integration of carbon emission costs into the total system cost minimization is a popular example (see, e.g., [218–223]) as CO_2 certificates have become a marketable commodity and so the considered CO_2 costs have practical implications. Other than that, approaches with theoretical penalty costs exist for non-financial objectives, e.g., minimizing land use along with total system costs. Graphically, the approach can be interpreted as a rotation of the objective function's gradient: as shown in Fig. 10b, the gradient would be horizontal in a case in which only x_1 is minimized, whereas it would be vertical if only x_2 was minimized. Linear combinations of these expressions of the form $\lambda x_1 + (1-\lambda)x_2, \lambda \in [0,1]$ allow the minimization of any trade-off between these two objectives. This means that theoretically, any point on the Pareto front can be found by repeating the optimization for infinitesimally varying values for λ an infinite number of times.

5.3. ε-constraint method

The ε-constraint method is shown in Fig. 10c, and it only considers a single optimization criterion in the objective function, whereas the remaining criteria are integrated by means of side constraints. This approach is frequently applied in the context of reduction targets for CO_2 emissions (see, e.g., [224–229]). In these cases, the objective is only given by the minimization of total costs of the energy system model, but subject to a side constraint imposing a maximum permissible CO_2 emission level (e.g., 95% reduction compared to 1990 as aspired to by many European countries by 2050) or requiring a minimum amount of energy from renewable energy sources known as a renewable portfolio standard (RPS) (see, e.g., [222,230]). This method also yields Pareto-efficient solutions, which coincide with the ones obtained using the weighted sum approach (i.e., yielding the same solution on the Pareto front), but they always differ with respect to the optimal objective function value due to the different objective function. The ε-constraint method shown in Fig. 10c constrains the feasible solution space instead of modifying the objective function gradient, i.e., in the case that x_1 represents total system costs and x_2 CO_2 emissions, the emissions limit shrinks the feasible space, and the minimum of x_1 is found at the maximum admissible value for x_2. As long as CO_2 emission reduction causes additional system costs, the emission constraint is a binding one, and the corresponding optimal solution is Pareto-efficient.

5.4. Modeling to generate alternatives

Modeling to generate alternatives (MGA) seeks to find maximally heterogeneous but near-optimal (or near-Pareto-efficient) solutions. The multitude of different technologies and allocation options often leads to a plethora of near-optimal alternative system designs, motivating this approach. As input data such as capacity-specific costs and future demand assumptions are uncertain, the analysis of near-optimal solutions sheds light on aspects such as the cost sensitivities of alternative designs and flexibility options during the capacity expansion process. A simple MGA approach is shown in Fig. 10d, for which the core objectives are removed from the objective function and replaced by constraints that allow for some degree of sub-optimality, e.g., 5% of additional costs compared to the cost-optimum given a 95% emission reduction target. The original objective function can be adapted to maximize or minimize other system aspects depending on the alternative to be generated, e.g., "maximize wind capacities", "minimize wind capacities", etc. More complex methods strive for a diversification of technology mixes by limiting the number of technologies used by means of binary variables and a permutation of available technologies. For any of these methods, however, a significant deviation from the Pareto-efficient solutions is avoided by the respective ε-factor.

Among others, the search directions in the solution space can be defined by the hop-skip-jump (HSJ) algorithm [231], which minimizes the weighted sum of variables of prior solutions. Others maximize the distance between new solutions and previous ones using the ε-method to find near-optimal solutions that are as diverse as possible [232–234]. Some further unique MGA approaches can be found in the literature, which combine the usually deterministic MGA technique with Monte Carlo simulations for key input parameters to take uncertainties into account [235,236]. Furthermore, portfolio constraints can quantify the benefits of technologies. This approach leaves the objective function unmodified, and during each iteration, it forcibly excludes a certain technology from the portfolio or restricts the capital costs of technologies [237]. Schyska et al. [238] used portfolio constraints to assess the sensitivity of linear optimization problems on chosen model parameters. While the ε-constraint usually includes costs, some articles considered multiple impact categories [239], i.e., they replaced multiple objectives with constraints in the optimization problem. In recent studies, MGA has been extended to include spatially distinct configurations of energy systems [240,241]. Pedersen et al. [242–244] tried to capture not only numerous but all near-optimal solutions in the solution space by constructing the feasible polyhedron using the quickhull algorithm to obtain a convex hull. Grochowicz et al. [229] extended previous approaches by intersecting the near-optimal solution spaces of different optimization problems for the same energy system but with different weather years in order to obtain a solution space with only weather-robust near-optimal solutions. In addition to exact methods, metaheuristics that store all solutions until finding an optimum (e.g., by using particle swarm optimization [245]) were also used for MGA.

In recent years, MGA has faced a strong uptake in energy system optimization, as shown in Table 6, because it offers a computationally efficient method for handling scenario-driven uncertainty in capacity expansion planning that is easy to implement, reproducible, and can be solved in a parallelized way.

6. Complexity handling

The preceding sections have shown that many additional model features can be integrated into frameworks by using mixed-integer linear formulations. However, given the NP-hardness of this type of problem, runtime grows exponentially with the number of additional constraints and variables, which is a major drawback compared to linear problems, which are, on the other hand, less versatile and not able to depict all system aspects. For large energy systems, the level of detail in the model must therefore be tailored to the specific research focus of the application. This is necessary to keep runtimes within practicable ranges, from multiple hours to a few days. Besides omitting certain model features, e.g., linear optimal power flow or piecewise linear cost functions, several methods exist to systematically decrease the model size. The most common approaches are spatio-technological and temporal aggregation, as well as myopic investment planning, which will be presented in the following.

Table 6
MGA in the energy system optimization literature.

Authors	Year	Method
Brill et al. [231]	1982	ε-method
DeCarolis [246]	2011	ε-method
Trutnevyte et al. [247]	2012	ε-method
Trutnevyte [248]	2013	ε-method
DeCarolis et al. [249]	2016	ε-method
Trutnevyte [236]	2016	ε-method combined with Monte Carlo simulations
Berntsen and Trutnevyte [234]	2017	ε-method based on minimizing and maximizing a particular attribute
Li and Trutnevyte [235]	2017	ε-method combined with Monte Carlo simulations
Price and Keppo [232]	2017	ε-method with maximized distance between solutions
Yue et al. [250]	2018	Review of MGA based on ε-method
Jing et al. [237]	2019	ε-method with portfolio constraints
Nacken et al. [233]	2019	ε-method with maximized distance between solutions
Lombardi et al. [240]	2020	ε-method with inclusion of spatial dimension
Sasse and Trutnevyte [251]	2020	ε-method
Neumann and Brown [252]	2021	ε-method with search direction based on minimizing and maximizing a particular attribute
Pedersen et al. [242]	2021	ε-method combined with even sampling of the near-optimal solution space (polyhedron)
Pedersen et al. [243]	2021	ε-method combined with even sampling of the near-optimal solution space (polyhedron)
Schyska et al. [238]	2021	ε-method with portfolio constraints
Weber et al. [253]	2021	Review of modeling uncertainties addressed by MGA
Chen et al. [254]	2022	ε-method with search direction based on minimizing and maximizing a particular attribute
Fioriti et al. [245]	2022	Metaheuristics (Particle Swarm Optimization) plus storing all solutions
Pickering et al. [241]	2022	ε-method with inclusion of spatial dimension
Grochowicz et al. [229]	2023	ε-method with intersecting near-optimal solution spaces of various different problems
Lombardi et al. [255]	2023	ε-method with inclusion of spatial dimension
Millinger et al. [256]	2023	ε-method with search direction based on minimizing and maximizing a particular attribute
Neumann and Brown [257]	2023	ε-method with search direction based on minimizing and maximizing a particular attribute
Pedersen et al. [244]	2023	ε-method combined with even sampling of the near-optimal solution space (polyhedron)
Sasse and Trutnevyte [239]	2023	ε-method with multiple impact constraints
Vågerö and Zeyringer [258]	2023	Review of MGA as a method to implement justice in energy system models

6.1. Spatio-technological aggregation

The number of considered spatial regions directly increases the complexity of a model. As is shown in Section 2.2, the number of variables and constraints of a model is approximately proportional to the number of regions assuming weak connectivity (i.e., the number of transmission lines does not increase disproportionately with the number of regions). Consequently, reducing the number of regions through spatio-technological aggregation techniques can effectively decrease model complexity.

