Doctoral Thesis

Optimization of Sustainable Urban Energy Systems: Model Development and Application

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List of Abbreviations

APC	article processing charge
API	application programming interface
ASHP	air source heat pump
BMBF	German Federal Minsistry of Education and Research
CBC	COIN-OR Branch-and-Cut
CC-BY 4.0	Creative Commons Attribution 4.0
CHPP	combined heat and power plant
DH	district heating
DALY	disability-adjusted life years
EU	European Union
GCHP	ground coupled heat pump
GHG	greenhouse gas
GIS	geographical information system
GPLv3	GNU General Public License Version 3
GUI	graphical user interface
IEP	Institute of Energy and Process Engineering
LCA	life-cycle assessment
MES	multi-energy system
oemof	Open Energy Modelling Framework
openmod	Open Energy Modelling Initiative
PV	photovoltaic
RAM	random-access memory
R2Q	Resource Planning for Urban Districts
RES:Z	Resource-efficient Urban Districts
SESMG	Spreadsheet Energy System Model Generator

Abstract

Urban energy systems will need to be completely transformed to meet climate protection goals and be robust to changing external conditions, such as the 2022 energy crisis in Europe. These systems are extremely complex and interconnected due to the highly decentralized energy supply, the use of volatile renewable energies, energy storage systems, sector coupling, and the increasing importance of new energy and demand sectors.

Multi-objective optimization approaches are well suited for the design of urban energy systems, with financial costs and greenhouse gas emissions as optimization targets, with holistic consideration of all relevant energy and demand sectors. An important aspect for the development of modeling tools is the goal of making novel models broadly applicable through low entry points, open and transparent methods, and data management.

When modeling and optimizing urban energy systems, challenges arise with respect to the (1) model properties and features, (2) model complexity affecting the (2a) applicability and (2b) required computing effort, (3) openness of models and input data, (4) quality and availability of input data, (5) model uncertainties, as well as (6) communication of model insights. Challenges regarding the selection of appropriate model properties and features, assuring data quality, and enabling openness of applied modeling methods are straightforward to address and, in some cases, allow for parallel improvement of other challenges. Challenges regarding models' complexity are more difficult to solve and come along with the need for trade-offs.

All of these challenges have been addressed in this work. With the Spreadsheet Energy System Model Generator (SESMG), a tool was developed that enables the automated modeling of urban energy systems. It is applicable without any programming knowledge, automatically defines the model parameters and structure, processes and visualizes the model results, and comes with a broad set of standard (but still customizable) technical, environmental, and economic parameters. The SESMG also includes a standard procedure for model-based complexity reduction, which enables the modeling of urban energy systems at high spatial resolution using standard personal computers. Just like all other developed methods and applied input data, the SESMG is published under an open-source license. All assumptions, uncertainties, and insights are communicated transparently.

The developed methods were applied to a typical reference urban energy system. The results obtained can be transferred to other urban energy systems, while the limitations of the transferability of the results to other real-world systems are well considered. Assuming energy prices (electricity, natural gas and hydrogen) as they were before the 2022 energy crisis in Europe, in the financially-optimized scenario the heat supply is primarily based on (centralized) natural gas technologies, and the electricity supply is based on heat-driven natural gas combined heat and power plants and photovoltaic systems. Large shares of produced electricity are exported. When energy prices rise, the financially-optimized scenario of the analyzed reference system approaches the least-greenhouse gas-emission scenario; in this emission-optimized scenario, the heat demand is significantly reduced by building insulation. The remaining heat demand is provided by air source heat pumps, ground coupled heat pumps and solar thermal systems. Photovoltaic systems and hydrogen operated combined heat and power plants are used for electricity supply and battery storages for load shifting.

Several other scenarios allow a compromise between these two extremes. Starting from the financial optimum, about 40 % of the possible greenhouse gas emission reduction can be saved at low cost, while another 40 % can be achieved at mid-range expenses, and the remaining 20 % requiring significant additional costs, mainly due to high investment costs of battery storage and hydrogen technologies.

Technologies and measures that are robust for use in optimized systems under expected trends such as increasing energy prices, increasing greenhouse gas emission reduction requirements, and decreasing greenhouse gas emissions from imported electricity are recommended. These include photovoltaic systems, decentralized heat pumps, thermal storages, electricity exchange between subsystems and with higher-level systems, and reducing energy demand through building insulation, behavioral changes, or reduction of living space per inhabitant. On the other hand, solar thermal systems, decentralized natural gas technologies, high capacity battery storages, hydrogen for building energy supply, and natural gas-based district heating bear the risk of not being viable under expected trends. It can be assumed that the maximum profitability of natural gas technologies has already been reached with the current natural gas purchase prices and that natural gas will be less and less considered in optimized urban energy systems.

The modeling approach developed and applied has some limitations, model uncertainties based on assumptions about input parameters, or the non-inclusion of the mobility sector and respective sector-coupling effects. However, as these gaps are transparently classified, both the method and the resulting findings are highly relevant for practice. There are related issues which will be addressed in future research. In particular, the integration of the mobility sector, the stakeholder-specific cost optimization, the conceptualization of local energy markets, and ways to enable the modeling of even more complex systems are important aspects for future research.

1 Introduction

Traditional urban energy systems need to be completely restructured to meet modern requirements [1, 2]. National and international climate protection targets and changing external conditions such as the 2022 energy crisis in Europe pose new challenges for modern, sustainable energy systems [C]. Further requirements result from the ongoing urbanization, which leads to increasing energy demands in cities [3].

Urban energy systems can be defined as "the 'combined process of acquiring and using energy in a given' [4] spatial entity with a high density and differentiation of residents, buildings, commercial sectors, infrastructure [5], and energy sectors (e.g., heat, electricity, fuels) [6]" [B]. They are also called mixed-use multi-energy systems [B].

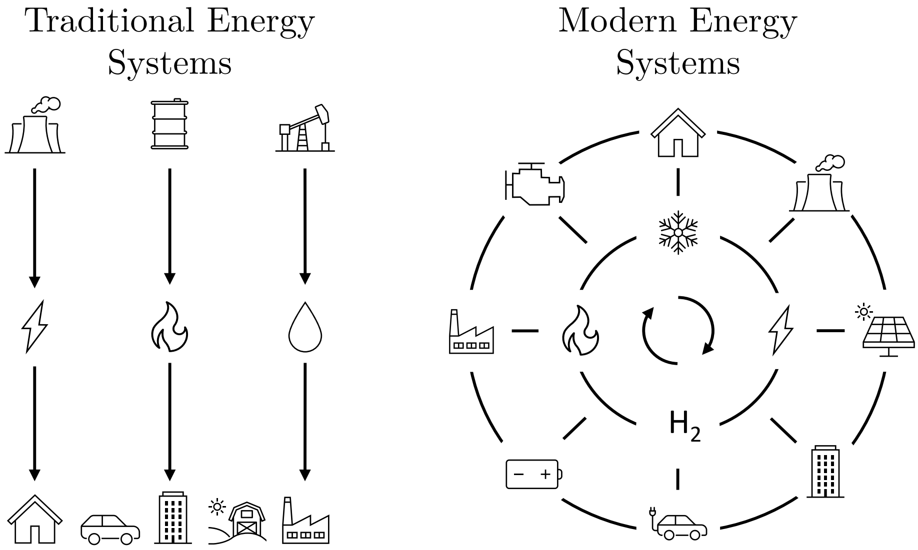

Figure 1.1: Schematic representation of traditional (left) and modern (right) energy systems. Adapted from [1].

Traditional urban energy systems are characterized by linear, sector-separated, area-wide homogeneous, and, in the electricity sector, centralized energy supply (Fig. 1.1) [C, 1]. Modern urban energy systems in turn are increasingly complex and entangled due to a widely decentralized energy supply, the use of volatile renewable energies, energy storage systems, sector coupling, and increasing relevance of new sectors such as the e-mobility and hydrogen sectors [C, 1].

In the past, traditional urban energy system planning was usually driven by financial interests only, and individual system parts (individual buildings, consumption sectors, and energy sectors) were planned independently of each other by comparing a limited number of possible supply scenarios [D, 7]. In contrast, the planning of increasingly entangled modern energy systems requires a much more holistic approach [D, 1]. When all system components are planned and optimized together, synergies can be exploited and conflicting objectives avoided. The use of optimization algorithms allows the comparison of all theoretically possible scenarios [D]. In addition to financial interests, it is recommended that other objectives such as the minimization of greenhouse gas (GHG) emissions are addressed as well. Therefore, the planning and optimization of urban energy systems and the respective models become more and more complex [D].

There is a lack of research and planning practice for methods being able to meet these criteria.

No modeling tool is available which is widely applicable for modeling and optimizing urban energy systems that (1) generates spatially high resolution results, (2) works with multi-objective optimization methods, (3) takes diverse energy and consumption sectors into account, (4) can be applied on standard personal computers, and (5) can be used without programming knowledge. To close this gap, a modeling tool for the optimization of sustainable urban energy systems is developed and applied within this work. A special focus lies on the analysis of challenges that arise during this process and how they can be handled. The developed modeling methods are able to represent all relevant aspects of modern urban energy systems. Further, they can be applied by a broad user community of planners and engineers. The tool is therefore published under an open-source license, applicable without any programming knowledge, and executable with standard personal computers.

Table 1.1: Publication overview of the cumulative thesis.

ID	Publication
[A]	Klemm, C. and Vennemann, P. "**Modeling and optimization of multi-energy systems in mixed-use districts: A review of existing methods and approaches**". *Renewable and Sustainable Energy Reviews*, 135, 110206 (2021). DOI: 10.1016/j.rser.2020.110206.
[B]	Klemm, C. and Wiese, F. "**Indicators for the Optimization of Sustainable Urban Energy Systems Based on Energy System Modeling**". *Energy, Sustainability and Society*, 12, 3 (2022). DOI: 10.1186/s13705-021-00323-3.
[C]	Klemm, C., Wiese, F., and Vennemann, P. "**Model-based run-time and memory reduction for a mixed-use multi-energy system model with high spatial resolution**". *Applied Energy*, 334, 120574 (2023). DOI: 10.1016/j.apenergy.2022.120574.
[D]	Klemm, C., Becker, G., Tockloth, J. N., Budde, J., and Vennemann, P. "**The Spreadsheet Energy System Model Generator (SESMG): A tool for the optimization of urban energy systems**". *Journal of Open Source Software*, 8, 89 (2023). DOI: 10.21105/joss.05519.
[E]	Klemm, C., Vennemann, P., and Wiese, F. "**Potential-Risk and No-Regret Options for Urban Energy System Design - A Sensitivity Analysis**". *Sustainable Cities and Society* (under review).

This work is a publication-based cumulative thesis and includes five peer-reviewed publications[1] (Tab. 1.1). The individual publications build on each other (Fig. 1.2). In publication [A], an extensive literature review was conducted to provide a detailed knowledge base for further investigation. Previous studies in the field of modeling and optimization of urban energy systems were evaluated, and approaches to build upon were identified. In publication [B], a greater basis was created by reviewing and evaluating indicators, system boundaries, and more. Methods for multi-objective optimization and emission balancing were selected, adapted and applied for a simplified test case. Publication [C] is primarily concerned with model-based simplification with the aim of reducing the computing resources (random-access memory (RAM) and run-time) required for solving energy system models. Only with these methods was it possible to solve the following models with sufficient spatial resolution to answer the research question.

Various versions of the Spreadsheet Energy System Model Generator (SESMG) were used in publications [B], [C], and [E]. The SESMG itself is described in publication [D]. The development of the SESMG took place in parallel and iterative to publications [B] and [C]. Finally, in Publication [E], all developed methods were combined and applied within a case study. The

[1]Transparency disclose: A first version of publication [A] was written and submitted for publication as part of Christian Klemm's master's thesis. The further publication process, including two extensive revisions, was carried out as part of the presented work.

result is a list of measures and technologies that are particularly robust to optimization, as well as those that are explicitly not. The studied system has a particularly transferable structure, so that the findings can also be applied to other urban energy systems.

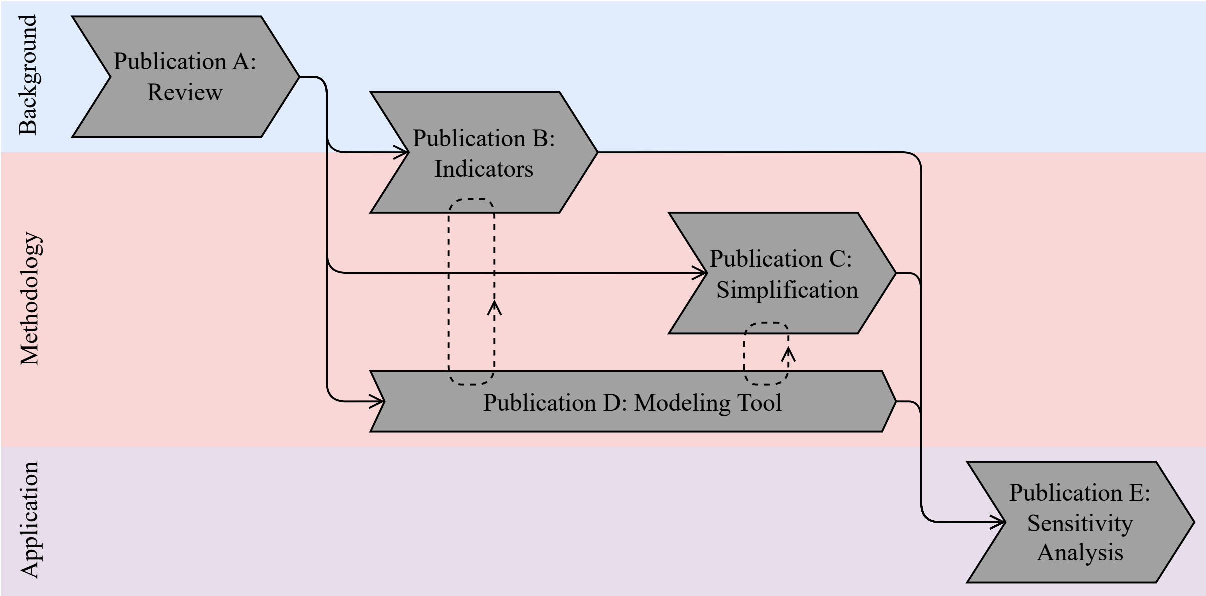

Figure 1.2: Structure of the individual publications listed in Tab. 1.1.

This work was conducted in conjunction with the research project Resource Planning for Urban Districts (R2Q) and the related interdisciplinary research network Resource-efficient Urban Districts (RES:Z). While the main publications of this work are listed in Tab. 1.1, further publications describing related side aspects and technical issues are listed in Tab. 1.2.

The content of this document is based on the publications listed in Tab. 1.1. Accordingly, content and verbatim transcriptions have been adopted from these publications. This is indicated in each case by letter references, as shown in Tab. 1.1. The publications are given in Appendices A–E in their published format, or as a manuscript version for the submitted publication under review. The following sections describe how the individual publications address various challenges of modeling and optimizing urban energy systems (Sec. 2), the modeling workflow of the SESMG (Sec. 3), and the results obtained from a case study (Sec. 4). Finally, both developed methods and obtained results are critically evaluated and classified (Sec. 5 and 6).

Table 1.2: Overview of selected publications related to this work.

Type	Publication	Ref.
Software	SESMG Developer Group. "**Spreadsheet Energy System Model Generator (SESMG) - Software**". *GitHub* (2023). URL: `https://github.com/SESMG/SESMG`.	[8]
Documentation	SESMG Developer Group. "**Spreadsheet Energy System Model Generator (SESMG) - Documentation**". *ReadTheDocs* (2023). URL: `https://spreadsheet-energy-system-model-generator.readthedocs.io`.	[9]
Documentation	Klemm, C., Budde, J., Becker, G., Tockloth, J. N., and Vennemann, P. "**Energy system model parameters - Potential-Risk and No-Regret Options for Urban Energy System Design - A Sensitivity Analysis**". *Zenodo* (2023). DOI: `10.5281/zenodo.7896185`.	[10]

Table 1.2: continued.

Type	Publication	Ref.
Project Report	Klemm, C., Budde, J., Becker, G., Arendt, R., Bach, V., Finkbeiner, M., and Vennemann, P. "**Leitfaden RessourcenPlan – Teil 2.4: Ressourcenmanagement Energie. Ergebnisse des Projekts R2Q RessourcenPlan im Quartier**". *Münster University of Applied Sciences* (2023). DOI: 10.25974/FHMS-15756.	[11]
Conference	Budde, J., Klemm, C., Tockloth, J. N., Becker, G., and Vennemann, P. "**Automatisierte Modellierung und Optimierung urbaner Energiesysteme**". *6. Regenerative Energietechnik Konferenz in Nordhausen* (February 09-10, 2023), pp. 150–159. URL: https://www.hs-nordhausen.de/fileadmin/Dateien/Forschung/2021/Tagungsband_RETCon_2023_Web.pdf.	[12]
Peer-Review	Becker, G., Klemm, C., and Vennemann, P. "**Open Source District Heating Modeling Tools—A Comparative Study**". *Energies*, 15, 8277 (2022). ISSN: 1996-1073. DOI: 10.3390/en15218277.	[13]
Documentation	Klemm, C., Budde, J., Becker, G., Tockloth, J. N., and Vennemann, P. "**Energy system model parameters: Model-based run- time and memory optimization for a mixed-use multi-energy system model with high spatial resolution**". *Zenodo* (2022). DOI: 10.5281/zenodo.6997547.	[14]
Peer-Review	Quest, G., Arendt, R., Klemm, C., Bach, V., Budde, J., Vennemann, P., and Finkbeiner, M. "**Integrated Life Cycle Assessment (LCA) of Power and Heat Supply for a Neighborhood: A Case Study of Herne, Germany**". *Energies*, 15, 5900 (2022). ISSN: 1996-1073. DOI: 10.3390/en15165900.	[15]
Peer-Review	Hörnschemeyer, B., Söfker-Rieniets, A., Niesten, J., Arendt, R., Kleckers, J., Klemm, C., Stretz, C. J., Reicher, C., Grimsehl-Schmitz, W., Wirbals, D., Bach, V., Finkbeiner, M., Haberkamp, J., Budde, J., Vennemann, P., Walter, G., Flamme, S., and Uhl, M. "**The ResourcePlan—An Instrument for Resource-Efficient Development of Urban Neighborhoods**". *Sustainability*, 14, 1522 (2022). ISSN: 2071-1050. DOI: 10.3390/su14031522.	[16]
Conference	Klemm, C. and Vennemann, P. "**Modellierung und Optimierung urbaner Energiesysteme im Projekt R2Q**". *4. Regenerative Energietechnik Konferenz in Nordhausen* (February 18-19, 2021), pp. 177 –188. URL: https://www.hs-nordhausen.de/fileadmin/daten/fb_ing/inret/PDFs/tagungsband_retcon21_web_aa3__1_.pdf.	[17]
Conference	Klemm, C., Vennemann, P., and Wiese, F. "**Sustainability indicators for the assessment of urban energy systems - A practical comparison**". *Energy Modelling Platform for Europe* (October 06-10, 2020). URL: https://www.youtube.com/watch?v=qXQkUUBgc7k.	[18]
Conference	Klemm, C. and Vennemann, P. "**Optimization of resource efficiency in mixed-use quarters**". *Oemof User Meeting in Oldenburg* (March 15-19, 2019). DOI: 10.25974/fhms-11036.	[19]

*SESMG Developer Group: Besides the four main developers Christian Klemm, Gregor Becker, Janik Budde, and Jan N. Tockloth, eight other persons (as of September 2023) have contributed to the development of the SESMG by writing smaller parts of the documentation or code segments.

2 Challenges and Solutions

When modeling and optimizing urban energy systems, a number of challenges arise. Some of them are general problems of energy system modeling, while others occur for the specific case of urban energy systems. The challenges described in the literature [2, 7, 20–38] were reviewed and summed up into the categories of

- Model properties and features,
- Complexity,
- Openness,
- Data,
- Uncertainties, and
- Communication.

Since many of the challenges, as well as their sub-aspects, overlap or interact, other categorizations can be reasonable as well. Each challenge category, how it interacts with the other categories, how it can be solved theoretically, and how it has been solved practically within the scope of this work are discussed in the following sub-sections.

2.1 Model Properties and Features

Challenge Energy system models may have a multitude of scopes to which a wide variety of model properties and features can be applied [A]. Choosing inappropriate modeling approaches or model parameters can lead to the amplification of problems in model complexity (Sec. 2.2) and model uncertainty (Sec. 2.5).

Only a small proportion of commonly used modeling tools come with properties required for modeling and optimizing urban energy systems [A]. Especially if further requirements apply, such as being available under an open-source license (Sec. 2.3), or being applicable without any programming knowledge (Sec. 2.2.1), it becomes more difficult to find appropriate tools [A].

Traditional tools for the planning of urban energy systems are typically focused on traditional energy systems and rather simplified energy supply scenarios. They do not match the requirements of optimizing modern urban energy systems (Sec. 1) so that a development of new or further development of existing tools is required.

Theoretical Solution It is recommended to define a clear research question and to choose model properties and features based on that, rather than the other way around [20]. The objective evaluation of the selected properties and features during the modeling process can help to correct inappropriate choices [20]. To keep the complexity of a model within manageable limits (Sec. 2.2), modelers often have to choose between high resolution and great horizons, both temporal and spatial. For urban energy systems, high resolution is particularly important [C].

Tab. 2.1 lists recommendations for the selection of model properties, features, and system boundaries for the optimization of urban energy systems. These were developed within the scope of literature reviews and subsequent analyses of the two background publications of this work ([A] and partly [B], see Fig. 1.2).

Practical Application With the SESMG a model generator based on the Open Energy Modelling Framework (oemof) [39] was developed, which enables the modeling and optimization of urban energy systems. It comes with all the features needed to model and optimize urban energy systems. At the same time, it provides the flexibility to customize model properties, features, and system boundaries for the purpose of modeled energy systems (Sec. 3) [D].

Besides the theoretically developed recommendations, Tab. 2.1 shows practically applied model parameters and system boundaries in the models of publications [B, C, E]. In addition, the following specifications were applied in the models of this work:

- Linear programming was used for dispatch and investment optimization. It was supplemented by the use of mixed-integer programming for investment decisions for technologies with high capacity-independent investment costs (e.g., district heating (DH) pipes) [B, C, E].
- Holistic optimization was considered by consulting the multi-energy system approach [37], several energy demands (residential, commercial, and industrial), as well as a multitude of technologies, including demand-side management measures [B, C, E]. The mobility sector, which is a complex system in itself, was excluded from the scope of the studies.
- For multi-objective optimization, the epsilon-constraint method [36] was applied, where the model is optimized in several runs for a primary optimization criterion with steadily tightening restrictions of a secondary criterion. The reduction of financial costs was used as the primary optimization criterion, with GHG emissions as the secondary criterion [B, E].
- The reduction of energy demands is a suitable third optimization criterion [B] which can be applied with the SESMG. However, behavioral-based demand reduction "is an opportunity, which simultaneously provides a reduction in financial costs and GHG-emissions [...] and therefore provides" [B] a quasi-automatic improvement of the other two indicators, independently from their further optimization. Therefore it was not necessary to use this third indicator.
- For the consideration of GHG emissions, "a global view is required to fully consider the respective effects" [B]. Therefore, clear system boundaries were defined based on the emission scopes of the World Resource Institute [B].
- The "energy balance boundary for the conversion processes to be considered in urban energy systems" were limited to "all conversion processes up to final energy. Further transformations from final energy into effective energy take place within subsystems of buildings or plants. Although these subsystems are, strictly speaking, part of the urban energy system, they are also complex systems in their own, the interrelationships of which lie outside the scope of research on holistic urban energy systems [40]" [B]. Energy types were considered according to definitions provided by VDI guideline 4600 [41].
- Further aspects, such as the coupling and integration of other sector and resource models ("model integration" [21]), were not directly included in the modeling process but were addressed separately as part of handling the communication challenge (Sec. 2.6).

Table 2.1: Model properties, features, and system boundaries which are recommended and used in the presented studies. Abbreviations: air source heat pump (ASHP), combined heat and power plant (CHPP), district heating (DH), ground coupled heat pump (GCHP), greenhouse gas (GHG), photovoltaic (PV).

Model Property, Feature, or System Boundary	Recommendation	Model used in [B]	Model used in [C]	Model used in [E]
Analytical Approach	bottom-up or hybrid [A]	bottom-up	bottom-up	bottom-up
Mathematical Approach	(mixed-integer) linear or dynamic programming [A]	linear programming	(mixed-integer) linear programming	(mixed-integer) linear programming
Methodology	dispatch and investment (multi-objective) optimization [A, B]	single-/multi-objective optimization (investment and dispatch)	single-objective optimization (investment and dispatch)	multi-objective optimization (epsilon-constraint method) (investment and dispatch)
Assessment Criteria	financial, environmental or energy efficiency criteria [A], particularly suitable indicators are total GHG emissions, financial costs and final energy demands [B]	primary energy efficiency, share of renewables, self-sufficiency, GHG emissions, energy demand	financial costs	financial costs, GHG emissions
Sectoral Coverage	various energy (e.g., electricity, heating, fossil resources, cooling, mobility) and demand (e.g., residential, commercial, industrial) sectors [A]	energy sectors: electricity, heating, fossil fuels; demand sectors: residential, commercial	energy sectors: electricity, heating, fossil fuels; demand sectors: residential, commercial	energy sectors: electricity, heating, fossil fuels, hydrogen; demand sectors: residential, commercial
Temporal Resolution	min. 1 hour [A]	1 hour	1 hour	1 hour
Spatial Resolution	plant to city specific [A]	district specific	building specific	building specific
Temporal Horizon	min. 1 year [A]	1 year	1 year	1 year (temporally simplified, Sec. 2.5)

Table 2.1: continued.

Model Property, Feature, or System Boundary	Recommendation	Model used in [B]	Model used in [C]	Model used in [E]
Technical Coverage	all technologies relevant for the purpose of investigation [A]	PV system, natural gas CHPP, biogas CHPP, natural gas heating, sub-system electricity exchange	central natural gas heating plant, natural gas CHPP, natural gas heating, GCHP, ASHP, PV system, battery storage, solar thermal collector, thermal storage, roof insulation, wall insulation, window insulation, DH network, sub-system electricity exchange	central natural gas heating plant, natural gas CHPP, natural gas heating, electric heating, GCHP, ASHP, PV system, battery storage, solar thermal collector, thermal storage, roof insulation, wall insulation, window insulation, DH network, electrolysis, hydrogen CHPP, methanation, natural gas storage, hydrogen storage, sub-system electricity exchange
Geographical Coverage	local or regional geographical coverage [A], as narrow as possible [B].	500 buildings	9 buildings	20 buildings
Demand-Side Management	can optionally be considered [A]	–	insulation	insulation, bevioral demand reduction
Change of Properties	can optionally be considered [A]	–	–	energy prices, GHG emissions, energy demands
Energetic Boundaries	all conversion processes up to final energy [B].	all conversion processes up to final energy	all conversion processes up to final energy	all conversion processes up to final energy
Balance Boundaries	life-cycle accounting for applied target values (e.g., costs and emissions), considering Scope 1 to 3 emissions [B].	life-cylcle consideration	life-cycle consideration	life-cycle consideration

2.2 Complexity

Rapidly increasing complexity and entanglement of energy system results in likewise increasing complexity of energy system models, which is one of the most frequently mentioned challenges of energy system modeling (see e.g., [2, 20–28]).

This challenge especially applies for models for the optimization of modern urban energy systems, as they include a particularly large number of interacting (renewable) technologies, energy sectors, and consumption sectors [28]. Increasing complexity in turn results in increasing effort (1) to create respective models or apply modeling tools, and (2) to meet increasing computing requirements caused by increased mathematical complexity [A]. The complexity of models thus represents a clear limitation on the applicable model size and model detail [2].

Both complexity challenges can be reduced by selecting the model properties and features during model conceptualization in such a way that the model is as "simple as possible and as complex as necessary" [20]. For this purpose, it is recommended to build up a model gradually, start with a simple model and add spatial, temporal, and sectoral detail as required [20].

2.2.1 Applicability

Challenge The high level of system complexity requires a high degree of prior knowledge about the structure of energy systems on the one hand, and great effort during the definition of the model as well as during processing and interpretation the results, on the other hand [17]. High system complexity requires high technical, spatial and temporal resolution of models (Sec. 2.1). This in turn leads to high data requirements (Sec. 2.4) but also the necessity to enter the different system structures into the model in a complex way [A].

In many cases, the requirements of programming skills for the application of modeling tools are a further entry threshold [A]. The training time for modeling tools is typically a few weeks up to several months [29]. Even for simpler models, the results are often difficult for non-experts to understand, making it difficult to communicate (Sec. 2.6) insights transparently [22].

Theoretical Solution Intuitively applicable tools are required to lower entry thresholds. For example, graphical user interfaces (GUIs) and spreadsheet or geographical information system (GIS) based data inputs [A], which require as little as possible prior knowledge on energy systems, are valuable in this context. By documenting all functions in detail and demonstrating them using real-world examples, the training time for modelers can be further reduced [42]. Communication and understanding of model results can be eased, if they are processed automatically in a descriptive form (Sec. 2.6).

Practical Application The developed SESMG comes with a low entry threshold. "Compared to other tools for the modeling and optimization of urban energy systems [...] the SESMG provides several advantages regarding user-friendliness due to [...]

- Applicability without any programming knowledge through a browser-based graphical user interface (GUI),
- Automatically conceptualizing individual urban energy systems of any size,
- Automatic result processing and visualization of complex relationships in form of system graphs, Pareto fronts, energy amount diagrams, and more, [...]
- A broad set of standard (but still customizable) technical and economic modeling parameters including description and references" [D], as well as
- "Detailed documentation, including step-by-step instructions, explanations of all modeling methods and troubleshooting with known application errors" [D].

However, the SESMG is still an expert tool, which requires “certain basic knowledge of energy systems and energy engineering” [D]. The target groups are “(urban) energy system planners and researchers in the field of energy engineering” [D].

2.2.2 Computing Effort

Challenge Modern urban energy systems include (decentralized) renewable energies with hardly predictable and volatile production, energy storage systems, and sector coupling [C]. In order to model these accurately, particularly high temporal, technical and spatial resolutions are required (Sec. 2.1) [C]. High model resolution causes high mathematical complexity, leading “to a rapid increase of required computing resources” [C] (run-time and RAM requirements) for energy system models. The run-time “increases quadratically with increasing model complexity” [C]. The use of binary variables in the context of mixed-integer programming has a particularly large influence. The RAM requirements “increases linearly with increasing model complexity” [C]. In order to limit the model complexity to a handable extend, “modelers must compromise between the computational effort on the one hand and the accuracy of the results on the other hand by creating simplified models [43]” [C] (Sec. 2.5).

Theoretical Solution Computing requirements can be reduced “by solver-based or by model-based methods [24]. Solver-based approaches deal with the mathematical optimization of the solving algorithm” [C], while model-based approaches deal with the simplification of the real-world representation of the model [C]. Solver-based optimization approaches are usually not within the expertise of energy system modelers [C]; therefore, the focus is often on using solvers optimized for respective models. Commercial solvers (e.g., gurobi [44]) often allow a significant reduction of the required computing resources compared to open solvers (e.g., COIN-OR Branch-and-Cut (CBC) [45]), but come with limitations in openness (Sec. 2.3).

Model-based approaches are more in the expertise of energy system modelers, with which modelers “make use of their deep understanding of the structure of energy systems” [C] to reduce the systems’ complexity to be solved by the solver. Model-based methods can be divided into temporal model adaptions which aim to reduce the number of modeled time-steps [C], and into techno-spatial methods, which aim to reduce “the number of possible combinations of investment decisions” [C].

However, model-based adaptions may cause uncertainties (Sec. 2.5), for example, based on temporal concurrency and continuity problems [30], incorrect balancing based on spatial clustering, or miscalculation due to technical linearization [C]. Furthermore, some methods require deeper knowledge of the system (Sec. 2.2.1). To achieve the best possible balance between reducing model complexity and losses in model accuracy or resolution, it is recommended to apply model simplifications in a structured manner [C].

Practical Application For the first modeling application, a model with low spatial resolution, with a small number of linear investment decisions, and containing no binary investment decisions was applied. For further models, the complexity was increased gradually (Tab. 2.2). This procedure ensured that the complexity of the models was manageable at any time with the available computing resources.

The significantly increased model complexity was successfully managed by implementing a five step procedure for model-based simplification. The procedure enables a significant reduction of computing requirements for high spatial-resolution multi-energy system models [C]. The suggested steps are sequential. Only as many steps as absolutely necessary should be applied to avoid model uncertainties [C]:

Table 2.2: Comparison of applied model complexity.

Model used in	Spatial Resolution	Linear Investment Decisions	Binary Investment Decisions
[B]	district sharp	4	0
[C]	building sharp	79	20
[E]	building sharp	373	47

model development ↓ increasing complexity ↓

1. **Keeping the model as simple as possible:** All system components that are not relevant to "the purpose of the study should be removed from the model. This applies in particular to (binary) investment decisions" [C].
2. **Pre-modeling:** "With the help of a time-simplified model (slicing/averaging of every 10th week is recommended), preliminary results can be obtained and incorporated into the main-model" [C]:
    a) **Technological pre-selection:** "Technologies not considered within [...] pre-modeling should be removed from the main-model" [C].
    b) **Technological boundaries:** "Investment limits can be reasonably limited based on the pre-model results" [C]. Technological boundaries of 500 % of the pre-model result investment values are recommended. "If the investment limits are fully used in the main-model, the technological boundaries should be enlarged" [C].
3. **Spatial sub-modeling:** "The model can be decomposed and the results subsequently aggregated. The boundaries of sub-models should be strategically aligned, for example at network nodes. Especially for models without interaction between sub-systems (i.e., without local energy markets or bi-directional heat networks), only small model deviations are to be expected" [C].
4. **Temporal simplification:** Temporal slicing is recommended, "using days as sample periods. The degree of slicing should be as low as necessary, with a maximum of every fifth day" [C].
5. **Further simplifications:** "If further model simplifications are necessary, [...] spatial clustering of sub-systems" is recommended. "The clusters should be kept as small as possible" [C].

For a reference case model, this procedure enabled a reduced run-time "by more than −99 % and the memory usage by up to −88 %" [C]. At the same time, however, uncertainties occurred. Sector coupling technologies, heat pumps, and battery storages were "undersized with decreasing number of modeled time steps", and central heat supply tended to be oversized with a decreasing number of modeled time steps [C].

The SESMG comes with functions to implement all five steps of this procedure. While the first step is covered by the automatic conceptualization of urban energy system models, the further steps can be selected and adjusted in their level of intensity. Beyond that, other model-based simplification methods can be applied with the SESMG, which may be better suited for other types of energy system models [D, 9]. Finally, the SESMG is applicable with both open or commercial solvers.

2.3 Openness

Challenge Models and modeling tools can be divided into the categories "open" and "closed", depending on the "public accessibility of their source code, their underlying assumptions, and the data they use [26]" [A]. While open models and modeling tools are partially or fully publicly accessible, closed models are "subject to fees, or even completely confidential [26]" [A].

Whether models and modeling tools are open or closed is defined by the selected license. Open-source licenses guarantee partial or complete public access to the source code, assumptions and data used via the copyright. In addition, the copyleft can prescribe that changes and further developments must also be made available openly [46]. Different license types are sometimes incompatible with each other based on their copyright and copyleft terms. This can unintentionally prevent the further development or linking of modeling approaches [32].

The majority of models and modeling tools are closed, which "generally hinders progress in energy system modeling" [A]. However, there are four major reasons why energy system models should be open [A, 31]:

- "The fundamental scientific principles of transparency, peer review, reproducibility and traceability can only be guaranteed if data, methodology and results are openly accessible [31, 33].
- Policymakers often have to fall back on models that are not quality-assured with academic practice or that provide incorrect results. With increasing transparency in energy system research, policymakers will gain access to more high-quality information [31].
- Research funding and researchers' time are limited resources. A great deal of time and money can be saved by avoiding duplication of work [31].
- The transparency of arguments based on scientific justifications are necessary in social and political debates [47]. Furthermore, the full results of publicly funded research should be available to the public" [A].

However, there are also a number of reasons why models often remain closed which have to be overcome to enable open accessibility of models, their assumptions and results:

1. "The hesitation among individuals or institutions may [...] be a cause for failing to open models and their results" [A].
2. There are not enough resources (working time or financial) available. Writing legible and reusable code "as well as comprehensible documentation and bug reports is time-consuming" [A]. In addition, open-access publication often requires the payment of an article processing charge (APC).
3. Releasing code carries the risk "that other researchers could expose flawed code sections or erroneous data and thus discredit the results" [A] and the authors.
4. Models "may contain sensitive commercial data or personal information, which is not permitted for public disclosure" [A].
5. Licenses of used models and modeling tools may be incompatible with open publication [32, 46].

Theoretical Solution It is recommended to define transparency as a goal of any modeling project to ensure that the need for open research and modeling is met [20]. In particular, the above-mentioned reasons, favoring closed models and their results, should be faced at an early stage. Taking necessary steps from the beginning, such as documenting the model code, can significantly reduce the overall effort. The use of an open-source guide such as presented by Becker [46] may help to realize open modeling in a structured manner.

Practical Application The individual partial hurdles of open modeling were handled in the following way:

1. The commitment to open-source development and open-access publication was defined as a goal in the exposé of this work and was followed in all steps.
2. Additional time and effort for open publication was scheduled from the beginning. APCs for publications were financed by the German Federal Minsistry of Education and Research (BMBF) and Münster University of Applied Sciences' Institute of Energy and Process Engineering (IEP).
3. The software was created according to current software open-source development standards [46] and underwent a peer-review process [D] to ensure quality.
4. Within the developed data standard only open data was used (Sec. 2.4).
5. Only modeling approaches and programming libraries were used, which allow open distribution. For the publication of the modeling approaches, licenses were selected (Tab. 2.3) that exclude any incompatibilities with used programming libraries [D, 8, 46].

Applied input data, modeling methods and results are openly published, as shown in Tab. 2.3.

Table 2.3: Overview of accessibility of applied model code, input data and assumptions. Abbreviations: application programming interface (API), Creative Commons Attribution 4.0 (CC-BY 4.0), GNU General Public License Version 3 (GPLv3).

Modeling Element	Reference	License
Modeling Tool (SESMG) - Code	[8]	GPLv3
Modeling Tool (SESMG) - API Documentation	[8, 9]	GPLv3
Modeling Tool (SESMG) - User Documentation	[9]	GPLv3
Models - Structure, Parameters, and Assumptions	[B, 10, 14]	CC-BY 4.0
Models - Model Input Data	[48–50]	CC-BY 4.0
Insights - Peer-Review Publications	[A, B, C, D, E]	CC-BY 4.0*

*Publication [E] has not been published yet. However, it is submitted to a peer-review journal, and as of now it will be published under a CC-BY 4.0 license.

2.4 Data

Challenge High temporal and spatial resolutions of urban energy system models (Sec. 2.1) require data at correspondingly high resolution [A]. This applies to the data for the area to be analyzed (e.g., building data, technology stock, energy consumption), technical parameters (efficiencies and other plant-specific operating parameters), price structures (e.g., investment and operating costs, fuel costs, sales prices, fees), GHG emissions (direct and indirect), and other influences (e.g., weather data). The acquisition of appropriate data is associated with considerable effort for the reasons of insufficient availability and data quality.

Data may not be publicly available because of a lack of openness (Sec. 2.3) [21], data protection hurdles, or that data has not yet been collected. For high spatial resolution systems, privacy issues are much more likely to arise than at coarse resolutions, as personal information can be drawn from them.

Available data may have insufficient or inconsistent quality. Often, data has too low spatial resolution (e.g., energy consumption), is subject to uncertainties, or was collected with divergent (e.g., accruing GHG emissions) or flattering methods (e.g., measurement obtained under laboratory conditions). Changes in data may occure based on behavior and social factors (e.g., individual consumption profiles) [22], future changes (e.g., weather data) [37], or geo-political issues (e.g., wars or material shortages) [E].

A significant amount of time spent on modeling projects is needed for data collection. If this process can be simplified, especially through widespread open availability of data, the time spent could be used for other important tasks, [22], such as meeting model disclosure requirements (see section 2.3).

Theoretical Solution Defining data standards to be implemented by regional and local governments would ensure the availability of data of high and consistent quality and resolution. If data is openly available under uniform data interfaces, it can be fetched by modelers in an automated manner. However, publicly available data and its standards are usually not in the hands of modelers, so they must take steps to obtain required data.

The development and application of quality assurance procedures can help to ensure that input data is of sufficient quality [20]. Homogenizing data, for example by clarifying which system boundaries are to be applied when considering life-cycle emissions [B], helps to objectively compare different technologies.

Statistical or stochastic estimation procedures may be applied to substitute missing real-world data. These include, for example, the annual energy demand of individual buildings and its distribution over time at hourly resolution [10, 14]. Respective models will lead to parametric uncertainties (Sec. 2.5) [E]. However, these limitation are necessary in order to guarantee the basic operability of models for systems with limited availability of data [10, 14].

Data that cannot be accurately predicted is subject to aleatory uncertainty. It is recommended to at least select this data on a transparent basis or ideally evaluate it through an uncertainty assessment (Sec. 2.5) [E].

Practical Application The data collection process for the applied modeling projects [B, C, E] and the developed modeling tool [D] was guided by the following data standards:

- **Sources:** Emphasis was placed on using data sources that are themselves quality-checked. These include official data, peer-reviewed literature, recognized databases, and technical standards that describe data collection methods. As far as possible, multiple data sources were used to validate the values with each other.
- **Uniformity:** Particular emphasis was placed on the consistency of data with respect to uniform data definitions and collection methods. For example, it was ensured that the complete life-cycle was considered, including production, operation and disposal, when collecting GHG emissions caused by technologies.
- **Assumptions:** Statistical and stochastic substitution methods were used for data that was not available (e.g., estimation of annual energy demands based on building data and temporal distribution with standard load profiles [51, 52] or stochastic methods [53]). Whenever no statistical values were available, they were estimated on a reasoned basis (for example, averaging from neighboring buildings). Future data was substituted by choosing historical reference values (for example, particularly comparable weather data sets were chosen).
- **Uncertainties:** All uncertainties known from estimation procedures or uncertain data sources were described and communicated transparently. Parameters that are likely to change in the future due to external system changes and that have a particularly large

influence on system optimization were investigated and discussed in detail through a series of sensitivity analyses [E].

All collected input data was made openly available (Sec. 2.3, Tab. 2.3) to simplify the collection process for future modeling projects.

2.5 Uncertainties

Challenge Uncertainties arise based on the above described challenges of selecting appropriate model properties and features (Sec. 2.1), reducing modeling complexity (Sec. 2.2), and collecting high quality data (Sec. 2.4).

Applying incorrect model properties, such as too coarse spatial or temporal resolution, can lead to structural model uncertainties. Simplifying a model, especially to reduce the computing effort, introduces the risk of uncertainty (Sec. 2.2). Last, inaccurate or uncertain data can cause parametric uncertainties.

Model uncertainties can be categorized into aleatory and epistemic uncertainties [E, 54]. While epistemic uncertainties are caused by insufficiently defined data or model structure, aleatory uncertainties have their origin in real-world uncertainty itself, for example by uncertain future behavior. For further clarification of epistemic and aleatory uncertainties, the theoretical solution approaches have to be carefully described [54]:

Theoretical Solution "Epistemic uncertainties can be avoided by improving the model quality through the use of additional data (parametric uncertainties) or by refining the model (structural uncertainties) [20]. Improving the model quality is the only way of quantifying epistemic uncertainties [22]. Aleatory uncertainties cannot be reduced by improved model quality [54], yet they can be quantified by deterministic or stochastic approaches [20]" [E]. When deterministic approaches are applied, model parameters are varied. Such approaches include methods of (global) sensitivity analysis, near optimal solution approaches, and scenario analysis [20]. With stochastic approaches, uncertainties are incorporated directly into the model, including approaches of stochastic optimization [20], robust optimization, and monte carlo analysis [34].

Presenting information on uncertainties transparently with any results is an essential part of the principles of open research (Sec. 2.3) [31] and the communication of insights (Sec. 2.6) [20].

Practical Application Structural epistemic uncertainties were reduced to an unavoidable minimum by selecting appropriate model properties (Sec. 2.1) and model structures [10, 14]. To reduce the necessary computational resources, model simplifications had to be made, which led to uncertainties, especially in the context of sizing energy storages and sector coupling technologies [C]. These uncertainties were quantified by a detailed investigation [C].

Parametric epistemic uncertainties were reduced to a minimum by assuring data quality standards during data collection (Sec. 2.4). However, assumptions had to be made to cover partly poor data availability (Sec. 2.4), which are associated with parametric epistemic uncertainties (Sec. 2.4).

Aleatory uncertainties were investigated through a series of deterministic sensitivity analyses [E]. The focus was on the impact of hardly predictable system changes due to varying energy prices, GHG emission structures, and energy consumption on the model results. The results of these sensitivity analyses were discussed and disclosed in detail.

All known epistemic and aleatory uncertainties are transparently communicated with the respective publications and associated data documentation [B, C, E, 10, 14]. In addition, all assumptions (data and structures) are openly communicated (Sec. 2.3), so that previously unknown uncertainties can be uncovered at any time.

2.6 Communication

Challenge: Insufficient communication can lead to a number of model-related problems, even though communication is not a direct part of the actual modeling process. Tab. 2.4 lists communication issues that need to be avoided by modelers during model design and application. The interaction with other modelers, interdisciplinary researchers, urban planners, policymakers, and the public are important to be addressed at all stages of model development and application. Tab. 2.4 also lists the solutions realized within the applications of this work.

Theoretical Solution It is recommended to strive for open and transparent communication with all stakeholders before, during, and after the actual modeling.

Transparent communication of methods and insights consists of several “layers” [20]. The “outer layer” includes general information which is appropriate for a public audience [20]. This layer presents key results in simple language [20]. It includes clear policy recommendations, for example by drawing a clear picture of how an ideal urban energy system could look like [21]. More detail may be incorporated to the “inner layer” [20]. This layer also addresses and eliminates possible misunderstandings, such as inconsistently defined wording [A, 35]. All layers should be characterized by openness and transparency (Sec. 2.3) and unconditionally disclose all relevant uncertainties (Sec. 2.5) and assumptions (Sec. 2.4).

Stakeholders have different interests with respect to the modeling results [A, 55]. Therefore, discussions and feedback with stakeholders during the modeling process is important. However, transparent communication includes disclosing which stakeholders had influence on assumptions and modeling.

Practical Application Communication in a scientific context was a secondary aspect in all the papers of this work [A, B, C, D, E]. Further publications (Tab. 1.2), as well as presentations for the general public, policymakers, engineers and urban planners, interdisciplinary researchers, and modelers covering both inner and outer layers of communication were accompanying actions during the preparation of the presented work. Possible communication problems where handled as shown in Tab. 2.4.

Table 2.4: Problems of lacking communication with various stakeholder groups and how they have been met. Abbreviations: life-cycle assessment (LCA), Open Energy Modelling Framework (oemof), Open Energy Modelling Initiative (openmod), Resource Planning for Urban Districts (R2Q), Resource-efficient Urban Districts (RES:Z), Spreadsheet Energy System Model Generator (SESMG).

Stakeholder Group	Problem	Practical Application
Modelers	Insufficienct communication of modeling projects can lead to parallel developments and lack of bundling competencies with other modelers [56].	Suitable communities have been identified for exchange (oemof user community and openmod); modeling project and tool development was announced in an early stage [19].
	Insufficienctly communicated assumptions and uncertainties (Sec. 2.5), as well as unclear or even contradictory definitions of terms or methods [A, 35] can lead to misinterpretation and follow-up errors.	All assumptions (Sec. 2.4) and uncertainties (Sec. 2.5) were communicated transparently. Modeling terms and goals were clearly defined and potential contradictions clearly named [A, B].
Interdisciplinary Researchers	Failure to match energy system modeling results with planning objectives for other urban resources (e.g., water, space, building materials [16]) and unaddressed environmental impacts (e.g., through an LCA [15]) can lead to planning conflicts and unused synergies [21].	Regular interdisciplinary exchange was attended within the R2Q [57] project and RES:Z [58] network. Integration of the energy system modeling results (model integration) via soft-coupling was carried out. Interdisciplinary studies were carried out using coupled models, addressing interactions with other resources and sustainability aspects were co-authored and published [15, 16, 59].
Engineers and Urban Planners	If modeling tools are not presented in a way that they can be used by engineers and urban planners, a transfer of practice will be hindered and the actual impact on the transformation of energy systems is limited [20].	The SESMG and further developed methods are openly available. The methods were presented to numerous planners and energy utilities at various events and integrated into the teaching activities at Münster University of Applied Sciences and Europa-Universität Flensburg.
Policymakers	If policy-relevant questions are not coordinated with decision-makers at early project stages or incorporated to the model, gaps between theoretical analysis and real-world policy debates and conclusions [20] may arise.	In the context of the R2Q project [57], there was regular exchange with various stakeholders and political decision-makers, which had a significant impact on the orientation of the modeling methodology.
Public	Failure to adequately prepare methods and findings for a non-specialist audience may cause that the results are not accessible to the general public, even though they often pay for the modeling (Sec. 2.3) [31].	The SESMG includes a browser-based "demo tool" which can be used for low-threshold training and information events (Sec. 3). It has been used in various public events to introduce energy system modeling of urban energy systems to non-specialist audiences.

3 Modeling Tool

In the energy system modeling landscape, a distinction is made between "models", "model generators", and "modeling frameworks" [A]. Models are simplified representations of real world energy systems [A, 60], "model generators are tools that can create models with certain predefined analytical and mathematical properties [26]", and "modeling frameworks are structured toolboxes that include several model generators and specific sub-models [26]" [A]. While the use of modeling frameworks and especially model generators makes creating models much easier and requires less knowledge than creating them from scratch, they also have limitations in terms of their flexibility and adaptability [A].

The SESMG is a model generator based on the modeling framework oemof. The modeling process shown in Fig. 3.1 enables the efficient modeling of (urban) energy systems with a low entry threshold and applicability without programming knowledge. At the same time, the typical inflexibility of model generators (e.g., fixed temporal and spatial resolution, optimization criteria, or model structure) has been counteracted by the ability to adapt the modeling process and to access intermediate results.

The modeling and optimization of energy systems using the SESMG consists of several process steps and sub-process steps. Note that some process steps include several smaller (sub-)steps, that are not shown for the sake of clarity.

Based on several user decisions, the modeling workflow may follow different pathways. These decisions (blue circles in Fig. 3.1) are made at the beginning of the process via the browser-based GUI.

During the modeling process, intermediate results and data are saved at several points. Mostly xlsx and csv spreadsheet formats are used, in some cases log files and visually prepared results (png and jpg). These commonly used file formats allow an intuitive handling and therefore do not require any special (programming) knowledge for further processing the data. Furthermore, these are open formats, which can be processed with various programs (e.g., LibreOffice, Excel, Numbers). All intermediate results and data (Fig. 3.1) can be manually customized by the user for the purpose of adapting standardized model structures.

Depending on the scope the SESMG is applied for, there are up to three entry points, which require manual input from the user:

With the "urban district upscaling tool" (1 in Fig. 3.1), the user must provide locally specific parameters for the investigated system through the "upscaling sheet". This includes the definition of spatial boundaries, energy demands and their spatial distribution, and the availability of energy and spatial potentials (e.g., geothermal potentials, space availability for PV and solar thermal systems). Depending on the availability, data of different quality can be used. For example, if exact energy demands and their load profiles of individual buildings are known, they can be entered. If these are not available, building data (e.g., building area, year of construction, type of use) can be entered as an alternative, which will then be the basis for an estimation of the energy demands. Standardized model parameters that can be transferred between energy systems are stored in the "standard parameters" file. These include technological (e.g., efficiencies), economic (e.g., periodic and variable costs), and environmental (e.g., direct and indirect emissions) parameters. The SESMG comes with a complete set of such standard parameters, which can be adapted to meet specific conditions. Based on the given values, the model structure of an default urban energy system [10, 14] is automatically created and a "model definition" (see below) is generated. This model definition can be adjusted if the model has to consider specific aspects that are not included in the default urban district upscaling tool.

The steps up to this point may be skipped when using the second entry point (2). In that case, the model definition is completely created by the user. This enables the modeling of energy systems with structures different from default urban energy systems. However, this approach requires more effort in model design and a deeper knowledge of the structure of energy systems.

The “demo tool” is the last possible entry point (3). In contrast to the applications described so far, the purpose of this demo tool is the demonstration and communication (Sec. 2.6) of the methodology and capabilities of the SESMG. The user can select energy supply technologies for a given urban energy system and observe their impact on the overall system. All decisions described below are predefined in the demo tool.

The model definition contains a parametrization of all components of the energy system and how they are connected to each other. According to the structure of oemof, this includes the definition of the optimization objective, a time system (start date, end date and temporal resolution of the model) and components of buses, sinks, sources, transformers and storages. Furthermore, custom components may be created, for example for the modeling of heat networks or building insulation. For each component, all relevant technical, economical and environmental parameters are defined. In addition to existing components, possible investment decisions for new components can be defined, which will be taken into account during the subsequent investment optimization process (Sec. 2.1). Time series of weather data and components (e.g., energy consumption or energy input) are either stored in the model definition, or calculated during later steps of the modeling process.

Based on the model definition, various methods for temporal and techno-spatial model simplification can be applied (Sec. 2.2.2). These methods are used to adapt time series for temporal simplifications, and model structure or parameters for techno-spatial simplifications. The respective adaptations are stored in an “updated model definition”.

On the basis of the model definition, or the updated model definition, the energy system model is created. This step consists of several sub-steps. The first step obtains data that is not directly stored in the model definition. These include, for example, the (optional) automated retrieval of weather data using the Python library open-FRED [61], the calculation of energy supply or demand time series based on various oemof sub-packages (e.g., feedinlib [62]), the stochastic distribution of electrical load profiles using the Python library richardsonpy [53], or the calculation of grid connection points for a heating network. Based on the given inputs, an oemof energy system model is created that is subsequently transformed into an mathematical model using the Python library Pyomo [63].