Since reducing the number of model regions typically involves fewer grid nodes and fewer supply and demand technologies, it can be distinguished between spatial aggregation (related to grid topology) and technological aggregation (related to supply and demand technologies). These concepts are illustrated in Fig. 11.

The extreme case for spatio-technological aggregation is to reduce the number of spatial regions to a single region. This approach allows for optimizing the model's dispatch while ignoring the limitations on

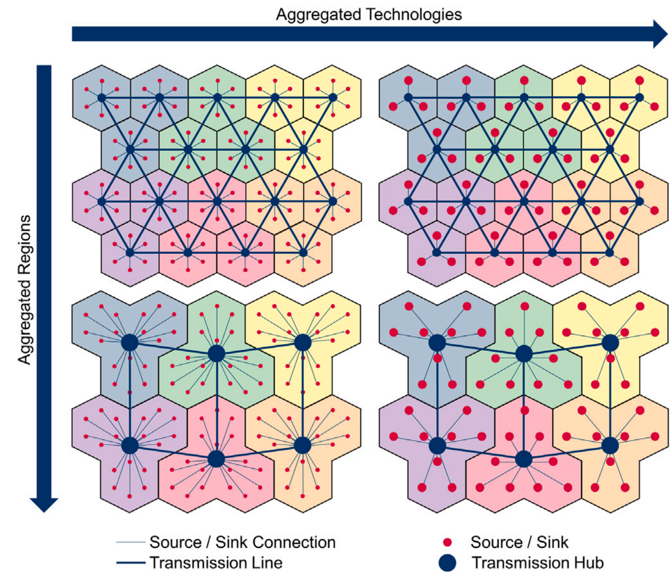

Fig. 11. Concept of spatial and technological aggregation. Spatial aggregation reduces the number of system nodes and thus simplifies the network topology, with side effects on the model's capability to mimic transmission bottlenecks, whereas technological aggregation reduces the number of components with a similar function in each region, which affects the model's capability to differentiate aspects such as more and less attractive sites for renewable electricity generation.

interactions between different spatial regions [24,51,259], and it is typically applied at large spatial scales, such as national or international levels [260–262]. This simplification is known as the copperplate assumption, as it disregards energy infrastructure and line congestion. In contrast, for multi-regional models, the copperplate assumption applies within each region but not between regions.

6.1.1. Spatial aggregation

Spatial aggregation reduces the number of network nodes, thereby altering the network topology. It can be conducted in a naive way, e.g., by using administrative [263,264] or square areas defined by longitude and latitude [265]. Apart from that, clustering techniques are popular in the modeling community [52], especially with existing algorithms such as k-means [24,266,267] or max-p [267,268] for defining the clusters. Clustering aims to maximize similarity within clusters and differences between clusters, preserving as much information from the original data set as possible when each cluster is represented by a single entity, in this case, a region. The clusters can be defined in terms of attributes such as market price zones [267], electrical distances [269,270], or capacity factors [270,271].

As pointed out by Cao et al. [272] and Frysztacki et al. [270], methods using nodal loads or capacities [273], marginal costs and nodal prices [274], electrical distances [270], or radial equivalent independent methods [272] have the limitation that they are based on current systems and thus may not be suitable for capacity expansion models. Instead, these methods are better suited to simplify dispatch models applied to existing systems. For capacity expansion models, approaches based on size-specific parameters such as capacity factor time series [270,271] are used for clustering because they are independent of the system layout.

The spatial aggregation of networks requires an interconnected network topology within each cluster. Depending on the attributes used for clustering, additional adjacency or connectivity constraints must be imposed to prevent two disjointed network parts from being assigned to the same cluster (see, e.g., [268,271]). Specialized algorithms for network clustering, such as those based on Dijkstra's shortest path algorithm [275,276], can also be employed. Table 7 presents a non-exhaustive review of spatial aggregation techniques applied in the literature.

Table 7
Spatial Aggregation in the Literature.

Authors	Year	Considered Attributes
Duque et al. [268]	2021	An MILP creating p clusters composed of adjacent candidate regions while maximizing intra-cluster homogeneity
Anderski et al. [277]	2015	Population Mean wind speed and solar irradiation Installed thermal and hydro capacity Agricultural areas (grasslands, etc.) Geographic locations of the regions
Hörsch and Brown [273]	2017	Demand and generation capacities Geographic locations of the regions
Unternährer et al. [278]	2017	Integer linear problem forming clusters for district heating networks minimizing intra-cluster distance and subject to minimum and maximum heating power
Cao et al. [274]	2018	Marginal costs of total power supply
Müller et al. [279]	2019	Same method as Hörsch and Brown [273]
Scaramuzzino et al. [280]	2019	Energy potentials Economic Sociodemographic Geographic locations of the regions
Siala and Mahfouz [281]	2019	Wind potential or photovoltaic potential or electricity demand
Biener and Garcia Rosas [269]	2020	Electrical distances between regions
Peters et al. [276]	2020	Assignment of generation sites to extra high voltage nodes using a Dijkstra algorithm proposed by Müller et al. [275]
Frysztacki et al. [266]	2021	Substation distance weighted by load and average capacity
Frysztacki et al. [270]	2022	Multiple methods: Clustering of geographic regions, annual capacity factors, hourly capacity factor and the electrical distance
Galván et al. [263]	2022	Assigning nodes with less electricity demand to larger adjacent ones or one node per country
Patil et al. [271]	2022	k-medoids with contiguity constraints using various techno-economic parameters for calculating the dissimilarity between candidate regions
Bogdanov et al. [264]	2023	Clustering based on geographic regions (Japan)
Klemm et al. [282]	2023	Similar building types or similar usage types
Phillips et al. [265]	2023	Geographical averaging using longitudinal and latitudinal square areas

6.1.2. Technological aggregation

Technological aggregation typically does not affect the network topology, and it is therefore not subject to additional connectivity or adjacency constraints. The simplest approach involves aggregating all generation sites of a kind into a single site per region (see, e.g., [68,265,274,281]). More complex approaches use clustering of techno-economic site attributes, such as LCOE [195], capacity factor time series [271], or different site-, technology-, and price-related values [283]. An overview of these methods is presented in Table 8.

Table 8
Technological aggregation in the literature.

Authors	Year	Considered Attributes
Welder et al. [68]	2018	Aggregating all the generation sites
Cao et al. [272]	2019	Aggregating all the generation sites
Siala and Mahfouz [281]	2019	Aggregating all the generation sites
Caglayan et al. [195]	2021	Clustering based on levelized cost of electricity (LCOE) of each generation site
Radu et al. [284]	2021	Running a simplified version of the ESOM to identify relevant generation sites
Frysztacki et al. [266]	2021	Aggregating all the generation sites within subregion groups
Klemm et al. [282]	2023	Weight-averaging roof orientations for PV and solar–thermal use
Phillips et al. [265]	2023	Averaging of technological time series within each square region
Pöstges and Weber [283]	2023	Simultaneous clustering of wind turbine sites and technologies using cost and revenue components (yield, resource-related, technology-specific, site-specific and grid-related values)

6.1.3. Trade-offs of spatial and technological aggregation

Straightforward geographical approaches often do not differentiate between spatial and technological clustering. Instead, they divide the area of interest into several regions and aggregate all generation sites of a technology type within each region into a single resource (see, e.g., [264,265]). In contrast, Frysztacki et al. [266] and Patil et al. [271] have analyzed the trade-off between spatial and technological aggregation. They both conclude that spatial aggregation underestimates the total annualized system costs by omitting some transmission bottlenecks, whereas technological aggregation overestimates them by averaging out the most profitable generation sites with high potential for capacity expansion. Simultaneous aggregation of nodes and generation sites can balance these cost effects but cannot fully address the system layout.

6.2. Temporal aggregation

The number of operational constraints and variables is proportional to the number of time steps, as shown in Eqs. (1a)–(1r), and typically exceeds the number of layout variables and constraints, such as capacities, by orders of magnitude. Most frameworks for energy system modeling use data from single years with hourly resolution due to the availability of datasets such as energy demands, prices, and net capacity factor time series [285]. However, this level of detail often remains computationally intractable for large-scale models. To address this issue, the number of time steps is reduced through a process known as temporal aggregation.

6.2.1. Temporal aggregation approaches

A straightforward method to reduce the temporal resolution is known as downsampling [285]. This involves merging every n time steps and representing them by their average value. This approach was applied, for example, by Pfenninger et al. [286], Stenzel et al. [287], Deane et al. [288], Beck et al. [289], and Yokoyama et al. [290].

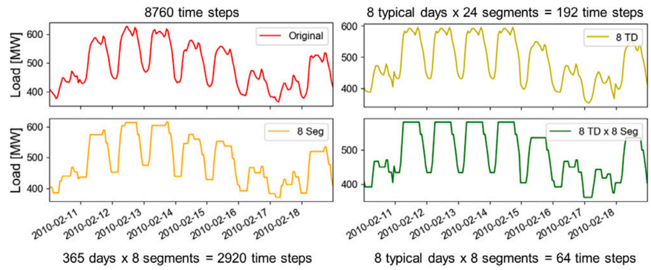

Fig. 12. Combination of typical days and irregular time step lengths adapted from Hoffmann et al. [312]. From the first to the second row, the number of inner-daily time steps is replaced by a smaller number of irregular segments, whereas the time series is replaced by a subset of typical days from the first to the second column. The effectiveness of the combination of methods is illustrated in the lower right graph.

Since high temporal resolution is not equally important for all time periods, using irregular time step lengths is a more effective way to reduce the temporal complexity of energy system models. Various methods in the literature address this by clustering [291–295], MILP optimizations [296], evolutionary algorithms [297], or other heuristics [298,299]. These methods aggregate adjacent time steps using a similarity measure, such as the difference between the adjacent time step values, based on the assumption that lower temporal resolution is sufficient for periods with smaller value gradients or variances. This technique is known as segmentation.

Another approach is to aggregate days, or sometimes weeks, to typical or representative days or weeks because most time series, such as solar capacity factors or demand time series, follow a daily or weekly cycle. A simple method uses a predefined ordering, e.g., by representing each month or season by a “mean day” or mean working days and weekend days. These methods are used in many established frameworks, including TIMES [73,74,300], THEA [301], LEAP [302], OSeMOSYS [303], and Syn-E-Sys [304], and are referred to as time slices.

Similar to the direct reduction of temporal resolution, typical days or weeks can also be determined irregularly based on the mutual similarity of periods within the original time series using clustering algorithms. This relatively new method was applied in the majority of recent publications addressing temporal aggregation techniques, such as [293,305–311].

6.2.2. Method combination and implementation

The irregular aggregation of typical periods using clustering algorithms typically results in smaller aggregation-induced errors than an aggregation solely based on a predefined ordering. This explains the growing popularity of clustering in recent years [285]. Additionally, this approach can be freely combined with a reduction in temporal resolution within the considered periods to further enhance the effectiveness of the aggregation [312], as illustrated in Fig. 12.

To incorporate a temporal aggregation approach with irregular time step lengths into a mathematical model or framework, all constraints involving a time step length Δt must be adapted to the irregular lengths of the respective time step. In the model in Section 2.2, this adjustment affects Eqs. (1l), (1p), (1q), and (1r).

In an aggregation to typical periods, each period in the aggregated model represents multiple periods in the original model, while the length of each time step remains unchanged. The number of original periods represented by a typical period must be weighted with a corresponding factor for time-dependent and cost-driving variables in the objective function. Therefore, Eq. (1a) is modified as follows:

$$\min \left(\sum_{c} \sum_{r} \left(c^{cap}_{c,r} x^{cap}_{c,r} + \sum_{p} w_p \sum_{\tilde{t}} c^{op}_{c,r,\tilde{t}} x^{op}_{c,r,\tilde{t}} \right) \right) \tag{39}$$

w_p represents the weighting assigned to the respective period p, and $\tilde{t}$ denotes the aggregated time steps within each period. Consequently, the total number of time steps considered in an aggregated model, involving typical periods, is $|p| \times |\tilde{t}|$. However, the aggregation to typical periods has a drawback: the temporal order between periods is lost because each typical period encompasses multiple periods of the original time series. As a result, a chronology of time steps is maintained only within each period, particularly affecting Eq. (1m). This means that the cycle length of the storage operation is generally restricted to that of the typical periods. Therefore, multiple publications have aimed to link state variables across periods using additional sets of auxiliary variables and constraints [77,306,313]. For the sake of brevity, these approaches are not discussed in detail within the scope of this study.

6.3. Investment pathway coupling

Decoupling the investment periods along the transformation pathway is another way to decrease model complexity. The most extreme simplification is to use a series of uncoupled investment periods, as depicted in the top row of Fig. 13 [27,314]. While this method enables parallelization, it lacks a smooth transition between investment periods because the optimal system design may vary significantly with each run, rendering it uncommon in the literature.

A more prevalent approach is the myopic foresight method, wherein the design solution of an investment period serves as the initial system for the subsequent investment period [27,314]. Consequently, a series of brownfield analyses is run consecutively. An extension of the myopic modeling approach is backcasting, where the target system is first solved and then used to define boundary conditions in the penultimate investment period before reaching the target system [315–317]. This process is repeated recursively until the first investment period is optimized. While the overall optimization involves one additional optimization run compared to the forward approach, it is less prone to delayed and thus disproportionately expensive investment decisions.

The rolling-horizon approach yields a smoother transition in the energy system but is more complex. In this method, optimization runs overlap each other [27,314], meaning that a single optimization spans at least two periods. After one optimization terminates, the design decisions are fixed for the first investment period covered by the respective optimization. Investment decisions in subsequent periods are re-evaluated in the next run, which starts one investment period later. As a result, this approach allows for less myopic decisions. The total number of optimization runs equals the number of investment periods minus the overlap between two consecutive optimization runs, as illustrated in the fourth and fifth rows of Fig. 13.

Models considering the entire investment horizon at once, depicted at the bottom of Fig. 13, are called perfect foresight models and are computationally the most expensive [27,314]. This approach is more complex than solving multiple smaller energy system models consecutively due to the growth of computational complexity with the model size, which is at least polynomial for LPs and exponential for MILPs.

Several studies in the literature have examined the impact of foresight modeling on results, as listed in Table 9. While perfect foresight always results in the most complex model runs, other modeling approaches are preferred for various reasons. Firstly, myopic foresight or rolling horizons always lead to investment inefficiencies, resulting in more expensive and suboptimal solutions. However, these solutions are often more realistic than perfect foresight solutions and can yield more robust cost projections or more conservative technological transformations. Secondly, only a subset of reviewed frameworks offers the option to optimize systems using perfect foresight. The others lack an investment period index, potentially due to an organic evolution of the respective program, and are thus limited to iterative, myopic approaches.

Table 9
Transformation pathway analyses in the literature.

Authors	Year	Model	Region	Myopic	Rolling Horizon	Perfect Foresight
Keppo and Strubegger [318]	2010	MESSAGE	Global	✗	✗	✗
Leibowicz et al. [319]	2013	MARKAL	US		✗	✗
Babrowski et al. [320]	2014	PERSEUS-NET	Germany	✗		✗
Poncelet et al. [321]	2016	LUSYM	Belgium		✗	✗
Fuso Nerini et al. [322]	2017	UK TIMES	UK		✗	✗
Gerbaulet et al. [323]	2019	dynELMOD	Europe	✗		✗
Löffler et al. [324]	2019	GENeSYS-MOD	Europe	✗		✗
Thomsen et al. [325]	2021	DISTRICT	district	✗		✗
Lambert et al. [326]	2021	N/A	Germany	✗	✗	✗