The mathematical model is solved by an external solver. Either the open-source solver CBC or the commercial gurobi solver can be used. Afterwards, the solver results are further converted and processed. The processed results include both system-wide values (e.g., cumulative system costs and GHG emissions) as well as results for each system component. These include optimized system capacities for components with investment decisions, incurred variable and periodical costs and GHG-emissions, energy inputs and outputs, and more. In addition, for each input, output, and status (e.g., storage content) time series are provided for each component.

If the user has specified to use pre-modeling to reduce computing resources (Sec. 2.2.2) or the epsilon-constraint method (Sec. 2.1) for multi-objective optimization, iteration loops are started by adapting the model definition based on the results of the first model run.

The inner iteration loop implements the optional pre-modeling. In the first run, a highly temporal simplified model is optimized, on the basis of which techno-spatial simplifications can be adopted for a second model run with higher temporal resolution [C]. A maximum of one iteration is performed for pre-modeling.

The outer iteration loop is used to perform the epsilon-constraint method. Here, a user-defined number of model runs with different weights of the optimization criteria are carried out (Sec. 2.1). An optimized energy supply scenario as described above is returned for every model run. The results of the individual model runs are subsequently combined to comprehensive results.

After completing all scheduled model runs, the results are visualized. Among others, a Pareto front, energy amount diagrams, system graphs, and time series plots are automatically generated. Alternatively, the user can manually access all (partial) results and process them in any form.

To further visualize the user experience, screenshots of the SESMG's interfaces (spreadsheets, decisions via GUI, results) are shown in Appendix F. A detailed description of all inputs, decision options, results as well as a detailed troubleshooting (description of known errors and how to fix them) is available in the documentation of the SESMG [9].

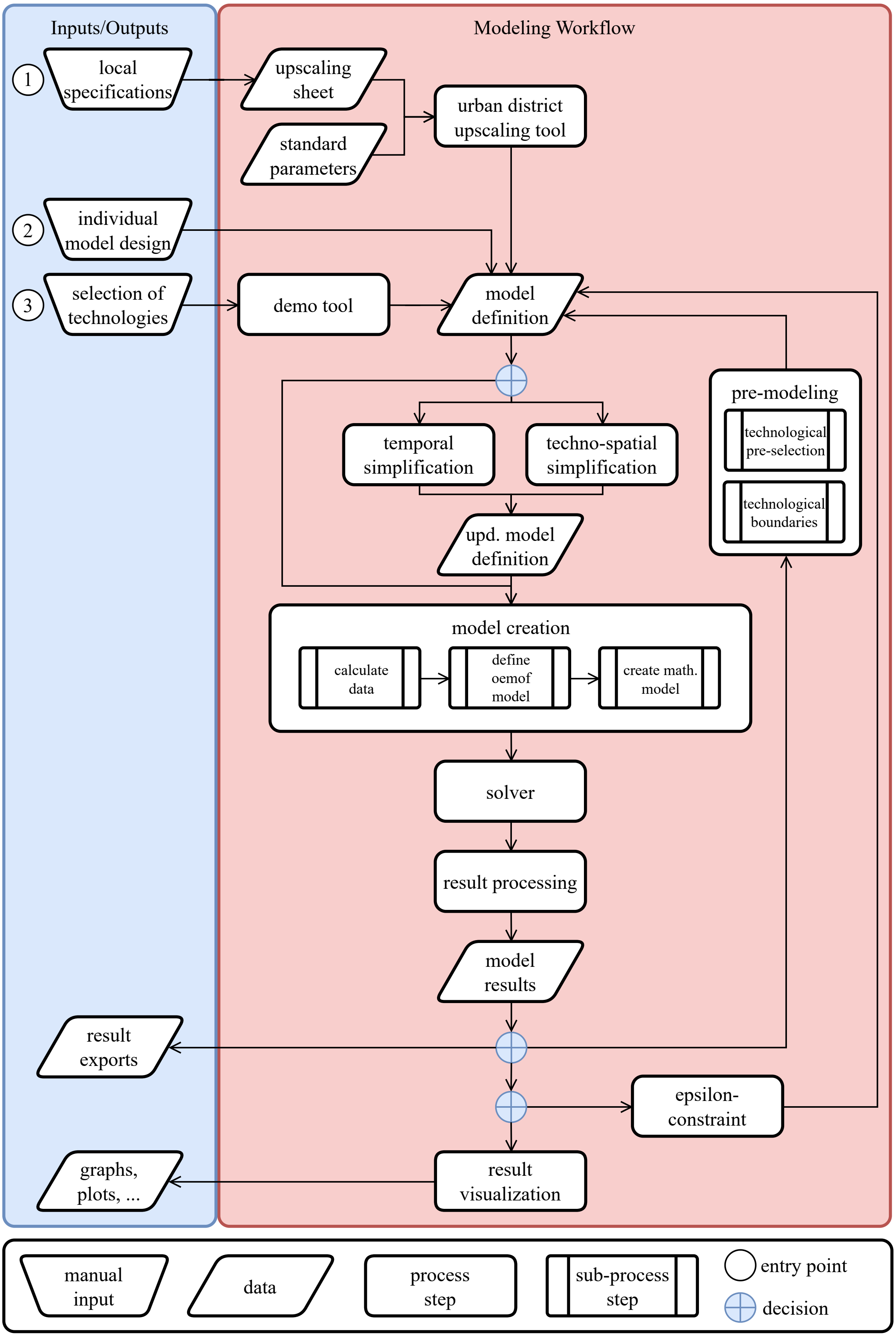

Figure 3.1: Modeling workflow of the SESMG. Decisions shown as circles are made via the GUI. Data represented as trapezoids can be accessed. Partly adapted from [9, 64]. Abbreviations: upd. = updated, math. = mathematical.

4 Case Study

The SESMG was applied in a case study to optimize a sustainable real-world urban energy system. The system is "considered sustainable if its negative impact on the society, environment, and economy is within the scope of the respective capacities [65]" [B]. Therefore a multi-objective optimization was applied to minimize both GHG emissions and financial costs. Compliance with legal regulations and technical security of energy supply were considered as unconditional requirements.

Several sensitivity analyses were then performed to determine which technologies and measures recommended for optimization are particularly robust or sensitive to changing system conditions. Based on these results, conclusions could be drawn about differentiating no-regret planning options from those with potential risk to future viability.

The system under study is a typical urban energy system and is highly transferable. It "consists of several sub-systems, i.e. buildings of various usage types (residential, commercial, sports facilities, garages), different types of residential buildings with differing population densities, roof orientations, and geothermal potentials" [E]. The results "are particularly applicable to urban energy systems in European Union (EU) member states, especially for western and central Europe, based on the characteristics of market structures, transition goals [66], climate conditions, consumption structures, and energetic potentials [67–69]" [E].

4.1 Multi-Objective Optimization

The optimization criteria were weighted differently for several scenarios by applying the epsilon-constraint optimization method (Sec. 2.1). The Pareto front in Fig. 4.1 shows that there is a clear conflict between minimizing financial costs and GHG emissions in the reference case. While the purely financially-optimized scenario causes comparatively high GHG emissions (+1 340 % as compared to the emission-optimized reference case), the emission-optimized scenario is way more expensive (+160 % as compared to the financially-optimized reference case). Starting from the financially-optimized system (uppermost point in Fig. 4.1), and moving towards the emission-optimized system along the Pareto front, the system change can be roughly divided into three phases. The phases differ in the magnitude ($<$ 100 €/t, $\geq$ 100 €/t, and $\geq$ 500 €/t) of the costs incurred to reduce GHG emissions (negative slope of the Pareto front). In the following, they will be referred to as phases of low, medium, and high GHG reduction costs (Fig. 4.1). For the reference case, the low GHG reduction cost phase includes the change from the financially-optimized scenario to P4 (4–19 €/t), the medium GHG reduction cost phase includes the change from P4 to P8 (160–274 €/t), and the high GHG reduction cost phase includes the change from P8 to the emission-optimized scenario (812–2 424 €/t).

Scenarios to the left and below the Pareto front are not technically feasible [B]. Scenarios to the right or above the curve are technically possible, but mean a violation of the optimization goals. In related studies, the status quo, i.e. the non-optimized traditional energy system, was located to the upper right of the financial optimum, which means that it is more expensive and causes more emissions than the purely financially-optimized scenario [11, 12].

The optimized energy supply mixes are shown in Fig. 4.2 for each of the scenarios presented in Fig. 4.1 with the financially-optimized scenario on the left of Fig. 4.2, the emission optimized scenario on the right side, and the differently weighted scenarios P1 to P9 in between.

Assuming energy prices (electricity, natural gas and hydrogen) as they were before the 2022 energy crisis in Europe, "within the **financially-optimized scenario**, the heat supply is primarily

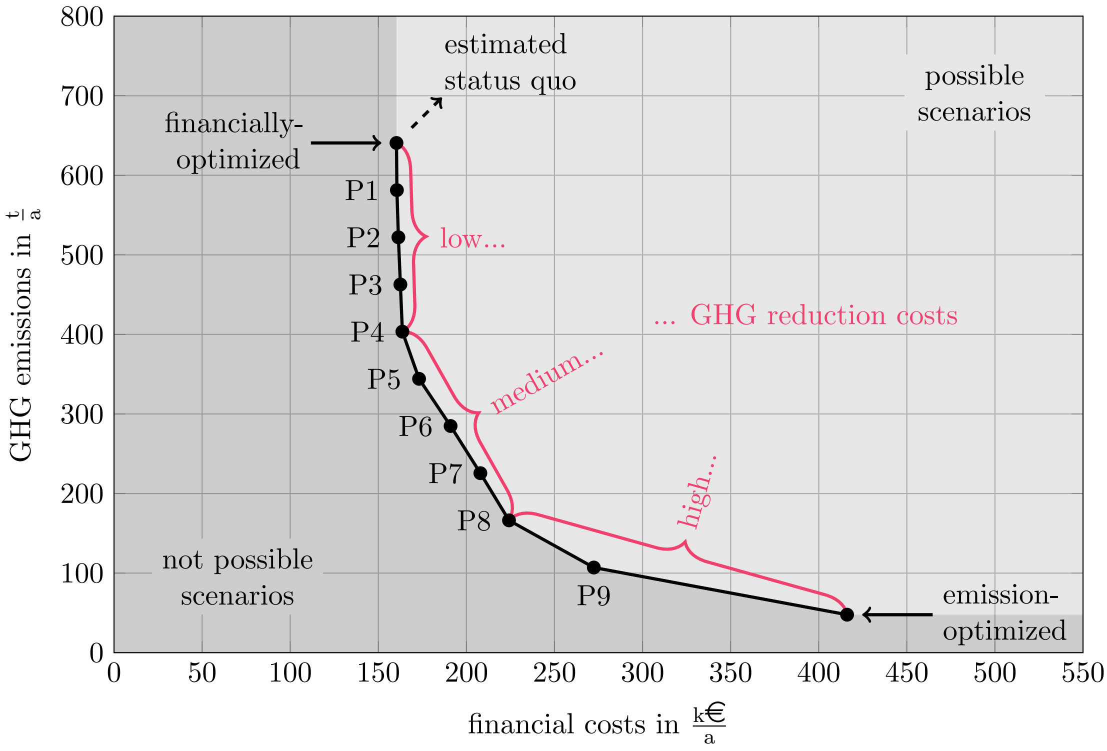

Figure 4.1: Pareto front and distinctive sections of an optimized reference urban energy system, considering financial costs and GHG emissions as optimization criteria. Adapted from [E] and [B]. Abbreviation: greenhouse gas (GHG).

based on (centralized) natural gas technologies, and the electricity is supplied by a heat-driven natural gas CHPP and PV systems. The net internal electricity production exceeds the electricity demand; therefore, large shares are exported. However, electricity still needs to be imported in small quantities at times when the internal production is insufficient" [E]. With increasing relevance of the GHG minimization criterion, the heating demand is steadily "reduced due to building insulation, and electricity demand increases due to electrification of the heat supply" [E]. The phases of low (financially-optimized scenario to P4) to medium (P4 to P8) GHG reduction costs are characterized by a progressively decentralized heat supply and increasing use of heat pumps.

In the phase of **medium GHG reduction costs**, internal electricity production due to reduced natural gas CHPP usage is not sufficient to cover the increased electricity demand from heat pumps. Therefore, the total costs increase due to (expensive) electricity imports [E]. The heat production of heat pumps is adjusted to the load profiles of PV systems and "thermal storages are utilized more frequently [...] to match heat supply with consumption" [E]. Increased financial costs in the phase of **high GHG reduction costs** (P8 to emission-optimized scenario) are mainly caused by high investment costs of hydrogen technologies and battery storages.

Finally, "in the **emission-optimized scenario**, the remaining heating demand of maximum possible insulated buildings is provided by ASHPs, GCHPs and solar thermal systems" [E]. Decentralized ASHPs are preferred over centralized ones for this scenario, since the heat source is available both centrally and decentrally, and the DH pipes must be newly installed. This avoids heat losses and life-cycle emissions for the construction of DH pipes [E]. "PV systems and hydrogen CHPP are used for electricity supply and battery storages for load shifting. The PV potential is not fully utilized in any of the scenarios, especially with respect to PV modules deviating more than 65° from the south axis. Solar thermal systems were only considered in the emission-optimized scenario on surfaces without PV potential" [E].

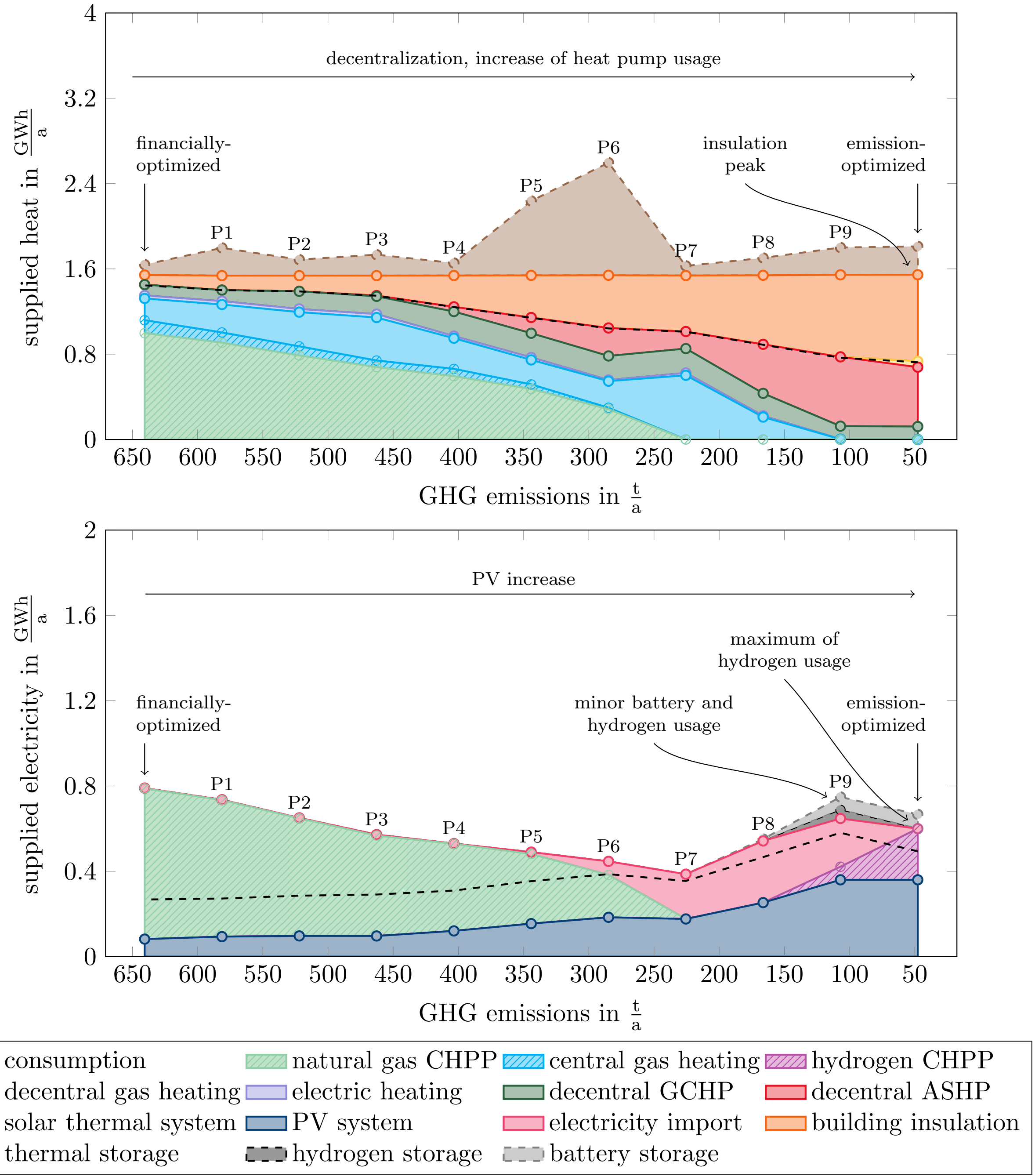

Figure 4.2: Heat (top) and electricity (bottom) supply in the optimized reference case scenario in dependency of weighting the two optimization criteria (financial costs and GHG emissions). The shown values represent aggregated energy amounts supplied in each scenario. Technologies that were not designed during optimization are not shown. Adapted from [E]. Abbreviations: air source heat pump (ASHP), combined heat and power plant (CHPP), ground coupled heat pump (GCHP), greenhouse gas (GHG), photovoltaic (PV).

4.2 Sensitivity Analysis

A set of sensitivity analyses were applied to analyze the impact of changing conditions with regard to GHG emissions (total GHG emissions, GHG emissions of imported electricity and hydrogen), energy prices (natural gas, electricity, hydrogen, and a combination of all), and effective energy demands (electricity, demand, heating demand, and population density) [E]. The variations of these parameters were each applied to the financially-optimized scenario and the GHG emissions-optimized scenario of the multi-objective optimization [E].

Both steady and sudden changes in boundary conditions can have a significant impact on the optimization of urban energy systems. For example, the sharp increase of energy prices during the 2022 energy crisis in Europe (particularly natural gas) had significant impact on the optimized design of urban energy systems. While pre-crisis values were assumed for the financial analysis in Sec. 4.1, the sensitivity analyses of changing energy prices showed that the viability of natural gas technologies significantly decreased with a respective price increase. In fact, the analyzed reference systems financially-optimized scenarios approached the GHG-optimized scenario with rising energy prices.

To ensure that optimized energy systems will be viable in the future, even under changing boundary conditions, it is recommended that they are suitable for both financial and emissions-based optimization, and that they are robust at least with expected trends of increasing GHG mitigation requirements, rising energy prices, and declining GHG emissions from imported electricity [E]. Based on the sensitivity analyses, the following technologies and measures have proven to be robust to the expected changing boundary conditions and are therefore particularly recommended for the optimization of urban energy systems:

- **Demand Reduction:** Reducing relative and absolute energy demands positively improves both financial costs and GHG emissions [E]. Demand reductions can be realized by building insulation, behavioral changes, and reducing living space per inhabitant [E]. However, modeling and implementation of the latter two aspects are separate research fields in their own right.
- **Decentralized heat pumps:** In optimized systems, “the usage of decentralized heat pumps for heat supply [...] steadily increases or at least remains at the same level” [E], under expected changing boundary conditions. “As far as heat potentials can be used both central and decentral, decentralized heat pumps allow a more viable use compared to centralized heat pumps due to less heat losses, investment costs, and life-cycle emissions of DH pipes” [E].
- **PV systems:** “The optimum size of the PV systems varies, but a certain amount with a region-specific maximum azimuth deviation from the south axis is highly robust. This maximum azimuth deviation increases with additional restrictions on total GHG emissions and increasing energy prices” [E].
- **Thermal storages:** Thermal storages are mostly more suitable for shifting volatile electricity supply than battery storages. This applies especially for systems with electrified heat supply. “Depending on the type of heat supply, either centralized or decentralized thermal” [E] storages are preferable.
- **Electricity exchange:** The exchange of electricity with higher-level energy systems (import, export) “reduces the need for local electricity storage capacities and oversized plants to meet peak loads. However, this approach may be limited due to transmission capacities and the ability of neighboring and higher-level systems to provide the necessary load exchange. [...] Fewer restrictions apply to the local exchange of locally produced (renewable) electricity between sub-systems. It [...] reduces necessary storage capacities and, by

avoiding electricity imports, financial costs and GHG emissions" [B].

On the other hand, some technologies and measures are particularly sensitive to changing boundary conditions and are therefore less suitable for robust optimized urban energy systems:

- **Solar thermal systems:** Solar thermal systems and PV systems compete with each other for suitable roof surfaces. PV systems are mostly preferred over solar thermal systems in optimized energy systems. Therefore, it is recommended to consider solar thermal systems only for surfaces where PV use is not viable [E].
- **Decentralized natural gas technologies:** "The use of decentralized natural gas technologies for heat supply is very sensitive to the analyzed system changes, and [...] their usage is partially or even completely reduced in optimized scenarios" [E].
- **Generalized implementation of DH networks:** "The viability of implementing new DH networks is very sensitive on total GHG emissions, energy prices, and heating demands" [E]. Therefore it is recommended to analyze and plan the exact connectability of buildings to DH networks in detail and with caution. "The generalized implementation of DH networks for entire areas, for example, in the context of a connection obligation" [E], is highly sensitive to changing boundary conditions.
- **High capacities of battery storages:** The usage of battery storages are preferably used in the emission-optimized scenario. Their usage is "sensitive on GHG emissions of imported energy (electricity and hydrogen) and the system's energy demands (electricity and heat)" [E]. Furthermore, battery storages with large capacities cause environmental impacts in other categories than GHG emissions, such as terrestrial eco toxicity. This causes, in some cases, an environmental damage according to the disability-adjusted life years (DALY)-index which is greater than the benefit gained through saved GHG emissions [15].
- **Hydrogen for building energy supply:** The usage of green hydrogen for building energy supply "is not viable from a financial perspective. It is especially sensitive to the system's absolute energy demands, and its capability for emission reduction is only viable if GHG emissions of imported electricity are higher than electricity supplied by the hydrogen CHPP" [E]. The use of green hydrogen is therefore highly sensitive, and "the use of non-green hydrogen is no option for system optimization at all" [E].

Note that all of the above recommendations apply to optimized energy systems. Compared to non-optimized systems, even non-robust technologies can bring an improvement. For example, it can be assumed that the use of solar thermal systems on a suitable roof surface is better than not using the roof surface for energy supply at all. If an energy system to be optimized consists of existing facilities or infrastructure not considered in the reference case, this can have a significant impact on the optimization results. For example, if a system consists of an existing and possibly depreciated DH network, centralized heat supply technologies may be more valuable, especially if they can utilize heat sources that cannot be used decentrally (e.g., river water or industrial waste heat).

5 Discussion

5.1 Interactions of Challenges

All common challenges of modeling and optimization of urban energy systems have been addressed in this thesis and the related publications. Synergies and trade-offs between the overlap of individual challenges have emerged, as well as aspects and gaps which should be addressed in future modeling projects.

There are several challenges in modeling and optimizing urban energy systems. Because of the interactions of these challenges, some solutions can address more than one challenge, while others require trade-offs among multiple challenges.

Reducing model **complexity** is necessary to reduce computing effort, to lower the entry threshold for applying energy system modeling tools, and to enable the communication of results to a wide audience. Approaches to reduce the computing effort to a tolerable level poses many conflicts with other challenges. The most straightforward way to reduce model complexity is to utilize knowledge of energy systems in order to keep the model as simple as possible. The required knowledge increases the entry threshold to energy system modeling and is therefore a hurdle in terms of applicability for a wide range of potential users. On the other hand, any automated application of model-based methods for complexity reduction, which are applicable without in-depth knowledge of energy systems, will, in most cases, reduce the spatial and temporal resolution and coverage of a model. This may lead to a reduction of the required effort for data collection, but primarily increases the model uncertainties and subsequently the risk of misinterpretation, especially with respect to the sizing of sector-coupling technologies and energy storages.

There is a general trend in scientific research towards **openness** of methods and data. Only open science is truly reproducible science and allows transparent communication of input data, assumptions, uncertainties, and results. Open models will facilitate the selection of model properties and features as well as the collection of data in subsequent projects. However, there are limitations associated with this concept, mainly related to the choice of modeling tools (including mathematical solvers) and the use of input data. For example, efficient mathematical solvers used to reduce computing effort are often not available under open-source licenses. Also, non-open input data is often of higher quality than open data. Therefore, a compromise must be made where non-open tools or data may be used to a very limited extent.

Poorly chosen **model properties or features** lead to an amplification of other challenges. For example, too low defined resolutions or system boundaries can lead to structural uncertainties. On the other hand, overly ambitious resolutions or system boundaries of a model can lead to a significant increase in computing effort, limited applicability of the model due to high input effort, and excessive demands on data quality.

Great effort during **data** collection and quality assurance will largely reduce parametric uncertainties.

The analysis of challenges and their interactions shows that the challenges of model properties and features, input data, and openness are associated with the fewest trade-offs. They are straightforward to address and, in some cases, allow for parallel improvement of other challenges.

The complexity challenge is much more difficult to address because it conflicts with several other challenges. The reduction of complexity is particularly relevant for high spatial resolution optimization of modern urban energy systems. The inevitable trade-off between complexity and uncertainty is particularly difficult and, overall, poses the greatest challenge in modeling and optimizing urban energy systems. Therefore, it has received great attention in this work. During model development, the model complexity was increased step by step (Tab. 2.2), increasing the need to simplify the model itself. With the model-based simplification methods developed in publication [C], much larger and more complex systems could be modeled with the same computing resources. Associated uncertainties, especially in the design of sector coupling technologies, storage technologies, and district heating (DH), have been quantified, classified, and transparently communicated.

5.2 Model Limitations

The SESMG has significantly lowered the **entry threshold** for modeling urban energy systems. However, users still "must have a certain basic knowledge of energy systems and energy engineering" [D], and the "target groups of the SESMG [...] are (urban) energy system planners and researchers in the field of energy engineering" [D]. By further automating the modeling process through the definition of system boundaries with GIS interfaces, perhaps the entry threshold could be lowered to a point where non-specialist users could benefit. However, necessary regional specific data sets are not available in a uniform format and, furthermore, are often not openly available. This hinders the implementation of such a feature.

The applied multi-objective optimization approach refers to the goals of global GHG emission reduction and system-wide **economic costs**. For GHG emissions, in the sense of climate protection as a global phenomenon, this is the correct chosen optimization goal. However, system-wide financial cost optimization involves minimizing the aggregated costs for all stakeholders. The distribution of these savings amongst stakeholders is not considered. The actual distribution may even result in additional costs for some stakeholders while others have dramatically reduced costs. To avoid such bias, stakeholder-specific costs can be optimized separately to ensure that costs are distributed fairly. However, this would introduce a new level of complexity.

Another limitation is the model **uncertainty** and its impact on the relevance and applicability of the model results. The impact of known uncertainties, such as the use of standard load profiles or model-based temporal simplifications, can be well estimated and classified by modelers. Unknown uncertainties, on the other hand, pose a much greater problem because it is not known how they will affect the model results.

This work makes the greatest effort to follow open-science strategies in all aspects. However, for some of the applied models, the commercial gurobi **solver** was used for solver-based reduction of computing efforts. Theoretically, the models can be solved with open solvers such as CBC, but with a significantly increased run-time. At this point, a compromise was made at the expense of openness. However, in this way, the results obtained and the respective uncertainties and assumptions could still be communicated transparently.

Various consumption sectors of building types in urban energy systems were considered in the individual models of this work. The **mobility sector**, however, was excluded. This is justified by the need to model social behavior patterns in order to generate consumption profiles and utilization potentials. Due to the increasing relevance of sector-coupled electric mobility with decentralized charging options in urban energy systems, this aspect is highly relevant for future modeling. In this way, it will be possible to investigate whether and how the electricity demand for mobility can be covered locally, and how the battery storage of electric vehicles can be used during parking times for load balancing within urban energy systems.

Coupling the results of an urban energy system optimization model with models from other urban resources [16] and a LCA model [15] has shown that there are relevant interactions and feedback mechanisms. Automated **model integration** of all urban planning aspects and global environmental impacts that potentially intersect with urban energy systems would ensure that all synergies and conflicting goals could be identified. However, this will, again, lead to increased model complexity and associated increased data requirements.

To ensure the best possible impact of the modeling results, further communication is needed even after the modeling project has ended. The development of concrete recommendations for **legislative adjustments** together with policy experts, by also taking social aspects into account, can enable nation-wide or even EU-wide impact.

5.3 Practical relevance

With the SESMG and the methods used in it, a modeling procedure is provided, that (1) produces outcomes with high-spatial resolution, (2) applies optimization methods involving multiple criteria, (3) considers a wide range of energy and consumption sectors, (4) is applicable on standard personal computers, and (5) is applicable without any programming knowledge. Thus, an important gap in the landscape of models for the optimization of sustainable mixed-use multi-energy systems is closed.

The developed modeling methods are suited for investigations regarding feasibility of energy supply concepts, for the recommendation of a technology mix, and for the identification of savings potentials. The final planning and practical implementation follows such modeling and is carried out by the respective planners. The SESMG and further methods developed are regularly applied in research projects [57], privately and publicly funded planning projects (one completed, two ongoing studies), as well as academic theses [46, 64, 70–75]. The theses included (1) analyzes of modeling methods, such as the modeling of residential load profiles or DH systems, (2) general investigations on the viability of certain technologies in urban energy systems, or (3) concrete planning projects ranging from small groups of buildings to entire neighborhoods. Both in research projects and in practical planning projects, the applied methods have proven to be relevant and suitable for the optimization of urban energy systems. The SESMG will also be used in planned and upcoming projects. Suggestions for future research strategies are presented in Sec. 6.

The recommended technologies and measures for optimized urban energy systems (Sec. 4) are widely transferable and can be an important decision-making support for the planning of urban energy systems. If the recommendations are implemented on a widespread basis, the resulting transformation can make a significant contribution to meeting national and international climate protection targets. However, there are some practical challenges. The need to invest, in combination with a lack of willingness of individual stakeholders to adapt, can be an obstacle, especially in existing systems. In addition, there are legal constraints on the implementation of some of the recommendations. For example, the local exchange of electricity within local energy markets is subject to a number of legal constraints. Removing these barriers through policy action is important to maintain the necessary pace of transformation of urban energy systems.

5.4 Comparison with Recent Literature

The challenges of energy system modeling have been extensively listed in the literature (e.g., [2, 7, 20–38]. These publications deal with the general challenges of energy system modeling, with challenges of specific types of energy system models, or with specific sub-challenges. This work fills a gap by providing a complete categorization of all the challenges relevant to the modeling and optimization of urban energy systems, and by providing concrete approaches to overcome them.

Studies with a focus on the design of (urban) energy systems have identified measures and technologies which are suitable to help achieving climate protection targets and/or to reduce financial costs. However, the model results provided by this work fill a gap by analyzing the full range between the competing objectives of financial minimization and minimization of GHG emissions, and further communicating the impact of changing external boundary conditions. The focus lies on urban energy systems, and all local interactions synergies and trade-offs between sub-systems and various energy sectors are considered [E]. This leads partly to similar results, but partly also to contradictions with the existing literature.

Consistent findings are about (1) **reducing energy demands** by high levels of building renovation [76, 77] and adjusting consumption patterns [78], (2) (partial) phase-out of **natural gas technologies** [76], (3) increasing electrification of the heat supply [77, 79], especially by **heat pumps** [76, 79], (4) using **thermal storages** for electric load shifting [79, 80], and (5) preferring the usage of **PV systems** over **solar thermal systems** on suitable surfaces [81]. Also, the findings that (6) the use of **hydrogen technologies** for buildings will only become viable under significantly lowered prices [82], but that they could nevertheless enable a reduction in GHG emissions under certain circumstances [77], are in consensus with recent literature.

Regarding the recommendation for more **exchange of electricity** between sub-systems and higher-level systems, there is no clear consensus in the literature. While some studies call for more autarky of sub-systems [83, 84], others call for an increase in the exchange between individual systems [79, 85]. This work provides further arguments and insights for this discussion by showing how relevant the exchange of electricity is both between sub-systems and with higher-level systems.

Partially deviating recommendations exist in the literature with regard to the viability of **DH networks** for optimized systems. This is generally due to two different assumptions concerning the boundary conditions. (1) DH networks can have a more positive effect on optimized systems if the building density is so high that decentralized heat pump usage is not possible, or if heat sources are available that can only be used centrally, such as deep geothermal energy [86], waste heat [87], or river and sea water [88]. (2) If DH networks are already installed in a system and may be depreciated, neither investment costs nor emissions may be included in models. However, new DH networks may also become more relevant in the future, when so-called “5th generation DH and cooling systems” gain relevance in planning practice [89, 90]. These systems can be used to exchange thermal energy between a number of sub-systems, similar to the local exchange of electricity [91].

When residential building energy systems are considered in isolation, the use of **battery storages** is often recommended, usually focusing on increasing self-sufficiency or financial costs of individual buildings [92–94]. Battery storages may in principle provide an improvement over a non-optimized system. However, the ability of battery storages to robustly optimize urban energy systems is very limited when competing with sector-coupled thermal storages and local electricity exchange. This discussion could take new directions if bi-directional charging of electric vehicles becomes technical standard and if battery storage of electric vehicles can be used for urban load shifting.

6 Conclusion and Outlook

With the developed methods and the Spreadsheet Energy System Model Generator (SESMG), a modeling procedure was created in this work that allows the modeling and optimization of urban energy systems. The SESMG provides a low entry threshold for modelers and planners, is very flexible, is applicable to existing and newly planned urban energy systems, and can be operated on standard personal computers.

The findings of this work lead to the following recommendations for the modeling and optimization of urban energy systems:

- **Multi-objective optimization** approaches should be applied, including at least financial costs and greenhouse gas (GHG) emissions as optimization criteria, with holistic consideration of **all relevant energy and demand sectors**. Appropriate model properties, features and system boundaries should be selected.
- **Model complexity** should be reduced where possible to avoid issues with to high computing efforts, as well as limited accessibility of methods and results for non-experts.
- Emphasis should be placed on the **openness** of the applied methods, input data, assumptions, and results.
- **Data** standards should be defined and uniformity of data sets should be guaranteed. If assumptions are necessary, it is recommended that these are communicated transparently.
- **Uncertainty** assessments should be conducted. All known uncertainties are recommended to be transparently communicated.
- **Communication** with modelers, interdisciplinary researchers, planners, policymakers and the public should be carried out before, during and after a modeling project to ensure relevance and feasibility of the results.

Individual modeling for the energy system of each investigated area helps to account for all relevant system-specific effects. However, based on the model of a transferable reference case, there are measures and technologies, which can be particularly recommended for the optimization of urban energy systems. Assuming expected trends of increasing GHG mitigation requirements, increasing energy prices, and decreasing GHG emissions from imported electricity, the following ones are suggested:

- Relative and absolute **energy demand reduction** through building insulation, behavioral changes, and reductions in living space per inhabitant
- **Decentralized heat pumps** for heat supply
- **Photovoltaic (PV) systems** on (roof) surfaces with suitable orientations
- **Thermal storages** for electrical load shifting
- **Exchange of electricity** between sub-systems as well as with higher-level energy systems

On the other hand, some technologies and measures carry the risk of being not suitable for optimized urban energy systems under expected trends. These include:

- **Solar thermal systems** on (roof) surfaces that are suitable for PV usage
- **Decentralized natural gas** heating technologies
- Generalized and comprehensive implementation of new **district heating (DH) networks**
- **Battery storages** with high capacities
- **Hydrogen technologies** for building energy supply

The limitations of the applied models provide a basis for further projects. In particular, the integration of the mobility sector, the integration of interdisciplinary model aspects, the stakeholder-specific cost optimization and the conceptualization of local energy markets are highly relevant for future research. A further reduction in the computational resources required to enable modeling of even more complex energy systems and an even lower entry threshold for modeling and optimization of urban energy systems are desirable.

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Appendix

A Publication: Modeling and optimization of multi-energy systems in mixed-use districts: A review of existing methods and approaches

Table A.1: Fact sheet publication [A]

Title:
Modeling and optimization of multi-energy systems in mixed-use districts: A review of existing methods and approaches

Authors:
Christian Klemm, Peter Vennemann

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Authors contribution:
Christian Klemm: Conceptualization, Methodology, Investigation, Formal analysis, Software, Visualization, Writing – original draft. Peter Vennemann: Funding acquisition, Supervision, Writing – review & editing.

Abstract:
About 75 % of the world's energy consumption takes place in cities. Although their large energy consumption attracts a large number of research projects, only a small fraction of them deal with approaches to model energy systems of city districts. These are particularly complex due to the existence of multiple energy sectors (multi- energy systems, MES), different consumption sectors (mixed-use), and different stakeholders who have many different interests.
This contribution is a review of the characteristics of energy system models and existing modeling tools. It evaluates current studies and identifies typical characteristics of models designed to optimize MES in mixed-use districts. These models operate at a temporal resolution of at least 1 h, follow either bottom-up or hybrid analytical approaches and make use of mixed-integer programming, linear or dynamic.
These characteristics were then used to analyze minimum requirements for existing modeling tools. Thirteen of 145 tools included in the study turned out to be suitable for optimizing MES in mixed-use districts. Other tools where either created for other fields of application (12), do not include any methodology of optimization (39), are not suitable to cover city districts as a geographical domain (44), do not include enough energy or demand sectors (20), or operate at a too coarse temporal resolution (17). If additional requirements are imposed, e.g. the applicability of non-financial assessment criteria and open source availability, only two tools remain.
Overall it can be stated that there are very few modeling tools suitable for the optimization of MES in mixed-use districts.

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ABSTRACT

About 75% of the world's energy consumption takes place in cities. Although their large energy consumption attracts a large number of research projects, only a small fraction of them deal with approaches to model energy systems of city districts. These are particularly complex due to the existence of multiple energy sectors (multi-energy systems, MES), different consumption sectors (mixed-use), and different stakeholders who have many different interests.

This contribution is a review of the characteristics of energy system models and existing modeling tools. It evaluates current studies and identifies typical characteristics of models designed to optimize MES in mixed-use districts. These models operate at a temporal resolution of at least 1 h, follow either bottom-up or hybrid analytical approaches and make use of mixed-integer programming, linear or dynamic.

These characteristics were then used to analyze minimum requirements for existing modeling tools. Thirteen of 145 tools included in the study turned out to be suitable for optimizing MES in mixed-use districts. Other tools where either created for other fields of application (12), do not include any methodology of optimization (39), are not suitable to cover city districts as a geographical domain (44), do not include enough energy or demand sectors (20), or operate at a too coarse temporal resolution (17). If additional requirements are imposed, e.g. the applicability of non-financial assessment criteria and open source availability, only two tools remain.

Overall it can be stated that there are very few modeling tools suitable for the optimization of MES in mixed-use districts.

1. Introduction

About 75% of the world's energy consumption takes place in cities, which in turn causes 70% of worldwide carbon dioxide emissions [1]. These numbers will likely increase with a projected doubling of the urban population by 2050 [2]. To reduce the energy consumption associated with this growth, it is mandatory to increase the energy efficiency of urban systems. While the field has attracted significant research on the potential of reduction of energy use [3], only 14% of the documented research projects have addressed the subject of energy efficiency at the district level [4]. This contribution provides an overview of the methods and tools used to model the optimization of energy systems at urban district levels as these are manageable urban planning units.

An energy system is defined as a "combined process of acquiring and using energy in a given society or economy" [5]. The focus of this contribution lies on multi-energy systems (MES) of mixed-use districts, i. e. on the acquisition and consumption of various forms of secondary energy (e.g. electricity, heating, cooling) in urban districts characterized by diverse purposes (e.g. residential buildings alongside industry and/or agriculture).

Models are an essential tool for planning and operating energy systems. In this context, a model may be understood as a simplified representation of a real world's energy system [6]. While models may be developed in many different ways, we focus on mathematical and coded models [3]. In addition to the term "model", "model generator" and "modeling framework" are also frequently used in the modeling landscape. Although these terms seem to have similar meanings, it is important to make precise distinctions. Model generators are tools that can create models with certain predefined analytical and mathematical properties [7]. The use of model generators can save time. However, due to these predefined properties, there are also limitations with respect to the flexibility of the models they generate. Modeling frameworks are structured toolboxes that include several model generators and specific sub-models [7]. Due to the wider range of tools provided with them,

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List of acronyms

C	capital costs
CEA	City Energy Analyst
CED	cumulated energy demand
Cont	continental
Conv	conventional generation
D	disposal
DP	dynamic programming
E	energy
El	electricity
EE	energy efficiency
Em	emissions
EPT	energy payback time
F	fossil resources
Fi	financial
GIS	geographical information system
H	heat
Hyd	hydrogen
Int	international
LA	level of autonomy
LCE	levelized costs of energy
LESP	loss of energy supply probability
Loc	local
LP	linear programming
m	mass
MES	multi-energy system
MIP	mixed-integer programming
Nat	national
O	operation
P	production
p	share of energy
Reg	regional
Ren	renewable generation
S	social
Stor	storages
T	time

there are fewer limitations, but their use requires more coding effort than the use of a model generator.

This is the first contribution addressing the question whether any existing tools of energy system modeling are suitable for the optimization of MES in mixed-use city districts. For this purpose, existing modeling tools are identified, minimum requirements for these tools to be applicable are defined, and the tools are evaluated accordingly. The next phase of the review entails discussing general deficits and making recommendations for further research.

2. Review method

To answer the research question formulated in the introduction, it is first necessary to determine and examine the general features and properties of energy system models (Section 3). The first step thus meant researching review articles on energy system models using Google Scholar as well as FINDEX, Münster University of Applied Sciences' library system. Search terms such as "energy system modeling review" were used. Additional articles were uncovered by looking at these articles' citations as well as by using "cited by" functions. The next step was to search additional articles on the specific properties of energy system models by using the same search methods. A total of 33 review articles have been evaluated [8–41].

The following step required describing and elaborating on the specific characteristics of models for the optimization of MES in mixed-use city districts. This in turn meant identifying the relevant articles using the same methods as above, but including search terms such as "energy AND optimization AND (quarter OR district OR city OR neighborhood)". The corpus included studies published between January 2014 and October 2019. In total, 30 studies have been included [42–72].

The second part of the paper (Section 4) presents and evaluates existing modeling tools. Different reviews [12,14,22,36–41] as well as complementary research with the above mentioned search engines were used as data sources. Only tools that were mentioned in peer-reviewed literature were included in the study. For the specification of specific model properties, "grey literature" (websites, documentations of tools, theses) was also used.

Based on the characteristics of models for the optimization of MES in mixed-use districts (Section 3), we defined minimum requirements that the modeling tools had to have for this purpose. These requirements were then used to categorize and evaluate the various tools.

3. Properties of energy system models

Several reviews exist in the area of energy system modeling. They can be categorized into reviews discussing.

- energy system models in general,
- specific properties of energy system models,
- energy system models for a specific scope of application, and
- existing modeling tools.

Reviews discussing **energy system models in general** provide a broad overview of existing modeling approaches and properties of energy system models. For example, Herbst et al. [8], Jebaraj and Iniyan [9] and Subramanian et al. [10] have presented overviews about existing modeling approaches in general. Foley et al. [11] have reviewed electric system models, while Hall and Buckley [12] evaluated and categorized energy system models in Great Britain. Pfenninger et al. [13] as well as Lopion et al. [14] have discussed current challenges in energy system modeling.

Other reviews deal with **specific properties of energy system models.** For instance, Lund et al. [15] discussed differences between the methodologies of simulation and optimization; Weijermars et al. discussed the methodology of optimization [16] (see Section 3.1, "*Methodology*"); Stein [17] summarized several *assessment criteria* of electricity production technologies; van Vuuren et al. [18] reviewed the differences between the analytical approaches of top-down and bottom-up approaches (see Section 3.4, "*Analytical Approach*"). Moreover, Kalogirou [19] and Zahraee et al. [20] dealt with the *mathematical approach* of artificial intelligence, and Pfenninger et al. [21] provided an overview of the importance of open data and software in energy research (see Section 3.6, "*Reusability*").

There have also been various approaches to using **energy system models for a specific scope of application.** One widely discussed topic was the integration of renewables into existing energy systems (Ringkjøb et al. [22], Després et al. [23], Bhandari et al. [24], Olsthoorn et al. [25], Luna-Rubio et al. [26]). Gu et al. [27] and Fathima et al. [28] focused on the optimization of microgrids; Suganthi and Samuel [29] on energy demand forecasting; Mancarella [30] on models for multi-energy system (MES) concepts; and Hiremath et al. [31] on models for decentralized energy planning. In the context of this paper, modeling approaches of the energy systems of buildings and residential areas are also of interest. Harish et al. [32] reviewed building energy system models in general, Nguyen et al. [33] looked at different approaches to increasing the energy efficiency of buildings, and Ma et al. [34] reviewed methods of retrofitting buildings using models. Swan and Ugursal [35] analyzed techniques to model end-use energy consumption in the residential sector, while Keirstead et al. [3] provided a more general overview of the approaches, challenges and opportunities facing urban energy system models.

There are also reviews specifically focusing on **existing modeling tools**. Allegrini et al. [36] analyzed 24 existing modeling tools with a focus on the building sector. Ringkjøb et al. evaluated 75 modeling tools with regard to their suitability for modeling renewable energies [22]. Van Beuzekom et al. [37] discussed 13 optimization and planning tools on their suitability for sustainable urban development; Lopion et al. presented 24 currently used tools for energy system modeling [14]; Hall and Buckley classified 22 tools used in the UK [12]. Bhattacharyya and Timilsina [38] presented six tools with a wide scope of application; Connolly et al. [39] discussed 37 tools for analyzing the integration of renewable energies into various energy systems. Suresh and Meenakumari [40] looked at 17 tools, while Sinha and Chandel [41] presented 19 tools that modeled hybrid renewable energy systems.

These articles show that energy system models could be categorized according to their purpose, methodology, assessment criteria, and structural and technological detail. They also take different analytical and mathematical approaches, and vary according to their reusability. These categories are shown in Fig. 1 together with additional characteristics.

3.1. Methodology

The methodology of energy system models can be classified into the three main categories of.

- optimization,
- forecasting, and
- back-casting (Fig. 2).

Optimization models are used for the purposes of investment or operational decision support. The model simulates all possible scenarios of a system, and rates them according to an objective function. Minimizing or maximizing this function helps the researcher to then identify an "optimum" scenario [13,15]. The optimum scenario could, for instance, consist of a preferred mix of technologies [16] or of certain operation modes [73]. Optimization models are the most common type for district-level energy system modeling. Prieto et al. for instance, used models to analyze and optimize the district heating system of Vienna [42]. Fonseca et al. implemented "City Energy Analyst" (CEA), which is a model framework for the analysis and optimization of energy systems in neighborhoods and city districts [61]. Bakken et al. created a model generator for the quantification of the minimum total energy system costs to meet predefined energy demands of electricity, gas and heating [75].

Forecasting models are used for the purposes of system analysis and scenario analysis. They investigate the behavior of a system under given conditions and attempt to predict the system's future behavior or specific parameters of the system [15], such as the future energy demand [29]. Forecasting is often referred to as "simulation". However, since simulations are also components of optimization and back-casting models, this term is misleading. The term "forecasting" will therefore be used instead from here on. Forecasting models are not used very often in district-level applications. However, they are very useful when forecasting the demand for renewable energy. Powell et al. for instance, used forecasting models to predict the heating, cooling and electrical loads of a college campus up to 24 h in advance by using weather data as input variables [65].

Back-casting models are used for specific scenario analysis. The researchers lay out an envisaged future state or set of properties of a system, and the back-casting model develops realistic paths that would lead to these future conditions [12]. This kind of model comes into use during the planning or implementation of political goals [74]. The utilization of back-casting models is even less relevant for applications at the district level. They are more often used for larger system scales, e.g. for nationwide or worldwide energy systems. The World Energy Council, for example, regularly identifies pathways that policymakers should select to achieve specific goals in the world energy system [76].

Several model types may be combined within a single model. Kampelis et al. for instance, implemented a tool to predict the energy demand at the levels of individual buildings as well as district (forecasting) and which would customize the operation of available micro power plants and storage facilities to minimize the energy purchased from external sources (optimization). When they applied their tool to an industrial district in Italy, they found cost savings of up to 15.39% [51].

3.2. Assessment criteria

Identifying the "best" future scenario by optimizing MES in models of mixed-use districts means selecting and applying different assessment criteria. These may be categorized into.

- Financial,
- Energy efficiency,
- Environmental,
- Technical, and
- Social/economic criteria.

Financial criteria aim to identify the least expensive scenario. Useful criteria could include the annualized capital costs C_{cap_a}, the annual system costs C_a, the payback time, the annual net profit, or the levelized costs of energy *LCE*.

The annualized capital costs C_{cap_a} may be calculated using an estimated rate of interest i and an estimated service lifetime of the system components Y in years [28]:

$$C_{cap_a} = C_{cap} \cdot \frac{i(i+1)^Y}{(i+1)^Y - 1}$$

Next, the annual system costs can be calculated from the annual capital costs C_{cap_a} plus additional costs for operation (including maintenance) C_{O_a} [28]:

$$C_a = C_{cap_a} + C_{O_a}$$

The levelized costs of energy (LCE) are calculable from the annualized system costs C_a and the energy delivered over the same period E_a [77]:

$$LCE = \frac{C_a}{E_a}$$

Additional financial criteria could include total life cycle costs or total capital costs [17].

Energy efficiency criteria may measure energy balances such as primary energy use, secondary energy use or consumer (end-user) energy use [53]. Alternatively, criteria measuring the level of autonomy *LA* of the system or the loss of energy supply probability *LESP* [26,28] can aid in measuring the degree of self-sufficiency in a system.

We can study energy balances by determining cumulated energy demand *CED*, which in turn can be calculated by looking at the total value chain of an energy system's components. This means calculating the energy demands of production (P), of operation (O) (including maintenance), and of disposal (D) after the operational lifetime of the system [79]:

$$CED = CED_P + CED_O + CED_D$$

The energy payback period *EPP* describes how long it would take to break even on the cumulated energy demand *CED* [80]:

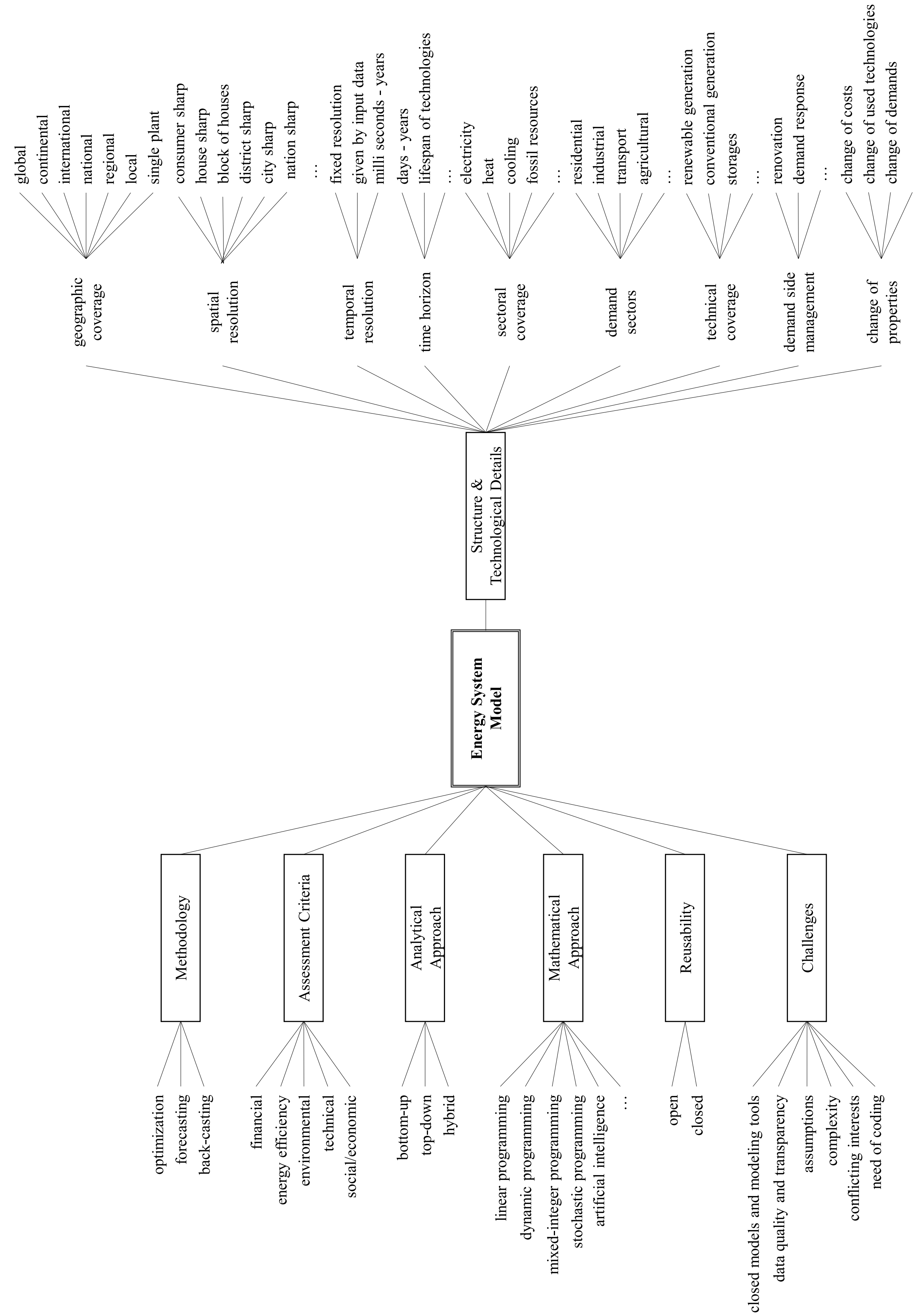

Fig. 1. Properties and possible categorizations of energy system models.