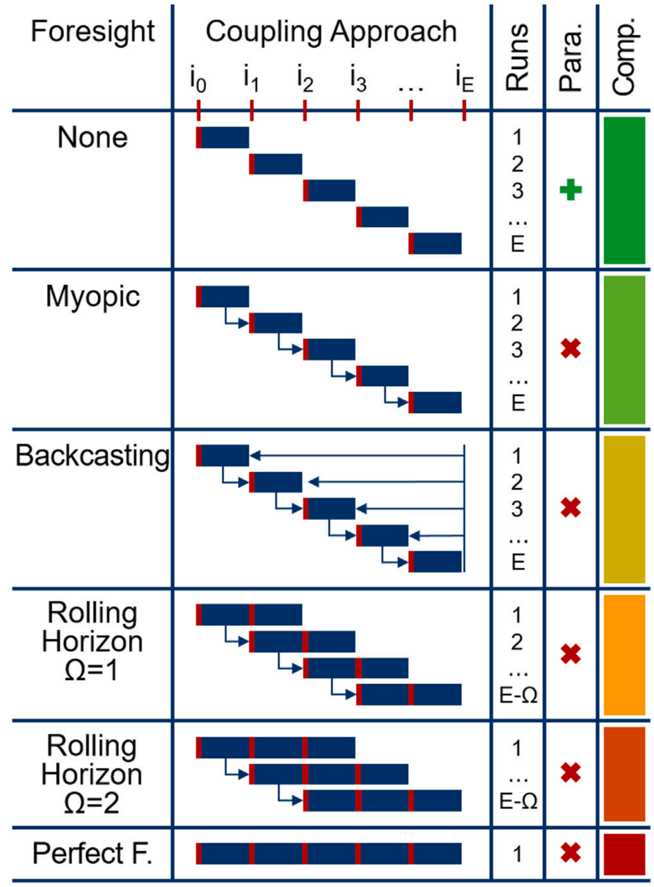

Fig. 13. Different foresight approaches for investment horizons adapted from [27,314]. With every row, the coupling between consecutive investment periods and likewise the computational complexity (Comp.) increase, whereas a parallelized solution for different target years (Para.) is not possible except for the first naive approach. E describes the total number of considered investment periods, and Ω describes the overlap of periods from one run to the next for the rolling horizon approach.

6.4. Trade-offs and computational tractability

Spatio-technological and temporal aggregation, along with the type of model coupling, represent only a subset of techniques to manage model complexity. As outlined in Section 3, additional component features can prolong model runtimes, whereas neglecting them can reduce computational complexity. Notably, high spatial, technological, or temporal model resolutions often result in disproportionately longer runtimes compared to the diminishing improvement in model accuracy. Hence, some researchers [24,282,327] have conducted sensitivity analyses by varying the resolution of multiple model aspects. Their consensus is that the efficacy of different simplification methods likely depends on the specific model. Moreover, model simplifications should be employed cautiously, with multiple methods tested to determine the most favorable balance between speedup and deviation from the original model. Considering that many current frameworks still lack adequate flexibility concerning the level of detail (see Martínez-Gordón et al. [267] in the case of spatial resolution), this observation presents a challenging demand for future framework development.

6.5. Parallelization

If accuracy losses due to reduced model resolution are unacceptable and high-performance infrastructure is available, energy system models can also be solved through parallelization. This is accomplished using decomposition methods that exploit the block-diagonal structure of the model, as illustrated in the two left-hand graphs in Fig. 14.

The block structure can be achieved by sorting the variables and constraints by one of the model dimensions, such as time steps or region indices. This approach leverages the sparsity of most model matrices, as most operational variables for a particular time step, region, scenario, commodity, and component only appear in the constraints associated with that specific time step, region, scenario, commodity, and component [328]. Depending on the dimension along which the model is decomposed, this method is referred to as decomposition with respect to time, space, or other dimensions [27,328]. The most commonly applied decomposition methods are listed in Table 10.

Typically, certain variables and constraints span multiple indices within the chosen dimension, known as complicating variables or constraints [328,329]. For instance, the capacity variable of a component appears in the capacity constraint (1l) of every time step, whereas the storage constraint in Eq. (1h) connects adjacent time steps. In temporal decomposition, capacity variables are therefore complicating variables, and storage constraints are complicating constraints.

With proper sorting, coupled systems can be restructured to solely include either complicating constraints at the top of the block-diagonal matrix in Fig. 14a or complicating variables on the left side of the block-diagonal matrix in Fig. 14b. For example, complicating variables can be converted into complicating constraints by defining a variable for each index and ensuring their equality through an additional set of constraints.

The mathematical solution algorithm depends on the shape of the matrix. For matrices with complicating constraints, the Dantzig–Wolfe decomposition is used. For matrices with complicating variables, Benders or Lagrangian decomposition are used. There are many additional algorithms, such as those solving models with both complicating variables and constraints in a nested approach or by reformulation using Karush–Kuhn–Tucker conditions and a parallel interior point algorithm [330]. However, Dantzig–Wolfe, Benders, and Lagrangian decomposition are the most commonly used, as shown in Table 10.

All three algorithms are iterative, as illustrated in Figs. 14c and 14d. In each iteration, a master problem defines cost coefficients for

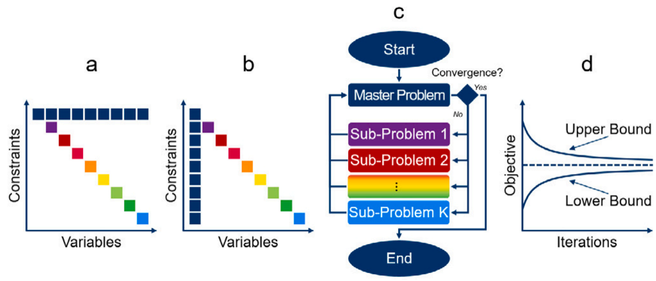

Fig. 14. (a): block-diagonal matrix with complicating constraints for Dantzig–Wolfe or Lagrangian decomposition; (b): block-diagonal matrix with complicating variables for Benders decomposition; (c): process of solving a decomposed model by iteratively solving the master problem and the sub-problems; (d): upper and lower bounds to the original model that are obtained in every iteration and successively approach each other until convergence is reached.

the sub-problems. The sub-problems consist of the problems of the diagonal blocks with modified objective functions. After solving the sub-problems in parallel, the solutions can either be infeasible (due to varying values for the same complicating variables in Benders decomposition or violated complicating constraints in Dantzig–Wolfe and Lagrangian decomposition), feasible and suboptimal, or optimal. Depending on the case, the master problem is adjusted until an optimality criterion is met. In each iteration, Benders and Dantzig–Wolfe decomposition provide both an upper and a lower bound to the original optimal objective function value, enabling early termination if a certain optimality gap is undercut. Lagrangian decomposition, however, provides only a lower bound.

7. Limitations of optimization frameworks

While we have shown that optimization-based frameworks for energy system modeling cover a wide set of applications, scales, and scopes, the modeling approach still has limitations with respect to certain aspects observed in real energy systems. In the following, we will divide out non-exhaustive discussion into technical, financial, environmental, and social aspects in the Sections 7.1, 7.2, 7.3, and 7.4, respectively.

7.1. Technical aspects

In general, technical aspects are well-addressed by optimization frameworks. Still, optimization never replaced simulation approaches in technical modeling, given the existence of popular hybrid or simulation-based energy system frameworks such as HOMER [365]. First, optimization models suffer from an exponential increase in computational complexity with model size, which naturally imposes limits on real-time applications or those with an extremely high level of detail, such as models with sub-hourly resolution [366]. Simulation, in contrast, is able to quickly and accurately compare the performance of alternative designs with options for sensitivity analyses but usually requires more or less predefined candidate systems to test their performance [367].

The perfect foresight paradigm of optimization frameworks can lead to additional drawbacks. On the one hand, real systems face uncertain future demand, whereas optimization frameworks have perfect information on the operational time horizon. Thus, the operational optimization of real systems relies on physical or non-physical foresight models and model-predictive control [368], and simulation models can be heuristically trained to capture real system behavior more accurately [369]. Lastly, despite the superiority of optimization-based operations over rule-based ones in systems such as microgrids, rule-based energy management systems are still the more widely used technology [370] due to their simplicity and lower data requirements. Optimization frameworks likewise fail to consider these historically developed, rule-based system limitations.

Table 10
Decomposition in the Literature.