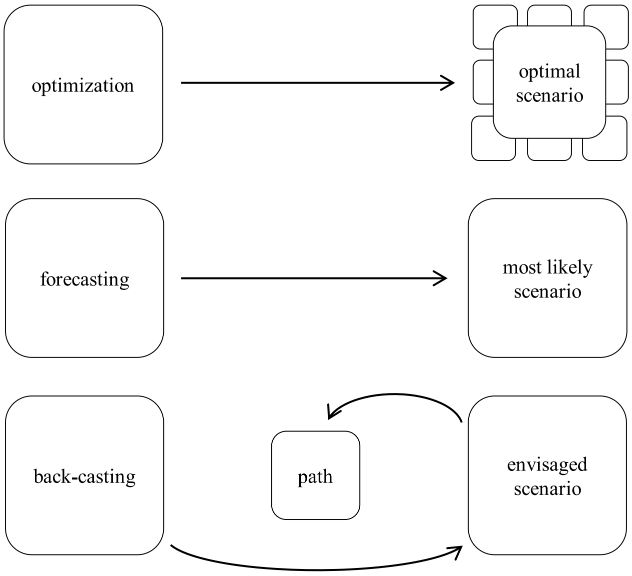

Fig. 2. Methodologies of optimization, forecasting and back-casting.

$$EPP = \frac{CED}{E_a}$$

The level of autonomy *LA* may be understood as the extent to which an energy system can be operated independently from external or upstream energy systems [26,81]. It can be calculated using the time in which loss of load occurs T_{LOL} and the total operation time T_{tot} [81]:

$$LA = 1 - \frac{T_{LOL}}{T_{tot}}$$

The loss of energy supply probability *LESP* is the share of energy that cannot be provided by the energy system itself [26] and which has to be obtained from external energy systems. It can becalculated by dividing the sum of energy deficits $E_{def}(t)$ by the total energy demands $E_{dem}(t)$ at any point in time t [26]:

$$LESP = \frac{\sum E_{def}(t) \cdot \Delta t}{\sum E_{dem}(t) \cdot \Delta t}$$

Possible **environmental criteria** could include the amount of greenhouse gases emitted, air pollutants such as NO_x or SO_x, the amount of freshwater used [22], land use, noise pollution, or human health impacts [17]. The amount of CO_2 emitted, m_{CO2}, for instance, may be calculated throughout the value chain of an energy system's components. Emissions issued by production (P), operation (O) (including maintenance) and disposal (D) after decommissioning all need to be included [82]:

$$m_{CO2} = m_{CO2_P} + m_{CO2_O} + m_{CO2_D}$$

Another useful environmental criterion would be the percentage of renewables. This is calculated using the percentages of energy supplied by renewable E_{ren} and conventional energy systems E_{conv}:

$$p_{ren} = \frac{E_{ren}}{E_{ren} + E_{conv}}$$

Other environmental criteria, such as health effects, are far less straightforward to quantify, and are thus less frequently applied in system analysis [17].

Technical criteria consider the safety, availability, reliability or overall technical feasibility in a system [17]. Since the processes and components entered to a model usually have to meet state-of-the-art standards of safety, availability and feasibility anyway, there is rarely any need to apply additional technical assessment criteria during the modeling process.

Social and economic criteria might include regional employment rates or technology-specific job opportunities, the risk of accidents, the availability of resources, the impact on local development and living standards, or foreign trade balances [17].

Financial criteria are probably the most common assessment criteria used to optimize MES at the district level. Environmental and energy efficiency criteria are also often integrated into the modeling. This is especially true of the amount of CO_2 emitted and the percentage of renewables.

Multi-objective optimization approaches – taking more than one criterion into consideration – are frequently used for the modeling of MES at the district level. Orehounig et al. [64], for instance, used the amount of CO_2 emissions (environmental criterion) and the end energy efficiency of buildings, as well as the degree of energy autonomy (energy efficiency criteria) to optimize the integration of decentralized energy systems into neighborhoods. One modeling framework, CEA, allows researchers to integrate financial criteria (levelized energy costs and total annual costs), energy efficiency criteria (amount of primary energy used), environmental criteria (greenhouse gas emissions) as well as social/economic criteria (percentage of renewables) [61].

3.3. *Structure and technological details*

The structure and technological details of energy system models can be summed up by their.

- Geographic coverage,
- Spatial resolution,
- Temporal resolution,
- Time horizon,
- Sectoral coverage,
- Demand sectors,
- Technical coverage,
- Demand-side management, and
- Change of properties,

as well as other additional properties.

Geographic coverage describes the spatial area that is included in the model. Coverage can range from the global to the continental, international, national, regional and local or even down to a single power plant [22]. The analysis of city districts requires local coverage. A recent model by Spielmann et al. for instance, identified the optimal energy supply scenario of a university campus [53].

The **spatial resolution** of the models could vary as well. For instance, it is possible to map the energy demand of a city district for the whole district, for every building, or even for every consumer. The **temporal resolution** specifies the time steps of the model. This could range from milliseconds to years (Table 1 [11]). The actual temporal resolution is fixed in some models and variable in others, for example depending on the resolution of the input data [22]. Ringkjøb et al. stressed that energy models with broad geographic coverage tend to have lower temporal resolution [22]. Models at the district level generally use an hourly resolution, less often a 15-min resolution. One-minute resolutions are used as well, but very rarely. Depending on the specific research question, more detailed results may be modeled by applying higher spatial and temporal resolution. However, the computing resources required increases quickly as spatial and temporal resolution of the model increases. Moreover, input data is usually not available at such high levels of resolution, so a better resolution of the model itself may not lead to better results [13].

Examples of the **time horizon** might include a day, a year, a decade, or the lifespan of the components used in the energy system [12]. Optimization models at the district level typically cover at least one full year.

Sectoral coverage describes which energy sectors are included in

Table 1
Applications of different temporal resolutions.[a].

Temporal Resolution	System Issues	Applications
ms → s	- Generator dynamics	- Stability management
	- Motor load dynamics	- Power-frequency regulation
	- Demand variation	
min → 1 h	- Power interchanges	- Economic dispatch
	- Maintain economic operation	- Generation control
	- Frequent control	- Power flow
	- Hourly generation planning	- Security analysis
		- Fault analysis
		- Voltage stability studies
h → 1 week	- Weekly generation planning	- Demand
		- Weather prediction
		- Unit commitment
weeks → months	- Seasonal generation planning	- Demand prediction
		- Maintenance planning
		- Hydro planning
		- Fuel planning
Years	- Demand growth	- Generation expansion planning
	- Plant Retirement/ refurbishment	- Reliability checks
	- Investment opportunities	- Scenario analysis
	- Long-term hydrological cycles	- Production cost modeling

[a] Reprinted from Energy, 35/12, A.M. Foley, B·P.Ó. Gallachóir, J. Hur, R. Baldick, E.J. McKeogh, A strategic review of electricity systems models, pp. 4522–30, Copyright (2010), with permission from Elsevier [11].

the model. These energy sectors typically include electricity, heating (district heating, low exergy networks, hot water), cooling, fossil resources, and commodities.

Possible **demand sectors** include the residential and commercial building sectors, industry, agriculture [22] and transport [12]. Models of mixed-use districts should incorporate at least two of these sectors.

Technical coverage refers to the specific technologies applied. Optimization models at the district level generally take into consideration solutions such as decentralized energy supply from combined heat and power plants (CHP), the renewable technologies of solar thermal plants, photovoltaics and heat pumps, and various types of heat and electricity storage methods, as well as boilers for heat supply. Occasionally, other technologies such as small hydropower plants [64], wind turbines [55,66], biomass boilers [54] and diesel engines [28] are also incorporated into models.

Demand side management comprises all measures on the consumer side of an energy system. They are typically intended to increase the energy efficiency of the system [83]. Measures may range from renovation (e.g. the installation of well-insulated windows) to demand-response measures (such as shifting energy demands from periods with high demand to periods with energy surpluses) [22]. Such measures can be especially helpful to balance the volatile production rates of renewable energy systems. They may be supplemented by energy storage facilities [22]. Only a very few studies have incorporated renovation measures into optimization models at the district level. One exception was a study by Falke et al. which dealt with the question of whether renovation measures in buildings could be an alternative to investment in new generation units [59]. Demand response has also taken on new importance in recent years, especially with the emerging application of artificial intelligence (see the section on *mathematical approaches below*). Kampelis et al. [51], for instance, developed an optimization approach for buildings and districts using demand-response measures in connection with artificial intelligence, and came to the conclusion that such measures could lead to cost savings of up to 15%.

Especially in long-term analyses, some of the **properties** of an energy system may **change** over the defined time horizon. In addition to changes in costs and components used, changes in behavior among residents could have profound effects on the demand side. Changes in system properties can be included in optimization models if the models include some kind of forecasting abilities. In current models, changes in system properties is only considered occasionally.

Additional properties of a model may, for instance, provide information about various cost aspects in the model [22] or how uncertainty and risk is treated [12].

3.4. Analytical Approaches

We can classify the analytical approaches that models of energy systems can take into three categories:

- Bottom-up models,
- Top-down models, and
- Hybrid models.

The first two are depicted in Fig. 3. In a **bottom-up** approach, several subsystems are modeled, and then these are merged onto an overlying system. Assembling the whole system from the bottom to the top makes it possible to create a model with a high level of technological detail, which allows for the evaluation of a wide range of technical options [84]. However, investment and cost aspects are usually limited to the technologies specifically included in the model. This leads to a lack of attention to macroeconomic interactions between the energy sector and other economic sectors. For example, changes in consumer behavior due to cost changes are hard to estimate [18]. Bottom-up energy system models are mainly used to identify technologies suitable for certain applications [84]. They are traditionally employed in the field of engineering [85], and are also known as techno-economic models [8].

The process of building a model with a **top-down** approach starts with a general overview of the entire system, and becomes more detailed by splitting the whole system into subsystems. Such models usually include the whole economy but take into account fewer technological details [18]. To compensate for this lack of detail, models often use historical parameters to estimate future system behaviors, which may cause imprecise results [84]. This approach is traditionally used for economic investigations (e.g. for the prediction of future energy demands, or conditional on macroeconomic interactions [8,18]) and is also known as the macroeconomic approach [8].

Hybrid models are created by linking a top-down model with a bottom-up one, combining the advantages of both approaches [8,12]. Despite the additional effort needed to apply this approach, more and more energy system models are based on hybrid approaches [8,18].

For the technical optimization of the holistic MES of urban districts, a modeling with high technical detail is mandatory. Such technical detail can only be guaranteed if the technical properties of various components are mapped in detail and then combined into an overall system. Therefore, models usually employ bottom-up approaches, and less often hybrid approaches. Top-down models are normally not applied for this purpose. Petrovic and Karlsson [57], for instance, implemented a model with the TIMES model generator, using the bottom-up approach. They investigated the role of heat pumps in residential energy systems to achieve Denmark's energy policy targets. They found that heat pumps in Denmark could supply 24–28% of total heat demand. On the other hand, they also determined that the energy targets could be met without using heat pumps at all. This would, however, increase total costs by 16%.

3.5. Mathematical Approaches

Different models take different mathematical or rather computational approaches as well. The most common include the following:

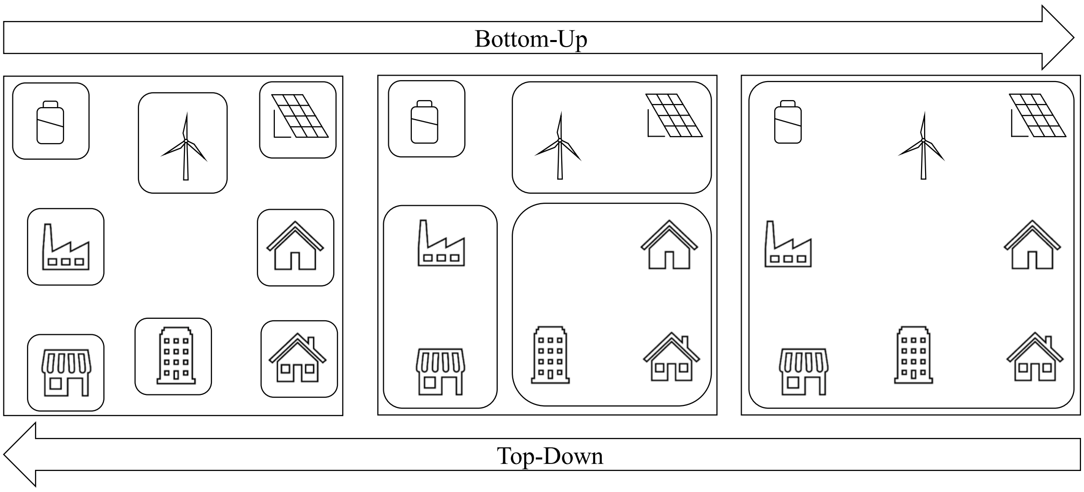

Fig. 3. Principle of bottom-up and top-down approaches.

- Linear programming,
- Dynamic programming,
- Mixed-integer programming,
- Stochastic programming, and
- Artificial intelligence approaches.

With the use of **linear programming** (Fig. 4 a), system behavior is described by linear mathematical functions, which in turn are summarized in an objective function. The model result is reached, for example, by finding and identifying the minimum or maximum of the objective function. Linear optimization models have a long history in energy system modeling [13,86], and are frequently used for the optimization of MES at the district level. Linear programming approaches are straightforward to apply. However, they are only appropriate in cases when all system relations can be thoroughly described with linear functions [87].

Non-linear relations either have to be linearized (Shao et al. for instance, transformed dynamic energy demands into piecewise-linear functions [88]) or instead treated with **dynamic programming** (Fig. 4 c). This is an algorithmic approach to solving problems by

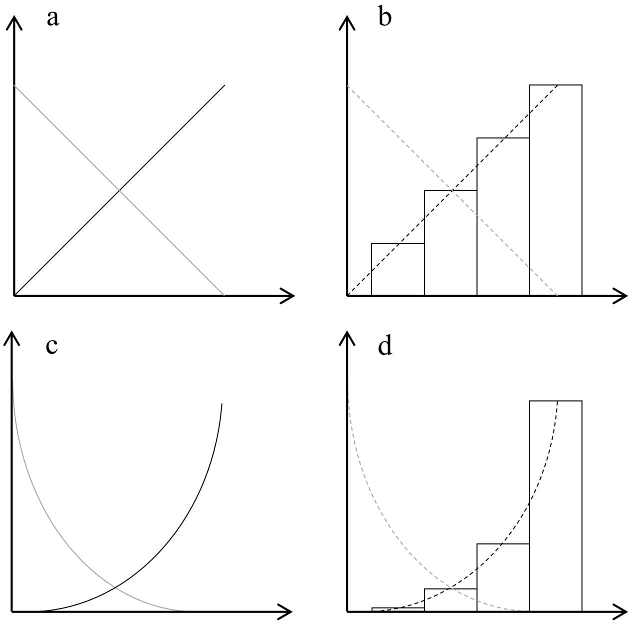

Fig. 4. Linear programming (a), linear mixed-integer programming (b), dynamic programming (c) and dynamic mixed-integer programming (d).

splitting them into sub-problems and systematically storing intermediate results. The subsequent combination of the intermediate results yields an overall solution [89].

Mixed-integer programming (MIP, Fig. 4 b, d) is a particular type of the three approaches mentioned above, but only allows outcomes with integer values [22,87]. These are useful in cases when it is helpful to identify an integer number, such as the ideal number of power plants, or storage facilities with predefined capacities.

The differences between linear and dynamic programming, as well as the differences between MIP and non-MIP are illustrated with a simplified example in Fig. 4. For example, the target values could be the point of intersection of the functions, or the minimum or maximum of the sum of the functions. Depending on the type of programming, these points would be different. For MIP functions, there is a limited number of solutions (represented by blocks), while for non-MIP functions, an infinite number of solutions is theoretically possible.

Stochastic programming approaches are linear and dynamic programming approaches that are not limited to the use of fixed parameter sets. Imprecisions in parameters and functions are coded into probabilistic elements, which in turn allow the generation of uncertainty estimates of the model output [11].

Artificial intelligence approaches are even further advanced and more complex approaches. Here, not only the imprecision of properties, but even a change of properties within a given time horizon is detected or predicted by the model itself. A decisive advantage of artificial intelligence is that it is fault-tolerant and can therefore also work with noisy or incomplete data. In addition, it is capable of working faster than conventional algorithms [19]. In addition, the results obtained from artificial intelligence can contribute to deeper understanding of the system. The implementation of artificial intelligence, however, is much more complicated than that of conventional optimization algorithms, and requires in-depth programming knowledge, especially as the number of parameters increases [20]. An additional challenge is that previous solved scenarios must be available and known to train the artificial intelligence [20,24]. Artificial intelligence approaches are based on fuzzy logic [12,24], agent-based programming [12], particle swarm optimization [20], genetic algorithms, or neural networks [24].

Mixed-integer programming is the approach most commonly used for the optimization of MES at the district level, while dynamic approaches are used less frequently. Artificial intelligence has only been used quite rarely so far, but has begun to receive more and more attention recently. Stochastic programming is used occasionally. Morvaj et al. [58], for instance, implemented a model using linear MIP to optimize district heating layouts. They identified measures to reduce the system's CO_2 emissions by 23% without any increase in costs. Stochastic models can also be used to determine how reliable an energy system would be under emergency conditions, as Najafi et al. [90] have done. Reynolds et al. [43] used artificial neural networks and genetic algorithms to predict multiple variables and to optimize operating schedules of heat generation units, thermal storage units, and heating set points. The optimization would allow a 45% increase in profit compared to a rule-based, priority-order baseline strategy. Schwarz et al. [45] used a stochastic linear MIP approach to support investment decision-making for technologies with unstable energy generation (photovoltaics and heat pumps) in a residential area. They predicted the required capacities of generation and storage to ensure reliable power supply under various probability and risk scenarios.

3.6. Reusability

Depending on their availability and reusability, it can be differentiated between models and modeling tools (model generators and frameworks) that are.

- Open and
- Closed [7].

Open models and modeling tools are characterized by the public accessibility of their source code, their underlying assumptions, and the data they use [7]. **Closed** models and modeling tools, on the other hand, do not publish their code or underlying assumptions [7]. Their use may be subject to fees, or even completely confidential [7]. The large majority of energy system models, model generators, and frameworks are closed. In light of calls for greater transparency and reusability of publicly funded research in Europe [90], there has been an increasing number of open models and modeling tools over the past few years [21].

In addition to motivations based on market strategies and economic considerations to keep commercially developed models and modeling tools closed, Pfenninger et al. [21] mentioned four reasons why models and modeling tools often remain closed. **(1)** Models and modeling tools may contain sensitive commercial data or personal information, which is not permitted for public disclosure. **(2)** The release of a code carries a risk that other researchers could expose flawed code sections or erroneous data and thus discredit the results. **(3)** The writing of legible and reusable codes as well as comprehensible documentation and bug reports is time-consuming. Not everyone is willing to invest this time. **(4)** The hesitation among individuals or institutions may also be a cause for failing to open models and their results.

Pfenninger et al. [21] also put forth four reasons why models and modeling tools should be published openly. **(1)** The fundamental scientific principles of transparency, peer review, reproducibility and traceability can only be guaranteed if data, methodology and results are openly accessible [21,92]. **(2)** Policymakers often have to fall back on models that are not quality-assured with academic practice or that provide incorrect results. With increasing transparency in energy system research, policymakers will gain access to more high-quality information [21]. **(3)** Research funding and researchers' time are limited resources. A great deal of time and money can be saved by avoiding duplication of work [21]. **(4)** The transparency of arguments based on scientific justifications are necessary in social and political debates [93]. Furthermore, the full results of publicly funded research should be available to the public.

3.7. Challenges

There seem to be six major challenges in the field of energy system modeling at present:

- Closed models and modeling tools,
- Data quality and transparency,
- Unreliable assumptions,
- Complexity,
- Conflicting interests, and
- The need for coding.

The high share of **closed models and modeling tools** generally hinders progress in energy system modeling. Data with high **quality** and with a sufficient temporal resolution are indispensable for the production of high-quality model results. Often, data to feed the models is not available, and often, the quality of the data is poor. Even in cases when data meeting the requirements exists, a lack of **transparency** and accessibility (arising for various reasons) are real problems [13]. Moreover, models are often based on **assumptions** that turn out to be more or less uncertain. Dealing with this uncertainty can be a challenge. Barely predictable power production from renewable energy systems [14] as well as human behavior, especially feedback between consumer behavior and policy decisions, introduce significant uncertainty into model codes and results [13].

The **complexity** of energy system models is increasing due to increasing geographic coverage, temporal resolution, and time horizons, as well as increasing numbers of relevant economic sectors and technologies. This in turn results in a drastic increase in the effort as well as the computing resources required from the modeler. To limit the need for those resources at acceptable levels, researchers need to strike compromises between the time and energy put into a model, the computing time necessary, and the informative value of the results [94].

Different stakeholders of energy system modeling may also have **conflicting interests**, which cannot be met within a single model. Therefore, models often represent tradeoffs, trying to combine various objectives, but yielding non-optimal results for any single stakeholder [16]. Policymakers could, for instance, aim to reduce costs (financial criteria), while local residents might instead focus on social or environmental criteria.

Energy system models are usually **coded** models, which means that even if researchers are working with model generators or frameworks, they can only take full advantage of energy system models if they have coding skills. To bring energy system models into widespread use among the public, it will be crucial to develop intuitive operable application surfaces (e.g. graphical user interfaces or spreadsheet/GIS (geographical information system) based applications).

All of these problems and challenges are relevant for the optimization of MES in mixed-use districts. Specific problems could, for instance, include a lack of high-quality load profiles, unreliable assumptions about future consumer behavior, increased complexity due to the inclusion of several economic sectors in the MES, or contradictory requirements for assessment criteria from policymakers or residents. The need for coding is also an obstacle to getting public officials to use models or modeling tools.

4. Existing modeling tools

The analysis of several reviews that discussed existing modeling tools [12,14,22,36–41] as well as an additional online search revealed a total of 145 energy system modeling tools. Not all of them were suitable for the optimization of MES in mixed-use districts. Based on our hitherto analysis and applying careful evaluation, we applied a cascade of criteria, to filter out the relatively small number of suitable modeling tools (Fig. 5):

1) In general, the **area of application** of a given tool has to be an energy system as it was defined at the beginning of this paper. Furthermore, the tool has to be useable for more than one such energy system.
2) The applied **methodology** has to include some kind of optimization.
3) A city district needs to be **geographically coverable.**
4) For the analysis of MES, **sectoral coverage** should include at least the electricity and heat sectors. To take mixed use into account, at least two different demand sectors have to be included.
5) The **temporal resolution** must generate at least hourly time steps.

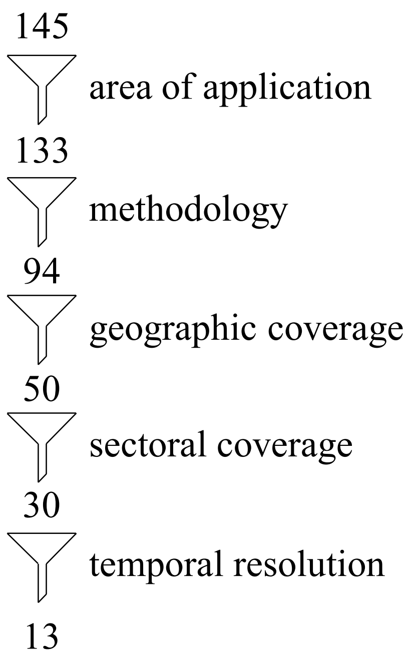

Fig. 5. Filtering of energy system modeling tools by applying the requirement for their suitability of optimizing multi-energy systems in mixed-use districts.

Fig. 5 shows how many tools were filtered out in each step. After applying all criteria, only 13 modeling tools were suitable for optimizing MES in mixed-use districts. These are listed in Table 2 with some of their properties. Table 3 lists the tools we filtered out, together with the criteria that lead to their exclusion.

In total, 132 of the 145 modeling tools analyzed here were not suitable for the optimization of MES in mixed-use districts. A total of 12 tools were designed for another area of application; 39 tools did not include any methodology of optimization; 44 tools were designed for either undersized or oversized geographic coverage (e.g. buildings, nations), 20 tools did not allow the consideration of more than one energy sector or demand sector; and finally, 17 tools had insufficient temporal resolution. Depending on the specific requirements for the envisaged application of a modeling tool, even more optional exclusion criteria may be necessary. If, for instance, assessment criteria other than financial criteria should be incorporated, only four tools are suitable (EnergyPLAN, eTransport, oemof, urbs). Note that five of the 13 suitable models come with an open source license. Two additional models are freely accessible. Six models are commercial, but none of the suitable models are completely inaccessible. Two tools (oemof, urbs) are available with an open source license and, at the same time, integrate various assessment criteria – in addition to financial ones. Overall, there are suitable tools, but only a small number of them. There is an inherent risk in a small number of suitable tools: there are hardly any possibilities to compare model outputs with each other, and thus both errors and potential for improvement are difficult to detect.

The “Open Energy Modeling Framework” (oemof) is a community-operated open-source modeling framework for the analysis and optimization of energy supply systems. It is designed as a modular python library consisting of a set of sub-libraries [123]. Examples of these sub-libraries include “oemof.solph”, which can be used to describe energy systems on the basis of mathematical graph theory, “oemof. demandlib”, which simulates consumers on the basis of standard load profiles, and “oemof.feedinlib”, which enables the modeling of renewable energy systems such as photovoltaic and wind power plants [123]. The community continuously develops new modules. The flexible modeling approach makes it possible to apply any geographical or temporal resolution and coverage; any energy or demand sector, and a variety of assessment criteria.

The modeling tool “urbs” focuses on energy systems that have a high proportion of renewables [189]. It was originally developed for the optimization of urban energy systems, but researchers have also employed it for continent-wide energy systems [189]. The tool was also developed in python and has a modular structure [134]. However, unlike oemof, the application does not require the use of a programming language. The model implementation takes place by entering spreadsheet files [134]. Financial costs and CO_2 emissions can be applied as assessment criteria.

All in all, oemof offers more sub-modules, and its flexible modeling approach makes it more accurate and versatile. On the other hand, urbs has a lower entry hurdle because there is no need to apply programming skills.

5. Conclusion

Energy systems of urban district are mixed-use multi-energy systems (MES). They include several energy sectors, such as electricity and heat,

Table 2
Modeling tools meeting the criteria for optimizing multi-energy systems in mixed-use districts. Acronyms: **Assessment Criteria:** EE = energy efficiency, Em = emissions, Fi. = financial, S = social. **Mathematical Approach:** DP = dynamic programming, LP = linear programming, MIP = mixed integer programming. **Geographic Coverage:** Cont. = continental, Int. = international, Loc. = local, Nat. = national, Reg. = regional. **Sectoral Coverage:** El. = electricity, F = fossil resources, H = heat, Hyd. = hydrogen. **Technical Coverage:** Conv. = conventional generation, Ren. = renewable generation, Stor. = storage (electricity and heat).

Tool	Calliope	DER-CAM	EnergyPLAN	energyPro	eTransport
Methodology	Optimization	optimization	optimization	optimization	optimization, forecasting
Assessment Criteria	Fi	Fi	Fi, EE, Em, S	Fi	Fi.
Analytical Approach	bottom-up	bottom-up	bottom-up	bottom-up	–
Mathematical Approach	LP[a]	MIP	LP	DP	DP, MIP
Geographic Coverage	user defined	buildings and microgrids[b]	Loc. to Cont.	Loc. to Reg	user-defined
Temporal Resolution	user defined	years[c]	hours	minutes	hours
Time Horizon	user defined	max. 20 years	1 year	max. 40 years	1–30 years
Sectoral Coverage	El., H, Hyd., F	El., H, C, F	El., H, F	El., H, C	El., H, C, F
Demand Sectors	any (aggregated)	any (aggregated)	any (aggregated)	any (aggregated)	any (aggregated)
Technical Coverage	Ren., Conv., Stor.[d]	Ren., Conv.,[e] Stor.	Ren., Conv., Stor.	Ren., Conv., Stor.[f]	Ren., Conv., Stor.[g]
Demand Response	yes	yes	no	no	no
Accessibility	open source	free	free	commercial	commercial
Website[h]	*https://calliope.readthedocs.io/en/stable/index.html*	*https://building-microgrid.lbl.gov/*	*https://www.energyplan.eu/*	*https://www.emd.dk/de/energypro/*	*https://www.sintef.no/en/projects/etransport/*
References	[14,22,95–100]	[12,22,101–103]	[12,14,22,40,104–108]	[12,22,36,107,109–112]	[37,75,113]

Tool	**ficus**	**HOMER**	**MARKAL**	**MARKAL-MACRO**	**oemof**
Methodology	optimization	optimization, forecasting	optimization	optimization	optimization
Assessment Criteria	Fi.	Fi.	Fi.	Fi.	Fi., EE, Em, S
Analytical Approach	bottom-up	bottom-up	bottom-up	hybrid	all applicable
Mathematical Approach	LP, MIP	–	LP, DP	DP	LP, MIP
Geographic Coverage	Loc. to Nat.	Loc.	Loc. to Reg.	Loc. to Nat.	user-defined
Temporal Resolution	15 min	minutes	user-defined	user-defined	user-defined
Time Horizon	1 year	several years	user-defined	user-defined	user-defined
Sectoral Coverage	any	any[i]	any	any (aggregated)	El., H, Hyd., F
Demand Sectors	any (aggregated)	any (aggregated)	any (aggregated)	any (aggregated)	any (aggregated)
Technical Coverage	Ren., Conv., Stor.	Ren., Conv., Stor.[j]	Ren., Conv., Stor.[k]	Ren., Conv., Stor.[l]	Ren., Conv., Stor.
Demand Response	no	no	yes	yes	yes
Accessibility	open source	commercial	commercial	commercial	open source
Website	*https://ficus.readthedocs.io/en/latest/index.html*	*https://www.homerenergy.com/*	*https://iea-etsap.org/index.php/etsaptool/model-generators/markal*	*https://iea-etsap.org/index.php/etsaptool/model-generators/markal*	*https://oemof.org/*
References	[22,114,115]	[12,22,36,40,41,116–118]	[12,14,22,119–122]	[12,119,123]	[7,14,22,124–126]

(*continued on next page*)

Table 2 (*continued*)

Tool	Temoa	TIMES	urbs
Methodology	optimization	optimization	optimization
Assessment Criteria	Fi.	Fi.	Fi., Em.
Analytical Approach	bottom-up	hybrid, bottom-up	bottom-up
Mathematical Approach	LP	LP, DP	LP
Geographic Coverage	user-defined	user-defined	Loc. to Nat.
Temporal Resolution	years[m]	years[n]	user-defined[o]
Time Horizon	user-defined	user-defined	user-defined
Sectoral Coverage	any	any	any
Demand Sectors	any (aggregated)	any (aggregated)	any (aggregated)
Technical Coverage	Ren., Conv., Stor.	Ren., Conv., Stor.	Ren., Conv., Stor.
Demand Response	no	–	yes
Accessibility	open source	commercial[p]	open source
Website	*https://temoacloud.com/*	*https://iea-etsap.org/index.php/documentation*	*https://urbs.readthedocs.io/en/latest/*
References	[12,14,22,127–129]	[12,14,22,130–133]	[22,134,135]

[a] MIP under development.
[b] Districts can only be modeled if they are assessed as microgrids.
[c] Temporal resolution of a year, but reference days with minute-level resolution may be defined.
[d] Tool designed for questions concerning the transition to renewable energy. The developers have pointed out that there are tools that are more suitable for other types of questions.
[e] Excluding nuclear power.
[f] Photovoltaic, wind turbines, batteries, electric boilers, electric absorption chillers, thermal storage units, geothermal energy, biomass, biogas and other fuels can be included.
[g] CHP, heat pumps, boilers, LNG plants, and power plants without emission flows can be included.
[h] Websites last accessed on June 9, 2020.
[i] The focus is clearly on the electricity sector.
[j] The focus is on renewable generation. Nuclear power cannot be included.
[k] Only hydropower, wind power, solar power and geothermal as renewables. Only night-day storage.
[l] Only hydropower, wind power, solar power and geothermal as renewables. Only night-day storage.
[m] Temporal resolution of multiple years, but a number of reference days for various seasons with undefined time steps may be defined.
[n] Temporal resolution of a year, but reference days with hourly resolution may be defined.
[o] Usually hours.
[p] Open source code, but commercial GAMS license required.

Table 3
Modeling tools that were not suitable for the optimization of multi-energy systems of mixed-use districts.

Exclusion Criterion	Tools		
area of application	BALMOREL [12,14,22,136–139]	Neplan [36,140]	ProdRisk [12,22]
	BESOM [14]	NetSim [36,144]	renpassG!S [21,22,141–143]
	Emcas [12,39]	ORCED [12,39]	SynCity [36,146]
	HYDROGEMS [12,39]	PLEXOS [11,12,22,148–150]	Termis [36,147]
methodology	AEOLIUS [12,39]	GridLAB-D [22]	Mesap PlaNet [12,39,151]
	ARES [40,41]	H2RES [12,39,152,153]	MEU [36,154]
	AURORAxmp [22]	HYBRID 2 [40,41,155]	OPENDSS [22]
	CASPOC [22]	HYBRIDS [41]	RAPSim [22]
	CIMS [14]	HybSim [40,41,156]	SAM [22]
	COMPOSE [12,22]	HySys [41]	SIMPOW [22]
	CYME [22]	INFORSE [12,39]	SIREN [22]
	DESSTinEE [22]	INSEL [41,157]	sivael [12,37,39]
	DIgSILENT/Power Factory [22]	INVERT/EE-Lab [12,22]	SOLSIM [40,41]
	Dymola/Modelica [41,94]	IPSA 2 [22]	TRNSYS [41]
	DynEMo [12,14]	IPSYS [40,41]	UKENVI [12]
	EMLab-Generation [22]	LOADMATCH [22]	UMI [36,158]
	ETM (2) [22]	MDM-E3 [12]	WEM [22]
geographic coverage (too small)	BCHP Screening Tool [39]	IDA ICE [36]	SCOPE [14,159,160]
	CitySim [36,161]	KULeuven IDEAS lib [36]	TRNSYS18 [22,36,162]
	EnergyPlus [36,163]	LBNL District lib [36]	
	ESP-r [36]	Polysun [36,164]	
geographic coverage (too big)	COMPETES [22]	GEM-E3 [12,22]	REMix [14,22,165–170]
	DIETER [22]	GENESYS [22]	REMod-D [14,171–174]
	DSIM [12]	IMAKUS [22]	SAGE [12,119]
	EMMA [22]	LIBEMOD [22]	SimRen [12,39]
	EMPIRE [22]	LIMES-EU [22]	stELMOD [22]
	EMPS [12,39]	LUSYM [22]	Stream [12,37,39]
	Eneertile [22]	MiniCAM [12,39]	WASP [12]
	ESME [12,14]	NEMO [22]	WeSIM [22]
	ETM [1,22]	PERSEUS [12,39]	WILMAR [12,39]
	ETSAP-TIAM [12,22]	POLES [12,22]	WITCH [22]
	EUCAD [22]	RAMSES [12,39]	
	EUPower-Dispatch [22]	REMIND [22]	
sectoral coverage	CEA [61,175]	Hybrid Designer [40,41]	PowerGAMA [22]
	DECC DDM [12]	HYPERSIM [22]	PyPSA [22,176–179]
	DIMOSIM [50]	iGRHYSO [40,41]	ReDS [22]
	EMPS [12,22,40,180]	iHOGA [22,40,41,181–183]	SOLSTOR [40,41]
	EnerGis [12,36,184]	IRiE [22]	SOMES [40,41]
	ENTIGRIS [22]	NEMS [12]	SWITCH [22]
	GTMax [12,39]	OSEMoSYS [12,14,22]	
temporal resolution	DECC 2050 calculator [12]	IKARUS [12,14,185–188]	REMIND-D [14]
	E3MG [12]	LEAP [12,14,22]	RETSCreen [12,22,36,40,41]
	E4cast [12,14]	MESSAGE [12,14,22]	SNOW [22]
	EMINENT [12,39]	MESSAGE-III [12]	TESOM [14]
	ENPEP-BALANCE [12,14]	NEMS [14,22]	UniSyD3 [12,39]
	GCAM [12,22]	PRIMES [12,14,22]	

and various consumption sectors, such as housing, industry and agriculture. Not least because of the structural change in the European energy system, the energy systems of city districts have become the focus of many planning activities. To meet the resulting challenges, tools for modeling and optimizing the energy systems of urban districts are needed. Although various studies have looked at increasing the energy efficiency of urban districts, or the development of general energy system modeling approaches in general, there is a lack of studies dealing with modeling tools for exactly this purpose.

To be suitable for the optimization of MES of mixed-use districts, modeling tools must be able to apply an optimization methodology. They have to address multiple energy and demand sectors, and operate with an at least hourly temporal resolution. Moreover, they have to follow a bottom-up or hybrid analytical approach. As the analysis presented in this article has shown, only 13 out of a total of 145 modeling tools meet these requirements. The other 132 tools where either created for another area of application (12 tools), used a different methodology (39 tools), were unable to consider the geographic coverage of city districts (44 tools), did not include enough energy and demand sectors (20 tools), or worked with overly low temporal resolution (17 tools).

We are fully aware that a direct comparison of the modeling tools presented here using a representative MES from a mixed-use district would be interesting. All 13 modeling tools meeting the requirements should be compared to each other. However, Connolly et al. have shown in their review [39] that the individual training time for each modeling tool is usually several weeks or even months. Therefore, carrying out such a comparison is outside the scope of this contribution. If readers are familiar with one or more of these tools, we would welcome the opportunity for a forthright joint study.

Going further and adding optional criteria such as the ability to use non-financial assessment criteria and open source availability, only two of the original 145 tools are suitable. Accordingly, oemof and urbs stand out from the crowd here.

Challenges in the field of energy system modeling, and therefore presumable reasons why the availability of models and modeling tools for urban districts are lacking, include the limited accessibility of supporting data as well as generally poor data quality. Another challenge is the need to find compromises between the preferably large system's complexity on the one hand, and the resources needed for coding and computing on the other. Conflicting interests among various stakeholders often produce difficulties as well. In our view, the lack of transparency is an avoidable problem. Existing databases and modeling approaches should be kept open. This would save time and effort, and eventually lead to a higher quality of energy system models. Fortunately, a significant share of the models analyzed in this review are available with an open source license or are at least freely accessible.

One problem in the literature on the topic of energy system modeling is the occasional contradictory use of terminology. For instance, the terms of "model" and "model generator" are frequently mixed up. While a "model" in our context is a simplified representation of a real world's energy system, a "model generator" is a tool that creates a model with predefined properties. Moreover, the term "simulation" is generally used for forecasting a model's behavior in a future scenario. Since "simulation" also takes place in optimization and back-casting operations, the use of the term is indeed misleading. To avoid misunderstandings, "forecasting" should be used instead when describing future scenarios.

In sum, there is a lack of tools for the modeling and optimization of MES in mixed-use districts. This is especially the case when optional criteria such as non-financial optimization and open source availability are required. Such a small number of suitable tools carries the risk that modeling results cannot be compared with each other, and thus errors as well as potential ways to improve the model are difficult to detect. Nevertheless, the availability of at least two tools shows that there is research and development in the area under consideration, although a wider variety would be desirable.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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B Publication: Indicators for the optimization of sustainable urban energy systems based on energy system modeling

Table B.1: Fact sheet publication [B]

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Abstract: Background: Urban energy systems are responsible for 75 % of the world's energy consumption and for 70 % of the worldwide greenhouse gas emissions. Energy system models are used to optimize, benchmark and compare such energy systems with the help of energy sustainability indicators. We discuss several indicators for their basic suitability and their response to changing boundary conditions, system structures and reference values. The most suitable parameters are applied to four different supply scenarios of a real-world urban energy system. Results: There is a number of energy sustainability indicators, but not all of them are suitable for the use in urban energy system optimization models. Shortcomings originate from the omission of upstream energy supply chains (secondary energy efficiency), from limited capabilities to compare small energy systems (energy productivity), from excessive accounting expense (regeneration rate), from unsuitable accounting methods (primary energy efficiency), from a questionable impact of some indicators on the overall system sustainability (self-sufficiency), from the lack of detailed information content (share of renewables), and more. On the other hand, indicators of absolute greenhouse gas emissions, energy costs, and final energy demand are well suitable for the use in optimization models. However, each of these indicators only represents partial aspects of energy sustainability; the use of only one indicator in the optimization process increases the risk that other important aspects will deteriorate significantly, eventually leading to suboptimal or even unrealistic scenarios in practice. Therefore, multi-criteria approaches should be used to enable a more holistic optimization and planning of sustainable urban energy systems. Conclusion: We recommend multi-criteria optimization approaches using the indicators of absolute greenhouse gas emissions, absolute energy costs, and absolute energy demand. For benchmarking and comparison purposes, specific indicators should be used and therefore related to the final energy demand, respectively, the number of inhabitants. Our example scenarios demonstrate modeling strategies to optimize sustainability of urban energy systems.

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Indicators for the optimization of sustainable urban energy systems based on energy system modeling

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Abstract

Background: Urban energy systems are responsible for 75% of the world's energy consumption and for 70% of the worldwide greenhouse gas emissions. Energy system models are used to optimize, benchmark and compare such energy systems with the help of energy sustainability indicators. We discuss several indicators for their basic suitability and their response to changing boundary conditions, system structures and reference values. The most suitable parameters are applied to four different supply scenarios of a real-world urban energy system.

Results: There is a number of energy sustainability indicators, but not all of them are suitable for the use in urban energy system optimization models. Shortcomings originate from the omission of upstream energy supply chains (secondary energy efficiency), from limited capabilities to compare small energy systems (energy productivity), from excessive accounting expense (regeneration rate), from unsuitable accounting methods (primary energy efficiency), from a questionable impact of some indicators on the overall system sustainability (self-sufficiency), from the lack of detailed information content (share of renewables), and more. On the other hand, indicators of absolute greenhouse gas emissions, energy costs, and final energy demand are well suitable for the use in optimization models. However, each of these indicators only represents partial aspects of energy sustainability; the use of only one indicator in the optimization process increases the risk that other important aspects will deteriorate significantly, eventually leading to suboptimal or even unrealistic scenarios in practice. Therefore, multi-criteria approaches should be used to enable a more holistic optimization and planning of sustainable urban energy systems.

Conclusion: We recommend multi-criteria optimization approaches using the indicators of absolute greenhouse gas emissions, absolute energy costs, and absolute energy demand. For benchmarking and comparison purposes, specific indicators should be used and therefore related to the final energy demand, respectively, the number of inhabitants. Our example scenarios demonstrate modeling strategies to optimize sustainability of urban energy systems.

Keywords: Energy system modeling, Urban energy systems, Multi-energy systems, Optimization indicators, Multi-objective optimization, Energy sustainability, Energy efficiency, Energy sufficiency, Energy consistency

Background

Introduction

Urban energy systems are the "combined process of acquiring and using energy in a given" [1] spatial entity with a high density and differentiation of residents, buildings, commercial sectors, infrastructure [2], and energy sectors (e.g., heat, electricity, fuels) [3]. They are also called mixed-used multi-energy systems. It is often

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challenging to clearly define spatial boundaries of urban energy systems. An often-used approach is to use legally defined city districts as balance entities.

The complexity of these systems, combined with the fact that urban energy systems are responsible for 75% of global energy consumption and 70% of worldwide greenhouse gas (GHG) emissions [4], results in the need for a profound transformation of urban energy systems. Different goals and strategies are discussed with respect to various sustainability aspects.

The most prominent goal is the fulfillment of national and international climate neutrality goals and thus the mitigation of GHG emissions [5–7]. Further widespread goals with respect to urban energy systems are the minimization of energy supply costs [5, 7], the non-use of fossil fuels [7], and the increase in regional value added [8]. The objectives of network access and security of supply [5, 7] are regarded as basic requirements of well-functioning urban energy systems.

Energy system models (ESM) are important tools for the design and optimization of existing or newly planned urban energy systems [9]. Various suitable indicators need to be identified in order to address a variety of sustainability aspects. These indicators can be used as target variables in optimization models. By mathematically minimizing or maximizing them [10, 11], sustainable urban energy systems can be designed.

In addition to being used for optimization purposes, indicators can also be used for benchmarking and comparison purposes. The broad application of a set of uniform indicators to a large number of different urban energy systems allows to identify structural problems (e.g., widespread use due to subsidies for less sustainable technologies) that can be remedied by national and international regulations.

We are oriented towards the three energy sustainability strategies of energy efficiency, energy sufficiency and energy consistency [12, 13], for the identification of suitable indicators to be applied in ESM. Particularly with the focus on climate neutrality objectives, it is advisable to thoroughly explore all existing options to mitigate climate change. This includes focusing not only on consistency, but also to examine efficiency and sufficiency demand-side solutions and their potential contribution [14]. Efficiency aims at the provision of the same service with lower input, thus a relative reduction of energy demands (final, secondary, primary), material goods, or financial values by technical means [15, 16]. Sufficiency aims at a reduction of energy service demand (e.g. lower room heat) which results in an absolute reduction of final energy demand and consequently lower resource demand [15, 17], and consistency describes the quality of the energy source [12]. These three strategies are no ends in themselves but different strategies to reach sustainability objectives. Both demand-side strategies, efficiency and sufficiency aim at a reduction of energy demand, yet their approaches differ substantially from each other, and both have their own specific advantages and drawbacks [18, 19]. Overall, each of the three sustainability strategies covers different aspects, and taking all of them into account leads to a broad and manifold picture of urban energy system optimization. We therefore use the categories of efficiency, sufficiency, and consistency, as orientation for the indicator search for a broad and comprehensive perspective.

While there are a number of different indicators for measuring and evaluating the efficiency of energy systems (e.g., [16, 20–22]), only few indicators for sufficiency and consistency are described in the literature (see "Sustainability of urban energy systems").

The majority of energy system models for the optimization of urban energy systems work single-criterial [23], using either economic (e.g., least costs) or environmental (e.g., least GHG emissions) indicators as target variables [24]. In light of the multitude of goals and challenges with regard to the optimization of urban energy systems, it is questionable whether this single-indicator optimization leads to satisfactory or sustainable solutions. Indicators representing more than one goal or multi-criteria optimization could support a more balanced optimization between different goals.

There are also multi-objective models, for instance, the studies by Rieder et. al [25], Sugihara et al. [26], Karmellos and Mavrotas [27], Fonseca et al. [28], and Jing et al. [29]. Usually, an indicator for minimizing system costs (cf. Eq. 5) and an indicator for reducing greenhouse gas emissions (cf. Eq. 4) are applied as optimization criteria. In some cases, third indicators, such as primary energy efficiency ([26], cf. Eq. 2), or degree of self-sufficiency ([28], cf. Eq. 10) are complemented.

Mostly, the selected indicators are set but not further evaluated for their suitability, or whether there are better suited indicators. Within this article, we will close this gap for the specific case of optimization of urban energy systems. Therefore, existing indicators for urban energy system optimization are evaluated, and new ones proposed (see "Sustainability of urban energy systems"). These indicators are then tested for their applicability in energy system modeling. Four different energy supply scenarios are modeled to evaluate the suitability of the new indicators in energy system models (see "Methods: single-criterion simulation" and "Results: single-criterion simulation"). The scenarios include the imports of energy (scenario 1), renewable energy technologies (scenario 2), sector-coupling technologies (scenario 3), and demand reduction (scenario 4). Subsequently, possibilities to combine the most suitable indicators using multi-criteria optimization approaches are presented (see "Methods: multi-objective optimization"). Finally, indicator usage including shortcomings and advantages are discussed and conclusions are drawn.

Sustainability of urban energy systems

Definitions

Energy is a fundamental physical quantity. However, when talking about energy systems, we tend to mean the production of "desired energy services, rather than [energy] as an end in itself" [30]. It is important to distinguish between the different forms of energy (primary energy (PE), secondary energy (SE), final energy (FE), and effective energy (EE)), as well as between direct and cumulative energy demands (CED). The use of different terms of "energy" will lead to considerably varying results during the assessment process [31]. Within this contribution we refer to the definitions of energy terms from the VDI 4600 directive ("Cumulative energy demand — terms, definitions, methods of calculation") [32].

We define the energy balance boundary for the conversion processes to be considered in urban energy systems as all conversion processes up to final energy. Further transformations from final energy into effective energy take place within subsystems of buildings or plants. Although these subsystems are, strictly speaking, part of the urban energy system, they are also complex systems in their own, the interrelationships of which lie outside the scope of research on holistic urban energy systems [31]. When applying methods of energy system modeling, such delimitations and simplifications of system complexity are necessary in order to minimize the input effort for the modeler as well as the computational effort [33].

Energy sustainability: An energy system is considered sustainable if its negative impact on the society, environment, and economy is within the scope of the respective capacities [34]. Energy sustainability can be achieved by the three strategies of energy efficiency, energy sufficiency and energy consistency [12, 13].

Energy efficiency aims at improving the input–output ratio of an energy system. It can be increased either by the reduction of the resource or energy input while maintaining the same energy service, or by the increase of the service with the same input [15].

Energy sufficiency aims at the absolute reduction of energy consumption through social innovations and behavioral changes [12]. An energy system is considered to be sufficient when just as much energy is consumed as is "enough for a particular purpose" [17]. Sufficiency therefore does not aim at reducing absolute energy consumption to zero, but at limiting or reducing it to a sustainable level [15]. Part of the literature also argue for not only upper, but also lower limits to reach a sustainable level of energy service demand, referred to as "enoughness" [35, 36]. A level of "enoughness" avoids excess, especially regarding planetary boundaries but still ensures a good life [37].

In some cases, the term "energy conservation" is used synonymous with "energy sufficiency" [38]. However, since "energy conservation" is mostly used to refer to efficiency-based measures [39], we will use the term "energy sufficiency" in the following.

Energy consistency makes a qualitative assessment of production patterns of supplied energy [40]. Often, this is understood as the distinction between renewable and non-renewable primary energy sources [12]. However, also any aspects referring to the origin of supplied energy may be assessed. For example, *where* or with the help of *which* renewable technology energy is provided.

Sustainability aspects of urban energy system optimization in ESM: In order to limit the complexity of energy sustainability to a level which can be handled by ESM, this contribution will be limited to technical, economical and particular environmental aspects of an energy system, which have regional (e.g., regional value, energy supply costs) or global (e.g., climate neutrality, non-use of fossil fuels) impact. Regarding environmental aspects, GHG are the main aspect considered. As an aside, we will discuss to which extent other environmental aspects like local emissions or resource usage could be directly or indirectly covered by indicators applicable in ESM. We consider security of supply as a basic prerequisite. Furthermore, the studies in this paper are limited to the energy sectors of electricity and heat and the residential, commercial and industry demand sectors.

Efficiency indicators for urban energy systems

Patterson [16] proposed to categorize indicators for the measurement of energy efficiency into:

- Thermodynamic indicators,
- Physical indicators,
- Physical–thermodynamic indicators,
- Economic–thermodynamic indicators, and
- Economic indicators.

Thermodynamic indicators (also denoted as "technical indicators" [41]) "rely entirely on measurements derived from the science of thermodynamics" [16], and express the ratio of useful energy output to the energy input [16]:

$$\text{energy efficiency} = \frac{\text{useful energy output}}{\text{energy input}} \quad (1)$$

Purely *physical indicators* have physical input/output values [16], for example the required amount of fuel per distance traveled by car (l/km or conversely km/l). *Physical–thermodynamic indicators* are hybrid indicators measuring inputs in thermodynamic values and outputs in physical ones, or vice versa. An example is the energy content per liter of fuel (kWh/l). As they are given in physical quantities they can be easily compared [16]. *Economic–thermodynamic indicators* are hybrid indicators as well, in this case using thermodynamic and financial quantities [16], e.g. the price per energy unit (EUR/kWh). For purely *economic indicators*, both input and output are measured with financial units [16], for instance, investments per revenue (EUR/EUR).

For the classification into these terms, it is debatable if the quantity of energy (in *J* or *Wh*) is a physical or a thermodynamic term. In the following, it will be considered as thermodynamic quantity.

The *primary energy efficiency PEE* is a thermodynamic indicator, which is the inverse value of the primary energy factor *PEF* and thus calculated as the ratio of the system's final energy demand *FE* over the cumulative energy demand *CED* [42, 43]:

$$\mathrm{PEE} = \mathrm{PEF}^{-1} = \frac{FE}{\mathrm{CED}} \quad (2)$$

The *secondary energy efficiency SEE* is a thermodynamic indicator as well. It is the ratio of the final energy demand over the secondary energy *SE* required for covering this demand [42]:

$$\mathrm{SEE} = \mathrm{SEF}^{-1} = \frac{\mathrm{FE}}{\mathrm{SE}} \quad (3)$$

In contrast to secondary energy efficiency, the primary energy efficiency takes into account upstream chains and their efficiency levels, which usually lie outside an urban energy system. For example, different production chains of purchased electricity with different primary energy factors (e.g., electricity from renewable sources vs. electricity from fossil-fuel power plants [32]) are considered, even though the processes lie outside the urban area. The outsourcing of an inefficient power plant to a location outside and the subsequent import of the energy would lead to an improvement of the balance sheet of secondary energy efficiency, while the primary energy efficiency would not be affected. We thus consider the primary energy efficiency to be better suited to assess energy efficiency of urban energy systems because it is a more holistic approach.

The *specific GHG emissions* m'_{GHG} are a physical–thermodynamic indicator, which relates the energy demand of the urban area to the related GHG emissions. However, this indicator is not used to calculate an input/output ratio (see Eq. 1), but an output/output ratio. Since GHG emissions should be minimized in order to avoid negative environmental impacts, we regard this indicator as an efficiency indicator. It is calculated as the ratio of the total GHG emissions m_{GHG} to the final energy demand *FE* (Eq. 4) [44]. We recommend life cycle assessments for the determination of the caused GHG emissions:

$$m'_{\mathrm{GHG,FE}} = \frac{m_{\mathrm{GHG}}}{FE} \quad (4)$$

Considering Eq. 1, the specific GHG emissions indicator is, strictly speaking, the *inverse value* of an efficiency indicator. We believe that the use of this indicator (g/kWh instead of kWh/g) is the more intuitive indicator, while it provides the same information content. Such inverse values are also regarded as efficiency indicators here and in the following.