Authors	Year	Dantzig–Wolfe	Benders	Lagrange	Schur Complement	Decomposition Dimension
Virmani et al. [331]	1989			✗		technology
Martínez-Crespo et al. [332]	2007		✗			time
Roh et al. [333]	2007		✗	✗		time
Khodaei et al. [334]	2010		✗			time
Flores-Quiroz et al. [335]	2016	✗				time
Wang et al. [336]	2016		✗	✗		space
Aghaei et al. [337]	2020		✗			time
Long et al. [338]	2020		✗			technology
Mahroo-Bakhtiari et al. [339]	2020	✗				space
Wakui et al. [340]	2020	✗				space
Wei et al. [341]	2020	✗				space
Asl et al. [342]	2021		✗			space
Hu et al. [343]	2021	✗				space
Kou et al. [344]	2021		✗			time
Moradi-Sepahvand and Amraee [345]	2021		✗			space
Shahbazi et al. [346]	2021		✗			time
Wang et al. [347]	2021		✗			time
Bakhtiari et al. [348]	2022		✗			space
Gan et al. [349]	2022		✗			time
Gan et al. [349]	2022		✗			space
Haghighi et al. [350]	2022		✗			space
Javadi et al. [351]	2022		✗			time
Li et al. [352]	2022		✗			time
Li et al. [353]	2022		✗			space
Mehrtash et al. [354]	2022				✗	scenario
Middelhauve et al. [355]	2022	✗				space
Rehfeldt et al. [330]	2022				✗	time
Wu et al. [356]	2023			✗		space
Zhang et al. [357]	2022		✗			time
Zhao et al. [358]	2022		✗			technology
Constante-Flores et al. [359]	2023		✗			time
Du et al. [360]	2023		✗			time
Paterakis [361]	2023		✗			time

(continued on next page)

Table 10 (*continued*).

Authors	Year	Dantzig–Wolfe	Benders	Lagrange	Schur Complement	Decomposition Dimension
dos Santos et al. [362]	2023		✗			time
Wirtz et al. [363]	2023	✗				space
Zhao et al. [364]	2023			✗		space

7.2. Financial aspects

The modeling of financial aspects has experienced a remarkable upswing over the last two decades, from pure investment decision support over cost minimization to dispatch optimization and the prediction of market-clearing prices. However, numerous aspects present in current energy markets are still not considered in modeling frameworks. According to different authors [17,197], the neglect of multiple stakeholders and trading options between them are among the most obvious. In the following, and without the claim of comprehensiveness, we provide a brief insight into two well-studied approaches to account for multiple stakeholders in energy systems, agent-based modeling and bi-level programming, which have not yet been integrated into the reviewed optimization frameworks.

7.2.1. Agent-based modeling

Agent-based models (ABMs) consist of autonomous decision-making entities [371] and are one option to account for the different stakeholder roles within modern energy systems, among which are energy consumers, providers and suppliers, distribution systems, transmission grid operators, and regulators [45]. Agent-based models are generally embedded into soft-coupled frameworks with interacting sub-problems, which can be based on both optimization and simulation. For example, Scheller et al. [372] present an agent-based model composed of a decision model for commercial actors, a bottom-up energy system optimization, and a sub-model to account for market principles to model municipal energy systems. Similar two-layer architectures consisting of energy system optimizations at the upper level and retail market models at the lower level have repeatedly been proposed in the literature (see, e.g., [373–375]).

7.2.2. Bi-level programming

Bi-level programming offers a way to integrate multiple agents into models with a single hard-coupled optimization, which uses the optimization problem of one or multiple agents as side constraints for another one. The nested optimization problem can then be transformed into an MILP using Karush–Kuhn–Tucker (KKT) conditions [376,377] for optimality of the sub-problem and an integer–linear formulation of complementary slackness conditions according to Fortuny-Amat and McCarl [378]. For example, this approach can be used to model the interaction between the price-setters of energy commodities and price-takers searching for the cheapest alternative, also referred to as Stackelberg pricing games [379].

Table 11 reveals that bi-level optimization has been applied to various energy sectors and scopes, often with investment decisions at the upper and market-clearing conditions at the lower levels. The most frequently employed approach is above-mentioned reformulation by Karush–Kuhn–Tucker conditions to so-called mathematical programs with equilibrium constraints (MPECs) [380–384]. However, due to the massive computational complexity of these models, some authors have avoided direct reformulation and relied on heuristic solvers such as teaching–learning-based optimizations (TLBOs) [385], non-dominated sorted genetic algorithms (NSGAs) [386,387], or a discretization of the model instead [388]. Apart from that, the simultaneous consideration of multiple lower-level problems as performed by Hoffmann et al. [388] has remained an exception due to computational limitations.

Table 11
Bi-level optimization in the literature.

Authors	Year	Upper Level	Lower Level	Method
Jenabi et al. [380]	2013	Investment in transmission by transmission grid operation	Market clearing	KKT (MPEC)
Feijoo and Das [381]	2015	Microgrid operation	Linear electricity dispatch	MPEC
Liu and Li [386]	2015	Electric dispatch	Load-control	NSGA
Valinejad and Barforoushi [382]	2015	Installments of new generation units	Market clearing	MPEC
Hu et al. [385]	2016	Fuel-cost and emission	Interval reduction for wind output	TLBO
Ju et al. [389]	2016	Maximize income of virtual power plant	Minimize operation cost of the day-ahead schedule	Models serially solved once
Škugor and Deur [387]	2016	Fleet-charging management	dynamic programming	NSGA
Li et al. [383]	2017	Electricity dispatch with wind and coal	Natural gas model	MPEC
Li et al. [384]	2019	Electricity and heating market	Market clearing and contracting	MPEC
Hoffmann et al. [388]	2023	District energy supplier	Residential prosumers	Discrete price constellations

Noteworthy, none of the reviewed frameworks in Table 12 incorporate KKT conditions given their significant mathematical complexity. Therefore, the reviewed literature in Table 11 used own models instead of frameworks, except for Hoffmann et al. [388] who discretized a bi-level program using multiple model instances of the ETHOS.FINE framework [69]. However, given the ongoing advancements of MILP solvers and the ubiquitous trend towards decentralized energy system models with many different providers and prosumers, future frameworks should strive to depict the different and, at times, conflicting objectives of different stakeholders.

7.3. Environmental aspects

In recent years, frameworks for energy system modeling have increasingly been used to account for ecological aspects such as CO_2-emissions [390], recycling [391], and life-cycle assessment [392,393]. Among others, the approaches involved modeling CO_2 and other material flows as commodities or integrating end-of-life emissions into the optimization.

However, energy systems interact with the environment on many more levels than by means of primary energy consumption, carbon emissions, and product life cycles alone. Renewable energy systems have a direct impact on land occupation [36] and the scenicness of the environment [189,394–396] with eventual second-order effects on assets such as real estate prices that are hard to quantify. Furthermore, large-scale capacity expansion of renewables such as wind turbines can cause feedback effects on micro-climates such as wake effects [192], thereby decreasing the anticipated profitability of planned large-scale wind parks.

Lastly, energy generation, whether fossil or renewable, can have direct and indirect impacts on biodiversity. Direct impacts can be observed, for instance, in the case of flooding due to hydroelectricity projects [397], whereas indirect effects involve increased mining activities [398] to secure the resource supply for new technologies. These local effects are difficult to quantify financially, which is why their inclusion in frameworks for energy system modeling has been widely neglected to date.

7.4. Social aspects

Social aspects such as fairness, social acceptance, behavioral adaptation, and political uncertainty are currently not sufficiently addressed by optimization-based modeling frameworks.

The transition of the energy sector has fundamental impacts on generation, distribution, and consumption concepts, and thereby price levels and volatility. Affordability and the empowerment of all social classes to participate in this transformation process are thus crucial to achieving both acceptance [399,400] and climate neutrality. This includes avoiding additional burdens on the poor [400], as quantified by the Gini-coefficient [401,402], and disproportionate benefits for some from feed-in tariffs [403], as can be quantified by Jain's fairness index [404].

Social acceptance is crucial to avoid a "not in my backyard" (NIMBY) mindset and local opposition [36,396,405]. For that, participation schemes and indirect benefits such as job creation [36] can be appropriate measures if efficiently offered and communicated.

Another aspect currently not covered in frameworks for energy system optimization are behavioral aspects that go beyond plain demand response modeling. Behavioral patterns are crucial for many aspects, such as residential electricity consumption [406,407] and mobility [408,409], which are partially non-financially motivated as well as stakeholder-dependent. Hence, they constitute another challenging modeling task to be considered endogenously in optimization models.