For the use in optimization models, it may be appropriate to use *absolute GHG emissions* of an energy system $m_{\mathrm{GHG,es}}$, instead of referring to a reference value. This simplifies the model, making it easier to use in ESM that are designed to minimize or maximize absolute values. A disadvantage is that the change of the final energy demand *FE*, for example by sufficiency measures, can influence the indicator, so that the indicator is no longer a pure efficiency indicator. For benchmarking and comparative purposes, a reference value should therefore certainly be applied.

The *specific energy costs* C' is an economic–thermodynamic indicator, calculated from the total system costs (including all costs for investment and operation) *C* and the final energy demand *FE* (Eq. 5). For optimization purposes the *absolute cost* of an energy system C_{es} may be considered (see above):

$$C'_{\mathrm{FE}} = \frac{C}{FE} \quad (5)$$

The *energy productivity EP* is also an economic–thermodynamic indicator and is calculated from the gross domestic product *GDP* and the final energy demand *FE* [45]:

$$\mathrm{EP} = \frac{\mathrm{GDP}}{\mathrm{FE}} \quad (6)$$

The energy productivity is usually used to assess national energy systems, and its significance decreases the smaller the energy system under consideration is. For example, the energy productivity of the small country of Luxembourg is strongly distorted by the strongly developed steel industry [46] and a high number of commuters and the resulting influences on the *GDP* [47]. Following analogous considerations, the suitability of this indicator for cities is doubtful.

In addition to the indicators mentioned, any other parameter can be divided by the discussed reference values, and thus be used as an energy efficiency indicator. In this way, other local emissions and resource requirements can also be included in ESM. Vera and Langlois [21] as well as Wang et al. [22], for example, list each about 30 indicators, divided into technical, social, economic and ecological aspects. In the context of energy system modeling, however, it is necessary to keep the number of indicators manageable and thus to choose a few meaningful and comparable indicators.

Sufficiency indicators for urban energy systems

The sufficiency strategy aims at limiting energy consumption to a sustainable level. There is no consensus of any value at which urban energy systems reach a state of sufficiency. There are, however, attempts to define such a level and apply them as indicator. One example is the Swiss 2000-Watt-certification standard for city districts [48]. Here, the primary energy demand including energy bound in building materials is related to the number of inhabitants [49] with the goal of reducing this value to 2 000 Watt per inhabitant.

Such absolute limits for energy consumption to a sustainable level may provide helpful orientation for the design and planning of urban energy systems. Determining those is, however, not only a complex research task on its own, but also requires a fair and detailed process that takes different city and district structures into account. The 2000-Watt-standard is applied to residential districts only [49], probably because urban areas with different sectoral structures (e.g., industrial, commercial or residential consumers) can hardly be compared with each other. We thus do not define absolute values for this indicator, but consider a reduction of energy demand generally as a contribution to sustainability.

Instead of using the primary energy demand to calculate the energy demand as done in the 2000-Watt-standard, we consider the use the final energy demand *FE* as more suitable. This excludes conversion processes from primary to final energy, and thus the efficiency of these processes, which are already represented by the efficiency indicators.

The *specific energy demand per inhabitant* ED'_{inh} is the ratio of the systems total final energy demand to the number of inhabitants n_{inh} (Eq. 7). The *absolute energy demand* of an energy system ED_{es} may be considered for optimization processes (see above):

$$ED'_{\text{inh}} = \frac{FE}{n_{\text{inh}}} \tag{7}$$

The reduction of the final energy demand can provide a rough assessment of many sustainability aspects, since the reduction of the demand leads to a reduction of resource needs. Although this is vague and not expressed in numbers here, it is conceivable that any reduction of the final energy demand reduces the environmental impact better than a sheer switch to another primary energy source. Note that renewable forms of energy also have certain resource requirements [50].

This particularly applies for demand reductions through sufficiency measures. However, the (specific) energy demand is influenced both, by the system's efficiency and sufficiency. In order to measure pure sufficiency effects with the help of this indicator, all efficiency parameters of the system must remain unchanged. For more precise statements regarding the system's energy sufficiency, parameters and indicators like heated living space per person, average room temperatures, electrical appliances per household or person, usage intensity of electrical appliances, volume of material production would have to be included. Those are beyond the scope of classic ESM, but could be included in sector models of the building or industry sectors.

Concluding, within the scope and possibilities of ESM, the indicator of (specific) energy demand (Eq. 7) provides a rough indication of sufficiency. When applying the indicator for comparison of different cities or districts, the sectoral structure needs to be taken into account.

Consistency indicators for urban energy systems

Energy consistency is mostly understood as the shift from fossil to renewable sources. Thus, the *share of renewables* (*SoR*), can be regarded as an appropriate energy consistency indicator [12, 51]:

$$SoR = \frac{\text{FE}_{\text{renewable}}}{\text{FE}_{\text{total}}} \tag{8}$$

In order to be considered sustainable, the utilization of an energy source should not exceed its *regeneration rate* [52, 53]. In this context, the consistency of an energy system could be assessed by considering the useful life t_{use} of materials used within an energy system in relation to its regeneration time t_{reg}:

$$t = \sum_{1}^{n} \frac{t_{\text{use,n}}}{t_{\text{reg,n}}} \tag{9}$$

Basically, this indicator is closely related to the *SoR* indicator, as both aim at the renewability (regeneration) of resources. However, this indicator goes into more detail than the *SoR* indicator and can, for example, also compare different renewable energy technologies (e.g. photovoltaic systems vs. biomass). However, in order to obtain a meaningful value, all materials used within an energy system, from the concrete in the foundation of a power plant up to the fuel, must be taken into account. Furthermore, emissions should also be considered as a "resource" and should be set in relation to the duration of mining. Such a balance would be extremely complex to compute and is a research field on its own.

Another aspect of consistency can be the locational origin of the energy source. A self-sufficient system can survive as a stand-alone unit, without any import of energy [54]. We use the location of energy supply as an evaluation of the energy origin and therefore the indicator *self-sufficiency SeS* to assess the degree to which a city or district can supply its own energy needs:

$$\mathrm{SeS} = \frac{\mathrm{FE}_{\mathrm{local}}}{\mathrm{FE}_{\mathrm{total}}} \tag{10}$$

Although the term sufficiency appears in the name of the indicator, it does not indicate a system's sufficiency in our understanding of this term. The self-sufficiency indicator is useful when considering the goals of strengthening the regional economy and reducing inter-regional grid capacities (e.g., from the wind-energy-intensive north to the south of Germany).

However, although local energy supply is indeed desirable [55], it must be questioned how an increase of self-sufficiency contributes to the fulfillment of sustainability goals in urban energy systems per se, or if a linkage to regionally connected systems is preferable from a broader sustainability perspective. Therefore, the regional reference of FE_{local} should be defined case-by-case.

Methods: single-criterion simulation

Based on the literature review and the arguments presented in the previous subsections, we consider

- Primary energy efficiency,
- (Specific) GHG emissions,
- (Specific) energy costs,
- Share of renewables,
- Self-sufficiency,
- (Specific) energy demand,

as basically suitable for the evaluation and optimization of urban energy systems. For the sufficiency indicator of specific energy demand, the restrictions discussed before need to be considered. We consider other indicators to be less suitable, due to their shortcomings of not including upstream chains (secondary energy efficiency *SEE*), their limited capability to compare small energy systems (energy productivity *EP*), or their excessive accounting expense (regeneration rate *t*). The chosen indicators will be further tested for use in energy system modeling.

The basically suitable indicators (see above) will be examined by applying them to an ESM. A real-world urban area will be simulated with different supply scenarios.

As long as the energy demand remains constant, there is a linear relationship between absolute emissions $m_{\mathrm{GHG,es}}$, costs C_{es}, and energy demand ED_{es} to specific emissions $m'_{\mathrm{GHG,FE}}$, specific costs C'_{FE}, and specific energy demand per inhabitant ED'_{inh}. Since we do not compare different systems in this case study (see "Efficiency indicators for urban energy systems"), we will use absolute values as long as the energy demand remains constant. When the energy demand changes (scenario 4), we will show both, absolute and specific values, in order to represent both efficiency and sufficiency effects.

The urban district "Strünkede" of the municipality of Herne (North Rhine-Westphalia, Germany) will be used as a real-world test area. This district has about 3 600 inhabitants and consists of 500 buildings (residential and non-residential).

We simulate a total of four energy supply scenarios and analyze how the chosen sustainability indicators behave depending on the intensity of the implementation of certain measures. Each of the four scenarios focuses on a different type of measure, all of them aiming to improve the district's energy sustainability. Namely, the share of renewable energy imports (scenario 1), the use of renewable energy technologies (scenario 2), the use of sector-coupling technologies (scenario 3), and the reduction of energy demands (scenario 4). Although the mobility/transport sector accounts for 30% of Germany's energy consumption [56], it is not examined in these scenarios. Due to its different structure, other indicators and model functionalities would be required to adequately cover the transport sector. Grey energy — i.e. the *CED* of consumer goods — is also not investigated due to similar reasons.

We use the "Spreadsheet Energy System Model Generator" (SESMG) v0.0.4, respectively v.0.2.0 [57], a model generator based on the "Open Energy Modeling Framework" (oemof) [58], for the simulation. The applied model uses a bottom-up analytical approach, methods of simulation and optimization, and the mathematical approach of linear programming. A district-sharp spatial resolution, a 1-hourly temporal resolution, and a 1-year time horizon is used. The operating modes of the plants in the model are dispatch-optimized with respect to the respective indicator under investigation. Investment optimization is not performed within this section. For detailed description of modeling methods, we refer to the documentation of oemof [59] and the SESMG [57]. The underlying Open

Energy Modelling Framework (oemof) and its sub-modules have undergone several validations [60].

Standard load profiles (SLP) are used to simulate the course of the electricity [61] and heat demand [62]. The annual electricity demand (11 000 MWh/a) and heat demand (32 000 MWh/a, see Table 2 in Appendix) are estimated on the basis of the type of building, building area, number of floors and number of residents. Photovoltaic systems (scenario 2 and 3) are simulated on the basis of weather data obtained from the German Weather Service [63]. The year 2012, an average solar year [64], was chosen as reference. We account for the GHG emission scopes listed in Table 1.

All other model parameters (plant efficiencies, costs, emissions) are estimated based on databases [63, 66, 67], legal bases [68], standards [32, 69], research articles [70], technical studies [71–73], comparison of market energy tariffs, data from the municipality of Herne and the German federal state of North Rhine-Westphalia as well as expert estimates. The model parameters used are listed in Appendix.

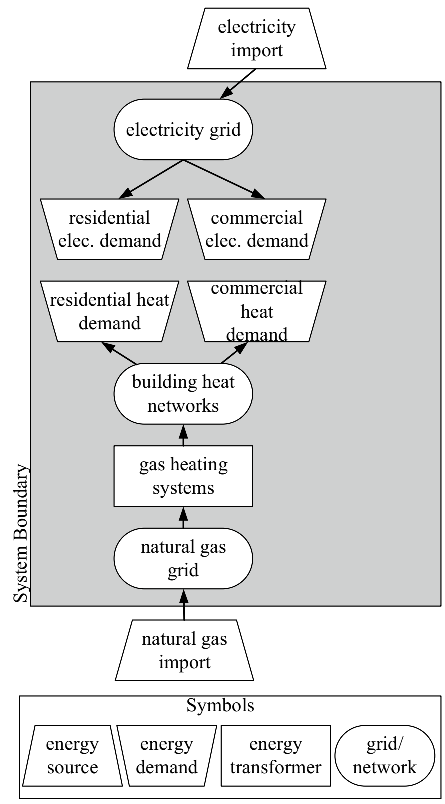

Fig. 1 Scenario 1

Results: single-criterion simulation

Scenario 1 — energy import

The first scenario (Fig. 1) reflects a typical current state of a German district energy system. It is assumed that the electricity demand is covered by electricity imports and the heat demand is covered by gas heating systems, operated with imported natural gas. The average German electricity mix (42% renewable energies [74]) is used.

We analyze the response of sustainability indicators to the share of renewable energies within the imported electricity (with an otherwise unchanged electricity mix) from zero (no renewable electricity) to one (100% renewable electricity) (Fig. 2). The indicators shown in Fig. 2 refer to the total energy supply, i.e. electricity and heat.

The primary energy efficiency increases from 0.68 to 0.88 due to the lower primary energy factor of renewable energies [32]. The share of renewables increases to a lesser extent than the share of imported electricity. The total share of renewables thus results from the share of renewables in the imported electricity, multiplied by the share of electricity in the total energy demand (about 2%). A further increase of this value is only possible if the heat supply (0% renewable) is substituted by renewable sources. The specific GHG emissions m'_{GHG} decrease due to the lower carbon footprint of renewables compared to other technologies of the German electricity mix. The required energy is still completely imported ($SeS = 0$) and thus remains the same. The energy demand ED_{es} remains constant because no changes have been made on the consumption side.

Table 1 Considered GHG emission scopes. Terms based on definitions of the World Resource Institute [65] and adapted for the purpose of analyzing urban energy systems

Scope	Definition
1	"Direct GHG emissions occur from sources that are" within the model domain, "for example, emissions from combustion in owned or controlled boilers, [...], etc." [65].
2	"GHG emissions from the generation of [imported] electricity", consumed within the model domain. "Scope 2 emissions physically occur at the facility where electricity is generated" [65]. For exported electricity a GHG emission credit is granted, accordingly.
3	GHG emissions of energy suply facilities which "occur from sources not owned or controlled" [65] within the model domain, e.g. for the production of photovoltaic modules.

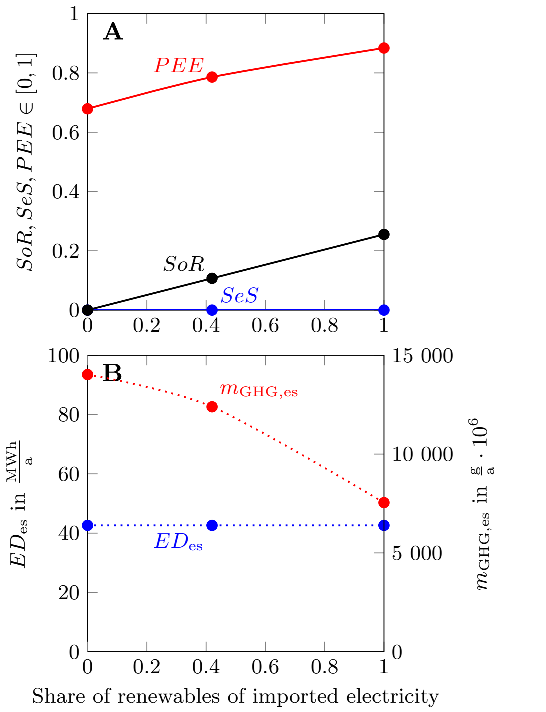

Fig. 2 Indicators in scenario 1. The simulated values are represented as dots and connected by lines. Abbreviations: *PEE* = primary energy efficiency, *SoR* = share of renewables, *SeS* = self-sufficiency, $m_{\mathrm{GHG,es}}$ = absolute GHG emissions, ED_{es} = absolute energy demand

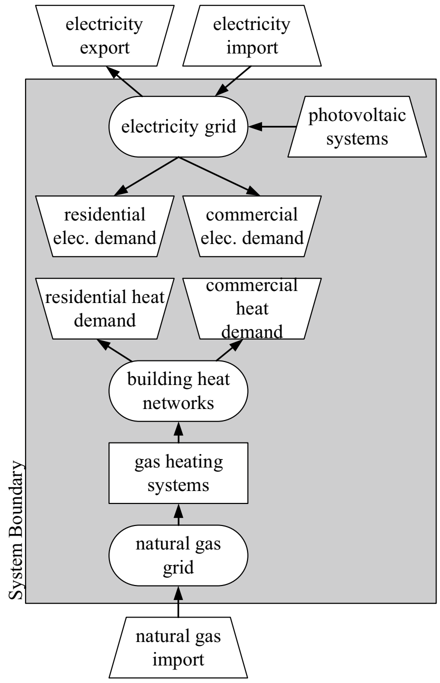

Fig. 3 Scenario 2. Symbol legend see Fig. 1

With the change in the share of renewable energies in the German electricity mix, the price of imported electricity will change due to macro-economic correlations. These relationships cannot be described with the model used in this study. For this reason, no curve for the energy costs C_{es} is presented for this scenario.

Scenario 2 — local renewable generation

In the second scenario, photovoltaic systems for decentralized provision of renewable electricity are added to the energy system. Energy required beyond that (electricity and natural gas) is imported like scenario 1. Electricity produced in excess of demand can be exported (Fig. 3).

Most indicators show a saturation effect after an installed PV capacity of 5 MW (Fig. 4). This is because PV systems only supply electricity at certain times. At times when no electricity can be supplied (e.g., at night), electricity still needs to be imported, no matter what PV capacity is installed. If in turn the demand of the system is exceeded (the maximum demand is 2.1 MW), electricity has to be exported. Exported electricity may have a positive influence on energy systems elsewhere. If the installed systems were thus to be related to a global energy system, no saturation behavior is expected.

The absolute energy cost curve does not show saturation effects, since electricity that is produced within the system boundary but not used by internal consumers, can be sold at a fixed rate due to the German renewable energies act (EEG [68]), and can thus be sold with profit. Although a credit is also granted for emissions, this does not generate any "emission profit" (the credit granted for exports is exactly the same as the emissions taken into account for production, see Table 1), which also leads to saturation behavior of the absolute emissions.

The decrease of the energy costs C_{es} is limited by the availability of space within the system area that can be used for installation. The exact cost values as well as the slope of the C_{es}-curve furthermore depend on the remuneration rate taken into account (changes for example, due to revised EEG frameworks). This remuneration is allocated to end-consumers in the form of the EEG compensation-fees. If the share of renewable energies in the electricity grid increases, this apportionment may rise. A nationally uniform expansion in the same proportion to the district under consideration could thus lead to an increase in the price of purchased energy, which in turn would increase the specific

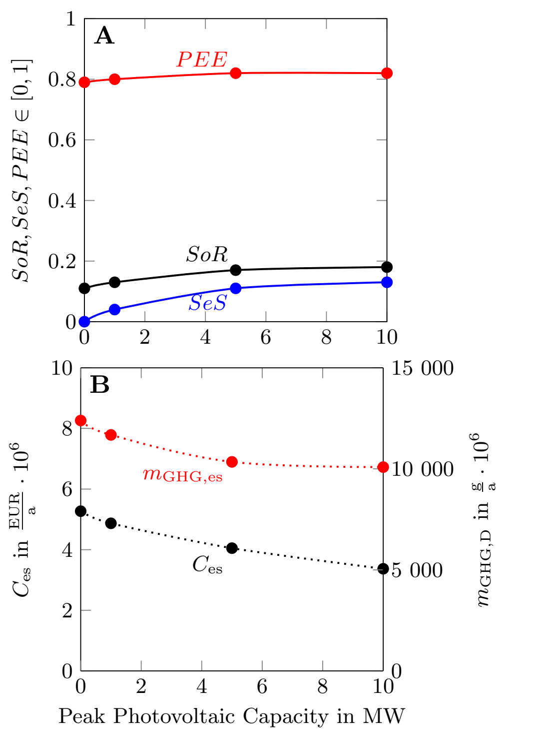

Fig. 4 Indicators in scenario 2. The simulated values are represented as dots and connected by lines. Abbreviations: *PEE* = primary energy efficiency, *SoR* = share of renewables, *SeS* = self-sufficiency, $m_{\mathrm{GHG,es}}$ = absolute GHG emissions, C_{es} = absolute energy costs

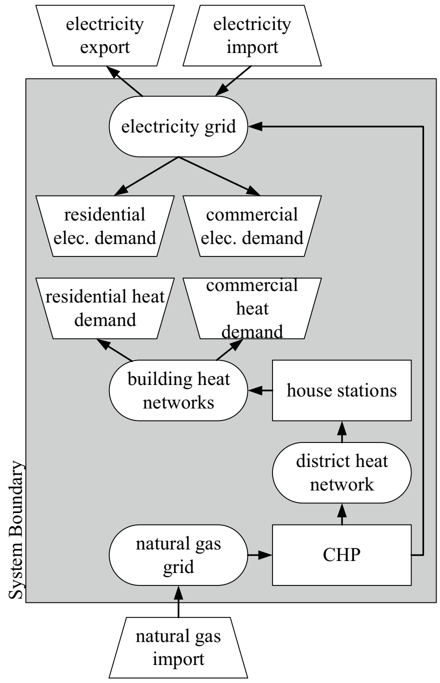

Fig. 5 Scenario 3. Symbol legend see Fig. 1

energy costs. A model with national balance limits is needed to investigate this relationship in more detail.

As in scenario 1, the (specific) energy demand remains constant and is for the sake of clarity not displayed here.

Scenario 3 — sector coupling

In the third scenario, a measure is considered which affects not only the electricity sector but also the heat sector. The entire energy supply is secured by combined heat and power plants (CHP) with an electric performance of 16 MW (thermal performance of 25 MW) in combination with a district heating network (Fig. 5). The CHPs can be operated either with biogas or natural gas. For the supply of both gases (natural gas import, biogas production) the same costs are assumed.

Figure 6 shows the development of the indicators depending on the share of (electrical) capacity of biogas, respectively natural gas-fired CHPs. Again, the specific energy demand remains constant and is therefore not displayed.

The primary energy factor of biogas CHPs is lower than that of natural gas CHPs [66]. Therefore the primary energy efficiency decreases with increasing biogas input, showing a saturation behavior. This can be explained by the fact that the lower capacity ranges are needed more frequently during the year than the higher ones (frequency quartiles of the CHP's electricity output: Q1: 1.7 MW, Q2: 3.6 MW, Q3: 6.0 MW, Q4: 16.0 MW). Thus higher biogas CHP capacities (especially above 6 MW) have less influence on the indicator.

In contrast to the scenarios discussed before, the increase of the share of renewables *SoR* and the self-sufficiency *SeS* is no longer limited to the share of the electricity sector. If the CHP units are solely operated with biogas which has its origin within the system area, both *SoR* and *SeS* increase to the maximum of 1. Again, there is a saturation effect for the same reason as for the primary energy factor. It has to be noted that in the real-world system, the availability of space for biogas production is probably limited and thereby restricts the increase of self-sufficiency *SeS* and share of renewables *SoR*.

Due to the higher purchase costs for biogas compared to natural gas, the energy costs C_{es} increase with increasing biogas usage. From approximately 8 MW electric biogas capacity on, the increase in costs becomes steeper. This can be explained by the above-mentioned frequency distribution of the CHP output and the dispatch optimization of the cost indicator (see "Methods:

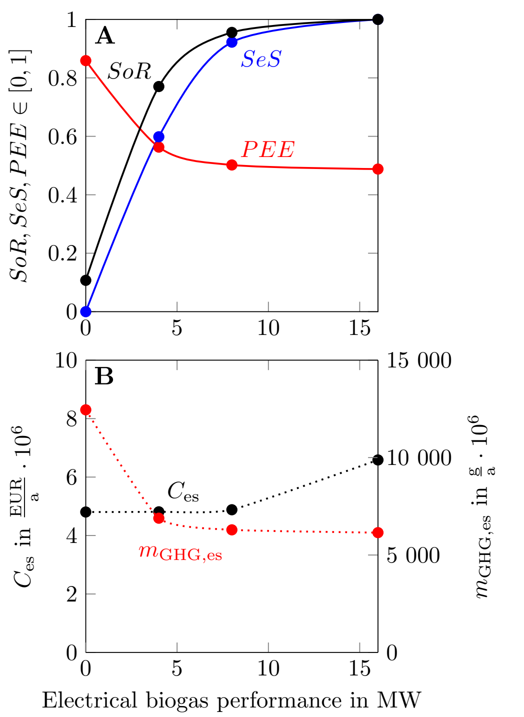

Fig. 6 Indicators in scenario 3. The simulated values are represented as dots and connected by lines. Abbreviations: *PEE* = primary energy efficiency, *SoR* = share of renewables, *SeS* = self-sufficiency, $m_{GHG,es}$ = absolute GHG emissions, C_{es} = absolute energy costs

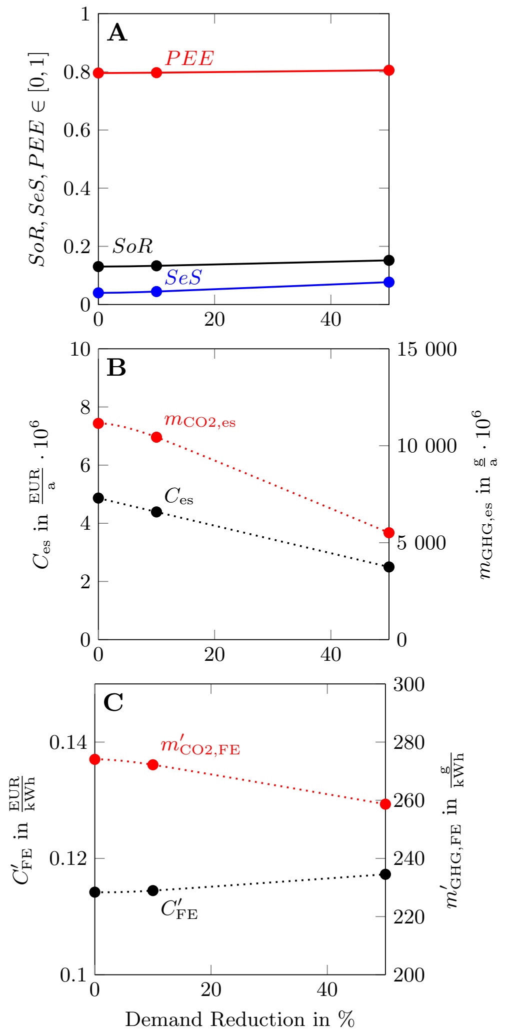

Fig. 7 Indicators in scenario 4: demand reduction, based on scenario 2 (1 MW photovoltaic systems). The simulated values are represented as dots and connected by lines. Abbreviations: *PEE* = primary energy efficiency, *SoR* = share of renewables, *SeS* = self-sufficiency, $m_{GHG,es}$ = absolute GHG emissions, $m'_{GHG,FE}$ = specific GHG emissions per final energy demand, C_{es} = absolute energy costs, C'_{FE} = specific energy costs per final energy demand

single-criterion simulation"). The (low-cost) available natural gas CHP capacity is used first, followed by the biogas CHP capacity. If the biogas CHP is only used to cover infrequent load peaks, the influence on the total system costs is relatively small, but if it is needed for the frequent base load capacities — which is the case in Fig. 6 above about 8 MW — the influence is correspondingly greater and causes the curve to rise more steeply.

Scenario 4 — demand Reduction

In the fourth scenario, the effect of changing energy demand on the district's sustainability indicators is analyzed. On the basis of scenario 2 (including 1 MW of PV systems), it is assumed that the energy demand is reduced by up to 50% for each simulated hour, both in the heating and electricity sector (Fig. 7).

The reduction in demand — which can be a result of sufficiency and efficiency measures lowers the energy demand (absolute and specific). The reduction in consumption ensures an absolute reduction in GHG emissions $m_{GHG,es}$ (Fig. 7, B). The GHG emissions are not only reduced linearly with the demand reduction, but also the GHG emissions per final energy $m'_{GHG,FE}$ (Fig. 7, C) are reduced, resulting in a exponential reduction of the total GHG emissions. This can be explained by the fact that a fixed capacity of PV systems (in this scenario we consider a fix capacity of 1 MW) can provide a higher share of the electricity supply when energy demand decreases. The reduction in consumption thus ensures that sources with high GHG emissions are used to a lesser extent, which leads to a reduction in GHG emissions. This effect also ensures a slight improvement in all other indicators (except for specific costs per final energy demand C'_{FE}).

With increasing PV capacity, the specific indicators (Fig. 7C) would change even more, and thus lead to an increasing de-linearization of the absolute indicators (Fig. 7B).

The reduction of the demand initially leads to a slight increase of the specific costs per final energy demand C'_{FE} (Fig. 7C). This is because higher consumption leads to an increased use of PV-electricity, which allows a higher profitability of PV electricity (import costs minus PV electricity production costs) than its sale (export price of PV electricity, see Appendix). However, this is a very small effect and becomes negligible when considering the absolute energy costs C_{es} (Fig. 7B).

Evaluation of the indicators

Energy efficiency indicators: The modeling results show that the primary energy efficiency *PEE* rather reflects the share of renewable than efficiency. Its increase in scenarios 1 and 3 is mainly due to the low primary energy factors used for (imported) renewable energies due to the VDI 4600 directive [32, 66]. Thus, the observed increase of primary energy efficiency is less driven by an improvement of the district's technical efficiency than by the accounting method, which grants an advantage to renewable energies. With increasing shares of renewables, the primary energy efficiency loses its original meaning of displaying efficient use of energy. Another criticism is that the primary energy efficiency factors to be applied according to the VDI 4600 directive do not distinguish between different forms of renewable energy.

With respect to the compliance with national and international climate protection targets, it is more appropriate to use the physical–thermodynamic indicator of (specific) GHG emissions as optimization criterion in ESM. Furthermore, it is not only suitable for the assessment of fundamental trends, but also for the identification of either limits that improvement measures may meet (e.g. saturation effect in scenario 3) or of a decrease of system performance.

Economic aspects play a significant role in planning practice. Economic indicators thus have a decisive influence on whether and which measures and technologies are implemented in urban energy systems. The indicator of (specific) energy costs is well suited for this purpose and should be taken into account.

Energy sufficiency indicators: The identification of suitable sufficiency indicators for ESM is difficult, since sufficiency targets at a reduction of energy service demand (e.g. heated living space per person), which is not directly considered in energy system models. However, the specific energy demand per inhabitant ED'_{inh} can give an impression of the contribution of demand-side measures. Although it cannot be distinguished between the contribution of efficiency or sufficiency, the indicator provides indications of absolute demand reduction, which is the more decisive information in terms of sustainability. Since this indicator is strongly dependent on external circumstances (sector structure, building efficiency, etc.), it should always be given together with structural information about the urban area under study. In addition, it is much less the *fixed value* of this indicator than its *change* that should be rated.

The increase of sufficiency of an urban energy system has several advantages: In addition to the absolute reduction of consumption and the associated savings, the specific costs and emissions are reduced. Since these values (consumption and its specific emissions or specific costs) are multiplied with each other to calculate the total emissions or total costs, the total savings through sufficiency measures not only exert a linear effect, but rather a quadratic effect on the savings (see "Scenario 4").

Energy consistency indicators: The share of renewables *SoR* is a clear and straightforward indicator. Nevertheless, increasing renewable energy is not a sustainability goal per se, but rather a way to reduce greenhouse gas emissions and conserve fossil fuels. The indicator does not provide any information on the improvement of these sustainability goals. Furthermore, it does not distinguish between different types of renewable energy and their different impacts on the main sustainability goals. Therefore, the indicator share of renewables is only conditionally suitable for measuring the energy sustainability of urban energy systems.

The indicator of self-sufficiency *SeS* is suitable for evaluating the increase of the local value. Nevertheless, it is questionable whether increasing self-sufficiency contributes to the sustainability of urban energy systems (see "Consistency indicators for urban energy systems"). The indicator is more suitable for evaluating entire regions, and less for individual urban areas or cities.

Methods: multi-objective optimization

As shown, there are a number of indicators that can evaluate various sub-goals of energy sustainability of urban energy systems in ESM, or can be used for optimization. But there is no single indicator for the evaluation of urban energy systems which combines various aspects and thus represents a broader perspective of different sustainability aspects. Therefore, multi-criteria optimization approaches are required for enabling such a broader perspective.

In classical single-criterion optimization, the scenario is determined which allows the minimization or maximization of the target value, other boundary parameters are completely left out [75]. Multi-objective optimization approaches in turn consider several, usually competing criteria for the optimization [75]. Therefore, the methods of combined indicators or adding constraints in single-criterion models (hereafter referred as "constraint optimization") may be considered.

By using the *combined indicator* approach, individual indicators are combined to a single value [76]. Two common approaches are the weighted sum (Eq. 11), and weighted product method (Eq. 12) [76].

Indicators formed by the *weighted sum approach* (Eq. 11) can usually be used in single-criterion optimization models. This is possible because the different indicator values (e.g., costs or emissions) — even if they occur at different process points — are simply added up to an overall indicator value. The original multi-criteria problem is thus transformed into a single-criterion problem. However, the drawback of the weighted sum method is, that the single indicators must have the same unit in order for Eq. (11) to be mathematically solvable [77]:

$$F(\vec{x}) = \sum_{i=1}^{k} w_i f_i(\vec{x}) \tag{11}$$

$F(\vec{x})$ multi-criteria function, $\vec{x}$ set of decision variables, k number of applied criteria, $f_i(\vec{x})$ function of criterion i, w_i weighting of criterion i.

The weighted product approach works similarly to the weighted sum approach [78], except that the individual indicators f_i are multiplied and the weights w_i are taken into account as potencies [76]:

$$F(\vec{x}) = \prod_{i=1}^{k} f_i(\vec{x})^{w_i} \tag{12}$$

The weighted product approach can possibly not easily be applied to single-criterion ESM tools, if the tool does not allow multiplying indicator values that apply at different process points (e.g. costs for purchasing natural gas vs. emissions from burning the gas). It has to be individually checked whether the respective modeling tool permits the use of such multi-indicators. Further note that multi-criteria functions could possibly complicate the system of equations to be solved by the model and thus increase the computing time. This may result in the need to simplify model structures in order to reduce the computing time, which may in turn reduce model accuracy.

With *constraint optimization* (also known as ϵ-constraint method [79]), the classical approach of single-criterion optimization is extended by restricting the possible solution space of the model. Therefore, for at least one additional criterion, limits (constraints) are defined by the modeler. A single-criterion solution algorithm can

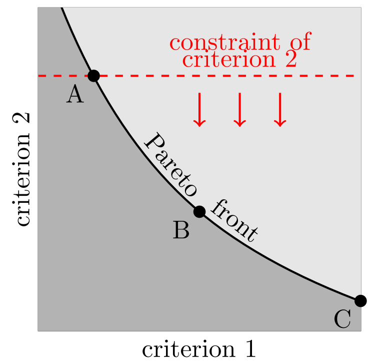

Fig. 8 Exemplary two-criteria Pareto front. Solution space in light gray (infinite number of possible scenarios), not realizable space respectively scenarios in dark gray. Three exemplary best-known Pareto points (A, B, C) are shown

then determine the remaining solution space for the minimum of the primary optimization criterion.

In this way, a multi-criteria optimization can be performed without using a multi-criteria indicator. Constraint optimization has the disadvantage that the modeling effort is greater, since each constraint limit must be set manually. In the case of an iterative reduction of this value, this can require a large number of model runs. Moreover, it should be noted that single-criterion energy system modeling tools sometimes can only apply constraints that are related to the main optimization criterion, but not for further criteria.

The solution of a multi-criteria solution function $F(\vec{x})$ does not — as in the case of a single-criterion function $f_i(\vec{x})$ — result in a single solution scenario $\vec{x}$, but in a set of (in the sense of the function) equivalent solution scenarios [80]. The function of these scenarios is known as *Pareto front* (Fig. 8, black) [81], which has one graphical dimension per selected sub-criterion.

By adjusting constraint optimization, several different scenarios, which lie on the Pareto front, can be determined. These are also often called "*best-known Pareto points*" [75]. By, for instance, successively moving the constraints shown in Fig. 8 (red) downwards, the scenarios A, B, and C could be determined.

Multi-objective optimization approaches are of particular importance in the context of sustainable optimization of urban energy systems, especially because the previous overview has shown that there is no single indicator for holistic quantification.

Combined indicator

In compliance with the design goals for urban energy systems (see "Introduction") and the discussion within "Evaluation of the indicators" Section, we consider specific energy costs, specific GHG emissions, and specific energy demand as the most appropriate indicators to be combined within an multi-objective optimization. Due to their shortcomings, the indicators of primary energy efficiency (unsuitable accounting method), share of renewables (not fulfilling climate protection goals per se and no differentiation of different types of renewables) and self-sufficiency (questionable impact on the overall system sustainability) will not considered further for the multi-criteria optimization approach.

Since the selected indicators have different units, they can only be combined using the weighted product method (Eq. 12):

$$F(\vec{x}) = \prod_{i=1}^{k} f_i(\vec{x})^{w_i} \tag{12}$$

$$F(\vec{x}) = (C'_{\mathrm{FE}})^{w_{\mathrm{C}}} \cdot (m'_{\mathrm{GHG,FE}})^{w_{\mathrm{m}}} \cdot (ED'_{\mathrm{inh}})^{w_{\mathrm{ED}}} \tag{13}$$

$$F(\vec{x}) = \frac{C^{w_{\mathrm{C}}}}{FE^{w_{\mathrm{C}}}} \cdot \frac{m_{\mathrm{GHG}}^{w_{\mathrm{m}}}}{FE^{w_{\mathrm{m}}}} \cdot \frac{FE^{w_{\mathrm{ED}}}}{n_{\mathrm{inh}}^{w_{\mathrm{ED}}}} \tag{14}$$

$$F(\vec{x}) = \frac{C^{w_{\mathrm{C}}} \cdot m_{\mathrm{GHG}}^{w_{\mathrm{m}}} \cdot FE^{w_{\mathrm{ED}}}}{FE^{w_{\mathrm{C}}} \cdot FE^{w_{\mathrm{m}}} \cdot n_{\mathrm{inh}}^{w_{\mathrm{ED}}}} \tag{15}$$

A further simplification is possible, if $w_i = 1$ applies for all weighting variables:

$$F(\vec{x}) = \frac{C \cdot m_{\mathrm{GHG}}}{FE \cdot n_{\mathrm{inh}}} \tag{16}$$

For the application of absolute values applies:

$$F(\vec{x}) = C^{w_{\mathrm{C}}} \cdot m_{\mathrm{GHG,es}}^{w_{\mathrm{m}}} \cdot FE^{w_{\mathrm{ED}}} \tag{17}$$

If nuclear power play a role in the energy system under study, it is recommended to additionally use either the share of renewables (Eq. 8) or the resources regeneration time (Eq. 9).

Constraint optimization model

For the optimization, the model used for the single-criterion simulations is extended by investment decision variables. Specifically, the model has the possibility to design the capacities of decentralized gas heating systems (scenario 1 and 2), photovoltaic systems (scenario 2, max. 10 MW) and central natural gas or biogas CHPs (scenario 3, max. 16 MW). As within the single-criterion model, dispatch optimization is performed as well.

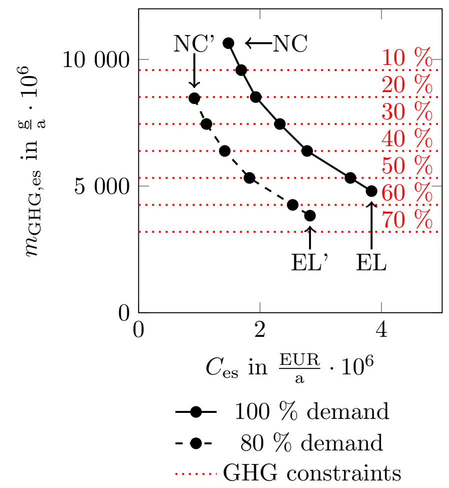

Fig. 9 Best-known Pareto points of a constraint optimization using absolute energy costs C_{es} as primary optimization criterion and absolute GHG emissions $m'_{\mathrm{GHG,es}}$ as well as absolute energy demand *ED* as constraints. The scenarios without an emission constraint (NC and NC') and the lower emission limits (EL and EL') of the solution space are marked separately. The constraint values are to be understood as percentage reductions of the initial value NC

As most of the optimization ESM [82], our modeling approach does not support the calculation of Pareto-curve functions from multi-criteria functions like shown in Eq. 16 or 17. For this reason and the advantages outlined in sec. 9, in the following we will use the constraint optimization approach and will determine best-known Pareto point. Therefore, we will first perform a purely cost-optimized model run (no constraint, NC). Based on the resulting scenario, the permitted GHG emissions are reduced in 10% steps until the value is so low that no target scenario can be determined. In a further model run, the lower emission limit of the solution space is determined, by using the GHG emission as optimization criterion. Subsequently, the energy demand is reduced, which is equivalent to a constraint of energy consumption, and optimized for the *same* GHG emission constraints as before.

Here, the demand reduction represents an opportunity, i.e., it is not a typical constraint limitation. However, this changes when the demand in systems is limited by planning regulations or individual target values. A demand constraint becomes particularly important if demand

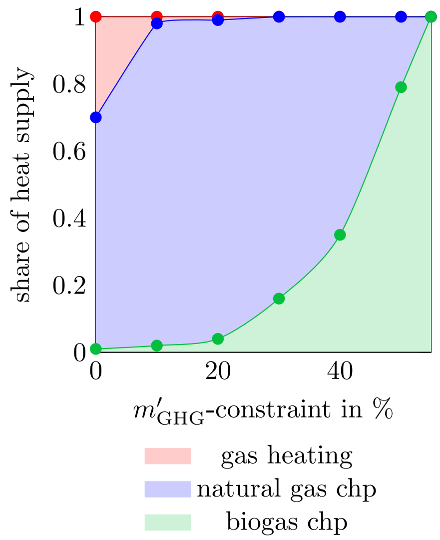

Fig. 10 Share of heat technologies available in the optimization model for heat supply with increasing GHG-constraint (in % from starting point NC, see Fig. 9)

can be reduced by an investment, e.g. by investing in better insulated windows/insulation or more efficient end-appliances (dryers, refrigerators, etc.). Then, the goal of minimizing costs would possibly get into a conflict with a demand constraint. This is a typical context for multi-criteria optimization.

Results: multi-objective optimization

The solution scenarios of the individual constraint optimization runs are best-known Pareto points. When the points are connected, the result is a typical Pareto front. In Fig. 9, slices of the actually three dimensional front (since three criteria are used) are shown. Without demand reduction, the model with 60% reduction of GHG emissions cannot be solved, because the set limits of emission free supply options are reached. Thus, such a scenario is outside the possible solution space. The lower emission limit (EL) of the solution space is below 5% of the emissions of the NC-scenario.

As the emissions constraint increases, the financial costs C' become higher. Thus, there is a conflict between cost and emission optimization in this system. The relationship is not linear.

However, the demand reduction is *not counteracting* for the other two optimization criteria, as no (investment) costs are incurred or GHG emissions are emitted for the demand reduction. Therefore, the demand reduction is an *opportunity*, which simultaneously provides a reduction in financial costs and GHG-emissions (dashed line in Fig. 7) and therefore provides a shift in the Pareto curve in Fig. 9 to the lower left. The demand reduction by 20% has the effect that even without emission constraint (NC' in Fig. 9) the emissions are lower compared to the point NC — with simultaneous reduction of costs. With the demand reduction, the solution space is extended downwards, so that also a scenario with 64% (EL') GHG emission reduction compared to NC can be enabled.

The change in the target scenarios can be attributed primarily to the cost/emission conflict in heat supply. The share of heat supply technologies available for optimization is shown in Fig. 10. Accordingly, without an emissions constraint, the heat supply is predominantly designed with natural gas CHPs with small shares of decentralized natural gas heating systems. With increasing emissions constraint, gas heating systems are not considered at all and biogas CHPs gain relevance compared to natural gas CHPs. As in the Pareto curve in Fig. 9, the progression is not linear. In each of the calculated scenarios, the investment limit of PV plants is completely used.

Discussion

The selection of suitable indicators for use in energy system modeling is influenced by several aspects. These include the selected spatial and energy system boundaries, the impact of individual indicators on the defined sustainability goals, whether indicators are used for optimization or benchmarking purposes, and whether single-criteria or multi-criteria modeling techniques are used.

System boundaries: The choice of system boundaries has decisive influence on sustainability indicators and have to be chosen carefully with respect to the effects the modeling should focus on. This applies to the used terms of energy, the applied geographical coverage, and the consideration of influences on resources other than energy. This can be used to direct the focus on certain aspects, but it can also lead to a “sham improvement” by outsourcing non-sustainable processes (see "Efficiency indicators for urban energy systems"). As outlined before, we consider upstream chains in the overall context of energy efficiency to be very important and therefore recommend the use of primary energy efficiency *PEE* over secondary efficiency *SEE*.

Awareness of the chosen system boundaries and respective effects are equally important for GHG emissions. Often the technologies used in the district have an influence outside the system boundaries, which may be considered to a given degree or neglected. This includes the emissions in the upstream chain of technologies used. Since climate change is not limited to the system boundaries of an urban area, the upstream chains need to be considered for providing a more holistic picture of emission reduction options.

Spatial system boundaries also exert an impact on the result. For example, the choice of a boundary limited to an urban area neglects positive effects of the export of renewable electricity to neighboring energy systems, national market impacts of raising energy prices due to increasing renewable energy production (see "Scenario 2 — local renewable generation"), or negative effects such as the indirect land use change effect (see below). In this case, the effect is outside the investigation area, but the *cause* is inside. Due to the limited space for energy generation, cities or districts can seldom fully meet their energy demands within their spatial boundaries. Thus, especially in the field of urban energy system modeling, system boundaries need to be carefully chosen to be able to assess sustainability of urban energy systems.

Another example of questionable sustainability contribution is the biogas usage displayed in scenario 3. There are doubts of the sustainability of land-use systems whenever a large portion of the managed land is used for biogas fuel production. A wider definition of the sustainability concept would lead to a different perspective since the choice of the balance limit neglects global impact of this scenario. In this case it can be assumed that considerable areas of land would have to be used for the biogas to be provided, which in turn may have a negative impact on the global climate balance via the indirect land use change effect [83].

Other sustainability aspects than GHG emissions (e.g., space, water, different raw materials) are not directly considered in this analysis as well. A global view is required to fully consider the respective effects. However, the indicator of (specific) energy demand can provide a first indication. Energy demand reduction in absolute terms generally leads to lower requirement of other resources as well. This might, on the one hand, be questionable for those efficiency measures which require resource-intensive technical measures and might therefore induce rebound effects, but is likely to be the case for sufficiency-induced demand reduction on the other hand. The combination of energy system modeling with complete life cycle assessment goes beyond the scope of most energy system analyses, but the various resource effects beyond GHG emissions should not be neglected in planning or political decision making. Thus, the indicator of specific energy demand and especially its change rate provides an important aspect of overall conservation of resources: the more the energy demand is reduced in absolute terms, the higher the likelihood that resource intensity and environmental impact in various aspects reduced as well.

Sustainability strategies: As a categorization of the examined indicators, we have used the trisection of efficiency, sufficiency, and consistency indicators. Thereby it became clear that there is no pure sufficiency indicator, since the indicators always depend on other strategies of energy sustainability. For example, efficiency (e.g. due to building insulation) has a significant influence on the specific energy demand ED'-sufficiency indicator. To actually measure energy sufficiency, all efficiency parameters must be kept constant, which is a quite unreasonable approach. Sufficiency rather needs to be measured on energy service level like, e.g., heated living space per person or electrical appliances per person. This requires more detailed sector models which in turn could be coupled with ESM.

Further difficulties arise when comparing different urban energy systems, as the structure (e.g. share of residential/commercial and industrial sectors) has a decisive influence on the total final energy demand of a system. A possible solution could therefore be to classify urban energy systems according to their structure so that homogeneous energy systems (e.g., purely residential areas) can be compared.

Reference values: Depending on the purpose of use, different reference values or absolute values may be used. We used final energy FE, the number of inhabitants n_{inh} as reference values, as well as absolute values. Absolute values are favorable for use in optimization models, since the equation of the respective indicators is usually rather simple. When compared to the reference value number of inhabitants n_{inh} (for the indicator specific energy demand ED'), absolute values are influenced by changes in the number of inhabitants. Thus, a decreasing number of inhabitants can improve this indicator value, although this does not provide a real sustainability benefit. Furthermore, compared to the reference value FE (e.g. for the indicators specific costs C' and specific GHG emissions m'_{GHG}), decreasing final energy demand has an influence on this indicator — thus also on sufficiency effects, although it is an efficiency indicator. Thus, absolute values ensure easy handling in optimization models, but for benchmarking and comparison purposes we recommend the use of the reference values of final energy demand *FE* and number of inhabitants n_{inh}.

Multi-criteria optimization: Energy sustainability of urban energy systems can be improved by various measures, e.g. by regenerative energy systems, sector coupling, demand reduction, demand-side management, energy storages and many more. Some of these measures have been exemplified within the modeling runs in this contribution. Depending on the weighting of the applied indicator, the combination of several measures and energy sustainability strategies in particular leads to the minimization of the applied optimization criterion.

If only a single target indicator is applied, the optimization of this value can simultaneously lead to a deterioration of other important indicators (as for example the cost and emission indicators in Fig. 6). While this conflict does not always become evident when using too few indicators in ESM, the application of a multi-criteria approach enables a more holistic view and trade-offs are quantified.

By applying multi-criteria optimization models, several equivalent scenarios in the form of a Pareto front can be compared and the conditions under which technology change occurs can be analyze (as shown, for example, in Fig. 10). Such an approach provides valuable insights for specialist planners, which can decide on a case-by-case basis which goals are most important to follow to which degree for urban energy systems.

Nevertheless, the number of indicators applied should be limited to a tolerable level: If too many indicators are used, it will be difficult to understand the interdependencies of the model and bears the potential of over-fitting. Furthermore, Pareto fronts with more than three indicators have more than three graphical dimensions. This in turn is difficult or impossible to visualize and thus also complicates the interpretation of the results. Further research on result communication of multi-objective optimization of various differently weighted indicators for urban energy systems is required.

As outlined in "Introduction", today's multi-criteria optimization models usually work with a cost and a greenhouse gas emission related indicator. In the context of urban energy system optimization, we recommend complementing them with the (specific) energy demand indicator. We further recommend that models that do not consider any measures of energy demand reduction, should be complemented. Due to the indirect effects of demand reduction (see "Sufficiency indicators for urban energy systems" and "Scenario 4 — demand reduction"), they will have decisive influence on the sustainability of urban energy systems.

Conclusion

Based on a theoretical evaluation and subsequent practical tests in an urban energy system model, various indicators were analyzed for the purposes of optimization as well as benchmarking and comparison of different urban energy systems.

As a result, there are indicators that are well suited for various aspects of the energy sustainability, but none that is able to represent overall energy sustainability of urban energy systems. The use of only one sub-indicator in the optimization process increases the risk that other important indicators will deteriorate significantly, leading to unrealistic scenarios in practice. To avoid this, multi-criteria approaches should be used to enable a more holistic optimization and planning of sustainable urban energy systems.

The evaluation of an exemplary urban energy system using the multi-objective ϵ-constraint optimization approach shows that a typical Pareto optimization curve (Fig. 9) and a clearly visible technology shift (Fig. 10) emerge for the competing optimization criteria of cost and greenhouse gas emission minimization. The optimization criterion of minimizing energy demand does not conflict with the other criteria, but actually supports them. Thus, minimizing demand provides an opportunity to improve the other objectives, within the available energy demand reduction potential. However, in subsequent studies it has to be examined to which extent costs and emissions, which are necessary for the reduction of the energy demand (e.g., investment costs of building insulation or financial incentives for consumption changes), impact the results of the multi-criteria optimization.

In conclusion, we recommend the use of multi-criteria models combining the indicators of absolute greenhouse gas emissions, energy costs, and energy demand, for the optimization of urban energy systems. For benchmarking and comparison purposes, specific indicators should be used and therefore related to the reference values of final energy (Eqs. 4 and 5), respectively, number of inhabitants (Eq. 7).

Appendix

Model parameters

See Table 2.

Table 2 System parameters used for modeling

Components	Periodical costs EUR/(kW·a)	Variable costs EUR/kWh	PEF	Periodical GHG emissions g/(kW·a)	Variable GHG emissions g/kWh	Efficiency
Electricity import (residential, 0% renewables)	0	0.3106	2.3	–	624	–
Electricity import (commercial, 0% renewables)	0	0.2156	2.3	–	624	–
Electricity import (residential, 42% renewables)	0	0.3106	1.6	–	474	–
Electricity import (commercial, 42% renewables)	0	0.2156	1.6	–	474	–
Electricity import (residential, 100% renewables)	0	0.3106	1	–	28	–
Electricity import (commercial, 100% renewables)	0	0.2156	1	–	28	–
Electricity export (PV)	0	−0.1293	−1.2	–	−56	–
Electricity export (CHP, biogas)	0	−0.0892	−2.91	–	−125	–
Electricity export (CHP, natural gas)	0	−0.0505	−1.91	–	−414	–
Natural gas import (residential)	0	0.0644	–	–	0	–
Natural gas import (commercial)	0	0.0455	–	–	0	–
Photovoltaic systems[a]	92	0	1.2	–[d]	56	[e]
Gas heating systems	30	–[c]	1.34	–	228	0.85
Natural gas CHP (electric output)	14	–[c]	1.91	–[d]	414	0.35
Natural gas CHP (thermal output)	–[b]	–[c]	0.76	–[d]	165	0.55
Biogas CHP (electric output)	14	–[c]	2.91	–[d]	125	0.35
Biogas CHP (thermal output)	–[b]	–[c]	1.42	–[d]	100	0.55
District heat network	30	0	–	–	0	0.85
Biomass cultivation & biogas production	–[g]	0.097	–[f]	–[f]	–[f]	–[f]
Biogas production	Taken into account through life cycle analysis in the CHP					
Building heat networks	Taken into account with the gas heating system respectively the district heating network					
Electricity grid	Considered as loss-free					
Natural gas grid	Considered as loss-free					
Demands	**Annual Demand** kWh/a	**Load Profile**				
Residential electricity demand	3600000.0	h0				
Commercial electricity demand	7312390.1	g0				
Residential heat demand	20810072.5	efh/mfh				
Commercial heat demand	10927989.6	ghd				

Parameters are estimated based on databases [63, 66, 67], legal bases [68], standards [32, 69], research articles [70], technical studies [71–73], comparison of market energy tariffs, data from the municipality of Herne and the German federal state of North Rhine-Westphalia as well as expert estimates. Annualized capital costs of investment are used

[a] Azimuth: 180°, tilt: 35°, albedo: 0.18, altitude: 60 m, latitude: 52.13°, longitude: 7.36°, module: Panasonic VBHN235SA06B

[b] Costs considered with the periodical costs of the CHP's electric capacity

[c] Costs are considered with the purchase costs of the fuels

[d] Through life cycle assessments, the periodic emissions are considered with the components variable costs

[e] Depending on the operating point

[f] Taken into account through life cycle analysis in the CHP

[g] Considered with the variable costs of the biogas process

Abbreviations
C: Energy costs; CED: Cumulative energy demands; CHP: Combined heat and power plant; ED: Energy demand; EE: Effective energy; EL: Emission limit; ESM: Energy system model(s); EP: Energy productivity; es: Energy system; *F*: Multi-criteria function; f_i: Function of criterion *i*; *FE*: Final energy; *GDP*: Gross domestic product; GHG: Greenhouse gas; inh: Inhabitant; *k*: Number of applied criteria; m_{GHG}: Greenhouse gas emissions; NC: No constraint; *PE*: Primary energy; *PEE*: Primary energy demand; *PEF*: Primary energy factor; PV: Photovoltaic; *SE*: Secondary energy; *SEE*: Secondary energy demand; *SEF*: Secondary energy factor; *SeS*: Self-sufficiency; SLP: Standard load profile; *SoR*: Share of renewables; *t*: Regeneration rate; VDI: Verein Deutscher Ingenieure; w_i: Weighting of criterion *i*; *x*: Decision variable.