Apart from that, legal regulations and subsidization schemes have occasionally been considered in energy system models, e.g., for public or residential buildings [171,199,206,207,410]. However, given the internationally diverse laws and regulations, standardized frameworks offer limited options for modeling legal constraints and opportunities beyond simple emission constraints or remuneration schemes, such as CAPEX subsidies or feed-in tariffs. Finally, geopolitical uncertainties such as the Russo–Ukrainian conflict are difficult to model but have inevitable implications on middle- and long-term energy supply pathways [411].

7.5. AI and risk of substitution

Lastly, the omnipresent ascent of artificial intelligence (AI) will likely also challenge computationally expensive bottom-up energy system modeling in general and frameworks in particular [412–415]. However, models based on machine learning, deep learning, and generative AI, including various forms of neural networks, are black-box models, which could make the identification of key drivers for a cost-efficient energy transition more opaque. Interestingly, a counter-approach using surrogate models can also be found in the literature. Surrogate models approximate complex black-box models with simpler white-box ones [416–419], often using data-driven approaches and a subset of data points derived from simulations. Given the continuously increasing complexity of energy systems, they may become an attractive alternative if abundant computational capacities are not available. In the future, energy system modelers will more than ever be confronted with the question of how much complexity is needed to find an answer to their problem at hand and what share of the solution process they need to understand or be able to reproduce results.

8. Discussion

Our review has shown that the underlying concept of optimization-based bottom-up frameworks for energy system modeling has stayed constant throughout the last 50 years. The vast majority of models and frameworks rely on the following aspects:

1. Linear or mixed-integer linear programming
2. A component logic
3. Energy balances (the first law of thermodynamics)

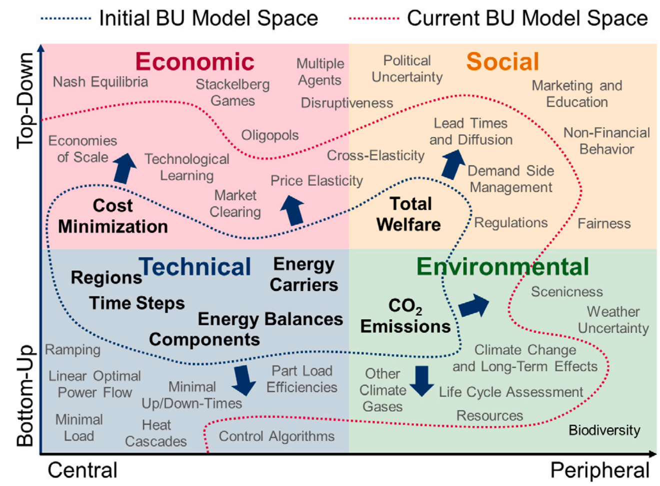

Fig. 15. Initial and current capabilities of bottom-up energy system optimization models. The blue dashed line encloses the nucleus optimization-based bottom-up of energy system models, whereas the red line encircles all features that are covered by many current models. The white terms reflect the features discussed in this work.

4. Cost minimization or profit maximization
5. A central-planner perspective

Against the backdrop of the number of bottom-up modeling frameworks that have grown from 25 between 1970 and 2014 to 63 in 2024, this implies two things: On the one hand, the underlying rationale of cost minimization while guaranteeing energy supply persists as the core task of energy system models. On the other hand, open-source framework development incorporates a significant share of redundancy. Likewise, the basic logic of reviews of bottom-up energy system models has remained unchanged. Most of them use a categorization of models and frameworks, or model features and system aspects. Hence, most reviews are status updates on current modeling trends but do not equip modelers with the knowledge to set up their own basic models. Our meta review addresses this issue and systematically introduces all basic as well as various extended model features and explains the respective mathematical formulations, sketching a picture of what is currently possible and how further system aspects could be incorporated or improved in future research.

In this context, our study demonstrates that many model extensions designed to capture economic, technological, or physical phenomena—such as economies of scale, technological learning, minimum up- or down-times, AC power flow, or energy flows in heat networks—introduce non-linearities. These non-linearities are frequently approximated using mixed-integer linear programming. The increased level of detail, however, comes at the cost of significantly higher computational complexity, often restricting model execution to high-performance computing environments, thereby limiting accessibility to a smaller number of research institutions. To address this challenge, our review presents methods for managing complexity through aggregation, decoupling, or parallelization. Aggregation reduces complexity by simplifying less critical parts of the model, for example, by merging non-critical time steps, regions, or technologies within the options portfolio. Decoupling, on the other hand, separates model components to solve them sequentially. Unlike these heuristic approaches, parallelization via decomposition is an exact method that allows models to be solved on distributed smaller resources, though it does not reduce the total cumulative runtime. These findings underscore that the trade-off between model detail and computational complexity remains a critical consideration.

Fig. 15 depicts the traditional core features of bottom-up energy system models with a blue line and the capabilities of many current models and frameworks with a red line. Starting from a mainly technical focus, recent models increasingly cover other system aspects, such as economic, socio-political, and environmental ones. We have addressed most of the model features listed in Fig. 15 by either presenting the mathematical formulations currently covered by energy system models (within the red dashed line) or by critically discussing the features not yet addressed by them.

With respect to economic aspects, frameworks for energy system modeling are currently not only capable of considering costs as a static attribute of components but can also capture complex laws of economics, such as economies of scale, technological learning, and demand elasticity. A remaining weakness of models with respect to these aspects is their prevalent central planner perspective, which usually underestimates the costs of multi-agent equilibria with deviating selfish behavior by stakeholders. The socio-political dimension has become part of many models, as regulatory schemes and flexibility options have become an important aspect of current systems with intermittent feed-in from renewables. However, non-financial aspects in particular of the societal interaction with energy systems, such as the impact of behavioral changes, also by means of education, and the aspect of fairness of energy affordability and distribution, have remained a widely neglected field for modern energy system modeling frameworks. Finally, the environmental aspects of energy systems have become a center of attention due to emissions and resource consumption, and they are currently already considered by the vast majority of models. In contrast, the non-technical aspects of the systems' interaction with the environment, among which are long-term climate uncertainty, the visual impact of modern energy sources on the landscape (scenicness), and the impact on biodiversity and wildlife habitats, are neglected by contemporal frameworks.

Overall, the fact that all the aspects named in this work have been studied in the literature but only a subset of them have been integrated into bottom-up energy modeling frameworks illustrates that mixed-integer linear programming and a modular framework logic impose limits on model adaptability and versatility. Given the steady evolution of bottom-up energy system models and the growing complexity of energy procurement, conversion, and consumption in the setting of a growing global population, destabilized climate conditions, intensifying resource scarcity, and a society that vacillates between unconditional support and counter-factual resentment, future modeling frameworks should become multi-objective, multi-agent, and partially non-financial.

9. Conclusions

Our study provides a comprehensive review of optimization-based energy system modeling frameworks, with a focus on their mathematical structures, particularly mixed-integer linear formulations. By analyzing 63 different frameworks and conducting a meta-review of 68 existing literature reviews, our study offers a dual perspective that bridges the gap between practical application and theoretical formulation in energy system optimization.

One of the primary outcomes of our work is that the basic concept of network-based energy flow optimization has remained consistent since the 1970s, despite the rapid propagation of new frameworks, particularly over the last decade. The significant growth in open-source frameworks, particularly in Europe, reflects the increasing demand for flexible, transparent, and easily customizable tools for energy system modeling. However, this growth also highlights potential challenges related to redundancy and fragmentation in the field, raising the need for improved documentation and collaboration among developers.

Despite the technological advancements in modeling tools, the underlying mathematical approaches have largely remained consistent, relying heavily on mixed-integer linear programming. This consistency underscores the importance of understanding these mathematical foundations, particularly for researchers and developers who seek to build or extend frameworks for specific applications. Thereby, ensuring the solvability of large-scale energy system models using complexity-handling techniques, such as temporal aggregation, spatio-technological aggregation, and parallelization, remains a critical cornerstone in the advancement of modeling techniques.

In addition to providing a detailed review, our study contributes to the field by offering a standardized set of mathematical formulations that can serve as a foundational reference for energy system modelers. These formulations aim to facilitate the development of new frameworks and enhance the transparency and comprehensibility of existing ones.

In summary, our study not only synthesizes the state of the art in energy system modeling frameworks but also provides practical tools and insights for advancing the field. By focusing on the mathematical underpinnings of these frameworks, we bridge a critical gap in the literature and offer valuable contributions for both academic researchers and practitioners engaged in the energy transition.

CRediT authorship contribution statement

Maximilian Hoffmann: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Bruno U. Schyska:** Writing – review & editing, Writing – original draft, Validation, Investigation, Formal analysis. **Julian Bartels:** Writing – review & editing, Writing – original draft, Validation, Investigation, Formal analysis. **Tristan Pelser:** Writing – original draft, Validation, Investigation, Formal analysis. **Johannes Behrens:** Writing – original draft, Validation, Investigation, Formal analysis. **Manuel Wetzel:** Writing – original draft, Validation, Investigation, Formal analysis. **Hans Christian Gils:** Writing – review & editing, Writing – original draft, Validation, Investigation, Formal analysis. **Chuen-Fung Tang:** Writing – original draft, Validation, Investigation, Formal analysis. **Marius Tillmanns:** Writing – original draft, Validation, Investigation, Formal analysis. **Jan Stock:** Writing – original draft, Validation, Investigation, Formal analysis. **André Xhonneux:** Supervision. **Leander Kotzur:** Methodology, Conceptualization. **Aaron Praktiknjo:** Supervision. **Thomas Vogt:** Supervision, Funding acquisition. **Patrick Jochem:** Writing – review & editing, Writing – original draft, Validation, Supervision, Investigation, Funding acquisition, Formal analysis. **Jochen Linßen:** Supervision, Funding acquisition, Conceptualization. **Jann M. Weinand:** Writing – review & editing, Writing – original draft, Validation, Supervision, Project administration, Investigation, Funding acquisition, Formal analysis. **Detlef Stolten:** Supervision, Project administration, Funding acquisition.

Declaration of competing interest

The manuscript has not been published and is not under consideration for publication elsewhere and we have no conflicts of interest to disclose.

Data availability

Data will be made available on request.

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Appendix A. List of reviewed frameworks

See Table 12.

Appendix B. MODEX-reviews

See Table 13.

Table 12
Energy system optimization frameworks according to 'Open Energy Platform' [2] and 'Open Energy Modelling Initiative' [3].

Acronym	Year	Country	Full Name	Mentioned in Review	Scope	Type	Language	Translator	Solver
AnyMOD [420]	2020	Germany	None	None	Large-scale multiple periods GEP for North America	GEP	Julia	JuMP	Gurobi
aristopy [421,422]	2021	Germany	None	None	Flexible scale and flexible periods	GEP	Python	Pyomo	Multiple
Backbone [82]	2019	Finland	None	[58]	Flexible scale flexible periods	Both	GAMS	GAMS	Multiple
Balmorel [423]	2001	Denmark	None	[1,13,15,18,21,25,29,30,40,44,45,47,50,51,53,54,56,58,60,424–426]	Large-scale flexible periods UC for multiple regions	Both	GAMS	GAMS	CPLEX
BESOM [427]	1974	USA	Brookhaven Energy System Optimization Model	[10,27,33,47,50]	Small-scale single period for US	Both	N/A	N/A	N/A
Breakthrough Energy Model [428,429]	2020	USA	None	None	Large-scale multiple periods production costs model for US	Dispatch/ UC	Julia	JuMP	Gurobi
Calliope [81]	2013	Great Britain	None	[1,27,30,44,47,49,51,53,60]	Flexible scale multiple periods UC for Europe and UK	Dispatch/ UC	Python	Pyomo	Gurobi
CapacityExpansion [430]	2020	USA	None	None	Flexible scale multiple periods GEP for California and Germany	GEP	Julia	JuMP	Gurobi
CAPOW [431,432]	2020	USA	California and West Coast Power System model	None	Small-scale single year market operation for California	Dispatch/ UC	Python	Pyomo	CPLEX
CLOVER [433]	2023	Great Britain	Continuous Lifetime Optimisation of Variable Electricity Resources	None	Flexible scale flexible periods GEP for multiple regions	GEP	Python	Python	None
DER-CAM [434]	2004	USA	Distributed Energy Resources Customer Adoption Model	[1,12,14,25,31,35,36,39,40,42,45,47,51,56,60,435]	Small-scale single periods UC for global microgrids	Dispatch/ UC	GAMS	GAMS	Multiple
DESOD [436]	2016	Italy	Distributed Energy System Optimal Design	[27]	Small-scale flexible periods GEP for residential and commercial districts	GEP	C#	C#	Multiple
DIETER [437]	2014	Germany	Dispatch and Investment Evaluation Tool with Endogenous Renewables	[1,18,25,29,30,44,47,51,56,59,60,163,438,439]	Large-scale single year GEP for Europe	GEP	Python	GAMS	CPLEX
Dispa-SET [440–442]	2015	Belgium	None	[25,29,30,51,60]	Flexible scale single year UC for Europe	Dispatch/ UC	Python	GAMS	CPLEX
EFOM [443]	1982	Belgium	Energy Flow Optimization Model	[10,13,20,27,28,32,33,58]					
eGo [444]	2017	Germany	Electricity grid optimization	None	Small-scale single year UC for Germany	Dispatch/ UC	Python	Pyomo	Gurobi
ELMOD [445]	2005	Germany	Electricity Model	[18,20,25,51,58,446–448]	Large-scale multiple periods UC for Europe	Dispatch/ UC	Python	GAMS	CPLEX
EMMA [449]	2013	Germany	The European Electricity Market Model	[1,25,30,44,47,51,59,60,450,451]	Large-scale single-year GEP	GEP	GAMS	GAMS	CPLEX
EnergyPLAN [452–454]	1999	Denmark	None	[1,12–14,21,25,28,29,31,35,37,39–45,47,49–56,58–60,435]	Mid-scale single year power simulation	Dispatch/ UC	Delphi, Pascal	Delphi, Pascal	Multiple
EnergyRt [455]	2022	Russia	Energy systems modeling toolbox in R	[51,60]	Large-scale multiple periods GEP for US	GEP	R	Multiple	Multiple
EnergyScope [456]	2014	Switzerland	None	[58,60]	Small-scale single year UC for Belgium	Dispatch/ UC	AMPL	AMPL	CPLEX
ESO-X [89]	2017	Great Britain	Electricity Systems Optimisation	None	Small-scale multiple periods GEP for Great Britain	GEP	Excel	GAMS	CPLEX
ESONE [457]	2020	Great Britain		None	Mid-scale multiple periods	Both	GAMS	GAMS	CPLEX
ETHOS.FINE [68,69]	2016	Germany	Framework for Integrated Energy System Assessment	[27,54]	Flexible scale flexible periods UC	Both	Python	Pyomo	Multiple
EU_REGEN [458]	2019	Germany	EU Regional Economy, Greenhouse Gas and Energy	None	Large-scale single year UC for Europe	Dispatch/ UC	GAMS	GAMS	CPLEX
ficus [459]	2017	Germany	VICUS for factories	[30,44,47,51,53,58]	Small-scale flexible periods GEP and UC for factories	GEP, Dispatch/ UC	Python	Pyomo	Multiple

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Table 12 (*continued*).