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Authors' contributions
CK evaluated the existing literature, created the model, evaluated the results, and drafted the manuscript. FW supervised the work, provided orientation, and edited the manuscript. Both authors read and approved the final manuscript.

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Availability of data and materials
The modeling scenarios generated and analyzed during this study are online available: https://doi.org/10.5281/zenodo.5410616. The used versions of the Spreadsheet Energy System Model Generator (SESMG) are available as well (v0.0.4: https://doi.org/10.5281/zenodo.5412027, v0.2.0: https://doi.org/10.5281/zenodo.5520513).

Declarations

Competing interests
The authors declare that they have no competing interests.

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Publisher's Note

C Publication: Model-based run-time and memory reduction for a mixed-use multi-energy system model with high spatial resolution

Table C.1: Fact sheet publication [C]

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Christian Klemm: Conceptualization, Methodology, Investigation, Formal analysis, Software, Visualization, Writing – original draft. Frauke Wiese: Funding acquisition, Supervision, Writing – review & editing. Peter Vennemann: Funding acquisition, Supervision, Writing – review & editing.

Abstract:
Local and regional energy systems are becoming increasingly entangled. Therefore, models for optimizing these energy systems are becoming more and more complex and the required computing resources (run-time and random access memory usage) are increasing rapidly. The computational requirements can basically be reduced solver-based (mathematical optimization of the solving process) or model-based (simplification of the real-world problem in the model). This paper deals with identifying how the required computational requirements for solving optimization models of multi-energy systems with high spatial resolution change with increasing model complexity and which model-based approaches enable to reduce the requirements with the lowest possible model deviations.
A total of 12 temporal model reductions (reduction of the number of modeled time steps), nine techno-spatial model reductions (reduction of possible solutions), and five combined reduction schemes were theoretically analyzed and practically applied to a test case. The improvement in reducing the usage of computational resources and the impact on the quality of the results were quantified by comparing the results with a non-simplified reference case.
The results show, that the run-time to solve a model increases quadratically and memory usage increases linearly with increasing model complexity. The application of various model adaption methods have enabled a reduction of the run-time by over 99 % and the memory usage by up to 88 %. At the same time, however, some of the methods led to significant deviations of the model results. Other methods require a profound prior knowledge and understanding of the investigated energy systems to be applied.
In order to reduce the run-time and memory requirements for investment optimization, while maintaining good quality results, we recommend the application of 1) a pre-model that is used to 1a) perform technological pre-selection and 1b) define reasonable technological boundaries, 2) spatial sub-modeling along network nodes, and 3) temporal simplification by only modeling every n-th day (temporal slicing), where at least 20 % of the original time steps are modeled. Further simplifications such as spatial clustering or larger temporal simplification can further reduce the computational effort, but also result in significant model deviations.

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Model-based run-time and memory reduction for a mixed-use multi-energy system model with high spatial resolution

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ABSTRACT

Local and regional energy systems are becoming increasingly entangled. Therefore, models for optimizing these energy systems are becoming more and more complex and the required computing resources (run-time and random access memory usage) are increasing rapidly. The computational requirements can basically be reduced solver-based (mathematical optimization of the solving process) or model-based (simplification of the real-world problem in the model). This paper deals with identifying how the required computational requirements for solving optimization models of multi-energy systems with high spatial resolution change with increasing model complexity and which model-based approaches enable to reduce the requirements with the lowest possible model deviations.

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In order to reduce the run-time and memory requirements for investment optimization, while maintaining good quality results, we recommend the application of (1) a pre-model that is used to (1a) perform technological pre-selection and (1b) define reasonable technological boundaries, (2) spatial sub-modeling along network nodes, and 3) temporal simplification by only modeling every *n*th day (temporal slicing), where at least 20% of the original time steps are modeled. Further simplifications such as spatial clustering or larger temporal simplification can further reduce the computational effort, but also result in significant model deviations.

1. Introduction

A total restructuring of energy systems are required as response to radical reduction of greenhouse gas emissions [1]. Thereby, local and regional energy systems are becoming more complex due to the introduction of renewable energies with hardly predictable and volatile production, of energy storage systems, as well as due to sector coupling and sectors with increasing relevance such as the e-mobility and the hydrogen fuel sectors. Traditionally, individual parts of energy systems, e.g., individual consumption sectors, energy sectors, or spatial regions, are individually planned [2]. The increasing entanglement and complexity of overall energy systems [3] make it necessary to carry out holistic planning [2]. This is the only way to fully exploit the potential for achieving various transformation goals of integrated energy systems [4]. Tools that utilize the multi-energy system (MES) approach [4] are suitable instruments for investment and dispatch optimization [5,6], as they take into account the complexity and interaction of different energy sectors.

The increase in system complexity leads to a rapid increase of required computing resources for energy system models. This applies in particular to the run-time and the required random access memory (RAM, hereafter referred to as memory) for solving the model. Consequently, modelers must compromise between the computational effort

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on the one hand and the accuracy of the results on the other hand by creating simplified models [7,8].

This paper deals with the challenge on reducing the computing resources required to solve high-spatial-resolution models of mixed-use MES without significant loss of quality of the results. Such reductions can basically be achieved by solver-based or by model-based methods [9]. While solver-based approaches deal with the mathematical optimization of the solving algorithm, model-based approaches are concerned with simplifying the real-world problem in the model [9].

Improving solvers which are tailored to be applicable to a wide variety of models from different domains is often out of the expertise of modelers. Instead, modelers should make use of their deep understanding of the structure of energy systems when modeling a real-world scenario. At this point, model-based adaptations can be incorporated in order to minimize the run-time on a given computer. This contribution investigates such model-based approaches.

Some research has been made on model-based run-time and memory reduction methods for energy system models. Several publications provide an overview of existing approaches to model adaptation [9–12] or focus on simplifying certain types of energy systems, e.g., power systems [13]. *Temporal model adaptions* are addressed by some publications in general [14–16] or for specific use cases, e.g., storage planning [17,18] or long time series of wind power and photovoltaic (pv) systems [19]. Others deal with specific methods, such as *temporal clustering* [7,20–22], *heuristic selection* [23–29], *multiple time grids* [30], *averaging* [29], or *variable time steps* [31]. Similarly, some articles deal with *techno-spatial model adaptions* more generally [32] and others are related to specific methods, such as *spatial clustering* [33], or specific use cases, such as urban energy systems [34].

However, most of the literature focuses on either temporal model adaptions (e.g., [14,15]) or techno-spatial model adaptions (e.g., [32, 33]), but does not compare the two. Further, most studies either deal with only one energy sector (electricity, e.g., [17,19,28], or heat, e.g., [24]) or with very large-scale spatial energy systems and correspondingly low spatial and technological resolutions (e.g., [9,29]). Since model results are affected by different effects depending on the energy sectors considered and on the spatial and technological resolutions (e.g., by the interaction of individual buildings), we suspect that model reduction methods may also affect different types of energy system models differently. For the case of spatially high-resolution multi-energy system models, it is therefore necessary to find out which parameters have a particularly large influence on the computing requirements. These can be, for example, the number of simulated time steps or the number of (binary) investment decisions. Furthermore, suitable methods of model reduction must be identified and their influence on the quality of results quantified. This paper aims to fill this gap. Several approaches are evaluated and categorized in Section 2, and new ones will be proposed. Subsequently, suitable approaches will be implemented in practice and examined using a practical example.

2. Overview of run-time and memory reduction methods

Run-time and memory usage reduction methods may be grouped in various categories as shown in Fig. 1. The categories of solver and model-based approaches, as mentioned above, can be subdivided into further categories.

Model-based methods aim at reducing the size of the system of equations to be solved by the solver. They can be divided into *temporal model adaptions* as well as technological and spatial model adaptions. Technological and spatial measures cannot always be clearly separated from each other and are combined in the category of *techno-spatial model adaptions*. Within those sub-categories further distinctions between model reduction methods (systematic reduction of the model complexity [10]) and decomposition methods (breaking up of the model and subsequent solving and coupling of the sub-models' results [10]) can be made [9]. In model reduction, the overall model is reduced in size, which reduces run-time and memory requirements. With decomposition, the overall size of the model can be retained, but the sub-models may have lower individual memory requirements. Further run-time improvements can be enabled by solving the individual sub-models in parallel. However, parallelization techniques are not the focus of this study.

Whether the individual model adaption methods can be transferred to a model without coding effort depends strongly on the modeling tool used. In some tools, e.g., *downsampling* can be applied by simply adjusting the models temporal resolution, whereas in others it is not possible. Also, clustering approaches (temporal or techno-spatial) can be implemented by adjusting the input data; on the other hand, automated adjustment of the input data requires coding effort or the use of external clustering tools.

2.1. Temporal model adaptions

Temporal model simplifications can be realized through model reductions or through decomposition. Model reductions include sampling ("reducing number of time steps by aggregating consecutive steps or by defining typical [periods]" [13]) and the adaption of the model structure (e.g., temporal resolution or time horizon). When using sampling methods, the applied modeling methodology must either be able to model specific time slices or time periods. Alternatively, the sample periods can be combined to a new shorter time series. In this case, as with the use of *averaging*, the modeling methodology must allow the use of a shorter time horizon.

Temporal model adaptions may lead to inaccuracies due to concurrency and continuity problems [19]. Concurrency arises when events that meet or overlap in reality are not adequately represented by the simplification in the model [19]. To avoid concurrency problems, reduced time series should be self-consistent and include all important events of the analyzed time series [19]. Continuity problems arise when the temporal change (e.g., the state of charge of a storage) cannot be adequately modeled because of the adapted time series [19]. This can involve intra-day, intra-week, and seasonal balancing [18]. To avoid continuity problems several consecutive days (e.g., weeks) rather than single days should be used when selecting suitable sample periods [19,25].

random sampling: In random sampling, a predetermined number of random periods (e.g., days or weeks) are selected and used as representative time periods [14].

averaging: In averaging, successive time periods (e.g., two consecutive days) are averaged and combined into one segment [14].

slicing: In slicing, every nth period is selected (e.g., every second day [14]) and subsequently recombined to a reduced time series.

k-clustering: The k-clustering algorithm divides a time series into a given number of k clusters so that the squared deviation of the cluster centers of gravity is minimal. The procedure is well described by Green et al. [7]. They also recommend using the time vector of a whole day (e.g., the temperature trend) as cluster criterion. Representative time periods can be extracted from the individual clusters by either calculating the mean cluster-vector or by selecting the medians or medoids of the cluster elements [20]. For energy system model time series simplification, the k-clustering algorithm is mostly carried out using mean values [18]. However, Helistö et al. rated k-medoids to be more suitable than k-means [20].

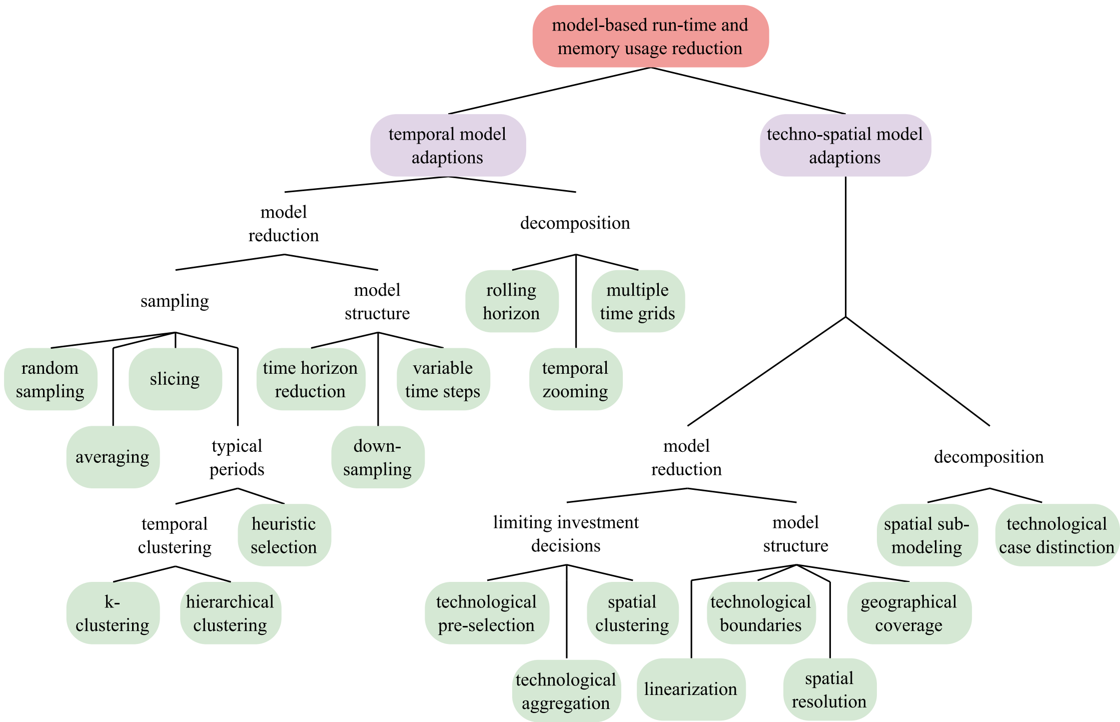

Fig. 1. Overview of model-based run-time and memory usage reduction methods discussed in this study.

hierarchical clustering: In hierarchical clustering, similar time periods (e.g., days or weeks) are grouped into clusters as well. In comparison to k-clustering, the number of periods per cluster varies, so that only similar periods are in a cluster. An appropriately representative period is then selected and weighted according to the cluster size [25]. Thus, the application of this method requires a modeling methodology allowing the weighting of single time steps or periods. Hierarchical clustering is more precise than k-clustering, but also involves more effort [7]. In addition, a weight must be assigned to the representative time periods, which cannot be easily implemented in every modeling approach. The exact procedure of hierarchical clustering is described in detail by Nahmacher et al. [25].

heuristic selection: In heuristic selection, representative time periods of a time series are selected from certain selection criteria [19]. For example, Poncelet et al. [23] propose a scheme to select between two and 24 reference periods from a year. The selection is based on seasons as well as extreme and average values of electricity demand, wind power feed-in and pv feed-in. Time periods which have not been selected are removed [19].

time horizon reduction: Depending on the length of the modeled time horizon, it should be examined whether a shorter model period would produce similar results, e.g., by modeling a single year instead of several years.

downsampling: The temporal resolution of an entire time series is changed. For example, the resolution can be changed from a 1-hourly to a 3-hourly temporal resolution [19]. For application, the modeling methodology used must allow the temporal resolution to be adjusted.

variable time steps: The variable time steps method defines critical time periods (as with *heuristic selection*) that are particularly important for the design of the investigated energy system. For these critical periods a high temporal resolution (e.g., hours) is used, for less important ones a coarser [31]. This method can enable more realistic modeling, especially with regard to energy storages [31]. For the application the applied modeling methodology must be able to use varying time steps within one model.

rolling horizon: Rolling horizon is a decomposition method in which the time series is divided into shorter intervals. Thus, several reduced sub-models are obtained, which are solved one after the other [9]. Rolling horizons come with the disadvantage that each sub-model is updated and coupled by a previous sub-model, so that parallelization of the process is not possible [9].

temporal zooming: To overcome the problem of the *rolling horizon* method to be incompatible with parallel solving, Cao et al. propose the method of temporal zooming [9], which is a decomposition method as well. Thereby, a model run with a reduced time series using *downsampling* is carried out. Afterwards, as with the rolling horizon method, several time periods are defined. Time-linking information between those periods are obtained from the first model run, so that the individual time periods can be modeled simultaneously. In contrast to rolling horizon, an additional run is necessary, but run-time can be saved by parallelizing the remaining runs [9].

multiple time grids: With the decomposition method of multiple time grids, the temporal resolution is varied for different model components and modeled in separate time systems [14]. Therefore, the applied modeling methodology must allow the application of varying time steps. Kotzur et al. [18] propose, e.g., a two-layer system when modeling seasonal storages. In the first layer, intra-day relationships (e.g., volatile production) are considered, while in the second, intra-season relationships (e.g., seasonal storage) are considered [14].

2.2 Techno-spatial model adaptions

Techno-spatial methods aim at reducing the number of possible combinations of investment decisions. Technological and spatial resolution are strongly related and they are often reduced together. Although the different methods described in the following usually have a technological or spatial focus (as the name often suggests), they may

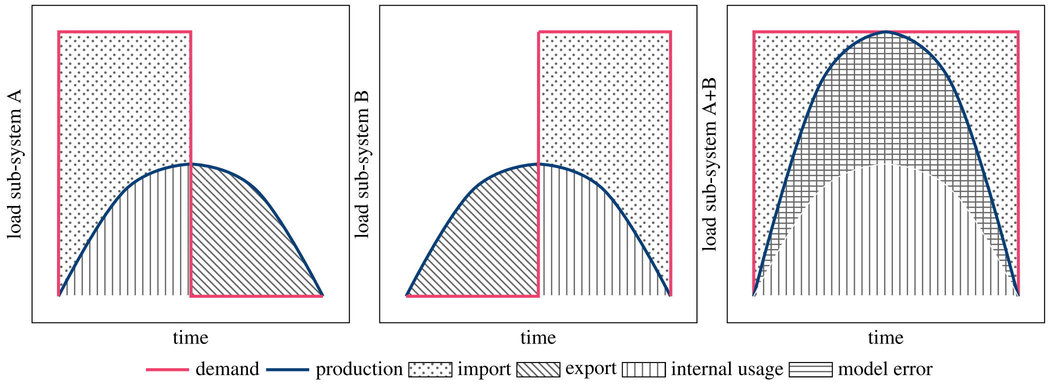

Fig. 2. Possible modeling error caused by spatial clustering. The fictional clustering of two sub-systems (A and B) with internal electricity production (e.g., by a pv system) and demands (e.g., electricity) of different load profiles. By clustering the profiles, the sub-systems balance each other out, resulting in an incorrect balance of imports and exports. With different system parameters (costs, emissions, …) for import and export, this leads to an overestimation of the share of own consumption and can lead to errors in investment decisions.

also influence the other aspect in each case. For example, a coarser sometimes unifies technologies with different technological parameters (e.g., differently oriented pv systems or heating systems with different efficiencies), while *technological aggregation* might combine technologies with a location focus (e.g., pv systems with different spatial references), in technological interactions between sub-systems are neglected (e.g., exchange of energy between subsystems), and in spatial parameters may be used for technological distinctions (e.g., spatial location of heating networks). Therefore, the reduction of both is combined in one category.

Techno-spatial model adaptions can be carried out by model reduction or decomposition (see Section 2). Model reduction can furthermore be divided into the limitation of investment decisions (i.e., reduction of the decisions to be included within the solved model) and adaptions of the model structure (e.g., coarsening of the spatial resolution or adjustment of the mathematical approach by avoiding binary decisions).

technological pre-selection: With the help of preliminary studies (e.g., solar potential, geothermal cadastres, or pre-models) or with the modelers deeper understanding of the investigated systems, non-profitable technologies can be identified with regard to the optimization criterion, which will certainly not be considered in the optimized energy system scenario. These technologies can be excluded from the model to reduce the number of investment decisions. If technologies are removed from the model due to of inaccurate or false assumptions, this automatically leads to model errors.

technological aggregation: If there are model components that differ only slightly from each other, they can be grouped together to reduce the number of investment decisions. For example, pv systems that supply for the same energy demand but have minor orientation (tilt and azimuth angles) differences may be grouped together.

spatial clustering: If there are repetitive or highly similar functional units in an energy system, the same investment and operational decisions are being made multiple times by the model. Comparable units (e.g., similar building types) may be clustered and aggregated into a grouped unit. For urban energy systems, Zhang et al. [33] recommend building clusters with a spatial diameter between 100 m and 1 km. If sub-systems are clustered which have insufficiently similar load profiles, this can lead to significantly varying model outputs. Fig. 2 shows, as an example, the fictional clustering of two sub-systems. To avoid this error, only similar sub-systems should be aggregated. Suitable cluster variables should be used [34], such as the year of construction, usage type, renewable energy potential (e.g., solar power potential), energy demand, and load characteristics [33,34].

linearization: As soon as an energy system model contains binary decisions, it is a so-called non-convex model. Such systems are generally harder to solve [35]. Therefore, modelers should aim to "stay convex where possible" [10], by avoiding non-linearities [13]. This can be done by "assuming linear relations or discrete steps" [13].

Linearizations can be applied to various aspects of the model, such as cost structures and modes of operation. Fig. 3 shows an exemplary linearization of binary investment decision between different pipe diameters of a district heating output with non-linear cost progression (black bars). Depending on which costs/pipe diameters are used as reference points (dots), significantly different linearized cost functions (red lines) may occur.

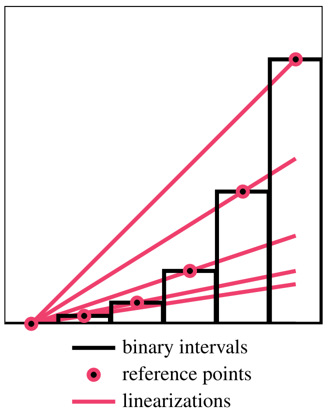

Fig. 3. Linearization of binary investment decisions: The choice of various reference points for linearization can lead to significantly deviating results.

technological boundaries: In order to limit the solution space to be investigated by the solver, boundaries (e.g., limits of possible plant capacities) should be set as tightly as possible [36]. This includes, for example, limiting the investment decision and not allowing any unrealistic investment decisions. This can improve the numerical behavior, as well as the solving time [36]. Technological boundaries can be defined based on preliminary studies, on pre-models or on the deeper understanding of the investigated system. If investment boundaries are defined to tight based on inaccurate or false assumptions, this may lead to modeling errors or even non-solvability of a model.

spatial resolution: By adjusting the spatial resolution, the number of sub-systems to be modeled can be reduced, just as with *spatial clustering*. In contrast to spatial clustering, however, the approach is less structured and sub-systems are aggregated solely according to their spatial location. Due to the spatial clustering error described above (Fig. 2), the structured approach of spatial clustering is therefore preferable over the simple adjustment of spatial resolution.

geographical coverage: Similar to the choice of the *time horizon reduction*, the geographical coverage of the model should be just as large as necessary for the research question. For example, it is not necessary to model an entire country for the design of a single building energy system. Possibly, it can be useful to divide the spatial area into several sub-models (see).

spatial sub-modeling: If there are completely independent investment decisions in the model, decomposition can be used to create spatial sub-models that are easier to solve. This may be the case, for example, if there is no technological connection between two spatial sub-areas. Sub-models can be solved in parallel.

technological case distinction: If there are central binary decisions which cannot be linearized, decomposition can be used to create technological sub-models that are easier to solve. This can, for example, be applied for the differentiation between centralized and decentralized heat supply. Case distinctions can be particularly useful if the individual model runs can be performed in a parallelized computing environment.

3 Materials and methods

3.1 Test case

The majority of the model simplifications described in Section 2 were applied to the test case area shown in Fig. 4. It is a real-world system (except COM2, which was added so that at least two non-residential are part of the system) which was selected to comply with the structure of larger urban areas. It therefore contains different buildings types (single-/two-family buildings, multi-family buildings, commercial buildings, buildings without energy demand) and roof orientations. Furthermore, the reference case of this system (model without simplification methods) is solvable with the computing resources available for this study with a run-time below 24 h and memory usage below 64 GB.

This test case area has already been used in previous studies [37–40] and has proven to be suitable for urban energy system modeling.

The modeled test case thus included a total of three semi-detached buildings, two multi-family buildings, two commercial buildings, and two garages. Only buildings that have an energy demand themselves or have at least one roof surface with pv potential (regarding to [41]) are considered. The garages have pv system potential but no energy demand of their own. All other buildings have both electricity and heating demands. The goal of the applied model was to optimize the financial costs of the systems' energy supply. For this purpose, an investment and dispatch optimization in different technologies of sector coupled electricity and heat supply was performed.

3.2 Model description

The "Spreadsheet Energy System Model Generator" (SESMG) [42] was utilized. The underlying "Open Energy Modeling Framework" (oemof) and its sub-modules have been widely validated [43,44]. The gurobi solver [45] was used.

A bottom-up analytical approach and the mathematical approach of (mixed-integer) linear programming ((MI)LP) were applied. Methods of simulation as well as dispatch and investment optimization were carried out. For the reference case, an hourly temporal resolution, a temporal horizon of one year, and a building-sharp spatial resolution were applied. A perfect foresight model is assumed, using weather data from the nearest station (ID 1078) of the German Weather Service (DWD) [46]. The year 2012 was considered, which was an average

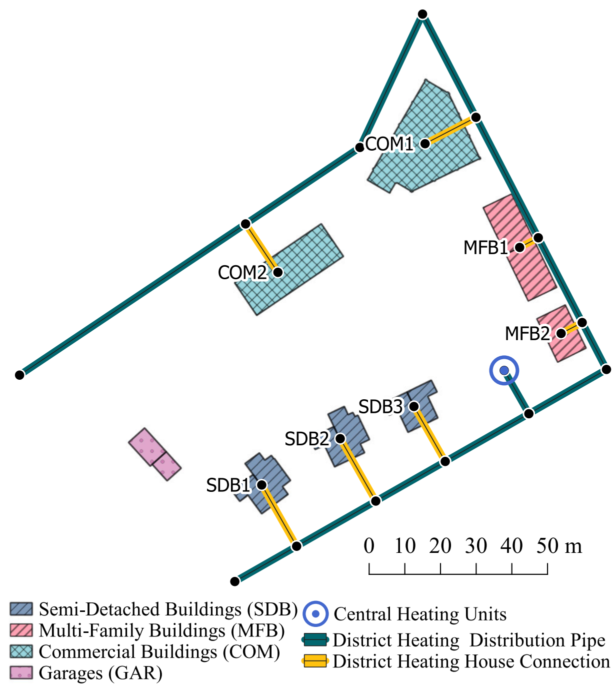

Fig. 4. Test case area to which the model simplification methods were applied.

solar year [47]. The minimization of financial costs were applied as optimization criterion. Therefore, the energy system configuration which enables the lowest system costs, was to be identified for the test case area.

The model included 79 linear and 20 binary investment decisions (see Appendix A). As long as there was no technological limitation for linear investment decisions, e.g., by available space, the model was allowed to design energy-converting technologies (e.g., heat pumps and gas heating systems) between 0 and 999 kW and storage technologies between 0 and 9999 kWh. Binary decisions could either be made with the predefined capacity or not at all.

There is area competition for the investment in pv and solar thermal systems on building roofs. This was considered within the model by using competition constraints. These allow investment in only pv systems, only solar thermal systems, or proportionately, e.g., half and half, yet no double investment for a specific area is allowed.

The investment costs for district heating pipes (−40%) and battery storages (−65%) were artificially reduced. Otherwise their investments would not have been considered in the reference case. This was necessary in order to study the influence of the various model simplifications on the use of these technologies in the model.

Furthermore, it is worth mentioning that the model included the possibility to exchange electricity between the individual buildings in exchange for grid fees and the like.

A complete description of the model, including the component structure, as well as all used model parameters is given in Appendix B. A Linux-operated computing cluster was used. The models were performed on an isolated computing node with 24 physical cores (2.5 GHz) and 64 GB of RAM. In this way, interactions with other processes on the computer cluster were avoided.

3.3 Run-time reduction

First, a reference model-run without any adaptions was carried out followed by several model simplifications. The results of these runs were then compared with the reference case. The time required to solve the model, the required memory, the determined target value (system costs) and the investment decisions made were compared as benchmarks. For the run-time and the memory usage we focus on the pure solving process, without pre-processing and post-processing, as the processing part is usually the bottleneck of large energy system models [9].

3.3.1 Temporal model adaptions

The methods described in Section 2.1 were applied to the test case. For sampling methods, days (e.g., recommended by [26]) and weeks (e.g., recommended by [27]) are tested for suitability as sampling periods. The number of modeled time steps was reduced with each method (as far as possible) reduced to 50%, 20%, 10%, 1.9% (only for reference weeks, equals to one week), and 0.8% (only for reference days, equals to one day) of the original time steps. The results were evaluated in terms of which methods show a converging behavior to the reference case with increasing number of time steps. For methods showing converging behavior, more accurate results with increasing number of modeled time steps can be expected. In contrast, for methods with results varying around the reference case depending on the number of time steps modeled, only certain configurations allow results with certain quality.

random sampling: Random sampling was carried out using random days, as well as weeks as reference periods. The“random”-library [48] was utilized for that purpose. To ensure reproducibility, a “seed” was defined, so that with each run the same random period is selected. A random time series of, e.g., ten periods therefore automatically makes up ten periods of a random time series of, e.g., 20 periods.

averaging: According to the above described degrees of reduction of time steps numbers of consecutive days and weeks were averaged.

slicing: Slicing of several numbers of days and weeks was carried out and applied. For the above described degrees of time step reduction, every nth sample period (reduction of the time series by more than 50%) was included in the modeling. In addition, the number of time steps modeled was reduced by only 25% by removing every fourth sample period from the time series.

k-clustering: k-means-clustering as well as k-medoids-clustering were carried out using the “scikit-learn” [49] and “scikit-learn-extra”-libraries [50]. Three different data types, for which the largest model influence was assumed (1. temperature, 2. solar radiation, 3. electricity demand) were applied as cluster criteria. The vectors of entire days, respectively weeks, were applied as cluster-vectors. The air temperature impacts the heat demand and investment decisions of the entire heat sector and thus exerts a great impact on the overall system. The solar irradiation has a strong impact on the performance of pv systems and the electricity demand. By taking electricity demand into account, deviations in the courses of the week and year can be mapped. Days and weeks were tested as sample periods. The number of time steps was reduced in each case by the degrees described above, with an exception for the k-medoids algorithm. Since at least three sample periods were contained in a cluster to form a medoid, the number was reduced by 67% instead of 50%.

heuristic selection: Based on the approach of Poncelet et al. [23], a heuristic selection scheme was carried out (see Table 1) considering different numbers n of reference periods. However, since they used this approach for simplifying time series of renewable electric feed-in, the selection criteria chosen there (1. total load, 2. wind load, 3. pv load) were replaced by criteria more suitable for the context of this study. Again, the criteria of 1. air temperature, 2. solar radiation and 3. electricity demand were applied. Days and weeks were used as reference periods. The number of time steps modeled differs from the above mentioned degrees of reduction due to the chosen schemes.

time horizon reduction: The time horizon was shortened and several time horizons (1/2 year, 1/4 year, 1/8 year) were applied.

Table 1
Heuristic selection scheme with up to three different selection criteria, based on Poncelet et al. [23] (adapted).

n	Season(s)	Criterion 1	Criterion 2	Criterion 3
2	Year	hp, lv	–	–
4	Year	hp, lv	ha, la	–
8	Summer, winter	hp, lv	ha, la	–
16	Winter, spring, summer, fall	hp, lv	ha, la	–
24	Winter, spring, summer, fall	hp, lv	ha, la	ha, la

Acronyms: hp = highest peak, lv = lowest valley, ha = highest average, la = lowest average.

downsampling: Different multiples of the original 1-hour resolution were applied and the number of modeled time steps reduced by the degrees described above.

For the applied temporal model adaptions, the model needed to be adjusted with respect to its temporal structure. To ensure the correct relationship between variable and periodical (annual) costs in the case of shortened time series, variable costs were multiplied by the variable cost factor:

$$\text{variable cost factor} = \frac{\text{original number of time steps}}{\text{new number of time steps}} \tag{1}$$

Furthermore, the modeled time series was shortened under certain conditions. For a time series' adjustment, the simplification factor should ideally be divisible by the length of the given time series without remainder. For example, out of 365 days, every fifth day can be selected via slicing without any problems (365/5 = 73), but every tenth day results in a remainder (365/10 = 36.5). In order to simplify the time series correctly in such cases, the given time series was shortened to the end, so that the calculation became executable error-free. For example, for slicing with every tenth day the time series would have been shortened to 360 days (360/10 = 36). In sampling methods (see Fig. 1), the selected periods were strung together and merged into a new time series. The individual sample periods were partially assigned new time stamps.

The methods of *multiple time grids* and *variable time steps* were not tested, because the applied modeling methodology does not allow the application of varying temporal resolutions within a single model run. Furthermore, *hierarchical clustering* was not applied, because in the model structure chosen, it is not possible to assign different weightings to individual time steps.

Within the *rolling horizon* method, investments are carried out based on only a part of the time horizon. Since we assume a perfect foresight model (see Section 3.2) this leads to continuity and competition problems. For other model types such as dispatch optimization models (see, e.g., [51–54]) and models that do not assume perfect foresight, rolling horizon can be useful.

Within the *temporal zooming* method, investment decisions are made on the basis of the first (downsampled) model-run and therefore offers no advantage over conventional downsampling for investment decisions. Due to this lack of suitability for investment optimization, rolling horizon and temporal zooming were neglected in the following parts of this study.

3.3.2 Techno-spatial model adaptions

The techno-spatial model adaptions described in Section 2.2 were applied to the test case. A full list of the applied techno-spatial model adaption schemes is listed in Appendix C.

technological pre-selection: Technologies for which no investment decision had been carried out within the reference case were removed from the model to reduce the number of investment decisions.

technological aggregation: Technological aggregation was used when a building had several differently oriented roof surfaces suitable for pv and solar thermal use. In this case, multiple investment decisions of pv or solar thermal systems were merged. Different model parameters (azimuth, tilt) were weight-averaged according to capacity fractions. In the test case, this applied to SDB2 and COM1 (see. Fig. 4).

spatial clustering: Sub-systems (buildings) were clustered according to their usage type. In different model tests, either similar building types (semi-detached buildings, multi-family buildings, commercial buildings and garages, as scheme C1), or similar usage types (residential buildings, commercial buildings, garages, C2), or all buildings of the system were clustered. For the building clusters, component types (e.g., pv systems, C2) and associated investment decisions were aggregated. An exception were the insulation measures, which could not be aggregated with the applied modeling methodology. Solar thermal and pv systems were aggregated into 45° groups according to their azimuth angle.

linearization: Within the reference case, district heating pipes were carried out as binary investment decisions. In total, the district heating network contained 20 possible pipe sections, each containing one binary investment decision. In five test runs, only the house connection pipes (as scheme D1), only the distribution pipes (D2), respectively all pipes with different linearization reference pipes (D3 to D5) were applied.

technological boundaries: The overwhelming share of linear investment decisions were considered with high investment caps (see Appendix A). In order to limit the resulting large solution space of the model, those investment caps were tightened, based on the results of the reference case. Unless there was a stricter restriction before (for pv systems and solar thermal systems) the investment caps were set at 500% (as scheme E1), 200% (E2), 150% (E3), and 100% (E4) of the value determined in the reference case. Binary decisions remained in the model as within the reference case.

spatial sub-modeling: The model was divided into two sub-models along the heating network starting from the heat source. The first sub-model (as scheme F1) included the three semi-detached buildings and garages. The second sub-model (F2) included the multi-family buildings and commercial buildings. The partial results were then combined. In the aggregation of plant outputs, the two partial results were added up. The central heat source is included in both sub-models. This was taken into account in the final consolidation of the results.

technological case distinction: A distinction was made between a system of centralized heat supply (G1) and a system of decentralized heat supply (G2). The investment decisions were then taken from that model run, for which the lower optimization value (system cost) had been calculated.

No modification of the *geographical coverage* was tested. A reduction of the *spatial resolution* was not reasonable due to the limited size of the test case area.

3.4 Combined model adaptions

After individual tests, the methods with the best results, i.e., those that allowed the best run-time/memory usage improvements with the least result deviation, were combined. A total of five method combinations were tested.

4 Results

4.1 Reference case

The reference case model with cost-based optimization resulted in the investment decisions listed in Table 2. Solving the model took 22:12:15 h and required a maximum of 12.24 GB of memory. The model results show, that only decentralized battery and thermal storage systems were designed, but no centralized storage systems. While the buildings connected to the district heating network (MFB1, MFB2, COM1) were completely centrally supplied with heat, all other buildings were supplied with decentralized heat.

Table 2
Model results for investment decisions of the reference case and the resulting system costs. Identical technologies in different sub-systems are aggregated in the presentation of results.

Technology	Model decision	Unit
Photovoltaic systems	52.31	kW
Gas heating systems	72.79	kW
Ground coupled heat pumps	12.57	kW
Air source heat pumps	1.68	kW
Combined heat and power plant	29.63	kW
Central heating plant	66.73	kW
Battery storages	3.39	kWh
Thermal storages	413.80	kWh
District heating house connection pipes	3	
District heating distribution pipes	5	
Wall insulation	0	m^2
Window insulation	0	m^2
Roof insulation	0	m^2
System costs	56 634	€/a

4.2 Temporal model adaptions

Fig. 5 shows the impact of the applied temporal model adaptions on the model run-time (left) and memory requirements (right) as a function of the number of time steps modeled. Note that only run-time and memory usage of the solver is shown. For the entire modeling process increased requirements may arise, depending on the computational resource intensity of the pre-processing and post-processing.

run-time: The quadratic regression ($R^2 = 0.80$) of the individual model runs shows that the run-time increased quadratically with an increasing number of time steps. However, the correlation cannot be generalized, individual points clearly fall above (e.g., slicing) or below (e.g., downsampling) the regression curve.

memory usage: The relationship between memory usage and modeled time steps can be described by a linear regression ($R^2 = 0.99$).

For the sake of clarity, the detailed results of the individual runs are only shown in the Appendix. In Appendix D all results are shown in tabular form. In Appendix E, the deviations of the optimized system costs and the aggregated investment decisions for different technologies depending on the selected temporal model simplification are plotted for the two most promising methods.

slicing: Investment decisions and system costs tended to converge well to the reference case with increasing temporal resolution. The choice of days as a sampling period is preferable, since the deviations are slightly smaller compared to the reference case than for weeks, especially as the number of modeled time steps increases (see Appendix D). On the other hand, in case of a very high temporal simplification (e.g., every 10th day or week), technologies that were designed in the reference case are taken into account more quickly when reference weeks are selected (e.g., Appendix E-5'). Useful results, i.e., no complete technology changes within individual sub-systems and more than half of all investment decisions with a deviation of less than 15%, occurred if at least 20% of the reference time steps were modeled. However, note that also in this case there are bigger deviations for some investment decisions, e.g., for battery storages (−67%, by slicing days).

averaging: The results tended to converge to the reference case with increasing temporal resolution. Advantages in the sample period to be averaged cannot be generalized. If days were chosen, the results for system costs (Appendix E-1), gas heating systems (Appendix E-3)

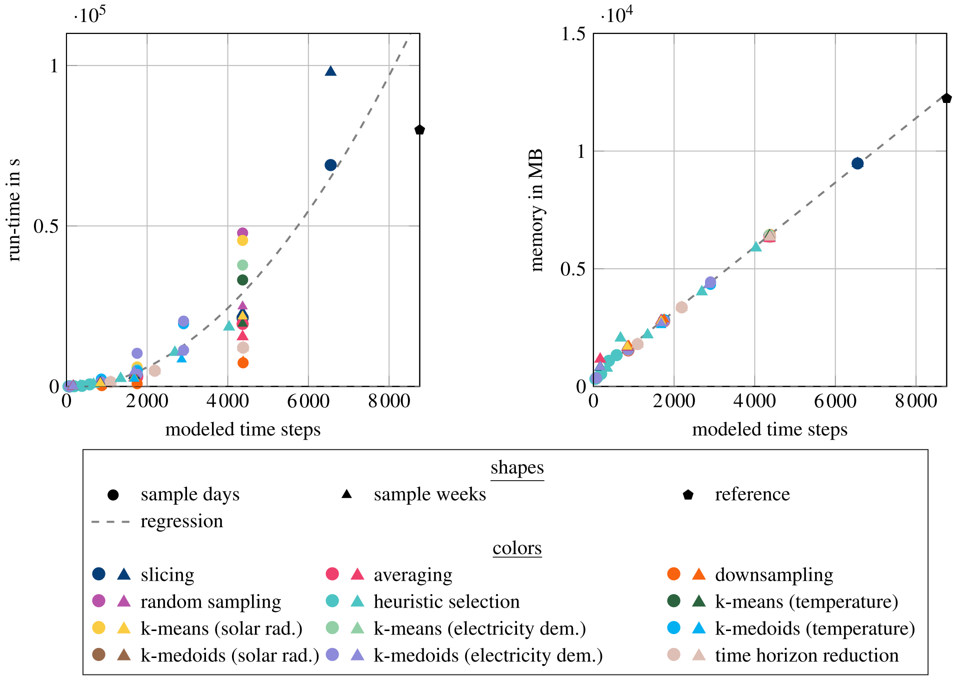

Fig. 5. Run-time and memory requirements depending on the number of time steps modeled. All values are also listed in Appendix D. The memory usage can be described by a linear regression (R^2 = 0.99) depending on the modeled time steps. The run-time can be described by a quadratic regression (R^2 = 0.80). The lower coefficient of determination shows that the run-time is also dependent on other parameters.

and central heating plant (Appendix E-7) converged faster or more accurately to the reference case. Weeks were more suitable for pv systems (Appendix E-2'), air source heat pumps (Appendix E-5'), and the combined heat and power (chp) plant (Appendix E-6). Useful results, i.e., no complete technology changes within individual sub-systems and more than half of all investment decisions with a deviation of less than 10%, occurred whenever at least 20% of the reference time steps were used. Note, that, also in this case, there are larger deviations for some investment decisions, e.g., battery storages (−84%, by averaging days).

downsampling: The downsampling result curves came closer to the reference values with increasing temporal resolution. However, the deviations from the reference case show significant deviations for the design of pv systems (−100% to +49%), chp plants (−31% to +376%) and district heating pipes (−20% to +133%) and for system costs (−1% to +1102%) and battery storages (−100% to +57 331%) even the largest deviations of all methods examined (see Appendix D).

random sampling: With random sampling, investment decisions for some technologies converged to the results of the reference case with increasing number of modeled time steps (e.g., thermal storages, district heating pipes, see Appendix D). However, other investment decisions deviated steadily from the reference results or even fluctuated around the reference values, regardless of the modeled number of time steps, e.g., for the chp plant (−100% to +64%), central heating plant (−100% to +119%), battery storages (−91% to +2052%), and thermal storages (−84% to +437%).

heuristic selection: Heuristic selection allows, depending on the applied scheme, for some investment decisions results with comparably small deviations to the reference case even with a small number of simulated time steps, e.g., at 192 modeled time steps for system costs (−2 %) and gas heating systems (−25%). For the same schemes, other investment decisions, however, had large deviations, e.g., for the case of 192 modeled timesteps heat pumps (−100%), thermal storages (+306%) and solar thermal systems (no investment in the reference case, see Appendix D). Overall, there are many outliers (e.g., thermal storage capacities oversized by up to +578%) and fluctuations in the results.

k-clustering: The results of k-clustering are, overall, noisy (see Appendix D). In the k-means-clustering (temperature criterion) of days, the investment decision of pv systems converged to the reference case; gas heating systems were about 80% under-designed and did not converge to the reference case. In the k-medoids clustering (solar radiation criterion) of days, some technologies that were relevant in the reference case were not considered at all (battery storage and ground coupled heat pumps (gchp)). In other schemes, decisions partly fluctuated around the reference decisions instead of converging to them. The clustering of weeks behaved somewhat more steady than that of days. Overall, for k-clustering no clear trend is discernible and it is unclear under which setting a consistently converging behavior can be expected.

time horizon reduction: Shortening the time horizon, led to large model deviations. In particular, if the time horizon was reduced by more than half, the ratio of winter to summer days is significantly changed, leading to undersizing of pv systems and related components, such as battery storages and heat pumps (all −100% for a quarter of the reference horizon). On the other hand other components are oversized, such as gas heating systems (+200%), thermal storage (+102%) and the chp plant (+308%). System costs were also greatly overestimated whenever the time horizon was shortened.

4.3 Techno-spatial model adaptions

The results show that the run-time depends largely on the number of binary investment decisions (Fig. 6, left) and that the memory depends largely on the sum of all investment decisions (Fig. 6, right). The memory requirement can be well described by a linear regression (R^2 = 0.74). The attempt to form a quadratic regression for the run-time is quite inaccurate (R^2 = 0.31), so that it can be stated that other parameters than the number of (binary) investment decisions play important roles as well.

For methods consisting of multiple model runs (spatial sub-modeling and technological case distinction), the run-time of all runs

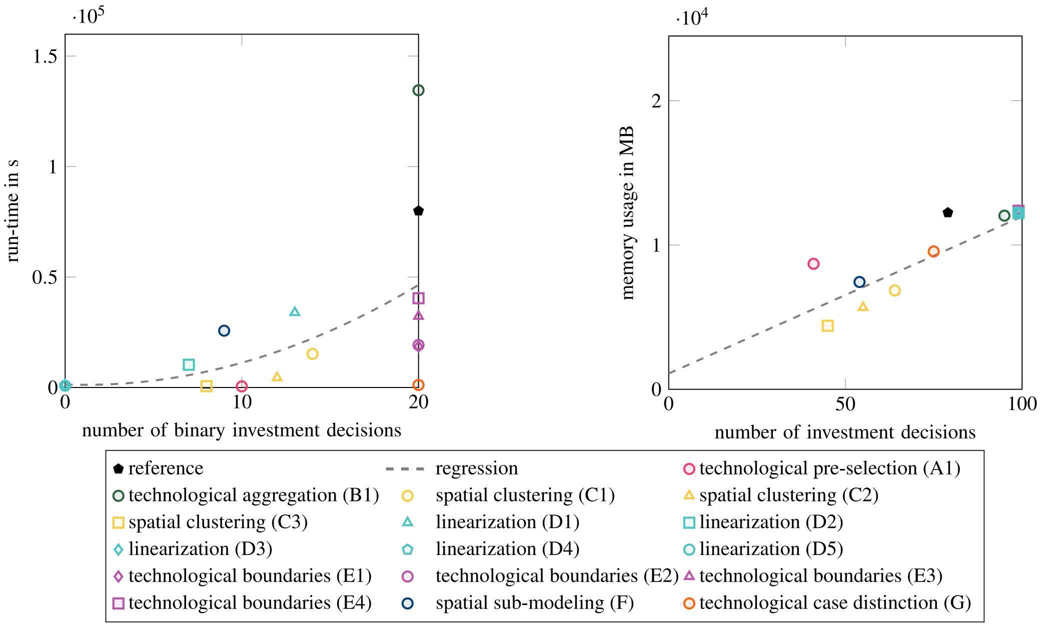

Fig. 6. Dependence of run-time on the number of binary investment decisions (left), as well as of the memory requirement on the number of total investment decisions (right) for the applied techno-spatial model adaptations. The run-time can roughly be described by a quadratic regression ($R^2 = 0.31$) depending on the number of binary decisions. The memory usage can be described by a linear regression ($R^2 = 0.74$) depending on the total number of investment decisions.

was added up for the consideration as benchmark, and the highest memory requirement of the individual model runs was taken into account. When balancing the number of investment decisions, the higher value of the two model runs is considered.

Detailed results for the investment decisions for all applied techno-spatial model adaptions are shown in Appendix F.

technological pre-selection: By technological pre-selection the number of linear investment decisions had been drastically reduced by −61% and the number of binary decisions by −50%. This led to a run-time reduction of −99% and lowered memory requirements of −29% without having impact on the modeling results.

technological aggregation: By aggregating the pv systems of individual sub-systems, investment decisions for higher capacities of pv systems (+5%), battery storage (+3%) and gchps (+3%) compared to the reference case were carried out. This can be explained by the fact that plants were aggregated according to their surface orientation (see Section 3.3.2). Within these aggregations, uniform angles were used. As a result of this change in the modeled orientation, certain pv systems for which an investment was not profitable with the original orientation in the reference case, probably moved above the break-even point. In turn, battery storages and heat pumps were dimensioned larger due to higher pv yields. However, technological aggregation led to a significant increase in computing time (+68%) and only a marginal reduction in memory requirements (−2%). Overall, technological aggregation thus led to a deterioration in computing performance.

spatial clustering: System costs were significantly underestimated between −44% and -64% compared to the reference run, within all clustering schemes. This is because plant capacities are shared by sub-systems and the modeled district heating distribution pipe lengths are shorter. Clustering of similar building types (C1) and similar usage types resulted in a lower configuration of central heat supply. This can be explained by the fact that buildings that were centrally supplied in the reference case (e.g., COM1) were partially clustered with buildings that were decentrally supplied in the reference case (e.g., COM2). In the fully clustered case (C3) there was a strong centralization. This can also be explained by the consideration of fewer district heating distribution pipe lengths and thus fewer costs taken into account. Spatial clustering, however, allowed a significant saving of run-time (up to −99%) and the largest reduction of memory (up to −64%), of all tested techno-spatial model adaptations.

linearization: All linearization schemes led to large model deviations compared to the reference case. The linearization increased the profitability of district heating networks by the option to partially (non-binary) design district heating pipe capacities. This led to a significant centralization of the heating supply and to an underestimation of the system costs within all linearization schemes. If linearization was applied to house connection pipes alone (D1), the underestimate was less yet also the run-time improvement (−58%) was lower than that of the other schemes (up to −99%). All linearizations had no effect on the memory requirements of the model.

technological boundaries: The application of appropriate technological boundaries allowed significant run-time improvements (up to −77%) while maintaining the same quality of results of the reference case. The memory was not significantly affected. Note, that the tightest technological boundaries (E4) led to smallest run-time savings. This may be explained by the fact that the model solution could only be approximated from one site due to particularly tight bounds. This resulted in fewer solution paths for the solver, which could have led to a higher run-time. Between the results with less tight technological boundaries (E1 and E2), there is no significant impact on the run-time.

spatial sub-modeling: The decomposition into two spatial sub-models affected the investment decisions of the pv systems, geothermal heat pumps, and battery storage. This can be explained by the fact that the electricity produced in each sub-model could no longer be delivered to all sub-systems, but only to sub-systems within the same sub-model. As a result, more battery storage capacities were required to use the produced electricity in an economically viable way, and gchps were less profitable because more electricity had to be imported at a higher price to operate them. However, this effect will probably lose significance, if the sub-models contain more sub-systems, which can exchange energy.

technological case distinction: Within the technological case distinction, the case of decentralized heat supply was evaluated to be more suitable than the case of centralized heat supply. Accordingly, central heat supply components (chp, central heating plant and district heating pipes) were not considered at all and more decentralized system capacity (gas heating, heat pumps, wall insulation) was designed. However, also pv systems and battery storage were dimensioned larger than in the reference case, probably due to the increased demand for electricity from the heat pumps. Overall, technological aggregation thus led to large model deviations and is therefore less suitable for the test case. However, technological case distinction allows a reduction of both total run-time (−99%) and memory requirements (−22%) despite the necessity to perform two model runs.

4.4 Combined methods

A total of five schemes of combined model reduction methods were applied (see Table 3). The following paragraphs refer to the results of these combined runs shown in Fig. 7 and Appendix G.

The combination of technological pre-selection and technological boundaries (X1) improved the run-time (−99.43%) and memory usage (−29%) without causing any model deviations regarding investment decisions and optimized system costs.

Building on scheme X1, temporal slicing of every second day (X2), respectively spatial sub-modeling (X3) were added to the model reduction scheme. Compared to X1, both methods allowed significantly greater memory usage savings (−62%, respectively −55%). X2 still allowed a greater saving in computing time (−99.57%), X3 somewhat less (−99.31%) due to the additionally required model run of the sub-modeling. Both schemes mainly influenced the design of heat pumps and battery storages. The battery storages were partly undersized (−38%, X2) and partly oversized (+29%, X3).

By combining the previous schemes (X4), the incorrect battery designs partially offset each other, but beyond that, similar model deviations occur. However, the scheme allows greater run-time savings (−99.70%) and memory usage (−77%) than before.

With the last scheme (X5) the temporal model reduction is increased to temporal slicing of (every fourth day). This led to further run-time (−99.89%) and memory savings (−88%), but also to significant model deviations for the investment decisions of pv systems, heatpumps, central heating plant and battery storages.

Table 3
Applied combined method schemes. For schemes consisting of several sub-models with different values, both values are given.

Scheme	Combined model adaptions	inv. decisions		Modeled
		Linear	Binary	time steps
X1	Technological pre-selection Technological boundaries (E2)	31	10	8 760
X2	Technological pre-selection Technological boundaries (E2) Temporal slicing (every second day)	31	10	4 368
X3	Technological pre-selection Technological boundaries (E2) Spatial sub-modeling	16/15	0/10	8 760
X4	Technological pre-selection Technological boundaries (E2) Temporal slicing (every second day) Spatial sub-modeling	16/15	0/10	4 368
X5	Technological pre-selection Technological boundaries (E2) Temporal slicing (every fourth day) Spatial sub-modeling	16/15	0/10	2 184

5 Discussion

Several temporal model adaptations and techno-spatial model adaptations, as well as five combined method schemes were applied to a real-world test case. The evaluation of these methods showed that model-based adaptations can significantly reduce run-time and random access memory (RAM) requirements of mixed-used multi-energy system models with high spatial resolution. At the same time, however, it became clear that some of the methods led to significant deviations of the model results. For the application of other methods, a profound prior knowledge and understanding of the energy systems under investigation is necessary.

The model reduction methods tested in this study were applied to a mixed-use multi-energy system optimization model with the focus on investment optimization. The test area with a total of nine buildings was selected to correspond to the structure of larger urban areas (see Section 3.1). We therefore assume that the results can also be applied to larger urban energy systems with several hundreds of buildings and similar multi-energy systems.

Interactions of the investigated methods to solver-based methods (this includes, for example, the choice of a different solver) were not investigated in this study. However, we assume that a similar

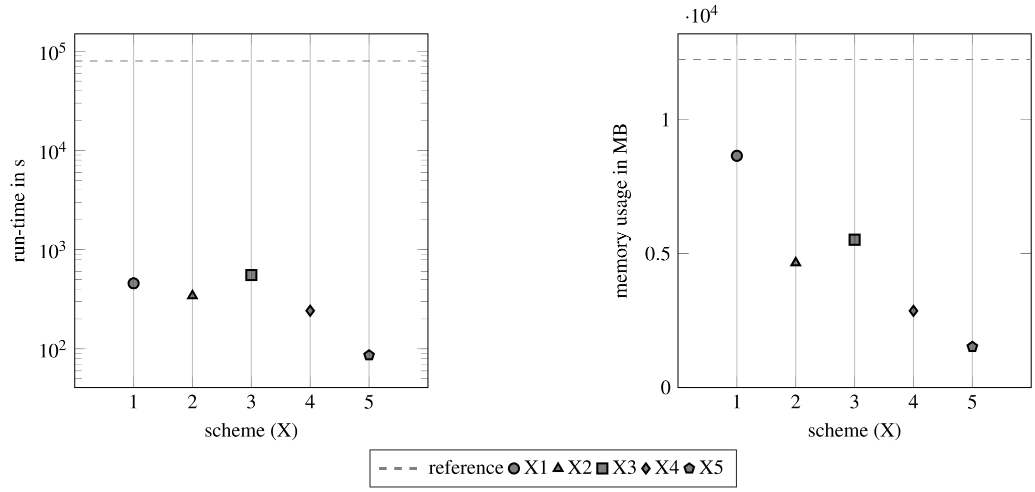

Fig. 7. Impact of the applied combined model reduction method schemes on the run-time (left) and the memory requirements (right).

improvement will be enabled with solver-based methods applied in parallel.

5.1 Temporal model adaptions

As expected in Section 1, the computing capacities required to solve energy system optimization models increases rapidly with rising number of modeled time steps. The memory requirement increases linearly, the run-time increases quadratically with a slightly lower coefficient of determination of the regression (see Fig. 5). It can thus be stated that the modeled number of time steps has a primary influence on the computing resources. However, the application of temporal model adaptations also causes model deviations in the investment decisions with respect to these technologies:

- **sector-coupling technologies**: Particularly heat pumps are undersized with decreasing number of modeled time steps.
- **battery storages**: The investments of battery storages are particularly vulnerable to (temporal) model simplifications. There is a rising over- or undersizing of the battery storage capacities with decreasing number of modeled time steps.
- **(de)centralized heat supply**: As the number of modeled time steps decreases, technologies for decentralized heat supply (gas heating systems, heat pumps) tend to be under-designed. Central heat supply, conversely, increases.

Methods that do not sufficiently represent the load and weather profiles of the entire year cause large model deviations, which do not converge to the reference case even with an increasing number of modeled time steps.

Further deviations may arise from the inappropriate ratio between days below and above the heating limit temperature. If the heating day ratio is too high, the model tends to consider investments into higher thermal storage capacities and technologies with low variable but high periodical costs. This must be taken into account, for example, in the choice of heuristic selection schemes and the number of reference days for slicing and averaging.

Overall, many deviations can thus be attributed largely to the previously discussed problems (see Section 2.1) of continuity (such as investment behavior for battery storages) and concurrency (e.g., shift between (de)centralized heating supply). None of the tested methods of temporal model reduction allowed a design without larger errors in the investment decisions. In fact, there was always at least one technology with major design errors of at least 10% compared to the reference case (see Appendix D). All in all, slicing and averaging provide the most reliable results of the tested temporal model adaptions. Slicing and averaging converge most reliably to the reference case results as the number of time steps modeled increases. Generally, useful results can be expected from the consideration of every fifth day or the averaging of a maximum of five days. Since slicing and averaging yield different model deviations for different technologies, one of the two methods should be selected depending on the application. Slicing is more reliable in the heat sector and for the design of storage systems, while averaging is more reliable for the design of sector-coupling technologies. This is probably due to the fact that maximum values (e.g., heat demand or pv production) are reduced in the course of averaging. At the same time, however, averaging more reliably takes into account combinations of energy consumption and supply that do not occur regularly across sectors (e.g., pv production and heat demand covered by heat pumps). In contrast to most of the other temporal model adaptations tested, slicing also allows only a slight reduction of the time steps (e.g., by one third). Overall, there are fewer deviations from the reference case when applying slicing.

In some cases, the heuristic selection produces usable results even with a very small number of days. The least useful results were obtained by time horizon reduction and downsampling. The least useful results with respect to investment decisions were obtained by time horizon reduction and downsampling.

The choice of whether reference weeks or reference days should be selected for temporal sampling also produces different results for different investment decisions. Reference days, for example, tend to provide a better cost estimate. Reference weeks, on the other hand, better reflect the design of thermal storage facilities, and are therefore more appropriate with respect to the continuity problem. However, in the specific case of slicing, better convergence behavior occurs when reference days are chosen, especially in the design of gchps, pv systems, chp plants, central heating plant, and district heating networks.

The variable cost factor applied to all temporal model adaptions (see Section 3.3.1) takes the ratio of periodical to variable costs well into account. For most temporal model adaptions a larger deviation of the modeled system costs is only recorded in the case of large temporal simplification. Only in the cases of downsampling, k-clustering (solar radiation and electricity demand criteria), and time horizon reduction the deviations were greater than 10%, as long as a minimum of 20% of the original number of time steps were modeled (see Appendix D).

5.2 Techno-spatial model adaptions

The tested techno-spatial model adaptions showed that the memory requirement is linearly related to the number of investment decisions (see Fig. 6). The run-time depends among other things on the number of binary investment decisions even though, the regression of this relationship has only a low coefficient of determination.

Some of the tested methods allow a significant reduction of the required computing resources without causing model deviations at all. This applies to technological pre-selection and the definition of appropriate technological boundaries (run-time only). Technological sub-modeling allows further improvements with, besides too high battery storage investments, negligible model deviations. Since the lack of compensation possibilities between the sub-systems mainly causes the undersizing of the battery storages, it can be assumed that this effect will become less important with increasing sub-system size. It is recommended to draw reasonable boundaries between the sub-models. For example, locations of central heat generation or grid nodes are particularly suitable for that purpose.

Spatial clustering, linearization and technological case distinction lead to significant model deviations. The previously, theoretically assumed problems with spatial clustering (Fig. 2) and linearization (Fig. 3) are thus confirmed. In the reference case, technological aggregation led only to minor model deviations, but to an increase of the run-time. The increase in run-time can be explained by the fact that systems with averaged parameters are closer to the profitability limit. For example, in the modeled reference case, the pv systems of building SDB1 were either fully designed (pv system 1 with 244° south-west orientation) or not designed at all (pv system 2 with 66° north-east orientation). This "all-or-nothing" decision indicates a clear and easily identifiable solution for the model. In the aggregated case, the parameters of the two plants are weighted averaged (aggregated pv system with 159° south-east orientation) and the investment decision is only partially sized. This partial design indicates that the investment decision is close to the profitability limit and the optimal capacity is harder to identify for the solution algorithm. Consequently, more run-time is required to solve the model. We therefore recommend not to use these methods.

Technological pre-selection, technological boundaries and spatial sub-modeling are suitable techno-spatial model adaptation methods to substantially improve the computing resources. However, these methods require either preliminary carried out studies or a profound knowledge and understanding of the energy system under investigation (see Section 2.2). If preliminary decisions are made on the basis of inaccurate or false assumptions, this will automatically lead to an inaccuracy in the main model as well.

5.3 Combined model adaptions

Before applying all the methods tested in this study, the conceptual design of energy system models should always avoid to include non-relevant system components and investment decisions that are not relevant to the research questions. Particular focus should be put on the avoidance of binary decisions.

A way to address lack of prior knowledge on the application of technological pre-selection and application of technological boundaries is the execution of a pre-model with temporal simplifications. Based on the results of this pre-model, investment decisions that were not used at all can be removed from the main model (technological pre-selection). In contrast to the temporal zooming approach, the investment decisions are thereby only limited within the pre-model, but the final decisions (dispatch and investment) are made entirely in the main-model. To ensure that no relevant technologies are mistakenly removed from the model, the method for temporal simplifying the pre-model should be chosen with care. The results of the applied case show that the shortening of the original time series by averaging each of ten consecutive weeks would be very suitable. More or less the same technologies were considered for investment decisions as in the reference case (see Section 4.2). Although the capacities of these investment decisions do not match those of the reference results, the decisions can be used for technological pre-selection. In addition, the pre-results can be used to reasonably constrain the technological investment limits. The test case results show that setting them to about 500% of the pre-results is appropriate. If subsequently the investment limits are fully utilized in the main model, the values should be increased and the main model repeated.

The application of pre-modeling with subsequent technological pre-selection and application of technological boundaries thus corresponds to the tested combined methods scheme X1 (see Table 3), which enabled a significant reduction of computing resources without causing model deviations.

The technological pre-selection considered manually in the model could have been made on the basis of a temporally simplified pre-model with averaging every 10th week (see Appendix D). Adding the solving time of such a pre-model of 840 s (see Appendix D) still a total run-time improvement of about −98% and a reduced memory requirements of −29% (see Appendix G) can be expected compared to the reference case.

Further savings of computing resources, especially memory usage, are possible through further method combinations. Based on the tested schemes, we recommend, the additional application of spatial sub-modeling, and temporal slicing. Temporal slicing should be applied only as much as absolutely necessary, because the model results deviate increasingly from the reference case with decreasing number of modeled time steps. Useful results with respect to the investment decisions made can be expected if at least 20% of the original time steps are modeled.

5.4 Evaluation of results

Although this study focuses on the specific case of reducing the computational requirements of mixed-use multi-energy systems with high spatial resolution through temporal and techno-spatial model adjustments, the results can be partially compared with other studies on run-time and memory reduction of energy system models.

Kotzur et al. [10] also recommend “a systematic reduction of the size of the model” and that “binary variables should be avoided and equations linearized where possible”. In addition, they also see potential in spatial clustering and draw attention to the risks of accounting mismatches.

In line with our results, Hoffmann et al. [14] came to the conclusion that “temporal aggregation methods are always based on the complexity reduction of not perfectly redundant input data and thus introduce deviations from fully resolved models" and that these should only be used if absolutely necessary.

Alimou et al. [28] analyzed a combination of heuristic selection and downsampling to select seven typical days, which are divided into six hourly time steps afterwards. Consistent with our results for heuristic selection and downsampling, they arrived at the conclusion that this procedure “tends to reduce the high variability of [...] wind and solar”, as well as to overestimate “the maximum load that must be supplied by [...] thermal power plants”.

Cao et al. [9] as well as Shirizadeh and Quirion [29] came to results regarding the downsampling method for the cases of nation scale models, which strongly differ from our results. They both identified downsampling to be the “most efficient speed-up approach” [9] of the time series simplification methods tested for their cases. The differences in the results can be attributed to the differences in the spatial scale and the technological and spatial resolution. We analyzed a comparatively small area with high spatial and technological resolution. In such areas, small-scale interactions between individual components and subsystems as well as the volatility of individual renewable energy plants are highly relevant. These points are not well represented by downsampling. However, these effects are less relevant for large energy system models with lower spatial and technological resolution (Shirizadeh and Quirion used only a single node). Accordingly, the weaknesses of the downsampling method have less influence on the results of such models. However, the different results underline how important it is to use appropriate methods of time series reduction depending on the application.

The methods considered in this study were applied to a real-world energy system with a total of nine buildings. However, we assume that the results can also be applied to other energy system models. The test area was selected to correspond to the structure of larger urban energy systems. We therefore assume that the results are transferable to urban areas with several hundred buildings.

We further assume that the results are particularly applicable to energy system models with a high level of technological detail and high spatial resolution. For spatially very large models (e.g., national scale) with low technological and spatial resolution, the results are not transferable without further ado.

The results for temporal model adaptations are particularly characterized by model deviations in the design of sector-coupling technologies, battery storage and the decision of (de)centralized heat supply (see Section 5.1). The results are therefore especially transferable to models that include such kind of technologies and decisions. For mono-sectoral models, the transferability has to be confirmed first. Furthermore, mainly short-term storages were considered within the test case, so that we cannot state the influence of the different temporal simplifications on long-term storages, which, e.g., have been described by Kotzur et al. [18].

The recommended techno-spatial methods of technological pre-selection and technological boundaries are expected to be highly transferable to most other types of energy systems, especially models with a high number of binary decisions. Rather, the uncertainties of these methods depend on the quality of the underlying preliminary investigations.

Lastly, the results are transferable for models where the solving process is the bottleneck of the whole modeling process. For models, where pre-processing or post-processing may be predominant, other approaches, which are not in the focus of this study, should be conducted.

6 Conclusion

The model runs performed in this study have shown that the computational requirements of run-time and (random access) memory usage to solve a model are influenced differently by increasing model complexity. The **run-time increases quadratically with increasing model complexity**. A correlation of the relationship with the number of time steps modeled proved to be particularly clear for the models used in this study, showing a coefficient of determination of $R^2 = 0.80$. Furthermore, in particularly the number of binary investment decisions had quadratic influence on the run-time, although this relationship showed up to be less clear ($R^2 = 0.31$). In turn, the **memory requirement increases linearly with increasing model complexity**. Again, the correlation to the number of modeled time steps was found to be particularly clear ($R^2 = 0.99$). Furthermore, the number of all investment decisions also had linear impact ($R^2 = 0.74$) on the memory requirement.

The application of model adaption methods can therefore significantly reduce computing resources. In the investigated test case, the run-time could be reduced by more than −99 % and the memory usage by up to −88 %, by using a combination of technological pre-selection, technological boundaries, temporal slicing (every fourth day), and spatial sub-modeling (scheme X5, see Table 3).

Based on our analysis, we recommend the following general procedure for the reduction of computing resources for multi-energy system investment optimizations models. The proposed steps are sequential. To avoid model inaccuracies, only as many steps as absolutely necessary should be applied:

1. **keeping the model as simple as possible:** All system components that are not relevant for the purpose of the study should be removed from the model. This applies in particular to (binary) investment decisions.
2. **pre-modeling:** With the help of a time-simplified model (slicing/averaging of every 10th week is recommended), preliminary results can be obtained and incorporated into the main-model (scheme X1, see Table 3):
   (a) **technological pre-selection:** Technologies not considered within in the pre-modeling should be removed from the main-model.
   (b) **technological boundaries:** Investment limits can be reasonably limited based on the pre-model results. We recommend technological boundaries of 500% of the pre-model result investment values. If the investment limits are fully used in the main-model, the technological boundaries should be enlarged.
3. **spatial sub-modeling:** The model can be decomposed and the results subsequently aggregated. The boundaries of sub-models should be strategically aligned, for example at network nodes. Especially for models without interaction between sub-systems (i.e., without local energy markets or bi-directional heat networks), only small model deviations are to be expected (scheme X3, see Table 3).
4. **temporal simplification:** We recommend temporal slicing, using days as sample periods. The degree of slicing should be as low as necessary, with a maximum of every fifth day (scheme X4 and X5, see Table 3).
5. **further simplifications:** If further model simplifications are necessary, we recommend spatial clustering of sub-systems. The clusters should be kept as small as possible.

Note that none of the tested methods of temporal model reduction allowed simplifications without model deviations. In fact, there was always at least one technology with major design errors of at least 10% compared to the reference case (see Appendix D). Due to large model deviations, we especially recommend avoiding the use of temporal downsampling, time horizon reduction, linearization and holistic spatial clustering, if possible.

The proposed procedure was tested for an urban area with a total of nine buildings. The test area was chosen to correspond to the structure of larger urban areas. Therefore, we presume that the procedure is also applicable to larger multi-energy systems, for example, of urban districts with several hundreds of buildings. However, the transferability still has to be finally confirmed in future research. In addition, we recommend the development of concrete instructions for solver-based methods and parallelization. In this way, the required computational resources can be further reduced or the possible model complexity can be increased while maintaining the same run-time and memory usage requirements.

CRediT authorship contribution statement

Christian Klemm: Conceptualization, Methodology, Investigation, Formal analysis, Software, Visualization, Writing – original draft. **Frauke Wiese:** Funding acquisition, Supervision, Writing – review & editing. **Peter Vennemann:** Funding acquisition, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

All modeling tools and input data used for this study are openly available. The "Spreadsheet Energy System Model Generator" (SESMG) v0.4.0rc1 (https://doi.org/10.5281/zenodo.6997542) was used for modeling. Scenarios files used for the modeling https://doi.org/10.5281/zenodo.6997372 and documentation of model structure and parameters (https://doi.org/10.5281/zenodo.6997547) are also available.

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Appendix A. Methods: Investment decision

A list of the investment decisions carried out in the test case is shown in Table 4.

Table 4
Investment decisions within the test case area. Unless otherwise indicated, the decisions are linear and the value to be determined can be between zero and the listed value.

	Unit	cent.	SDB1	SDB2	SDB3	MFB1	MFB2	COM1	COM2	GAR1	GAR2
Central heating plant	kW	999	–	–	–	–	–	–	–	–	–
Gas heating systems	kW	–	999	999	999	999	999	999	999	–	–
Chp plant	kW	999	–	–	–	–	–	–	–	–	–
gchp		–	27.8	18.4	21.6	21.5	30.1	–	–	–	–
Ashp	kW	999	999	999	999	999	999	999	999	–	–
Pv systems	kW	–	6.75	13.50[a]	7.02	14.04	7.29	14.96[a]	9.32	2.70	2.16
Battery storage	kWh	9 999	9 999	9 999	9 999	9 999	9 999	9 999	9 999	–	–
solar th. collectors	kW	–	27.71	55.42[a]	28.82	57.64	29.93	61.41[a]	38.27	–	–
Thermal storage	kWh	9 999	9 999	9 999	9 999	9 999	9 999	9 999	9 999	–	–
Roof insulation	m^2	–	163	162	125	297	138	527	323	–	–
Wall insulation	m^2	–	364	365	338	402	194	340	523	–	–
Window insulation	m^2	–	60	59	47	103	48	211	131	–	–
Dh network		20 pipe sections, each with a binary decisions of DN25 (max. 87 kW) for house connection pipes and DN35 (max. 165 kW) for distribution network pipes.									

Acronyms: ashp = air source heat pump, cent. = central, chp = combined heat and power, dh = district heat, gchp = ground coupled heat pump, ng = natural gas, pv = photovoltaic, th. = thermal.
[a]Aggregated capacity of two partial plants.

Appendix B. Methods: Model parameters

All parameters used for the modeling including sources and derivations are stored in the following directories:

- SESMG scenario-files: https://doi.org/10.5281/zenodo.6997372
- Model and parameter documentation: https://doi.org/10.5281/zenodo.6997547

Appendix C. Methods: Techno-spatial model adaptions

A list of the applied techno-spatial model adaptions is shown in Table 5.

Table 5
Applied techno-spatial adaptions.

ID	Method	Specification	Investment decisions	
			Linear	Binary
Ref.	Reference case		79	20
A1	Technological pre-selection		31	10
B1	Technological aggregation		75	20
C1	Spatial clustering	Similar building types (4 clusters)	50	14
C2	Spatial clustering	Similar usage types (3 clusters)	43	12
C3	Spatial clustering	All buildings of the system (1 cluster)	37	8
D1	Linearization	House connection pipes, reference value: DN25	86	13
D2	Linearization	Distribution pipes, reference value: DN32	92	7
D3	Linearization	All pipes, reference value: DN25	99	0
D4	Linearization	All pipes, reference value: DN32	99	0
D5	Linearization	All pipes, reference value: DN25 & DN32	99	0
E1	Technological boundaries	500% reference investments	79	20
E2	Technological boundaries	200% of reference investments	79	20
E3	Technological boundaries	150% of reference investments	79	20
E4	Technological boundaries	100% of reference investments	79	20
F1	Sub-modeling	Sub-model 1 (SDB1-3, GAR1-2)	39	8
F2	Sub-modeling	Sub-model 2 (MFB1-2, COM 1-2)	45	13
G1	Technological case distinction	Centralized heat supply	43	20
G2	Technological case distinction	Decentralized heat supply	75	0

Appendix D. Results: Temporal model adaptions

Deviations of temporal simplified models from the reference case are shown in Table 6.

Table 6
Deviations of temporal simplified models from the reference case. Green cells indicate a model improvement, respectively low model errors, red cells indicate negative deviations from the reference case, blue positive deviations.

Scheme	Modeled time steps	Run-time	Memory usage	System costs	pv systems	Gas heating systems	gchp	ashp	chp	Central heating plant	Battery storages	Thermal storages	House connection pipes	Distribution pipes	Roof insulation	Wall insulation	Window insulation	Solar thermal systems
Averaging (days)	72	−99.98%	−97%	−27%	−23%	−89%	−100%	−100%	53%	−100%	238%	120%	100%	60%	–	–	–	–
Averaging (days)	864	−98.67%	−88%	−6%	−8%	−33%	17%	−100%	3%	−40%	−92%	154%	0%	0%	–	–	–	–
Averaging (days)	4368	−75.64%	−48%	−1%	−1%	−1%	2%	4%	2%	−2%	−52%	−3%	0%	0%	–	–	–	–
Averaging (days)	1752	−96.38%	−77%	−3%	−3%	−12%	28%	−29%	12%	−16%	−84%	11%	0%	0%	–	–	–	–
Averaging (weeks)	840	−99.03%	−86%	−17%	0%	−47%	7%	−100%	−2%	−55%	−85%	−39%	0%	0%	–	–	–	–
Averaging (weeks)	4368	−80.63%	−49%	−2%	2%	−6%	9%	−3%	2%	−8%	−47%	−2%	0%	0%	–	–	–	–
Averaging (weeks)	168	−99.91%	−91%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
Averaging (weeks)	1680	−96.67%	−77%	−16%	0%	−45%	19%	−17%	−3%	−49%	−71%	−26%	0%	0%	–	–	–	–
Downsampling (days)	88	−99.99%	−97%	1102%	49%	−100%	−100%	−100%	376%	−100%	57 331%	−100%	133%	120%	a	a	–	–
Downsampling (days)	876	−99.69%	−87%	113%	49%	−100%	−100%	−100%	255%	−37%	5409%	5%	133%	120%	–	a	–	–
Downsampling (days)	4380	−90.79%	−47%	20%	49%	−69%	−100%	35%	65%	9%	1131%	−15%	100%	60%	–	a	–	–
Downsampling (days)	1752	−98.94%	−77%	57%	49%	−100%	−100%	−100%	191%	−9%	2501%	−16%	133%	120%	–	a	–	–
Downsampling (days)	2920	−89.44%	−61%	−1%	−100%	−67%	−100%	−100%	64%	61%	−100%	−56%	100%	60%	–	–	–	–
Downsampling (days)	2190	−91.61%	−64%	−1%	−91%	10%	−100%	−100%	−31%	−45%	−100%	−42%	0%	−20%	–	a	–	–
Heuristic selection (days)	48	−99.99%	−97%	0%	12%	−73%	−100%	−100%	163%	−100%	1201%	398%	100%	60%	–	–	–	–
Heuristic selection (days)	96	−99.98%	−97%	−4%	−32%	−78%	−100%	−100%	87%	−100%	−72%	578%	100%	60%	–	–	–	–
Heuristic selection (days)	192	−99.94%	−96%	−2%	−42%	−25%	−100%	−100%	−12%	−41%	43%	306%	0%	0%	–	–	–	a
Heuristic selection (days)	384	−99.78%	−91%	−4%	−42%	−25%	−100%	−100%	1%	−48%	−44%	305%	0%	0%	–	–	–	a
Heuristic selection (days)	576	−99.20%	−89%	0%	−59%	−77%	−100%	−100%	74%	−25%	−82%	296%	100%	60%	–	–	–	–
Heuristic selection (weeks)	336	−99.78%	−94%	14%	−3%	−66%	−100%	−100%	265%	−92%	148%	−16%	100%	60%	–	a	–	–
Heuristic selection (weeks)	672	−99.15%	−83%	9%	−51%	−66%	−100%	−100%	63%	12%	−71%	−16%	100%	60%	–	a	–	–
Heuristic selection (weeks)	1344	−96.90%	−82%	5%	−50%	−66%	−100%	−100%	49%	37%	−72%	−10%	100%	60%	–	a	–	–
Heuristic selection (weeks)	2688	−86.72%	−67%	−1%	−19%	3%	−7%	−61%	1%	−1%	−72%	0%	0%	0%	–	–	–	–
Heuristic selection (weeks)	4032	−76.84%	−52%	−2%	−9%	0%	2%	−11%	0%	0%	−55%	0%	0%	0%	–	–	–	–
k-means clustering (solar radiation) (days)	72	−99.98%	−97%	−31%	−18%	−89%	−100%	−100%	38%	−100%	332%	96%	100%	60%	–	–	–	–
k-means clustering (solar radiation) (days)	864	−98.55%	−87%	−31%	14%	−78%	39%	−16%	−40%	−70%	−27%	107%	0%	0%	–	–	–	–
k-means clustering (solar radiation) (days)	4368	−43.08%	−47%	−30%	28%	−80%	62%	120%	−38%	−88%	124%	312%	0%	0%	–	–	–	–
k-means clustering (solar radiation) (days)	1752	−92.40%	−77%	−35%	23%	−86%	29%	43%	−43%	−82%	112%	183%	0%	0%	–	–	–	–
k-means clustering (electricity demand) (days)	72	−99.99%	−97%	−32%	−33%	−91%	−100%	−100%	51%	−100%	479%	−2%	100%	60%	–	–	–	–
k-means clustering (electricity demand) (days)	864	−97.83%	−87%	−17%	−23%	−85%	−100%	−98%	63%	−66%	−19%	171%	100%	60%	–	–	–	–
k-means clustering (electricity demand) (days)	4368	−52.69%	−47%	−6%	−12%	−80%	−100%	19%	53%	−8%	53%	253%	100%	60%	–	–	–	–
k-means clustering (electricity demand) (days)	1752	−93.43%	−77%	−21%	−12%	−86%	−100%	−51%	53%	−59%	47%	65%	100%	60%	–	–	–	–
k-means clustering (temperature) (days)	72	−99.99%	−97%	−14%	−30%	−81%	−100%	−100%	95%	−100%	12%	242%	100%	60%	–	–	–	–
k-means clustering (temperature) (days)	864	−98.03%	−87%	−7%	−20%	−83%	−100%	−100%	46%	−52%	−76%	451%	100%	60%	–	–	–	–
k-means clustering (temperature) (days)	4368	−58.50%	−48%	−7%	−10%	−82%	−100%	−25%	48%	−22%	24%	353%	100%	60%	–	–	–	–
k-means clustering (temperature) (days)	1752	−94.79%	−77%	−8%	−13%	−79%	−100%	−81%	60%	−17%	−40%	263%	100%	60%	–	–	–	–
k-means clustering (solar radiation) (weeks)	840	−98.72%	−86%	−29%	15%	−64%	27%	−86%	−32%	−57%	−56%	−48%	0%	0%	–	–	–	–
k-means clustering (solar radiation) (weeks)	4368	−72.69%	−48%	−37%	38%	−16%	39%	298%	−100%	−100%	492%	−45%	−100%	−100%	–	a	–	–
k-means clustering (solar radiation) (weeks)	168	−99.92%	−93%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
k-means clustering (solar radiation) (weeks)	1680	−96.64%	−77%	−35%	36%	−25%	86%	155%	−100%	−100%	627%	−53%	−100%	−100%	–	a	–	–
k-means clustering (electricity demand) (weeks)	4368	−78.13%	−48%	1%	−11%	−68%	−100%	−21%	54%	66%	34%	1%	100%	60%	–	–	–	–
k-means clustering (electricity demand) (weeks)	168	−99.92%	−93%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
k-means clustering (electricity demand) (weeks)	1680	−94.97%	−77%	−16%	−2%	−46%	−6%	−19%	9%	−60%	−57%	−38%	0%	0%	–	–	–	–
k-means clustering (temperature) (weeks)	840	−98.91%	−86%	7%	−31%	−68%	−100%	−100%	45%	12%	−71%	−19%	100%	60%	–	a	–	–
k-means clustering (temperature) (weeks)	4368	−75.52%	−47%	4%	−27%	−67%	−100%	−61%	45%	38%	−15%	−9%	100%	60%	–	a	–	–
k-means clustering (temperature) (weeks)	168	−99.92%	−93%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
k-means clustering (temperature) (weeks)	1680	−96.09%	−77%	−1%	3%	−5%	17%	−76%	−4%	−5%	−59%	−2%	0%	0%	–	–	–	–
k-medoids clustering (solar radiation) (days)	72	−99.99%	−97%	−28%	−26%	−89%	−100%	−100%	48%	−100%	77%	99%	100%	60%	–	–	–	–
k-medoids clustering (solar radiation) (days)	864	−98.31%	−87%	−10%	−31%	−86%	−100%	−100%	69%	−95%	−60%	530%	100%	60%	–	–	–	–
k-medoids clustering (solar radiation) (days)	2904	−85.88%	−64%	3%	−42%	−66%	−100%	−100%	44%	38%	−50%	−6%	100%	60%	–	a	–	–
k-medoids clustering (solar radiation) (days)	1752	−95.26%	−77%	3%	−39%	−66%	−100%	−100%	41%	40%	−61%	−6%	100%	60%	–	a	–	–
k-medoids clustering (electricity demand) (days)	72	−99.98%	−97%	−33%	−35%	−91%	−100%	−100%	50%	−100%	868%	−54%	100%	60%	–	–	–	–

(continued on next page)

Table 6 (*continued*).

k-medoids clustering (electricity demand) (days)	864	−98.30%	−87%	−27%	6%	−76%	23%	−25%	−17%	−80%	127%	44%	0%	0%	–	–	–	–
k-medoids clustering (electricity demand) (days)	2904	−74.55%	−64%	−10%	−5%	−85%	−100%	25%	48%	−28%	48%	320%	100%	60%	–	–	–	–
k-medoids clustering (electricity demand) (days)	1752	−87.09%	−77%	−27%	8%	−74%	8%	−43%	−6%	−88%	64%	55%	0%	0%	–	–	–	–
k-medoids clustering (temperature) (days)	72	−99.99%	−97%	−23%	−26%	−86%	−100%	−100%	60%	−100%	110%	166%	100%	60%	–	–	–	–
k-medoids clustering (temperature) (days)	864	−97.13%	−87%	−9%	−55%	−85%	−100%	−100%	48%	−53%	−99%	395%	100%	60%	–	–	–	–
k-medoids clustering (temperature) (days)	2904	−75.56%	−65%	−9%	−47%	−88%	−100%	−100%	45%	−66%	−61%	477%	100%	60%	–	–	–	–
k-medoids clustering (temperature) (days)	1752	−93.88%	−77%	−10%	−52%	−85%	−100%	−100%	47%	−48%	−87%	391%	100%	60%	–	–	–	–
k-medoids clustering (solar radiation) (weeks)	2856	−86.75%	−65%	5%	−51%	−66%	−100%	−100%	65%	29%	−89%	−11%	100%	60%	–	[a]	–	–
k-medoids clustering (solar radiation) (weeks)	168	−99.92%	−93%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
k-medoids clustering (solar radiation) (weeks)	1680	−94.12%	−78%	−14%	−28%	−80%	−100%	−28%	33%	−10%	−55%	−12%	100%	60%	–	–	–	–
k-medoids clustering (electricity demand) (weeks)	2856	−85.70%	−65%	−11%	0%	−33%	6%	32%	−2%	−33%	−63%	−23%	0%	0%	–	–	–	–
k-medoids clustering (electricity demand) (weeks)	168	−99.92%	−93%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
k-medoids clustering (electricity demand) (weeks)	1680	−95.54%	−78%	−12%	8%	−41%	59%	−19%	−2%	−32%	−42%	−23%	0%	0%	–	–	–	–
k-medoids clustering (temperature) (weeks)	2856	−89.46%	−65%	0%	−30%	−68%	−100%	−80%	64%	52%	−26%	−2%	100%	60%	–	–	–	–
k-medoids clustering (temperature) (weeks)	168	−99.92%	−93%	−33%	−18%	−91%	−100%	−100%	49%	−97%	876%	−64%	100%	60%	–	–	–	–
k-medoids clustering (temperature) (weeks)	1680	−96.97%	−79%	0%	−17%	−68%	−100%	−74%	55%	56%	−23%	−2%	100%	60%	–	–	–	–
Random sampling (days)	4368	−40.19%	−48%	−2%	−18%	−69%	−100%	−38%	36%	64%	57%	39%	100%	60%	–	–	–	–
Random sampling (days)	864	−98.66%	−87%	−8%	−45%	−85%	−100%	−100%	60%	−60%	−40%	437%	100%	60%	–	–	–	–
Random sampling (days)	72	−99.99%	−97%	−8%	−72%	−81%	−100%	−100%	119%	−100%	−91%	232%	100%	60%	–	–	–	–
Random sampling (days)	1752	−94.00%	−77%	0%	−40%	−67%	−100%	−100%	45%	57%	−28%	57%	100%	60%	–	–	–	–
Random sampling (weeks)	1680	−95.04%	−77%	−16%	−14%	−44%	−20%	−50%	2%	−56%	−65%	−20%	0%	0%	–	–	–	–
Random sampling (weeks)	168	−99.96%	−93%	−66%	33%	−86%	−61%	−89%	−100%	−100%	2052%	−84%	−100%	−100%	–	–	–	[a]
Random sampling (weeks)	4368	−68.79%	−48%	−4%	−26%	−73%	−100%	21%	70%	31%	2%	6%	100%	60%	–	–	–	–
Random sampling (weeks)	840	−98.75%	−86%	−12%	−46%	−80%	−100%	−100%	98%	−48%	−49%	−20%	100%	60%	–	–	–	–
Slicing (days)	72	−99.99%	−97%	−29%	−81%	−69%	−100%	−100%	−30%	−100%	−100%	13%	0%	0%	–	–	–	–
Slicing (days)	864	−98.88%	−87%	−5%	−26%	−12%	−33%	−100%	1%	−21%	−60%	28%	0%	0%	–	–	–	–
Slicing (days)	4368	−73.35%	−48%	0%	−4%	−2%	0%	20%	2%	−3%	−38%	−1%	0%	0%	–	–	–	–
Slicing (days)	1752	−95.89%	−77%	−2%	−24%	−3%	−25%	−54%	0%	−10%	−67%	−4%	0%	0%	–	–	–	–
Slicing (days)	5808	+18.81%	−29%	0%	0%	−1%	2%	22%	2%	−1%	−16%	1%	0%	0%	–	–	–	–
Slicing (days)	6552	−13.71%	−23%	0%	−2%	0%	−2%	1%	0%	0%	−20%	1%	0%	0%	–	–	–	–
Slicing (weeks)	840	−98.64%	−86%	−29%	−22%	−59%	−50%	−74%	−17%	−75%	−60%	−43%	0%	0%	–	–	–	–
Slicing (weeks)	4368	−71.35%	−48%	−1%	−13%	0%	−8%	−23%	−1%	−4%	−55%	−5%	0%	0%	–	–	–	–
Slicing (weeks)	168	−99.94%	−93%	−18%	−100%	−87%	−100%	−100%	96%	−90%	−100%	−43%	100%	60%	–	–	–	–
Slicing (weeks)	1680	−95.65%	−77%	0%	0%	−4%	31%	−81%	−1%	1%	−43%	−1%	0%	0%	–	–	–	–
Slicing (weeks)	6552	+22.48%	−23%	1%	−5%	2%	−10%	−9%	−1%	0%	−23%	0%	0%	0%	–	–	–	–
Time horizon reduction	1095	−98.31%	−85%	300%	−100%	488%	−100%	−100%	380%	−100%	−100%	214%	67%	40%	[a]	[a]	–	–
Time horizon reduction	2190	−93.88%	−73%	113%	−72%	200%	−100%	−100%	380%	−100%	−100%	102%	100%	60%	[a]	[a]	–	–
Time horizon reduction	4380	−84.88%	−48%	46%	−7%	61%	−100%	−17%	166%	10%	93%	52%	100%	60%	–	[a]	–	–

[a] In the simplified model, an investment has taken place which was not taken into account in the reference case.

Appendix E. Results: Temporal model adaptions (Plots)

Deviations of investment decisions of slicing and averaging from the reference case are shown in Figs. 8–10. Investment decisions that did not prove suitable for system optimization neither in the reference case nor in the simplified model runs for system optimization (wall, window and roof insulation) are not shown.

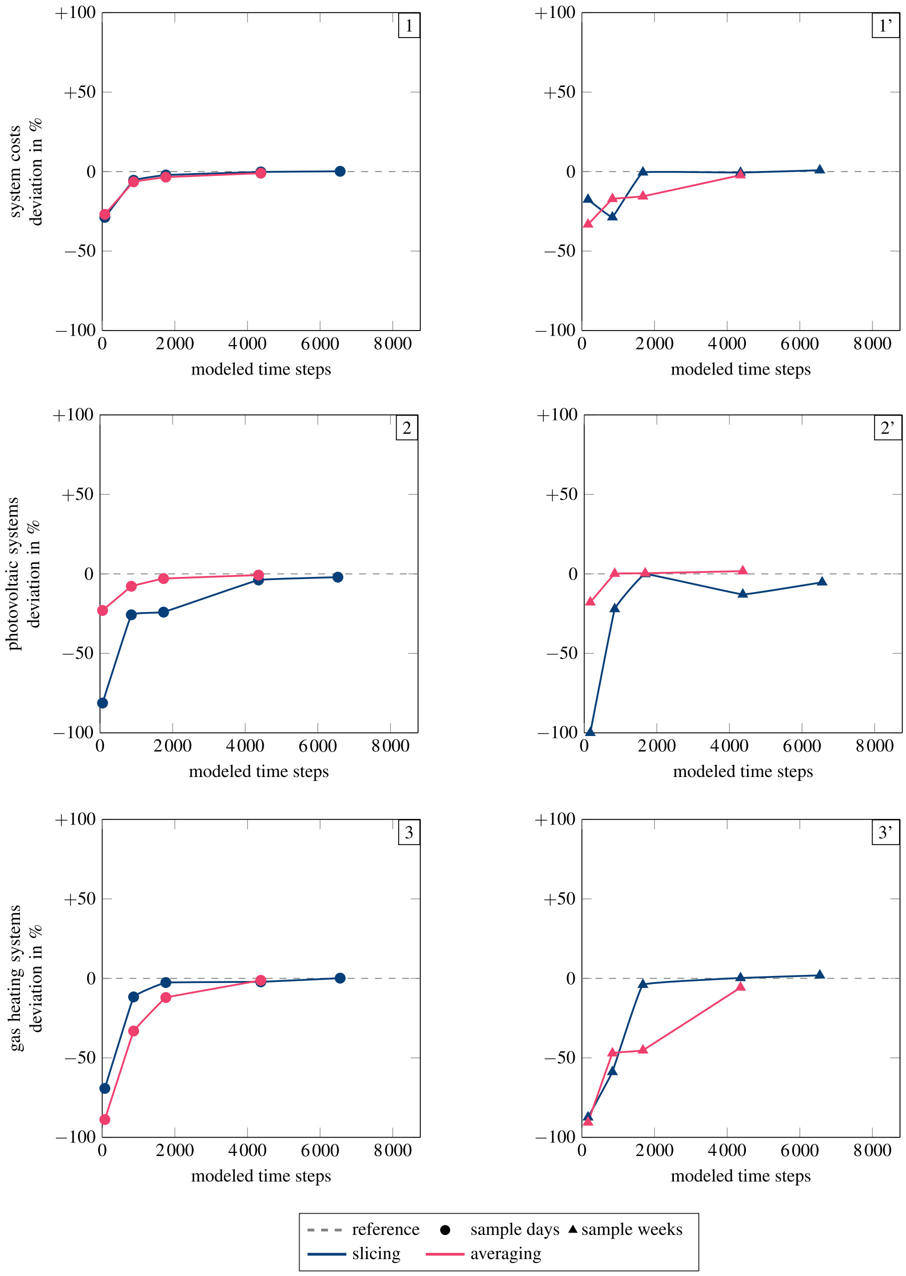

Fig. 8. Investment decision deviations of temporal simplified models from the reference case. Methods with sample days are shown on the left, sample weeks on the right. Modeled values are shown as full symbols.

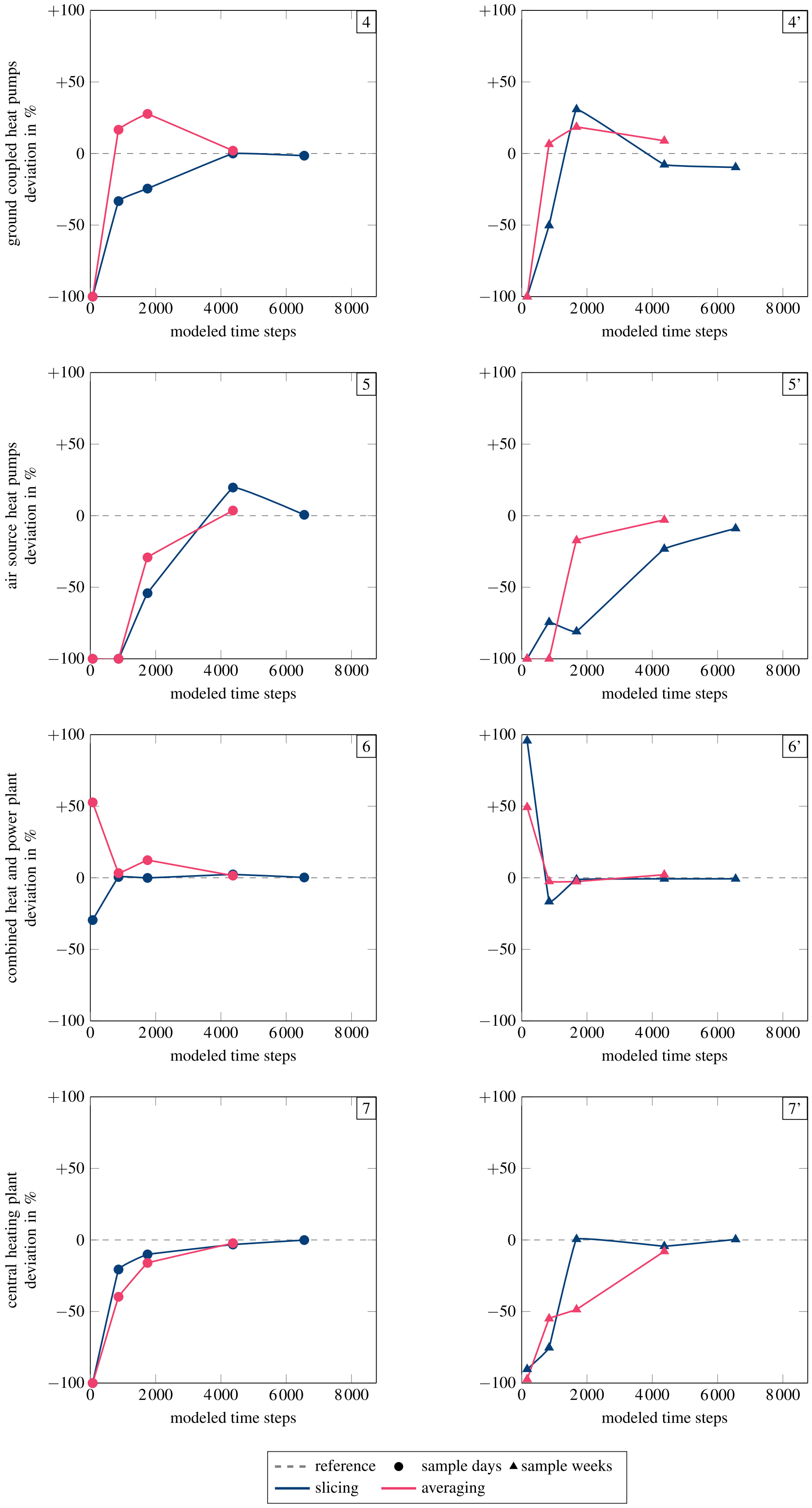

Fig. 9. Investment decision deviations of temporal simplified models from the reference case. Methods with sample days are shown on the left, sample weeks on the right. Modeled values are shown as full symbols.

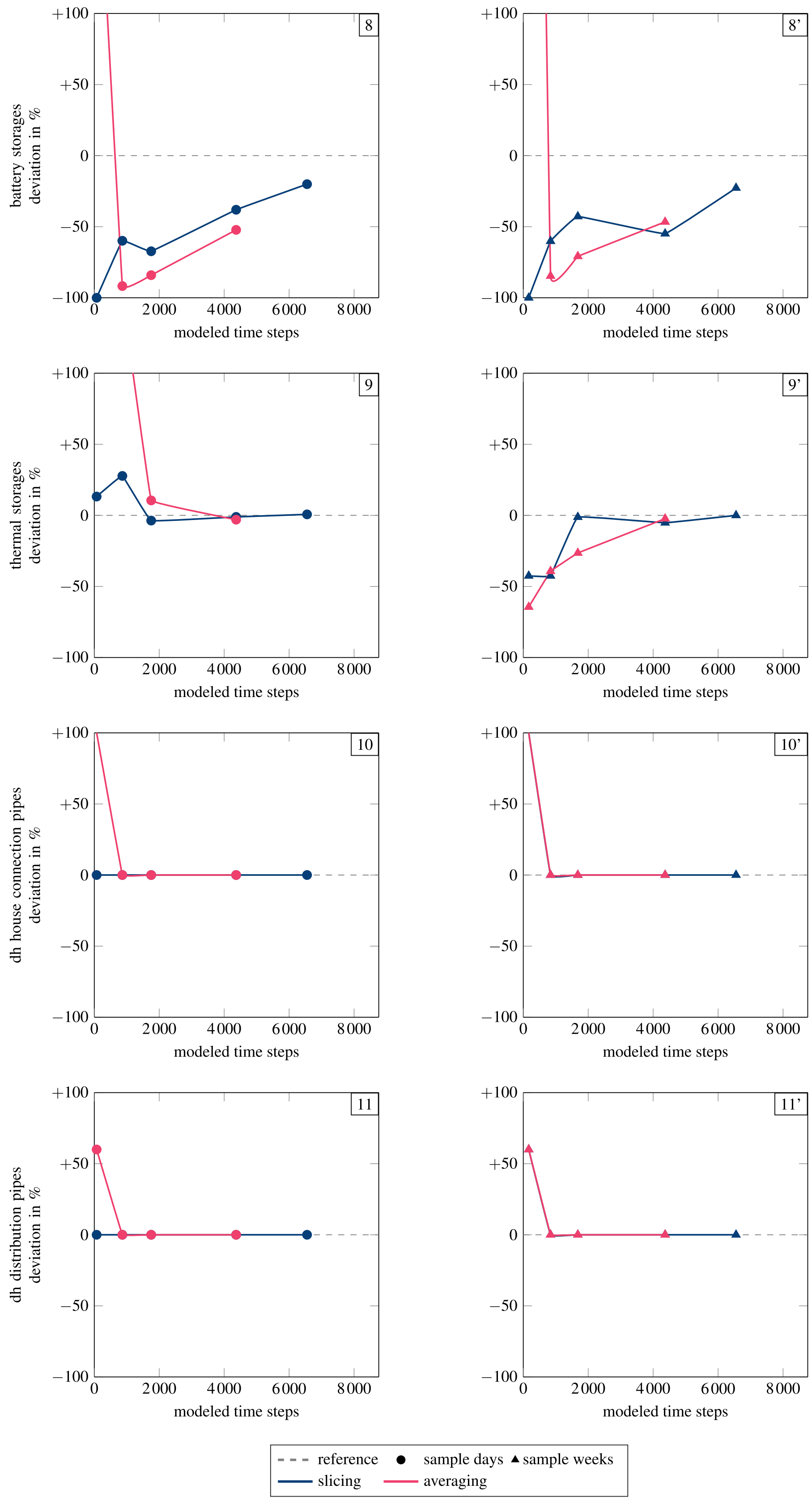

Fig. 10. Investment decision deviations of temporal simplified models from the reference case. Methods with sample days are shown on the left, sample weeks on the right. Modeled values are shown as full symbols.

Appendix F. Results: Techno-spatial model adaptions

Deviations of techno-spatial simplified models from the reference case are shown in Table 7.

Table 7
Deviations of techno-spatial simplified models from the reference case. Green cells indicate a model improvement, respectively low model errors, red cells indicate negative deviations from the reference case, blue positive deviations.

Method	Linear investment decisions	Binary investment decisions	Run-time	Memory usage	System costs	pv systems	Gas heating systems	gchp	ashp	chp	Central heating plant	Battery storages	Thermal storages	House connection pipes	Distribution pipes	Roof insulation	Wall insulation	Window insulation	Solar thermal systems
A1: technological pre-selection	31	10	−99.38%	−29%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
B1: technological aggregation	75	20	+68.27%	−2%	0%	+5%	−1%	+3%	0%	0%	0%	+3%	0%	0%	0%	0%	0%	0%	0%
C1: spatial clustering	50	14	−80.97%	−44%	−4%	+9%	+2%	−2%	+120%	−35%	−38%	+5%	−16%	−67%	−60%	0%	a	0%	0%
C2: spatial clustering	43	12	−94.51%	−54%	−10%	−7%	−7%	−100%	+121%	−10%	−15%	−26%	−15%	−67%	−60%	0%	a	0%	0%
C3: spatial clustering	37	8	−99.26%	−64%	−20%	−15%	−11%	−100%	−100%	+39%	−41%	−78%	−26%	−67%	−60%	0%	a	0%	0%
D1: linearization	86	13	−57.58%	0%	−4%	−16%	−68%	−100%	0%	+54%	+57%	+62%	−3%	+100%	+60%	0%	a	0%	0%
D2: linearization	92	7	−87.13%	0%	−9%	−18%	−40%	−100%	−100%	+55%	−9%	+62%	−17%	+133%	+160%	0%	a	0%	0%
D3: linearization	99	0	−98.49%	0%	−13%	−18%	+18%	−100%	−100%	+37%	−70%	+62%	−17%	+500%	−100%	0%	a	0%	0%
D4: linearization	99	0	−98.99%	0%	−14%	−18%	−28%	−100%	−100%	+59%	−22%	+62%	−17%	−100%	+300%	0%	a	0%	0%
D5: linearization	99	0	−99.01%	0%	−14%	−18%	−19%	−100%	−100%	+55%	−31%	+62%	−17%	+133%	+160%	0%	a	0%	0%
E1: technological boundaries	79	20	−76.79%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
E2: technological boundaries	79	20	−75.96%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
E3: technological boundaries	79	20	−59.71%	+1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
E4: technological boundaries	79	20	−49.47%	+1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
F: sub-modeling	39/45	8/13	−67.84%	−39%	+1%	0%	+1%	−6%	0%	0%	0%	+54%	0%	0%	0%	0%	0%	0%	0%
G: case-distinction	43/75	20/0	−98.56%	−22%	+1%	+13%	+81%	+33%	+122%	−100%	−100%	+55%	−16%	−100%	−100%	0%	a	0%	0%

[a] In the simplified model, an investment has taken place which was not taken into account in the reference case.

Appendix G. Results: Combined methods

Deviations of simplified models using combined methods from the reference case are shown in Table 8 and Fig. 11.

Table 8
Deviations of models with combined methods from the reference case. Green cells indicate a model improvement, respectively low model errors, red cells indicate negative deviations from the reference case, blue positive deviations.

Scheme	Linear investment decisions	Binary investment decisions	Run-time	Memory usage	System costs	pv systems	Gas heating systems	gchp	ashp	chp	Central heating plant	Battery storages	Thermal storages	House connection pipes	Distribution pipes	Roof insulation	Wall insulation	Window insulation	Solar thermal systems
X1	31	10	−99.43%	−29%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
X2	31	10	−99.57%	−62%	0%	−4%	−2%	0%	+20%	+2%	−3%	−38%	−1%	0%	0%	0%	0%	0%	0%
X3	16/15	0/10	−99.31%	−55%	+1%	0%	+1%	−5%	0%	0%	0%	+29%	0%	0%	0%	0%	0%	0%	0%
X4	16/15	0/10	−99.70%	−77%	+1%	−2%	−1%	−4%	+20%	+2%	−3%	+9%	−1%	0%	0%	0%	0%	0%	0%
X5	16/15	0/10	−99.89%	−88%	−1%	−21%	−2%	−29%	−54%	0%	−10%	−32%	−4%	0%	0%	0%	0%	0%	0%

In the simplified model, an investment has taken place which was not taken into account in the reference case.