Acronym	Year	Country	Full Name	Mentioned in Review	Scope	Type	Language	Translator	Solver
FOCUS	2023	Germany	Framework for Optimizing sector-Coupled Urban energy Systems	[18]	Residential to city-scale GEP	GEP	Python	Pyomo	Multiple
FlexiGIS [460]	2018	Germany	Flexibilisation in Geographic Information Systems	None	Small-scale single year UC for cities	Dispatch/ UC	Python	Oemof	CBC
GBOML [461]	2022	Belgium	Graph-Based Optimization Modeling Language	None	Flexible scale single year GEP	GEP	Python	Python	Multiple
GENeSYS-MOD [462,463]	2017	Germany	Global Energy System Model	[18,29,30,53,60,424–426]	Flexible scale single year UC	Dispatch/ UC	Excel, GAMS	GAMS	CPLEX
GenX [464]	2017	USA	None	None	Flexible scale single year UC	Both	Julia	JuMP	CPLEX, Gurobi
GridCal [465]	2016	Spain	Grid Calculator	[60]	Flexible scale flexible periods UC	Dispatch/ UC	Python	None	Multiple
GRIMSEL-FLEX [466–470]	2019	Switzerland	General Integrated Modeling environment for the Supply of Electricity and Low-temperature heat	None	Small-scale single year UC for Switzerland	Dispatch/ UC	Python	Pyomo	CPLEX
highRES [230,471]	2018	Great Britain	The high spatial and temporal Resolution Electricity System	None	Large-scale flexible periods	Both	Python	GAMS	CPLEX
IKARUS [472,473]	1994	Germany	Instrumente für Klimagas-Reduktionsstrategien	[14,15,27,47,50,52,55,59]	Mid-scale multiple periods	Both	Delphi, Pascal	Delphi, Pascal	Multiple
LEAP [474]	1980	Sweden	Long-range Energy Alternatives Planning	[1,20,27,28,34,37,41,44,47,50,52,55–59]	Flexible scale large periods GEP	GEP	GUI	GUI	Multiple
Lemlab [475]	2021	Germany	Local energy market laboratory	None	Small-scale real-time UC	Dispatch/ UC	Python	Pyomo	Multiple
MARKAL [476]	1978	USA	Market and Allocation	[14,17,20,21,27–29,34,36,37,42,44,47,49,50,52,53,55,57–59,61,425]	Flexible scale large periods	Both	GAMS	GAMS	Multiple
MATPOWER [477]	1997	USA	None	None	Flexible scale flexible periods UC	Dispatch/ UC	Matlab	Matlab	Multiple
Medea [478]	2019	Austria	None	None	Large-scale single year UC for Germany and Austria	Dispatch/ UC	Python	GAMS	CPLEX, Gurobi
MESSAGEix [479,480]	1981	Austria	Model for Energy Supply Strategy Alternatives and their General Environmental Impact	[29,60]	Large-scale flexible periods UC	Both	Python	GAMS	Multiple
MicroGridsPy [481–484]	2016	Belgium		None	Small-scale flexible periods	Both	Python	Pyomo	Multiple
NEMO (SEI) [485,486]	2018	Nemo	Next Energy Modeling system for Optimization	[1,30,44,47]	Flexible scale flexible periods	Both	Julia	Julia	Multiple
oemof-solph [80]	2017	Germany	Open Energy Modeling Framework	[29,30,426]	Flexible scale flexible periods	Both	Python	Pyomo	Multiple
OMEGAlpes [487–489]	2018	France	Generation of Optimization Models As Linear Programming for Energy Systems	[58]	Small-scale single year UC for districts	Dispatch/ UC	Python	PuLP	Multiple
OpenTEPES [490]	2021	Spain	Open Generation, Storage, and Transmission Operation and Expansion Planning Model with RES and ESS	None	Large-scale multiple peridos GEP for Europe	GEP	Python	Pyomo	Gurobi
OSeMOSYS [70]	2008	Sweden	Open Source Energy Modeling System	[1,15,17,28–30,44,47,49,50,52–54,56–60]	Large-scale large periods GEP	GEP	Python, GNU MathProg	Pyomo, GNU MathProg	Multiple
Pandapower [491]	2016	Germany	None	[18,30,44,289]	Small-scale multiple periods UC	Dispatch/ UC	Python	Python	PyPOWER
PERSEUS [492]	2008	Germany	Program-package for Emission Reduction Strategies in Energy	[18,29,47,59,306,446–448]	Mid-scale large periods UC	Both	GAMS	GAMS	Multiple
POMATO [493–496]	2019	Germany	POwer MArket TOol	None	Large-scale single year UC	Dispatch/ UC	Python, Julia	JuMP	CLP
PowerSimulations.jl [497,498]	2017	USA	None	None	Large-scale flexible periods UC	Dispatch/ UC	Julia	JuMP	Multiple
PowNet [499]	2019	Singapore	None	None	Large-scale single year UC for south-east Asia	Dispatch/ UC	Python	Pyomo	CPLEX, Gurobi

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Table 12 (*continued*).

Acronym	Year	Country	Full Name	Mentioned in Review	Scope	Type	Language	Translator	Solver
PyPSA [182]	2015	Germany	Python for Power System Analysis	[1,15,27,28,30,44,53, 59,60,446,448]	Flexible scale flexible periods UC for multiple regions	Both	Python	Python	Multiple
REMIND [390,500]	2006	Germany	REgional Model of INvestments and Development	[1,28,44,47,50,60]	Large-scale multiple periods GEP	GEP	GAMS	GAMS	Multiple
REMix [71]	2012	Germany	Renewable Energy Mix for sustainable electricity supply	[18,47,52,53,163,438, 439]	Large-scale flexible periods UC	Both	Python	GAMS	Multiple
ReEDS [501]	2007	USA	Renewable Energy integration and OPTimization platform	[1,60]	Large-scale flexible periods UC and GEP for north America	Dispatch/ UC and GEP	Python, R	GAMS	CPLEX
REopt [502,503]	2014	USA	Renewable Energy integration and OPTimization platform	None	Small-scale flexible periods UC	Dispatch/ UC	Python, Julia	JuMP	Multiple
SecMOD [392]	2020	Germany	None	None	Flexible scale flexible periods incorporating LCA	GEP	Python	Pyomo	CPLEX, Gurobi
SpineOpt [504]	2017	Belgium	None	None	Flexible scale flexible periods	Both	Julia	JuMP	Multiple
Switch [30,505–515]	2012	USA	Solar, Wind, conventional and Hydroelectric generation, and transmission	None	Large-scale flexible periods UC for multiple regions	Dispatch/ UC	Python	Pyomo	Multiple
Temoa [516]	2010	USA	Tools for Energy Model Optimization and Analysis	[1,17,29,44,47,50,53, 58]	Large-scale flexible periods GEP for multiple regions	GEP	Python	Pyomo	Multiple
TIMES [4,5,72–74]	1998	International	The Integrated MARKAL-EFOM System	[1,15,17,20,27–29,42,44,47,49,50,52, 53,55,58–60,446]	Flexible scale flexible periods	Both	GAMS	GAMS	Multiple
URBS [517–521]	2003	Germany	None	[1,18,27,30,44,47,56, 58,59,424–426]	Flexible scale flexible periods	Both	Python	Pyomo	Multiple

Table 13
Categorization of MODEX-based reviews.

Reference	Tools reviewed	Scope: Details	Focus		Type of models	Frame-works incl.	Description
			Models	Methodology			
				Approach #5: MODEX model comparison			
a. Scope: Geographically specific							
Raventós et al. [446], 2022	8	Municipal	✓	✓	BU, opt	✓	Workflows for disaggregation of time series in ESMs
Beck et al. [522], 2021	4	Germany	✓	✓	opt, sim	✓	Use of power grid-focused scenarios for the comparison of optimization models
van Ouwerkerk et al. [424], 2022	5	Germany	✓	✓	BU	✓	CO2 emission budgets applied to 2030 base scenario
Candas et al. [425], 2022	5	Germany	✗	✓	opt	✓	Mathematical implementations with results for 2050 CO2 budget
Hobbie et al. [447], 2022	8	Europe	✓	✓	sim, opt	✓	Congestion management in high-voltage grids
Syranidou et al. [448], 2022	8	Europe	✓	✓	TD, BU, opt, sim	✓	Quantitative and qualitative comparison for grid and power systems
van Ouwerkerk et al. [438], 2022	6	Europe	✓	✗	opt	✓	Differentiation in capacity expansion scenarios
Gils et al. [163], 2022	9	Europe	✓	✓	opt	✓	Technology representation, optimization approaches, and sector coupling
Gnann et al. [523], 2022	3	Germany	✓	✗	opt, sim	✗	Market diffusion of alternative fuels in passenger cars
Misconel et al. [62], 2022	3	Germany	✓	✗	opt, sim	✗	Mathematical approaches, myopic foresight perspective, and level of detail
Ruhnau et al. [450], 2022	5	Europe	✓	✗	opt	✓	Electricity market models for carbon pricing scenarios
b. Scope: Not specified/sector-specific							
Bucksteeg et al. [451], 2022	5	Combined heat & power	✓	✓	opt	✓	Decarbonization through power-to-heat scenarios
Gils et al. [439], 2022	8	n.a.	✓	✗	opt	✓	Model-related deviations with sector-coupling for 16 test cases
Berendes et al. [426], 2022 (?)	5	n.a.	✗	✓	opt	✓	Employment of user survey for the usability testing of ESM frameworks

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