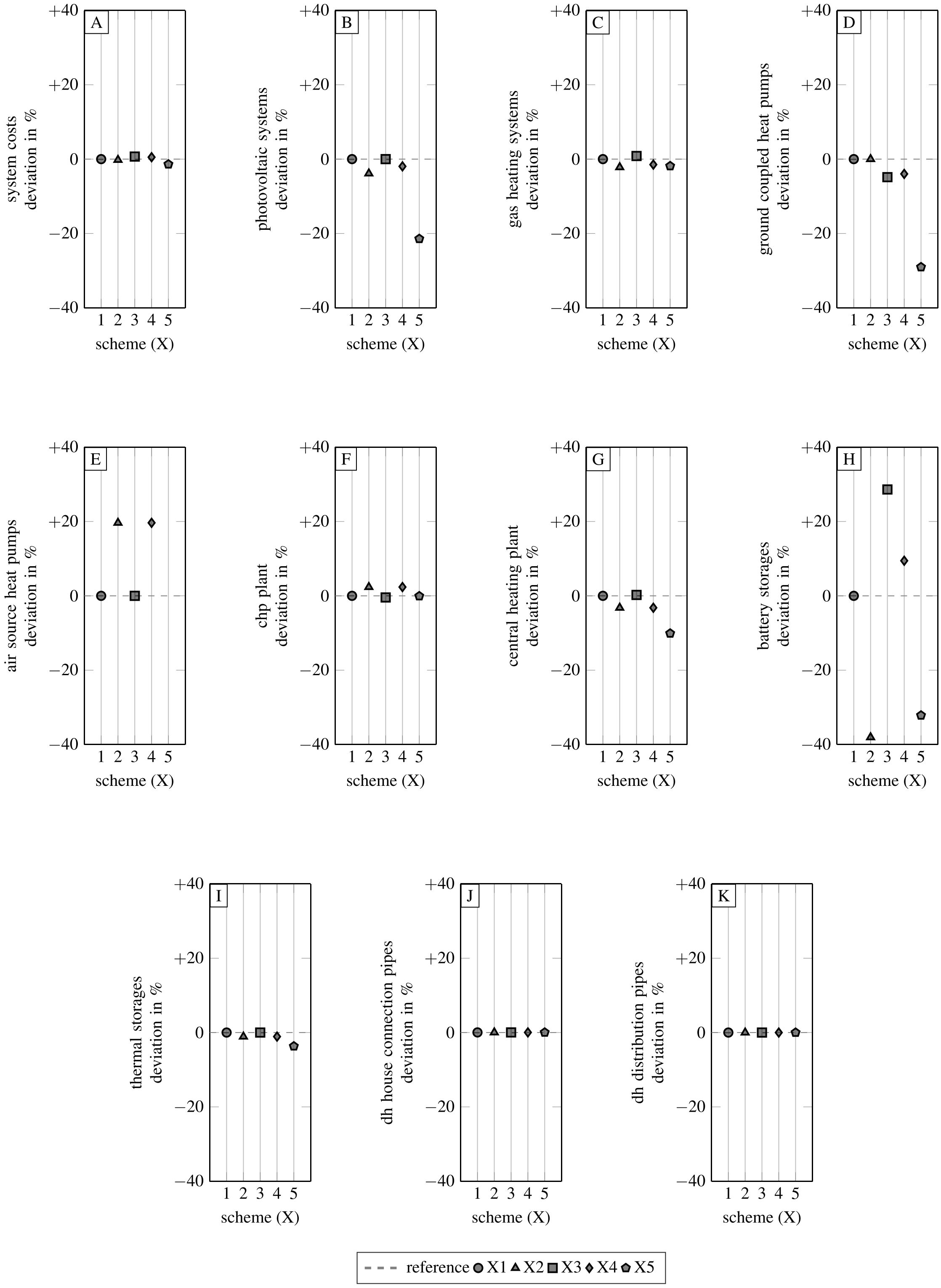

Fig. 11. Investment decision deviations of the applied combined model reduction method schemes from the reference case results.

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D Publication: The Spreadsheet Energy System Model Generator (SESMG): A tool for the optimization of urban energy systems

Table D.1: Fact sheet publication [D]

Title: The Spreadsheet Energy System Model Generator (SESMG): A tool for the optimization of urban energy systems
Authors: Christian Klemm, Gregor Becker, Jan N. Tockloth, Janik Budde, Peter Vennemann
Journal: The Journal of Open Source Software
Date: 09/2023
Digital Object Identifier (DOI): `https://doi.org/10.21105/joss.05519`
Authors contribution: Christian Klemm: Conceptualization, Software, Writing – original draft. Gregor Becker: Conceptualization, Software, Writing – review & editing. Jan N. Tockloth: Conceptualization, Software, Writing – review & editing. Janik Budde: Conceptualization, Software, Writing – review & editing. Peter Vennemann: Funding acquisition, Supervision, Writing – review & editing.
Abstract: The Spreadsheet Energy System Model Generator (SESMG) is a tool for modeling and optimizing energy systems with a focus on urban systems. The SESMG is easily accessible as it comes with a browser-based graphical user interface, spreadsheets to provide data entry, and detailed documentation on how to use it. Programming skills are not required for the installation or application of the tool. The SESMG includes advanced modeling features such as the application of the multi-energy system (MES) approach, multi-objective optimization, model-based methods for reducing computational requirements, and automated conceptualization and result processing of urban energy systems with high spatial resolution. Due to its accessibility and the applied modeling methods, urban energy systems can be modeled and optimized with comparatively low effort.

The Spreadsheet Energy System Model Generator (SESMG): A tool for the optimization of urban energy systems

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Software

- Review
- Repository
- Archive

Editor: Tim Tröndle

Reviewers:

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Summary

The Spreadsheet Energy System Model Generator (SESMG) is a tool for modeling and optimizing energy systems with a focus on urban systems. The SESMG is easily accessible as it comes with a browser-based graphical user interface, spreadsheets to provide data entry, and detailed documentation on how to use it. Programming skills are not required for the installation or application of the tool. The SESMG includes advanced modeling features such as the application of the multi-energy system (MES) approach, multi-objective optimization, model-based methods for reducing computational requirements, and automated conceptualization and result processing of urban energy systems with high spatial resolution. Due to its accessibility and the applied modeling methods, urban energy systems can be modeled and optimized with comparatively low effort.

Statement of need

The Spreadsheet Energy System Model Generator (SESMG) meets various challenges of modeling urban energy systems. Planning and optimizing the design of urban energy systems is becoming increasingly complex (Zhang et al., 2018) due to sector coupling, the use of decentralized renewable energy sources with volatile production, the use of diverse energy storage systems, the growing importance of new energy sectors such as hydrogen, as well as the increasing relevance of multiple planning objectives. In this context, urban energy systems are defined as "the combined process of acquiring and using energy in a given spatial entity with a high density and differentiation of residents, buildings, commercial sectors, infrastructure, and energy sectors (e.g., heat, electricity, fuels)" (Klemm & Wiese, 2022). Traditionally, such systems are designed by simulating and comparing a limited number of pre-defined energy supply scenarios without using optimization methods. Individual buildings, consumption sectors, or energy sectors are rarely planned and designed holistically, but rather separately from each other (Lukszo et al., 2018). Finally, planning processes are often only driven by financial interests, rather than considering additional planning objectives such as minimizing green house gas (ghg) emissions, or final energy demand. To fully exploit all synergies and to avoid conflicting interests due to interdependencies of increasingly entangled energy systems (Pfenninger, 2014), it is necessary to carry out holistic planning (Lukszo et al., 2018). Therefore, all energy sectors, planning objectives, as well as an entire spatial entity should be considered within a holistic analysis (United Nations Environment Programme, 2015). Not only certain, but all theoretically possible supply scenarios should be compared by using optimization algorithms (DeCarolis et al., 2017) in order to ensure that scenarios that allow

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the minimization of the planning objectives by a given ratio are identified (Klemm & Wiese, 2022). All these requirements for planning and optimization methods result in increasingly high computing requirements, especially in run-time and random access memory (RAM) (Klemm et al., 2023). To limit the necessary computing capacities to an acceptable extend, modelers may make decisions regarding the temporal and spatial resolution of the system. Alternatively, model-based or solver-based methods can be used to reduce the computational requirements (Cao et al., 2019), with only slight differences in the quality of the results.

Combining functions of the underlying Open Energy Modeling Framework (oemof) (Krien et al., n.d.) as well as its own functionalities, the SESMG overcomes these typical problems of modeling urban energy systems by

- considering the **multi-energy system (MES)** approach (Mancarella et al., 2016),
- carrying out **multi-objective optimization** by using the epsilon-constraint-method (Mavrotas, 2009), and by
- enabling high spatial resolution results through the applicability of **model-based** methods for the **reduction of computational effort** (Klemm et al., 2023).

The SESMG enables the optimization of multi-sectoral and spatial synergies of entire urban energy systems with an adaptable number of buildings. Due to the multi-criteria results in the form of a Pareto front, transformation processes between status quo, financial cost minimized and ghg emission minimized target scenarios can be identified.

The target groups of the SESMG are (urban) energy system planners and researchers in the field of energy engineering. As it is required for the application of the SESMG and the interpretation of the results, users must have a certain basic knowledge of energy systems and energy engineering. Compared to other tools for the modeling and optimization of urban energy systems, as they have been listed by Klemm and Vennemann (Klemm & Vennemann, 2021), the SESMG provides several advantages regarding user-friendliness due to

- being available under an **open-source license**,
- applicability **without any programming knowledge** through a **browser-based graphical user interface** (GUI),
- **automatically conceptualizing** individual urban energy systems of any size,
- **automatic result processing and visualization** of complex relationships in form of system graphs, Pareto fronts, energy amount diagrams, and more, as well as
- a broad set of **standard (but still customizable) technical and economic modeling parameters** including description and references.

The SESMG comes with a detailed documentation, including step-by-step instructions, explanations of all modeling methods, and troubleshooting with known application errors. In addition, the documentation includes an ongoing list of peer review publications, conference proceedings, study works, research projects, and other publications related to the SESMG.

Acknowledgements

The authors would like to thank the oemof user and developer community for the development of oemof and for discussions regarding the development of the SESMG. We would also like to thank all contributing users for their development work, bug reports, bug fixes, and helpful discussions. This research has been conducted within the R2Q project, funded by the German Federal Ministry of Education and Research (BMBF), grant number 033W102A.

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E Publication: Potential-Risk and No-Regret Options for Urban Energy System Design - A Sensitivity Analysis

Table E.1: Fact sheet publication [E]

Title: Potential-Risk and No-Regret Options for Urban Energy System Design - A Sensitivity Analysis
Authors: Christian Klemm, Peter Vennemann, Frauke Wiese
Journal: Sustainable Cities and Society (Under Review)
Date (Submission): 07/2023
Note: The manuscript was submitted for publication in an anonymized form as part of a double anonymized review process. For this appendix, the anonymization was removed and four typos were corrected. Apart from that, the manuscript was submitted for publication in this form (content and formatting).
Authors contribution: Christian Klemm: Conceptualization, Methodology, Investigation, Formal analysis, Software, Visualization, Writing – original draft. Peter Vennemann: Funding acquisition, Supervision, Writing – review & editing. Frauke Wiese: Funding acquisition, Supervision, Writing – review & editing.
Abstract: The optimization of urban energy systems considering the competing objectives of minimizing financial cost and greenhouse gas (GHG) emissions includes decisions that are sensitive to changes in energy prices, GHG emissions, and final energy demands. A high resolution sensitivity analysis of critical system parameters revealed several no-regret options that are robust to external conditions, as well as possible-risk options that are particularly sensitive to external conditions. No-regret options include photovoltaic systems, decentralized heat pumps, thermal storages, electricity exchange between sub-systems and with higher-level systems, and the reduction of energy demands through building insulation, behavioral changes, or reduction of living space per inhabitant. Potential-risk options include the use of solar thermal systems, decentralized natural gas technologies, high capacity battery storages, hydrogen for building energy supply, and natural gas-based district heating. When energy prices (electricity, natural gas and hydrogen) rise, financially-optimized systems approach the least-emission solution of system design.

Potential-Risk and No-Regret Options for Urban Energy System Design - A Sensitivity Analysis

September, 2023

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Abstract

The optimization of urban energy systems considering the competing objectives of minimizing financial cost and greenhouse gas (GHG) emissions includes decisions that are sensitive to changes in energy prices, GHG emissions, and final energy demands. A high resolution sensitivity analysis of critical system parameters revealed several no-regret options that are robust to external conditions, as well as possible-risk options that are particularly sensitive to external conditions. No-regret options include photovoltaic systems, decentralized heat pumps, thermal storages, electricity exchange between sub-systems and with higher-level systems, and the reduction of energy demands through building insulation, behavioral changes, or reduction of living space per inhabitant. Potential-risk options include the use of solar thermal systems, decentralized natural gas technologies, high capacity battery storages, hydrogen for building energy supply, and natural gas-based district heating. When energy prices (electricity, natural gas and hydrogen) rise, financially-optimized systems approach the least-emission solution of system design.

Key words: Sustainable Energy, Urban Energy System, No-Regret, Potential Risk, Climate Neutrality, Energy System Modeling

1. Introduction

The 2022 energy crisis in Europe [1] has shown how quickly some of the most relevant parameters for the design of energy systems may change. Compared to the pre-crisis year of 2021, the average wholesale price of electricity in the European Union (EU) has increased by an average of +220 % [2], and the wholesale price of natural gas by +300 % [3], while the natural gas consumption decreased by −10 % [3]. Such changes in system parameters are expected to have a strong effect on energy systems, their design, and their optimization [4].

This study analyzes the impact of aleatory uncertainties [5] on optimized urban energy supply systems. A multi-criteria approach was conducted, optimizing the energy supply of an reference urban energy system for both financial costs and greenhouse gas (GHG) emissions. Subsequently, sensitivity analyses were conducted by re-running the optimization with varying system parameters and examining the changes in investment and dispatch decisions. The focus of the sensitivity analyses lays on uncertainties of energy prices (natural gas, electricity, hydrogen, combined), GHG emissions (total GHG emissions, GHG emissions of imported electricity and hydrogen), various energy demands (electricity, heating), and population density on urban energy systems. The application of a reference case with representative structure with respect to different consumption and energy sectors, as well as investment and dispatch decisions, ensures transferability of the results to other urban energy systems. This especially applies to countries of the European Union which share similar challenges and strategies for energy supply and market structures for energy pricing, driven by decisions of the European Commission [6].

Parameter changes which exert a major impact on urban energy system design will be identified. Specifically, we will analyze which technologies and measures are particularly robust to parameter changes (**no-regret options**) and which are particularly sensitive (**potential-risk options**) in terms of both financial costs and climate protection targets.

Several studies identify no-regret options in terms of financial costs and the achievement of EU climate protection targets. For example, no-regret options for the heating sector include high levels of building renovation [7, 8], (partial) phase-out of natural gas technologies [7] and replacement by electrification technologies [8] such as heat pumps [7], and the use of biofuels [8]. Another no-regret measure is the reduction of heating demand by adjusting consumption patterns, providing absolute savings potential, and enabling both financial and GHG savings

[9]. However, the achievement of full climate neutrality requires the use of technologies such as synthetic hydrocarbons or hydrogen, which are considered to be associated with a higher financial risk [8]. The economic viability of hydrogen technologies in the building sector is only expected at very low prices [10].

This study fills a gap by analyzing not only financial minimization and net-zero boundary conditions, but also the full range in between these competing interests. Furthermore, dependencies on changing external conditions are communicated. The focus is on small-scale urban energy systems, taking into account all local interactions, synergies, and trade-offs of sub-systems and energy sectors. The findings provide a scientific foundation for urban energy system planning, specifically with respect to potential-risk and no-regret measures and technologies.

2. Material and Methods

2.1. Reference Case

Urban energy systems differ strongly from each other with regard to their building structure (e.g., building density or construction year), usage types (e.g., residential, commercial, or industrial), existence of energetic potentials (e.g., geothermal potentials), and many more. Therefore, it is not feasible to define a generally valid reference system. To ensure the highest possible degree of transferability, a real-world energy system (Fig. 1) was chosen as the reference case for this study. It meets numerous pre-defined requirements; it consists of several sub-systems, i.e. buildings of various usage types (residential, commercial, sports facilities, garages), different types of residential buildings with differing population densities, roof orientations, and geothermal potentials. It is assumed that up to three identical adjacent buildings share the same energy supply technologies. These buildings are therefore clustered in the model. The geographical coverage was chosen so that each optimization run could be solved in under 24 hours using the chosen methodology.

The aim of the model is to optimize the energy supply regarding both financial costs and GHG emissions. Various investment and dispatch decisions for several kinds of technologies can be carried out by the model. In the course of this optimization, it is assumed for simplicity that all buildings are in an unrenovated state and that investment costs apply for every technology

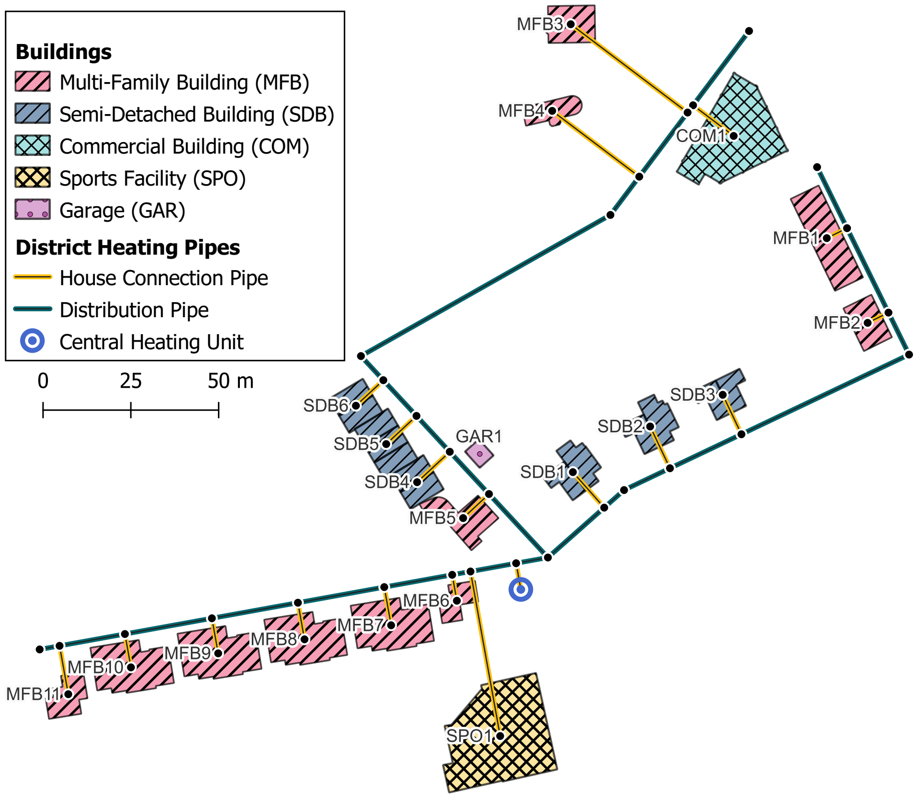

Figure 1: **Reference case area to which the sensitivity analyses were applied.** The shown district heating (DH) pipes corresponds to the position of pipes for which investment decisions could be carried out during the optimization process.

considered. Tab. 1 provides an overview of which technologies and measures can be considered. Electricity, natural gas and hydrogen imports can be carried out as dispatch decision. Financial costs and upstream GHG emissions occuring for the imported energy are taken into account. Electricity produced in individual sub-systems, i.e. buildings or central energy supply units, can either be used internally, transferred to other sub-systems in return for grid fees, or sold/exported to outside the system.

Table 1: **Technologies and measures which were considered for the optimization of the test cases energy supply.** *If photovoltaic (PV) and solar thermal systems may potentially be installed on the same surface, only one of the two technologies will be considered during the optimization.

Technology	Centr.	Decentr.	Technology	Centr.	Decentr.
natural gas heating	x	x	DH network	x	
ashp	x	x	natural gas chpp	x	
gchp		x	electrolysis	x	
electric heating		x	hydrogen chpp (fuel cell)	x	
PV system*		x	methanation	x	
solar thermal system*		x	natural gas storage	x	
battery storage		x	hydrogen storage	x	
wall insulation		x	battery storage	x	x
roof insulation		x	thermal storage	x	x
window insulation		x	sub-system electricity exchange	x	
DH connection		x			

Acronyms: ashp = air source heat pump, centr. = centralized, chpp = combined heat and power plant, decentr. = decentralized, gchp = ground coupled heat pump.

2.2. Model Description

The Spreadsheet Energy System Model Generator (SESMG) [15], a modeling tool based on the Open Energy Modelling Framework (oemof) [16], was used. The Gurobi solver [17] was employed.

Model properties: The applied perfect foresight model used a bottom-up analytical approach and mathematical approaches of linear programming and mixed-integer programming (for DH only) for investment and dispatch optimization. Several energy sectors (electricity, heat, natural gas, hydrogen) and demand sectors (residential, commercial, sports facilities) were covered. A house sharp spatial resolution, a hourly temporal resolution, and a time horizon of one year were applied.

Multi-criteria optimization: The epsilon-constraint method [18] is applied for multi-criteria optimization. Therefore, a primary optimization criterion (financial costs in €) is minimized by the models' solving algorithm. In a second model run, a secondary optimization criterion, GHG emissions in g CO_2-equivalents (in the following just referred to as g), is minimized. To combine both optimization criteria, the secondary optimization criterion is used as a constraint, which is tightened in several model runs until the minimum of the secondary criterion is reached. In consideration of this constraint, the model runs are minimized with respect to the primary criterion. The calculated semi-optimal scenarios act as "best-known Pareto points" and are combined to a "Pareto front" [19]. A reasonable third optimization criterion would be to minimize the effective energy demand [20]. However, demand reductions based on sufficiency measures do not counteract any of the other two optimization criteria and are usually very likely to improve them. Therefore, the reduction of the effective energy demand has not been used as a tertiary optimization criterion, but was separately treated in the sensitivity analysis.

Emissions approach: For the consideration of GHG emissions, the adapted territorial based emissions approach by Klemm and Wiese [20] was considered. All emissions that are caused for the provision of the energy consumed in the system were taken into account, but not for energy exported to neighboring systems.

Model simplification: The applied model is spatially and temporally highly resolved and contains a large number of linear and binary investment decisions. In order to solve this model with the available random-access memory (RAM) and run-time, it was necessary to make some model simplifications. By carrying out temporal simplified pre-models using weekly time-averaging (averaging and merging of ten weeks each), preliminary results were created for each model run ("pre-modeling" [21]). These preliminary results were used to identify technologies that are not profitable at all. Based on this, these technologies were removed from the main-model ("technical pre-selection" [21]). Within the main-model, temporal-slicing [21] considering every fourth day was used.

Data: Weather data from the German Weather Service for the year of 2012 [22], which was an average solar year [23], was used. A detailed description of all system parameters as well as how the individual components in the system are connected to each other is given in Appendix A. Due to the European energy crisis, energy prices were subject to strong fluctuations at the time this study was carried out. Pre-crisis values were therefore used for the entire model to take account of a settled market situation with regular ratios and proportions.

2.3. Sensitivity Analysis

Emerging uncertainties can be categorized into aleatory and epistemic uncertainties [5]. Epistemic uncertainties can be avoided by improving the model quality through the use of additional data (parametric uncertainties) or by refining the model (structural uncertainties) [24].

Improving the model quality is the only way of quantifying epistemic uncertainties [4]. Aleatory uncertainties cannot be reduced by improved model quality [5], yet they can be quantified by deterministic or stochastic approaches [24]. Within this study, the deterministic approach of sensitivity analysis was applied. This approach enables the identification of "critical model features that lead to important changes" [24] in system design and furthermore to "extract insights that are robust to" [24] changing system conditions. These insights can be used to better define system design with regard to changing key system parameters.

The financially-optimized energy supply scenario and the GHG emission-optimized supply scenario were calculated and used as reference scenarios for the sensitivity analyses. Several gradations were applied for each sensitivity parameter. For each of these gradations, a new optimization run was performed and thus an adjusted energy supply scenario was calculated. A total of 10 sensitvitiy analyses were applied, which can be divided into three categories:

- GHG emissions
  - total GHG emissions
  - GHG emissions of imported electricity
  - GHG emissions of imported hydrogen
- financial costs
  - natural gas price
  - electricity price
  - hydrogen price
  - combined energy price
- effective energy demands
  - electricity demand
  - heating demand
  - population density

For the variation of restrictions regarding the **total GHG emissions**, the epsilon-constraint method (see above) was applied to calculate a financially-optimized scenario (0 % GHG reduction), an emission-optimized scenario (100 % GHG reduction), and nine further scenarios in 10 % GHG reduction steps in-between. The financially-optimized and emission-optimized scenarios form the reference cases for the further sensitivity analyses

The average GHG emissions of the German electricity mix, considered as the **GHG emissions of imported electricity**, were initially varied in six gradations (0, 50, 75, 125, 150 and 200 %) and supplemented by a further gradation (25 %) for a more precise resolution.

Typical GHG emissions of green hydrogen were considered in the reference case for the **GHG emissions of imported hydrogen**. This value was initially varied in six gradations (0, 50, 75, 200, 500, and 1 000 %) and supplemented by two further gradation (300 and 400 %) for a more precise resolution.

The individual energy **prices of natural gas, electricity and hydrogen** were varied in six gradations (0, 50, 75, 200, 500, and 1 000 %) deviating from the respective reference value. As the interactions between the prices of individual energy forms are particularly strong [25], the prices have been varied together (combined energy prices). Therefore, it was assumed that the costs for the import of all energy carriers vary linearly with the same gradations as above.

The individual **electricity demand** as well as the **heating demand** for every individual building based on consumption behavior was varied in six gradations (0, 50, 75, 125, 150 and 200 %) deviating from the respective reference values.

The **population density** was varied by the number of inhabitants per housing unit in six gradations (0, 50, 75, 125, 150 and 200 %) deviating from the reference case. The number of inhabitants was rounded to integer numbers or zero for each housing unit.

3. Results

3.1. Reference Case and Impact of GHG Reduction Goals

The Pareto front in Fig. 2 includes the financially-optimized scenario, the GHG emission-optimized scenario, and nine further Pareto scenarios in between. A reduction of GHG emissions by −93 % may be realized compared to the financially-optimized case, but a reduction to zero is not possible due to life-cycle emissions of technical facilities.

Within the **financially-optimized scenario**, the heat supply is primarily based on (centralized) natural gas technologies, and the electricity is supplied by a heat-driven natural gas

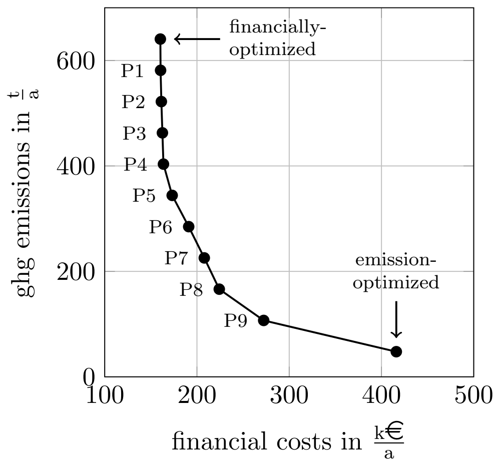

Figure 2: **Pareto front composed of optimized energy systems for an urban district with different weighting of primary (financial costs) and secondary (GHG emissions) optimization criteria.** The financially-optimized scenario causes financial costs of 160 k€/a and annual GHG emissions of 641 t/a. Starting from there, up to the P4 scenario a significant reduction in emissions (−37 %) with only a slight increase in financial costs (+2 %) is enabled. From P5 on, the additional costs increase more, with the largest increase occurring between P9 and the emission-optimized scenario. The emission-optimized scenario enables a significant reduction of GHG emissions to 48 t/a (−93 %), but also increased financial costs of 416 k€/a (+160 %).

combined heat and power plant (CHPP), as well as PV systems (Fig. 3). The net internal electricity production exceeds the electricity demand; therefore, large shares are exported. However, electricity still needs to be imported in small quantities at times when the internal production is insufficient.

With **decreasing total GHG emissions**, the heat supply is progressively decentralized. At the same time, the heating demand is reduced due to building insulation, and electricity demand increases due to electrification of the heat supply. In P5 and P6, flexible electricity supply is low while the heating demand is met by heat pumps that are adjusted to the load profiles of PV systems. Thermal storages are utilized more frequently, although not with a higher capacity than in other scenarios, to match heat supply with consumption. As the GHG emissions constraint increases, the natural gas CHPP production is designed to zero in P7, and the electricity demand increases to its maximum in P9 due to heat pump usage. In scenarios P6 through P9, major shares of electricity are imported. In the emission-optimized scenario, battery storages and hydrogen CHPP are considered instead. P9 is the only scenario, where a combination of electrolysis and hydrogen storage are used for electric load shifting.

In the **emission-optimized scenario**, the remaining heating demand of maximum possible insulated buildings is provided by air source heat pumps (ASHPs), ground coupled heat pumps (GCHPs) and solar thermal systems. Decentralized ASHPs are preferred over centralized ones, as heat losses (about 8 %) and life-cycle emissions for the construction of DH pipes are thus avoided. PV systems, hydrogen, and CHPP are used for electricity supply and battery storages for load shifting. The PV potential is not fully utilized in any of the scenarios, especially with respect to PV modules deviating more than 65° from the south axis. Solar thermal systems were only considered in the emission-optimized scenario on surfaces without PV potential.

3.2. Sensitivity: GHG Emissions of Imported Energy

Within two individual sensitivity analyses, the GHG emissions of (1) imported electricity and (2) imported hydrogen between 0 % and 200 %, respectively 1 000 %, of the reference values.

In the **financially-optimized scenario**, varying the GHG emissions of imported electricity (Appendix C) and hydrogen (Appendix D) has no effect on investment or dispatch decisions, as no financial parameters are changed. However, absolute GHG emissions are reduced, corresponding to the extent of respective energy imports.

Within the **emission-optimized scenario**, the import of electricity and the use of hydrogen CHPP for electricity supply are in direct competition (Appendix C and D). Electricity imports increase in emission-optimized scenarios when the GHG emissions of imported electricity (reference 366 g/kWh) drops below the footprint of electricity supplied by the hydrogen CHPP (120 g/kWh in the reference case) or even by PV systems (27 g/kWh). The hydrogen CHPP is applied within the optimization for GHG emissions of imported hydrogen up to 132 g/kWh (reference 44 g/kWh). However, if non-green hydrogen is imported, electricity imports are preferred over the hydrogen CHPP (this includes when the imported electricity is used for hydrogen production). The heat supply, apart from the cases of emissions-neutral imports of electricity or hydrogen, remains unchanged.

3.3. Sensitivity: Energy Prices

Within four individual sensitivity analyses, the prices for (1) natural gas, (2) electricity, (3) hydrogen, and (4) all together (combined energy prices) were varied between 0 % and 1 000 % of the respective reference values.

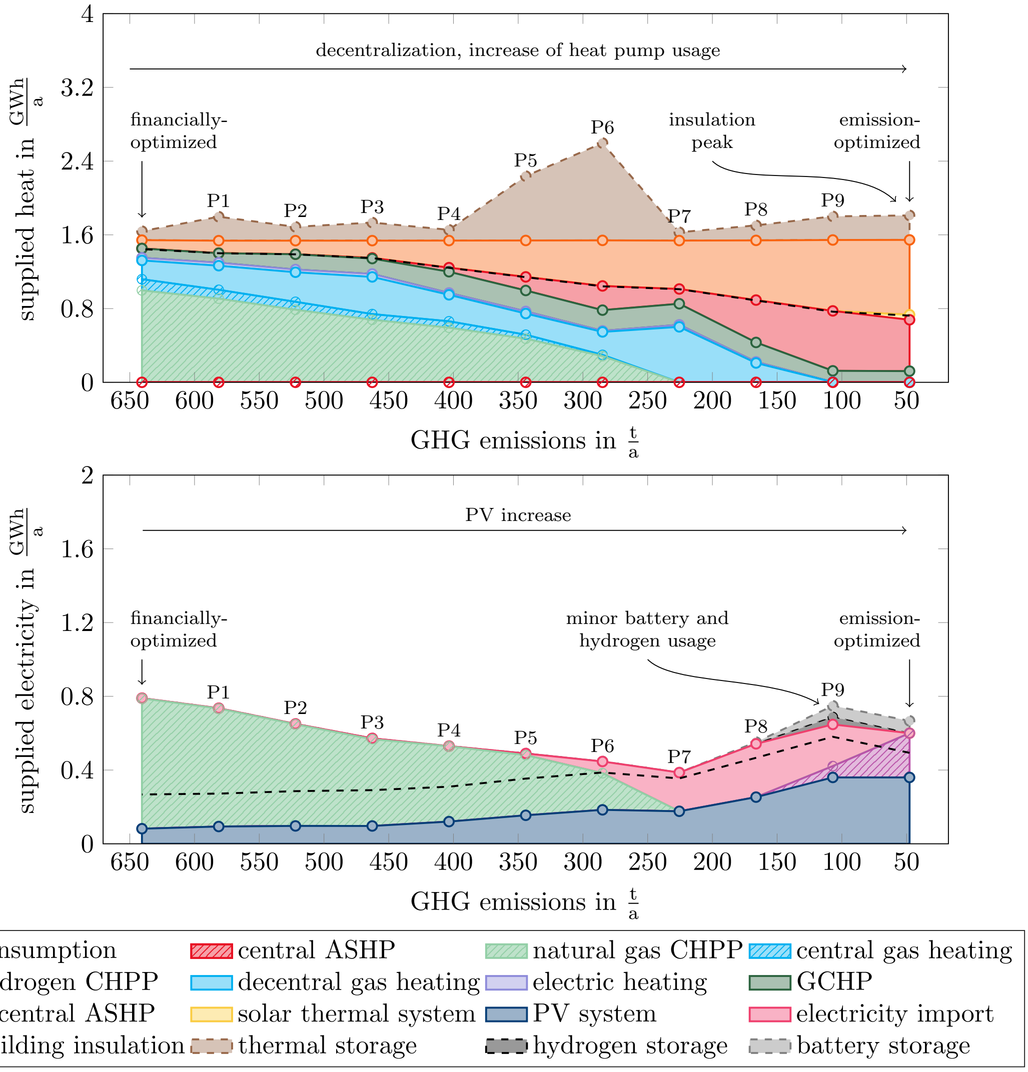

Figure 3: **Heat (top) and electricity (bottom) supply in the optimized reference case scenario in dependency on total GHG emissions.** In the financially-optimized case, the heat supply is primarily based on natural gas with a major share (13/19 buildings) of centralized heat supply. Building insulation (reducing the heating demand by 6 %), GCHPs (7 % of the heating demand), and electric heating (2 % of the heating demand) technologies are less important. In the emission-optimized case, the maximum possible building insulation enables a reduction of heating demand by −53 %, the remaining heating demand being covered by heat pumps (76 % ASHPs and 17 % GCHPs) and solar thermal systems (7 %). Electricity is supplied by PV systems (0.36 GWh/a) and a central hydrogen CHPP (operated purely electrically, 0.24 GWh/a) in combination with battery storages (0.07 GWh/a). Further results are presented in Appendix B.

The comparison of the effects of changes in combined energy prices (Fig. 4) with those in individual energy prices shows that the effect of changing natural gas prices (Appendix E) dominates the **financially-optimized scenario**. The centralized natural gas technologies have their maximum viability between 75 % and 100 % of the reference case. At higher natural gas prices, reduced CHPP capacities lead to higher shares of PV systems and electricity imports. However, the increase in electricity prices (Appendix F) has a damping effect on this trend, and even at 1 000 % of the reference combined energy prices, four buildings remain connected to the natural gas-based DH network. Reduced CHPP electricity supply is replaced by increased PV usage, small battery storages, and (only in the case of 1000 % combined energy prices) a hydrogen CHPP. In scenarios with the least internal electricity production, thermal storages

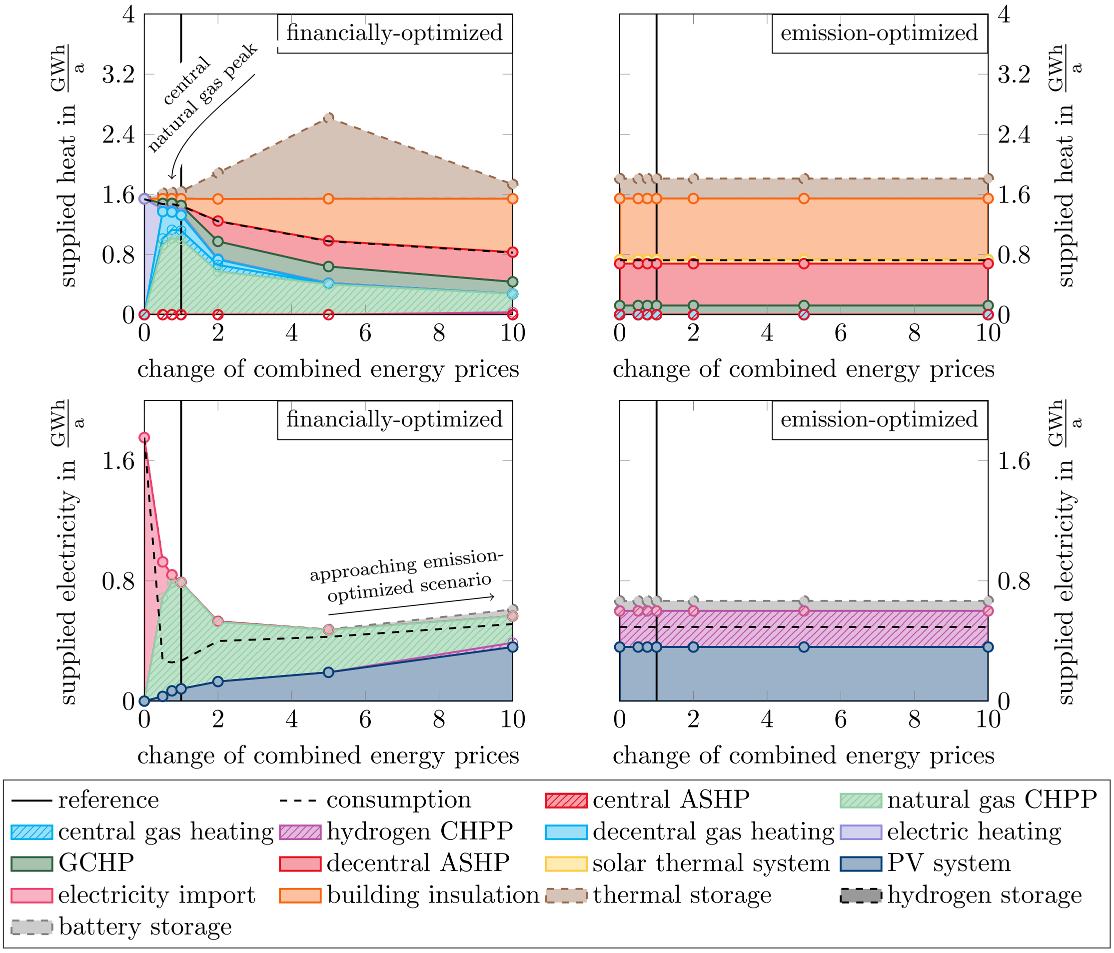

Figure 4: **Supplied heat (top) and electricity (bottom) in the financially- (left) and emission-optimized (right) reference case in dependency on changing combined energy prices.** The financially-optimized reference case corresponds to the maximum of natural gas-based central heat supply with 13 out of 19 buildings being connected and a heat supply share of 84 %. With energy prices ten times higher than the reference case, energy is supplied with building insulation (reducing demands by −46 %), thermal storages (shifting 23 %), GCHP (supplying 19 %), ASHP (48 %), natural gas CHPP (30 %), and hydrogen CHPP (4 %) for heat supply and PV systems (supply of 73 % of the internal demand with additional export of temporal surpluses), natural gas CHPP (34 %), hydrogen CHPP (6 %) and battery storages (shifting 9 %) for electricity supply. Further results of the sensitivity of combined energy prices are visualized in Appendix H. Results for individual variations of natural gas, electricity and hydrogen are shown in Appendices E, F, and G.

are again utilized more intensively by increasing storage frequency. Overall, with an increase of combined energy prices, the energy supply moves towards the emission-optimized scenario.

The usage of PV systems is replaced when electricity prices decrease below the production costs of PV (0.08−0.14 €/kWh, depending on orientation). For the hypothetical scenario of all energy prices decreasing to near-zero, the electricity price has a dominant effect and the use of electric heating systems for heat supply rises sharply shortly before the case of a cost-free energy.

The **emission-optimized scenario** is not affected, because changes in energy prices do not affect the minimization of GHG emissions within the applied model.

3.4. Sensitivity: Energy Demands

Within two individual sensitivity analyses, the (1) electricity demand and the (2) heating demands have been varied between 0 % and 200 % of the respective reference values.

Changing electricity demands (Appendix I) only affects the electricity supply, not the heat supply. The influence is limited primarily to the dimensioning of PV systems in the **financially-optimized scenario** and to hydrogen CHPP and battery storages in the **emission-optimized scenario**. If the behavioral based electricity demand is reduced to zero, the absolute electricity demand and thus the electricity supply has an offset which is caused by the electrified heat supply.

Changes in heating demand (Fig. 5) based on consumption behavior affect optimization for both heat and electricity supply. In the **financially-optimized scenario**, with decreasing heating demand, the shares of insulation, GCHPs, and decentralized gas heating systems increase. As soon as the electricity production through heat driven natural gas CHPP in combination with PV systems cannot meet the electricity demand from a certain state on, electricity imports increase. With increasing heating demand, the profitability of natural gas-based central heating supply increases due to increased spatial density of heating demands and more buildings being connected to the DH network. In the **emission-optimized scenario**, the usage of ASHP, GCHP, solar thermal systems, and thermal storages changes linearly with heating demand. The usage of hydrogen CHPP changes linearly for heating demands above 50 % of the reference value, due to the sector coupled system. Below this value, the system remains unchanged and

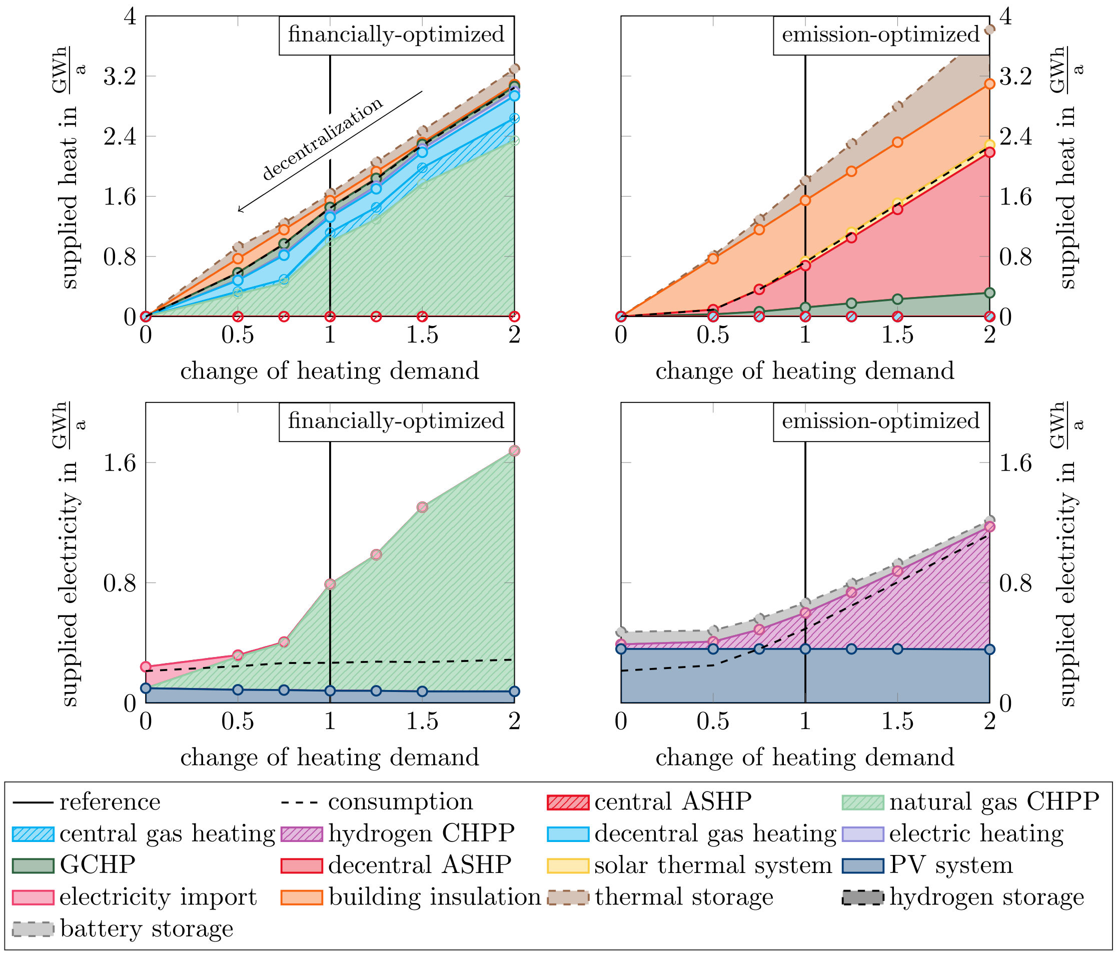

Figure 5: **Supplied heat (top) and electricity (bottom) in the financially- (left) and emission-optimized (right) reference case in dependency on changing heating demands.** In the financially-optimized scenario, the heat is primarily supplied by natural gas regardless of the heating demand, but the number of buildings connected to the DH network varies from five (at a maximum of 75 % of the reference heating demand) to 16 buildings (at a minimum of 150 % of the reference heating demand). At the same time, with higher heating demand based on consumption behavior, less insulation is considered, because the viability of natural gas-based central heat supply increases. In all emission-optimized scenarios apart 0 % heating demand, the maximum possible building insulation is used. The use of the considered supply technologies (ASHP, GCHP, solar thermal systems, and thermal storage) changes linearly with heating demand. Further results of the sensitivity of heating demands based on consumption behavior are visualized in Appendix J.

PV systems relatively dominate. As the heating demand increases, flexibility is mostly provided by increased thermal storages, leading to reduced battery storage usage.

Both reductions of electricity and heating demands enable a significant reduction in financial costs and GHG emissions. However, the reduction of the heating demand has a larger impact since it makes up a larger share on total energy demand.

3.5. Sensitivity: Population Density

Within this sensitivity analysis, the population density was varied between 0 % and 200 % of the respective reference values.

The population density primarily influences the absolute electricity demand (Appendix K) for both financially and emission-optimized scenarios. Therefore, the system design is rather robust against changes in population density. However, the specific energy supply per inhabitant changes significantly (Fig. 6), and the relative impact on both specific financial costs and GHG emissions is enormous.

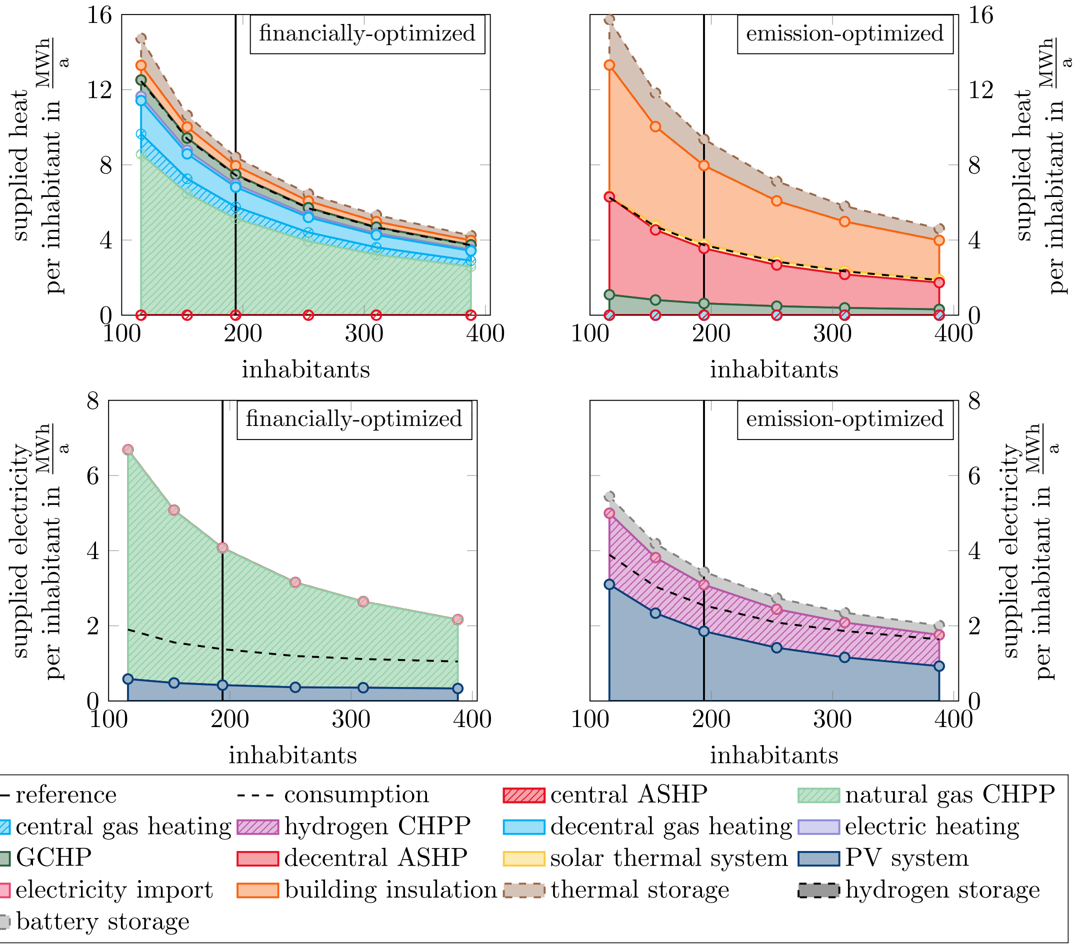

Figure 6: **Supplied heat (top) and electricity (bottom) per inhabitant in the financially (left) and emission-optimized (right) reference case in dependency on changing population density.** The curves are not linear, since the energy demand of non-residential buildings remains unchanged as a base demand. The change in population density has limited impact on the absolute optimized energy supply. Mainly the absolute use of PV systems in the financially-optimized case and hydrogen CHPP in the emission-optimized case change, but the specific use per inhabitant remains rather constant. Further results of the sensitivity of population density are visualized in Appendix K.

4. Discussion

4.1. Potential-Risk and No-Regret Options

The analysis showed that the level of system's permitted GHG emissions, the price of imported energy, especially natural gas, as well as absolute heat and electricity demands have the highest influence on the design of optimized urban energy systems. Measures and technologies for optimizing urban energy systems can be considered as **no-regret options** if the sensitivity analyses of this study have proven their suitability for both financial and emissions-based optimization and if they are robust to parameter changes. Expected trends such as GHG mitigation requirements, rising energy prices, or declining GHG emissions from imported electricity are particularly relevant. Measures and technologies that are particularly sensitive to these changes can be considered as **potential-risk options**.

The implementation of **building insulation** is a no-regret strategy for financially-optimized decarbonisation of urban energy systems. The optimal amount of building insulation used in a system is subject to trends of energy prices, requested reductions in total GHG emissions, and trends of energy demands, and will yet more likely increase than decrease under any predictable future scenarios. The obvious positive climate effect may be diminished by a high climate intensity of the material used for insulation. Reducing energy demands (heat and electricity) by **behavioral and structural changes** is a no-regret measure with regard to reducing both financial costs and GHG emissions. It is expected that the mix of supply options will remain largely unchanged, while the sizing of the technologies will change in response to demand. Only the share of central heating, which is dependent on the spatial density of heating demands, decreases with demand reductions. Reduction of **living space per inhabitant** by adapting the population density is a no-regret strategy, as both financial costs and GHG emissions per inhabitant are reduced while the design of optimized systems remains largely unchanged.

The use of **decentralized natural gas technologies** for heat supply is very sensitive to the analyzed system changes, and their usage is therefore a clear potential-risk option. With respect to predictable trends such as increasing total GHG emissions mitigation requirements and energy prices, their usage is partially or even completely reduced in optimized scenarios. The usage of **decentralized heat pumps** for heat supply in turn steadily increases or at least remains at the same level. As far as heat potentials can be used both central and decentral, decentralized heat pumps allow a more viable use compared to centralized heat pumps due to less heat losses, investment costs, and life-cycle emissions of DH pipes. The usage of heat pumps, especially decentralized ones, is therefore a clear no-regret option.

The viability of implementing new **DH networks** is very sensitive on total GHG emissions, energy prices, and heating demands. Therefore, the exact connectability of buildings to DH networks should be analyzed in detail and be planned with caution. The generalized implementation of DH networks for entire areas, for example, in the context of a connection obligation, carries a high potential-risk.

The optimum size of the **PV systems** varies, but a certain amount with a region-specific maximum azimuth deviation from the south axis is highly robust. This maximum azimuth deviation increases with additional restrictions on total GHG emissions and increasing energy prices. PV systems within the acceptable deviation are no-regret technologies. However, using **solar thermal systems** on surfaces where viable PV usage is an option is a possible-risk option. The usage of PV systems is superior to solar thermal systems with regard to both financial cost and GHG emission reduction.

Exchanging electricity with higher-level energy systems by exporting electricity surpluses and importing deficits is a no-regret strategy, which was applied in each of the optimized scenarios examined. It reduces the need for local electricity storage capacities and oversized plants to meet peak loads. However, this approach may be limited due to transmission capacities and the ability of neighboring and higher-level systems to provide the necessary load exchange. For emission optimized systems, the GHG emissions of imported electricity must furthermore be comparable to or lower than internal electricity production. Fewer restrictions apply to the **local exchange** of locally produced (renewable) electricity between sub-systems. It is a no-regret strategy which reduces necessary storage capacities and, by avoiding electricity imports, financial costs and GHG emissions.

As long as such local exchange of electricity between sub-systems is possible, **battery storages** are only suitable for certain cases of total GHG emission minimization, but not for financial optimization at all. Their usage in optimized systems is furthermore sensitive on GHG emissions of imported energy (electricity and hydrogen) and the system's energy demands (electricity and heat). In combination with the conflict with the robust measures of electricity exchange on various levels, the implementation of large battery storages thus carries a potential-risk. Due to lower life cycle GHG emissions, **thermal storage systems** are more robust for shifting volatile electricity supply with regard to system changes, especially in the case of electrified heat supplies. Depending on the type of heat supply, either centralized or decentralized thermal storage for electric load shifting is therefore a no-regret option.

Green **hydrogen-powered CHPP** is not viable from a financial perspective. It is especially sensitive to the system's absolute energy demands, and its capability for emission reduction is only viable if GHG emissions of imported electricity are higher than electricity supplied by the hydrogen CHPP. The use of hydrogen is therefore a potential-risk option, and the use of non-green hydrogen is no option for system optimization at all.

4.2. Transferability

The results of this study are particularly applicable to urban energy systems in EU member states, especially for western and central Europe, based on the characteristics of market structures, transition goals [6], climate conditions, consumption structures, and energetic potentials [11, 12, 13]. In a wider perspective, statements on (1) decisions between centralized and decentralized energy supply, (2) the requirement of sector-coupling, (3) the relationship between (non-)flexible energy provision and storage facilities, (4) the interaction between (sub-)systems for energy exchange, (5) the interaction between strategies of efficiency, consistency, and sufficiency for fulfilling sustainability goals, as well as (6) the identification of GHG reduction potentials at low financial costs are expected to be widely transferable independently of differing input conditions of other regions.

Although market structures are comparable in the mentioned regions, absolute energy prices may differ significantly. For instance, electricity prices for households are +75 % higher in Denmark and −60 % lower in France than in Germany (end of 2022, [14]). It can, however, be assumed that similar sensitivity effects occur, although they shift horizontally along the price scale. For example, there is also a maximum profitability of natural gas supported central heat supply (Fig. 4) if natural gas prices are lower than in Germany; it just requires a higher relative price increase for it to be exceeded.

To maintain transparency, all model parameters are accessible (Appendix A).

5. Conclusion

The analysis on design of financially- and emission-optimized urban energy systems has identified the following **no-regret options**, which are robust against external drivers such as changing energy prices and GHG emissions of imported energy:

- reducing **relative and absolute energy demands** by behavioral and structural changes, building insulation, and reducing living space per inhabitant
- preferred use of **decentralized heat pumps** for heat supply
- using **PV systems** on surfaces with suitable orientations
- using **thermal storages** for electric load shifting
- enabling **electricity exchange** both between sub-systems and with higher-level energy systems

On the other hand, the following **potential-risk options** are particularly sensitive to changes in permitted GHG emissions, the price of imported energy, especially natural gas, as well as absolute heat and electricity demands:

- using **solar thermal systems** on surfaces which are suitable for PV usage
- **decentralized natural gas** technologies for heat supply
- generalized implementation of **district heating (dh) networks**
- using **high capacities of battery storages**
- **hydrogen** for building energy supply

In order to be prepared for constant system changes in predictable trends, but also for sudden changes, for example in the context of a renewed energy crisis, it is advisable to focus on the mentioned no-regret options and to avoid the possible-risk options when planning urban energy systems. While those pathways are generalizable, detailed analyses of individual urban systems, taking into account all relevant energy sectors, demands and potentials to consider all area-specific synergies, financial constraints and GHG reduction targets are essential.

Furthermore, specific framework conditions that influence energy system planning but go beyond the scope of energy system modeling (like resource use, quality of living) might shift the focus in respective municipalities and thus the preferred supply options.

Acronyms

ASHP air source heat pump

CHPP combined heat and power plant

DH district heating

EU European Union

GCHP ground coupled heat pump

GHG greenhouse gas

oemof Open Energy Modelling Framework

PV photovoltaic

RAM random-access memory

SESMG Spreadsheet Energy System Model Generator

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Appendix

A. Model Parameters

The model is subject to the common problem in energy system modeling of uncertainty of input data [4, 24, 26]. The applied configuration of model-based methods for reducing computing requirements have led, in past studies, to underestimation of the viability of heat pumps and PV systems [21]. Therefore, their role as no-regret decisions may even have been underestimated in the presented analysis. The viability of battery storages has been underestimated in the past as well [21]. The fundamental decision whether a battery storage should be used or not is unaffected, but the question of what capacity to use is affected [21]. Therefore, the decision between thermal and battery storage is not affected and the recommendations derived remain valid.

All parameters and modeling methods used for this study are openly available within the following directories:

- Description of the model structure and all modeling parameters: `https://doi.org/10.5281/zenodo.7896185`
- Applied version of the Spreadsheet Energy System Model Generator (SESMG): `https://doi.org/10.5281/zenodo.8055828`
- SESMG model definitions: `https://doi.org/10.5281/zenodo.8042239`
- SESMG model results: `https://doi.org/10.5281/zenodo.8046254`

B. Results: Reference / GHG emissions

Table 2: **Optimized technology capacities in the reference case in dependency on total GHG emissions.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	decentral GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
P1	116	91	0	0	0	0	0	112	81	82	0	20	585	0	0	11
P2	100	90	0	0	0	0	0	95	104	84	0	30	628	0	0	8
P3	86	64	0	0	0	0	0	99	127	84	2	29	608	0	0	6
P4	74	92	0	0	0	0	0	43	105	105	11	45	668	0	0	5
P5	61	55	0	0	0	0	0	51	91	134	30	54	682	0	0	4
P6	39	27	0	0	0	0	0	17	124	158	55	54	734	0	0	3
P7	0	0	0	0	0	0	0	32	200	151	49	54	566	0	0	0
P8	0	0	0	0	0	0	0	23	123	216	100	50	728	33	0	0
P9	0	0	0	10	26	0	0	29	2	295	201	28	1392	222	236	0
EO	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

C. Results: GHG Emissions of Imported Electricity

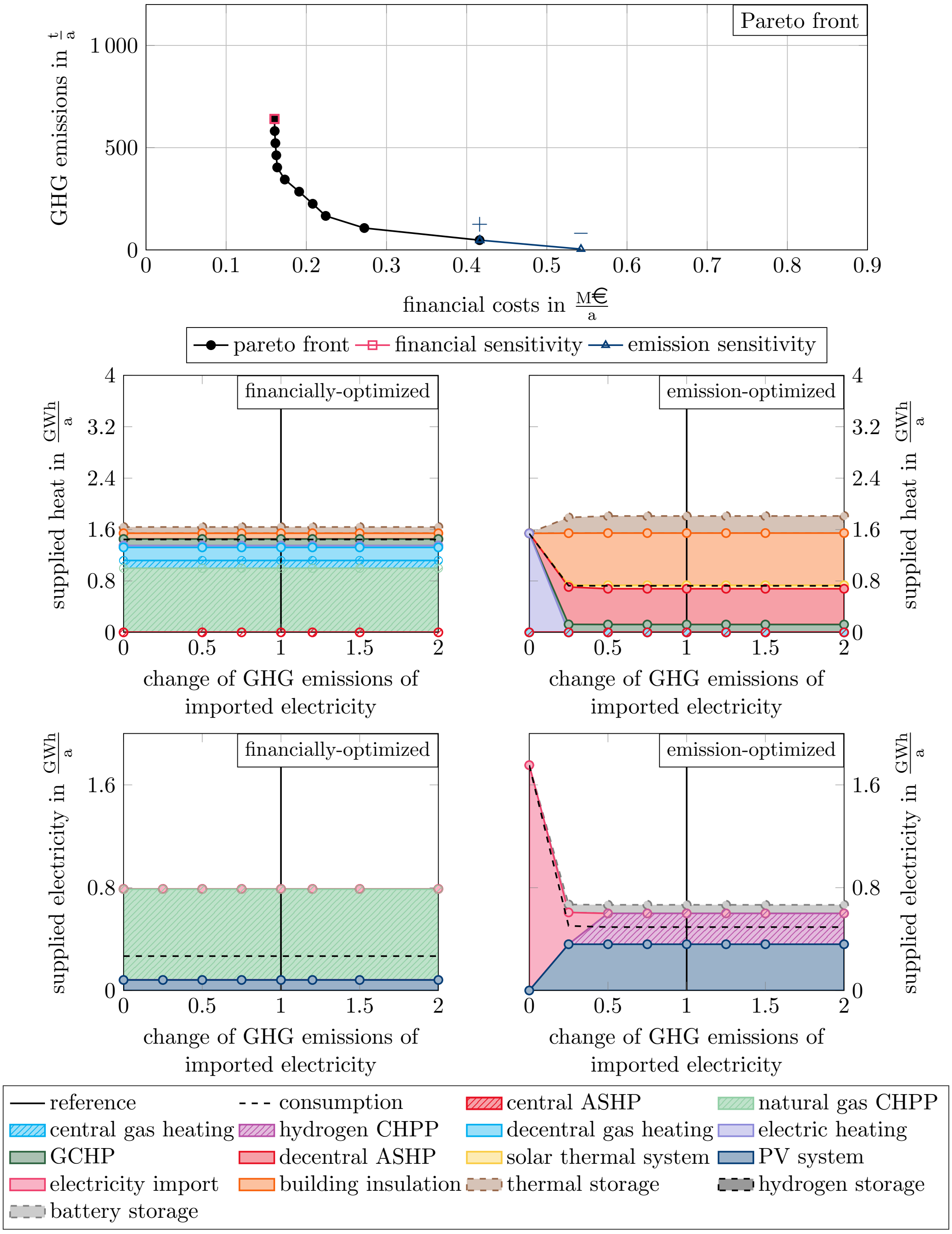

Figure 7: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (GHG emissions of imported electricity). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "−", the highest as "+". In the emission-optimized case the scenarios including 25 %, 50 %, 100 %, 125 %, 150 %, and 200 % lie on top of each other. **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 3: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of GHG emissions of imported electricity.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-0.25	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-0.5	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-0.75	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.2	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.5	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-2.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
EO-0.0	0	0	0	0	0	0	0	532	0	0	0	0	393	0	0	0
EO-0.25	0	0	0	0	0	0	29	0	0	295	200	28	1378	316	0	0
EO-0.5	0	0	0	185	0	0	56	0	0	295	218	28	1654	347	0	0
EO-0.75	0	0	0	185	0	0	56	0	0	295	218	28	1654	348	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.25	0	0	0	185	0	0	56	0	0	295	218	28	1654	347	0	0
EO-1.5	0	0	0	185	0	0	56	0	0	295	218	28	1654	346	0	0
EO-2.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	347	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

D. Results: GHG Emissions of Imported Hydrogen

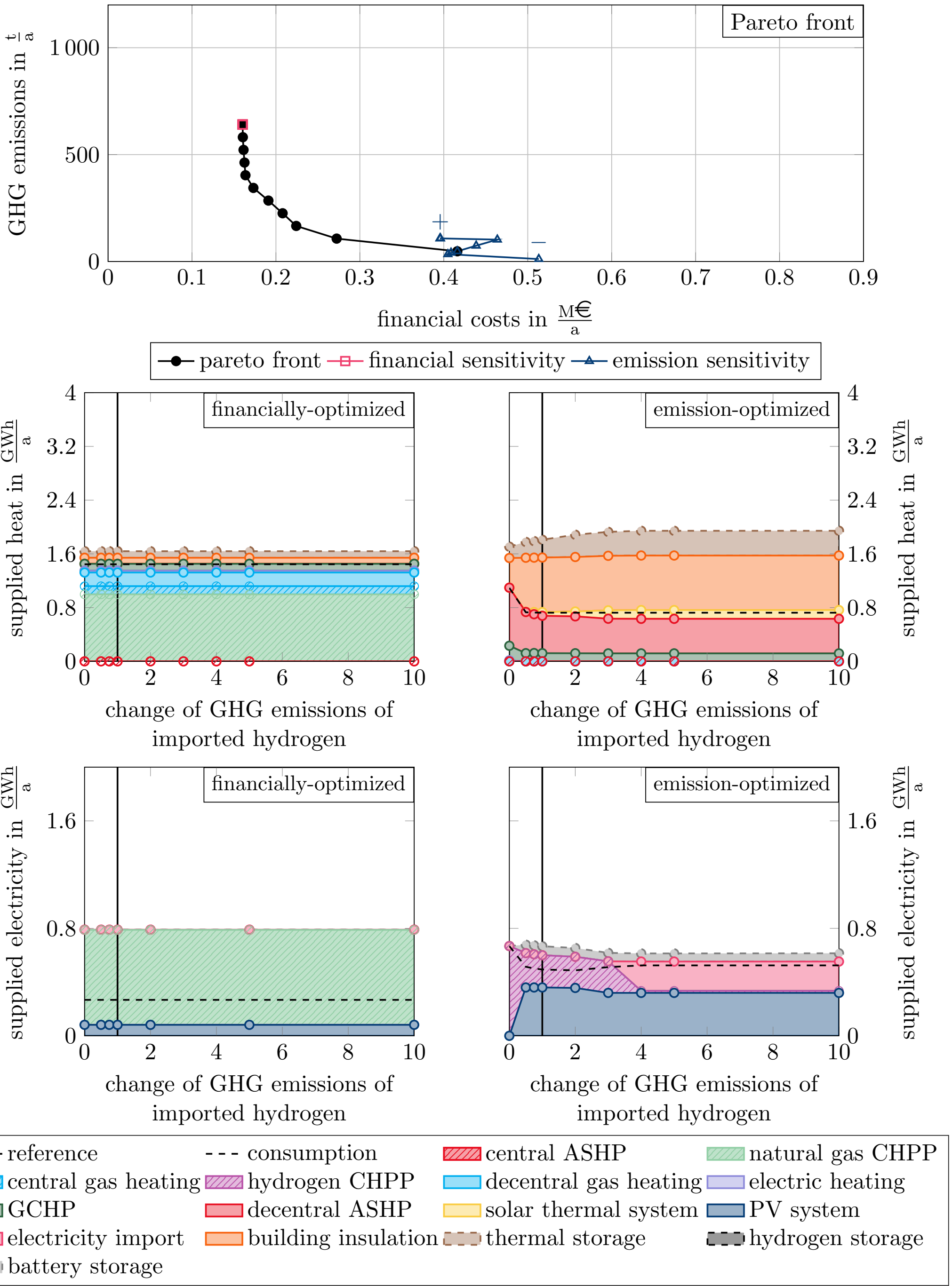

Figure 8: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (GHG emissions of imported hydrogen). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "−", the highest as "+". In the emission-optimized case the scenarios 400 %, 500 %, and 1 000 % lie on top of each other. **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 4: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of GHG emissions of imported hydrogen.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-0.5	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-0.75	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-2.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-3.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-4.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-5.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-10.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
EO-0.0	0	0	0	286	0	0	0	73	0	0	243	52	422	0	0	0
EO-0.5	0	0	0	168	0	0	2	0	0	295	196	28	1160	311	0	0
EO-0.75	0	0	0	172	0	0	33	0	0	295	202	28	1403	337	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-2.0	0	0	0	207	62	0	73	62	0	292	286	28	3131	328	167	0
EO-3.0	0	0	0	207	160	0	126	160	0	265	299	28	5962	326	7455	0
EO-4.0	0	0	0	157	160	0	132	160	0	265	320	28	6620	321	9999	0
EO-5.0	0	0	0	157	160	0	132	160	0	265	320	28	6620	321	9999	0
EO-10.0	0	0	0	157	160	0	132	160	0	265	320	28	6620	325	9999	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

E. Results: Natural Gas Price

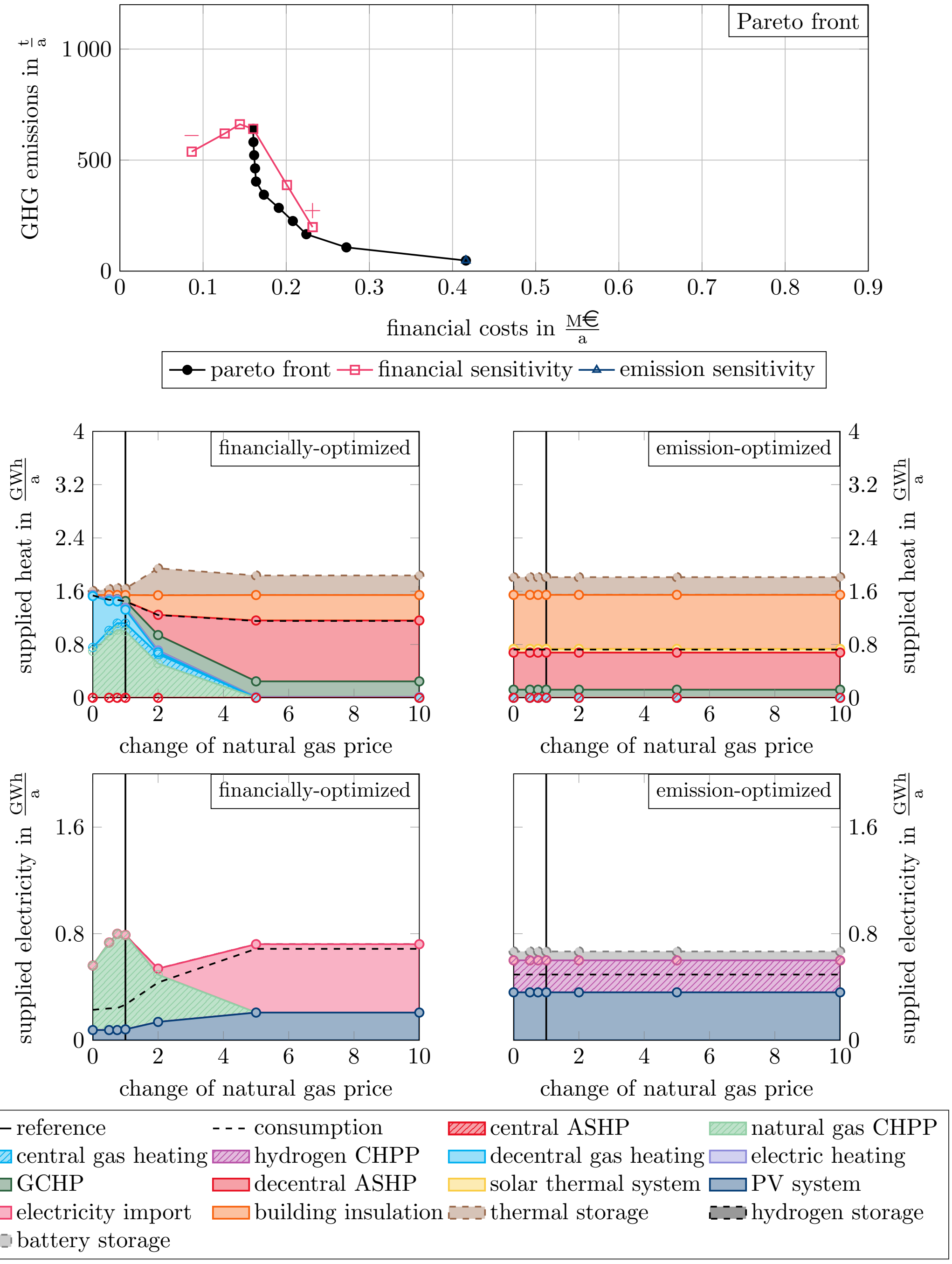

Figure 9: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (natural gas price). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "–", the highest as "+". In the financially-optimized case the scenarios 500 % and 1 000 % lie on top of each other. **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 5: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of natural gas prices.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	92	96	0	0	0	0	0	73	207	65	0	0	753	0	0	6
FO-0.5	121	81	0	0	0	0	0	116	119	66	0	0	710	0	0	11
FO-0.75	131	97	0	0	0	0	0	121	87	66	0	2	638	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-2.0	57	97	0	0	0	0	0	88	12	121	78	49	657	0	0	6
FO-5.0	0	0	0	0	0	0	0	37	0	176	272	55	1072	0	0	0
FO-10.0	0	0	0	0	0	0	0	37	0	176	272	55	1072	0	0	0
EM-0.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EM-0.5	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EM-0.75	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EM-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EM-2.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EM-5.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EM-10.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

F. Results: Electricity Price

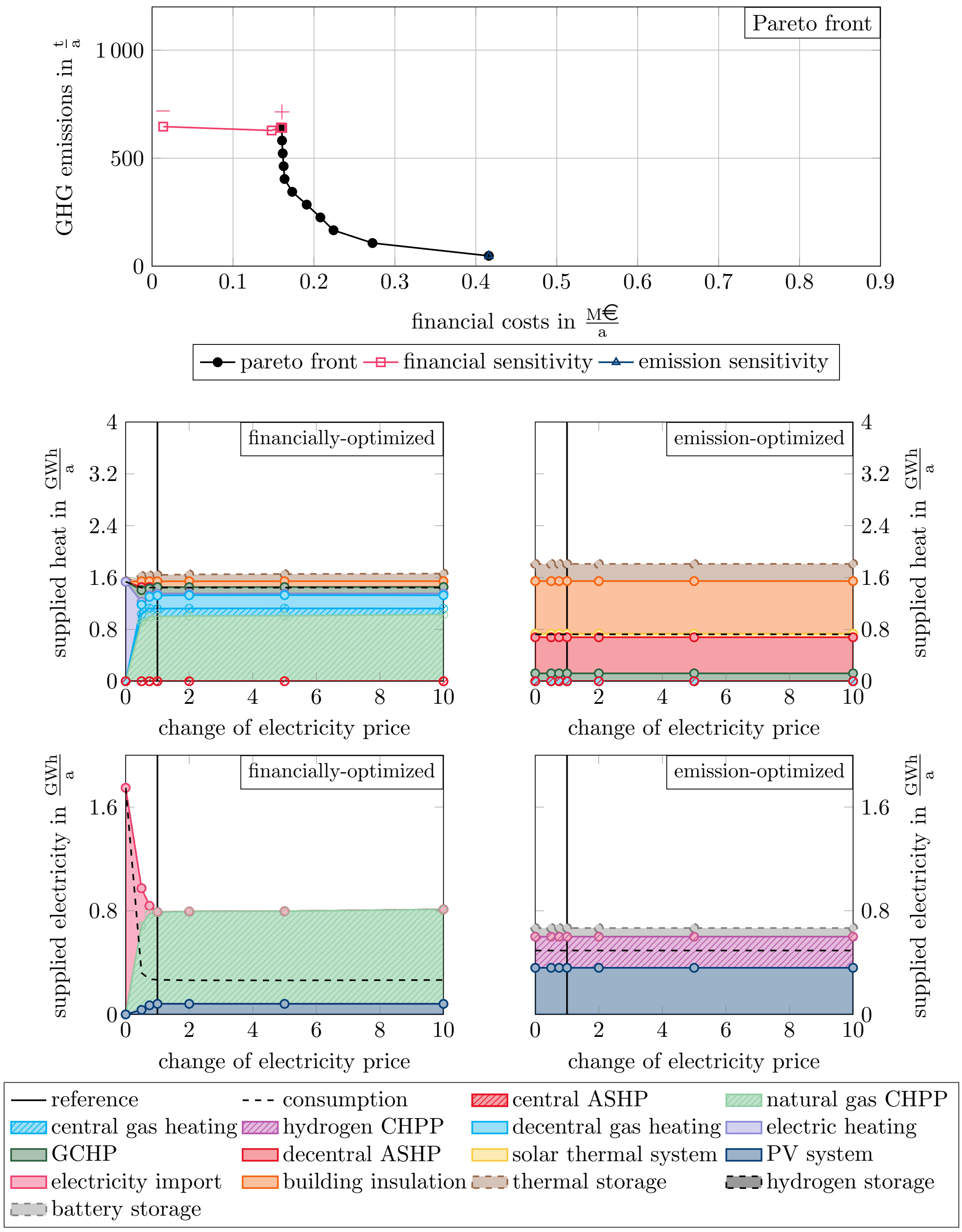

Figure 10: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (electricity price). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "–", the highest as "+". In the financially-optimized case the scenarios 75 %, 100 %, 200 %, 500 %, and 1 000 % lie on top of each other. **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 6: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of electrcity prices.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	0	0	0	0	0	0	0	539	0	0	0	0	340	0	0	0
FO-0.5	114	111	0	0	0	0	0	127	42	34	6	34	648	0	0	12
FO-0.75	123	131	0	0	0	0	0	94	56	62	3	19	697	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-2.0	127	117	0	0	0	0	0	100	66	70	0	17	662	0	0	13
FO-5.0	128	116	0	0	0	0	0	99	66	70	0	17	703	0	0	13
FO-10.0	134	94	0	0	0	0	0	111	67	70	0	17	739	0	0	13
EO-0.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-0.5	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-0.75	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-2.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-5.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-10.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

G. Results: Hydrogen Price

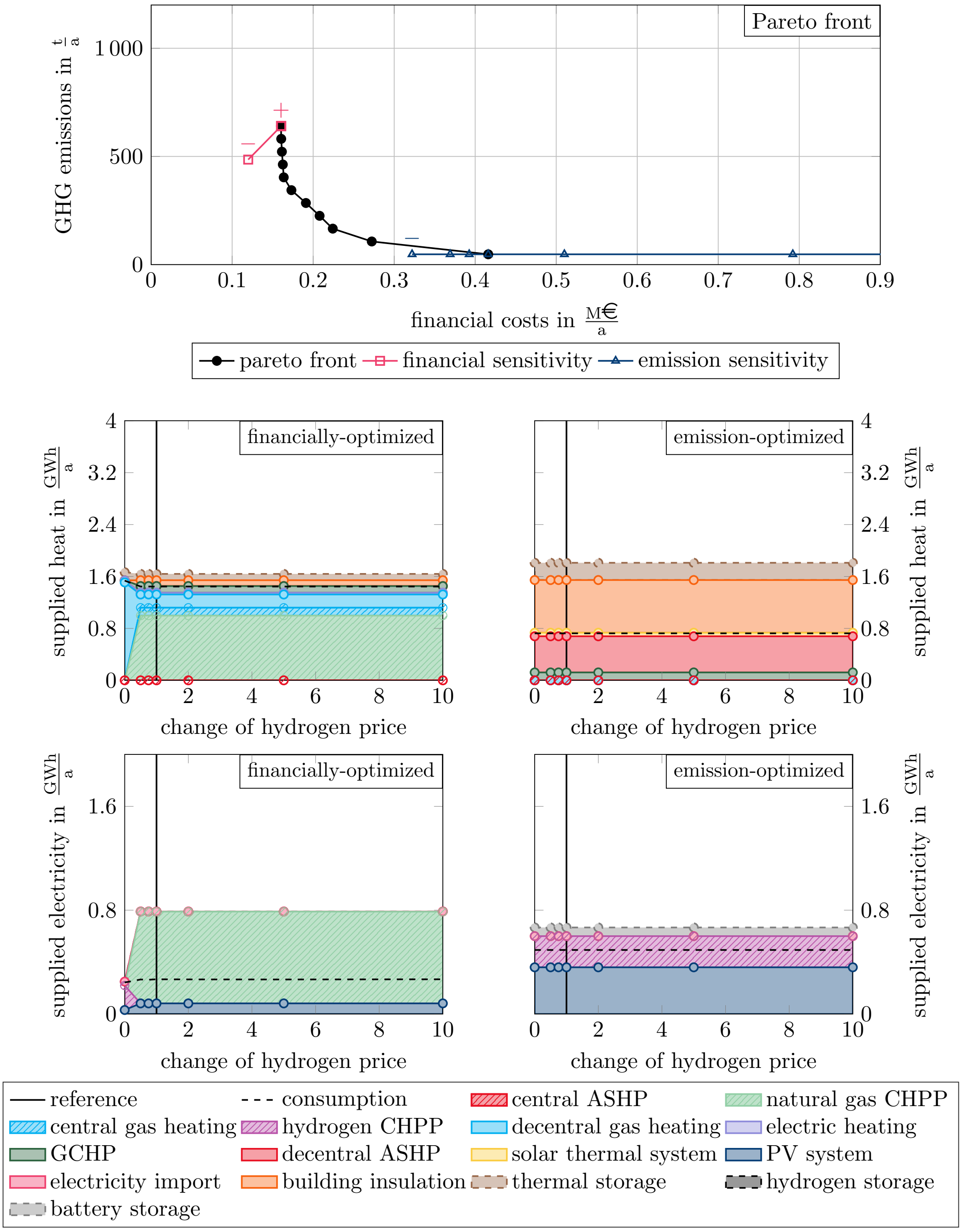

Figure 11: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (hydrogen price). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "–", the highest as "+". In the financially-optimized case the scenarios 50 %, 75 %, 100 %, 200 %, 500 %, and 1 000 % lie on top of each other. **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 7: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of hydrogen prices.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	0	0	0	30	0	331	0	127	386	29	0	0	706	0	0	0
FO-0.5	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-0.75	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-2.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-5.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-10.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
EO-0.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-0.5	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-0.75	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-2.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-5.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-10.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

H. Results: Combined Energy Price

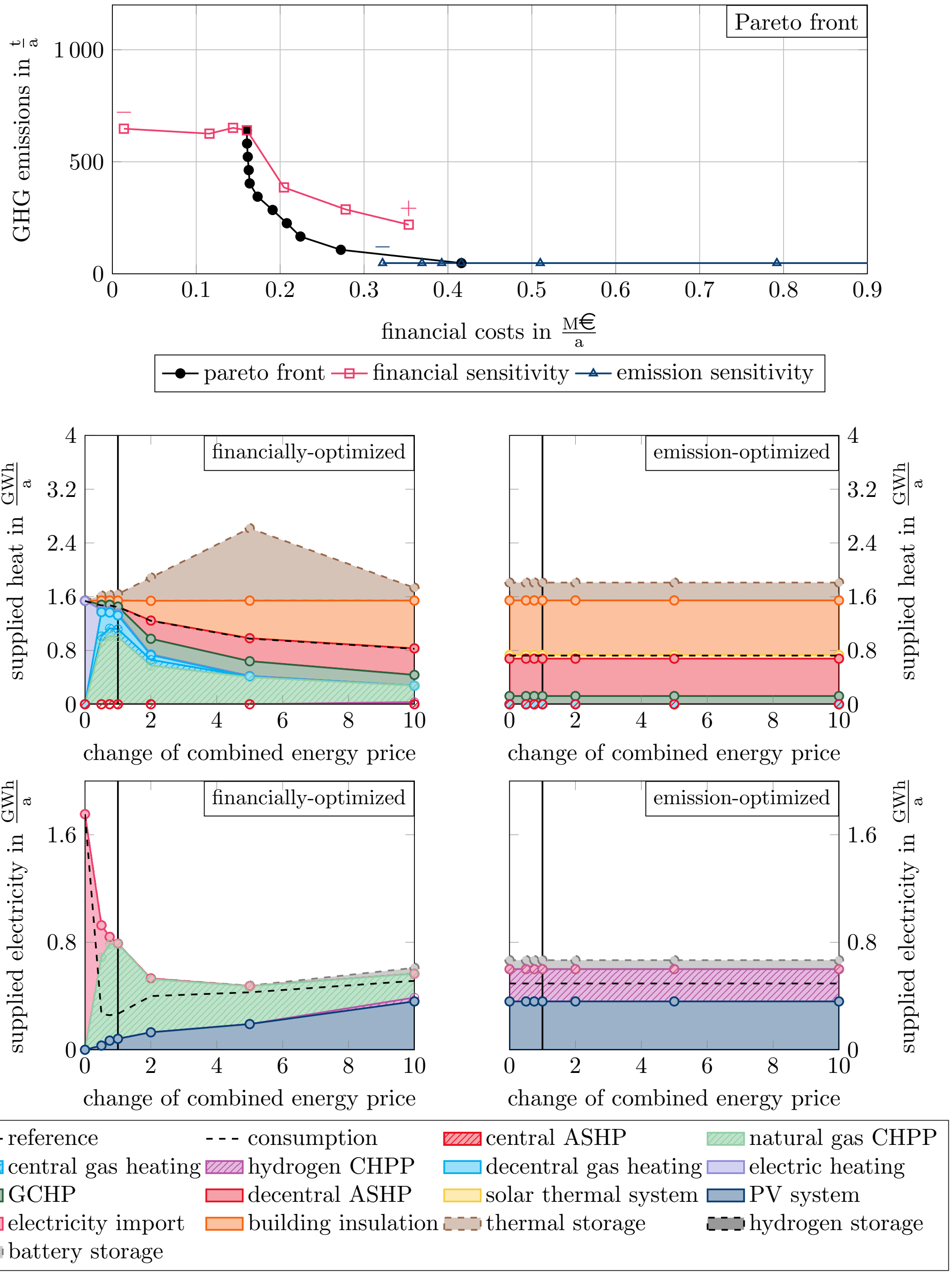

Figure 12: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (combined energy price). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "−", the highest as "+". **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 8: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of combined energy prices.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	0	0	0	0	0	0	0	539	0	0	0	0	340	0	0	0
FO-0.5	121	92	0	0	0	0	0	117	98	29	0	10	687	0	0	11
FO-0.75	129	130	0	0	0	0	0	87	73	60	0	15	728	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-2.0	69	100	0	0	0	0	0	31	59	114	58	51	758	0	0	5
FO-5.0	93	6	0	0	0	0	0	46	8	165	99	54	1138	12	0	4
FO-10.0	81	0	0	10	50	0	0	54	0	295	132	39	1303	175	438	4
EO-0.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-0.5	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-0.75	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-2.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-5.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-10.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

I. Results: Electricity Demand

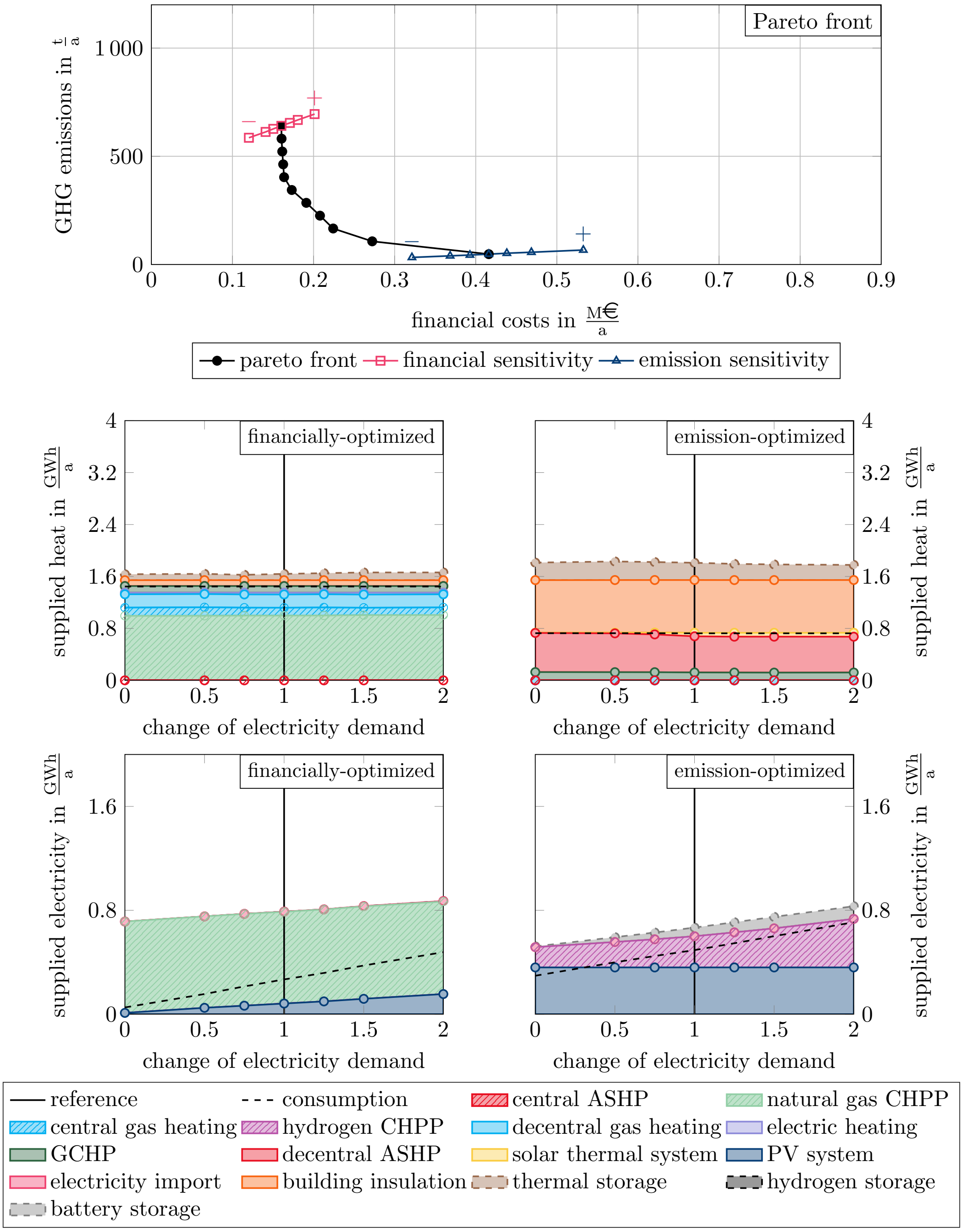

Figure 13: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (electricity demand). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "–", the highest as "+". **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter. If the behavioral based electricity demand is reduced to zero the absolute electricity demand and thus the electricity supply has an offset, which is caused by the electrified heat supply.

Table 9: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of electricity demands.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	124	114	0	0	0	0	0	111	65	8	0	17	633	0	0	13
FO-0.5	123	131	0	0	0	0	0	90	65	42	0	17	701	0	0	13
FO-0.75	125	110	0	0	0	0	0	113	65	56	0	17	635	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.25	125	119	0	0	0	0	0	102	65	84	0	17	649	0	0	13
FO-1.5	127	103	0	0	0	0	0	116	66	101	0	17	633	0	0	13
FO-2.0	127	117	0	0	0	0	0	97	65	132	0	18	720	0	0	13
EO-0.0	0	0	0	155	22	0	4	22	0	295	230	28	1422	36	22	0
EO-0.5	0	0	0	178	0	0	12	0	0	295	241	28	1592	172	0	0
EO-0.75	0	0	0	186	0	0	29	0	0	295	234	28	1658	263	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.25	0	0	0	185	0	0	62	0	0	295	202	28	1508	417	0	0
EO-1.5	0	0	0	191	11	0	62	11	0	295	194	28	1452	496	11	0
EO-2.0	0	0	0	209	33	0	63	33	0	295	187	28	1527	623	33	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

J. Results: Heat Demand

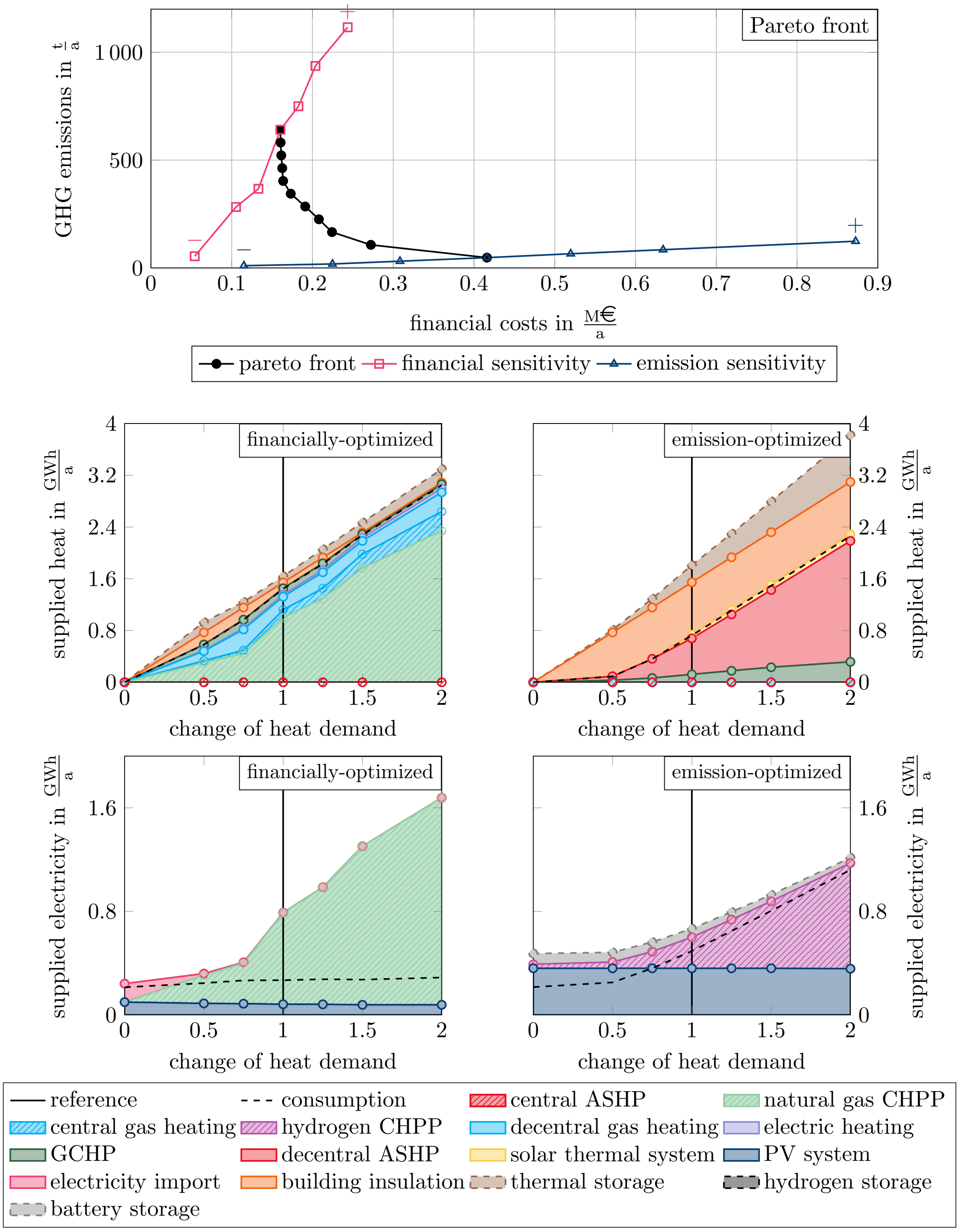

Figure 14: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (heat demand). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "−", the highest as "+". **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 10: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of heat demands.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	0	0	0	0	0	0	0	0	0	84	0	0	0	0	0	0
FO-0.5	39	44	0	0	0	0	0	22	49	75	0	18	314	0	0	5
FO-0.75	56	56	0	0	0	0	0	58	99	74	0	23	491	0	0	5
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.25	160	136	0	0	0	0	0	148	78	70	0	19	796	0	0	14
FO-1.5	218	182	0	0	0	0	0	187	66	66	0	9	975	0	0	16
FO-2.0	285	246	0	0	0	0	0	251	94	66	0	9	1304	0	0	16
EO-0.0	0	0	0	37	0	0	0	0	0	295	0	0	0	360	0	0
EO-0.5	0	0	0	57	26	0	0	26	0	295	51	5	292	332	26	0
EO-0.75	0	0	0	105	0	0	2	0	0	295	118	14	689	351	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.25	0	0	0	247	0	0	74	0	0	295	298	41	2074	323	0	0
EO-1.5	0	0	0	319	0	0	85	0	0	295	399	52	2623	311	0	0
EO-2.0	0	0	0	473	0	0	101	0	0	292	619	65	3797	304	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

K. Results: Population Density

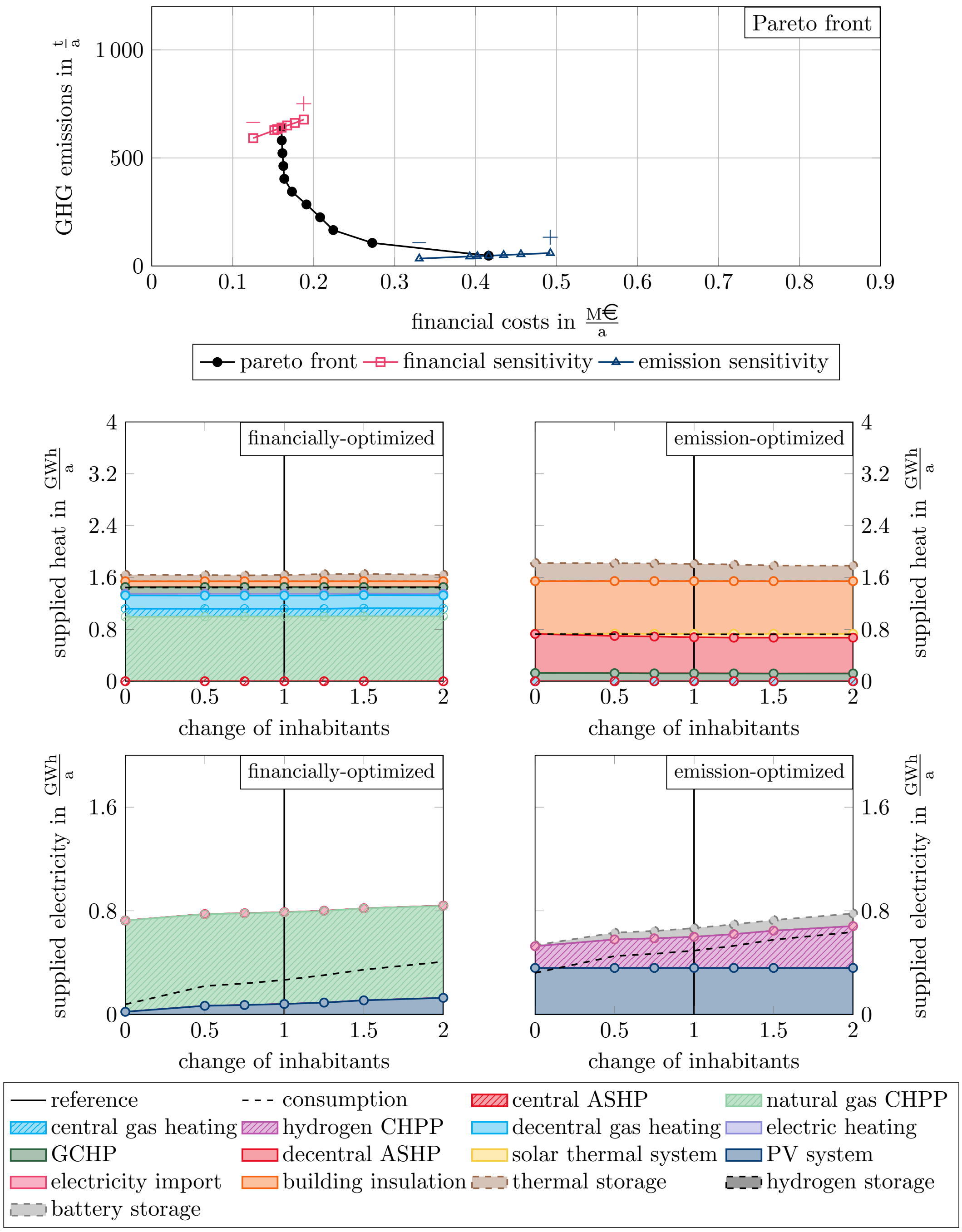

Figure 15: **Deviations financially-optimized and emission-optimized scenarios caused by changes of the sensitivity parameter (population density). Pareto front (top diagram):** Changes of the financially-optimized scenario are shown in red of emission-optimized scenario in blue. If no changes occur, the points lie on top of each other. Otherwise, the lowest value (0 % of the sensitivity parameter compared to the reference case) is marked as "−", the highest as "+". **Supplied energy (four diagrams below):** Supplied heat (top) and electricity (bottom) per inhabitant in the financially (left) and emission-optimized (right) reference case in dependency on the sensitivity parameter.

Table 11: **Optimized technology capacities in the finanically-optimized (FO) and emission-optimized (EO) reference case in dependency on changes of population density.** The results are aggregated for each technology type.

scenario	natural gas CHPP in kW	central gas heating in kW	central ASHP in kW	hydrogen CHPP in kW	electrolysis in kW	methanation in kW	solar thermal system in kW	electric heating in kW	decentral gas heating in kW	PV system in kW	decentral ASHP in kW	GCHP in kW	thermal storage in kWh	battery storage in kWh	hydrogen storage in kWh	DH buildings
FO-0.0	124	112	0	0	0	0	0	113	65	17	0	17	631	0	0	13
FO-0.5	125	106	0	0	0	0	0	117	66	57	0	17	628	0	0	13
FO-0.75	125	106	0	0	0	0	0	116	65	63	0	17	632	0	0	13
FO-1.0	125	106	0	0	0	0	0	116	65	70	0	17	632	0	0	13
FO-1.25	125	106	0	0	0	0	0	116	66	80	0	17	632	0	0	13
FO-1.5	125	128	0	0	0	0	0	90	65	95	0	18	699	0	0	13
FO-2.0	126	119	0	0	0	0	0	101	65	112	0	17	665	0	0	13
EO-0.0	0	0	0	165	4	0	4	4	0	295	239	28	1521	38	4	0
EO-0.5	0	0	0	182	0	0	38	0	0	295	228	28	1721	263	0	0
EO-0.75	0	0	0	184	0	0	45	0	0	295	225	28	1654	293	0	0
EO-1.0	0	0	0	185	0	0	56	0	0	295	218	28	1654	349	0	0
EO-1.25	0	0	0	186	16	0	62	16	0	295	208	28	1555	400	16	0
EO-1.5	0	0	0	187	0	0	61	0	0	295	194	28	1435	445	0	0
EO-2.0	0	0	0	203	0	0	62	0	0	295	194	28	1426	568	0	0

Acronyms: ashp = air source heat pump; centr. = central; chpp = combined heat and power plant; decentr. = decentral; dh = district heating; EO = emission-optimized; FO = financially-optimized; gchp = ground coupled heat pump

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F SESMG Interface

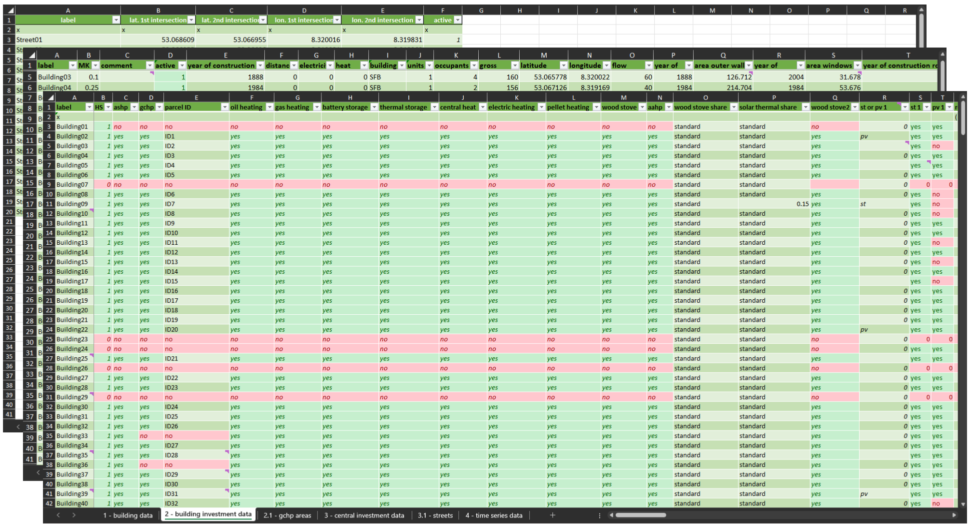

Figure F.1: Screenshots of the "urban district upscaling sheet" in which locally-specific parameters of an urban energy system are entered.

Figure F.2: Screenshots of the "model definition" spreadsheet. The spreadsheet consists of several sheets and contains all model parameters necessary for the creation of a model.

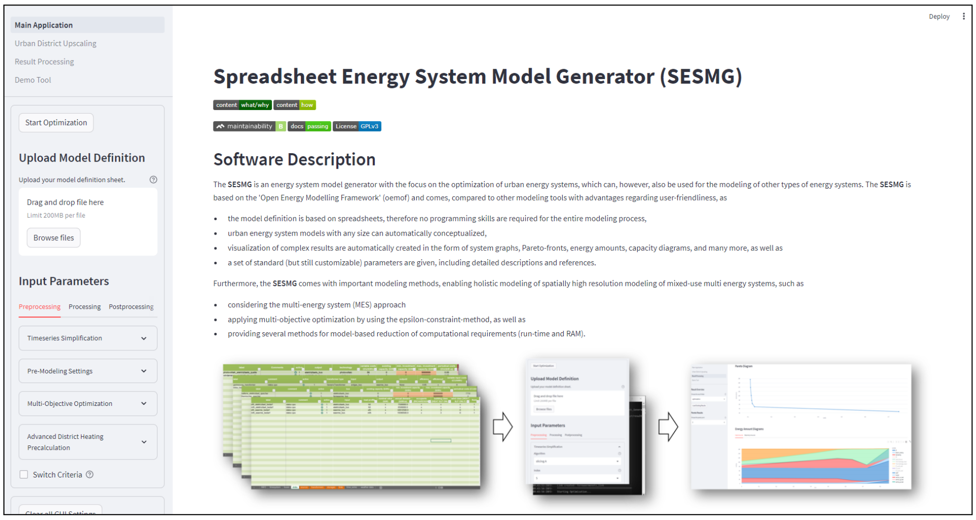

Figure F.3: Screenshot of the GUI. On the left side user inputs are made, on the right side descriptions and results can be accessed..

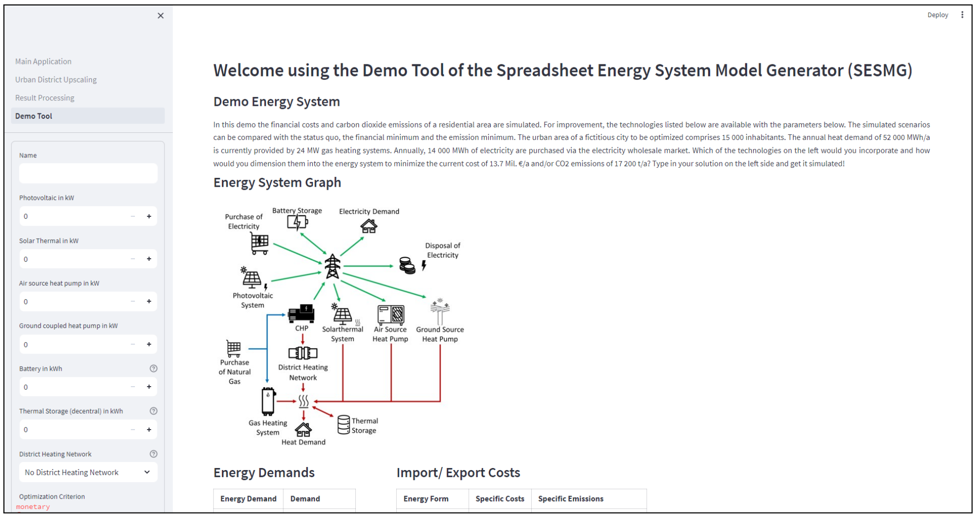

Figure F.4: Screenshot of the "demo tool", which can be accessed within the GUI. On the left side a technology mix can be selected, on the right side a description of the demo model (before the model run) and the model results (after the model run) are shown.

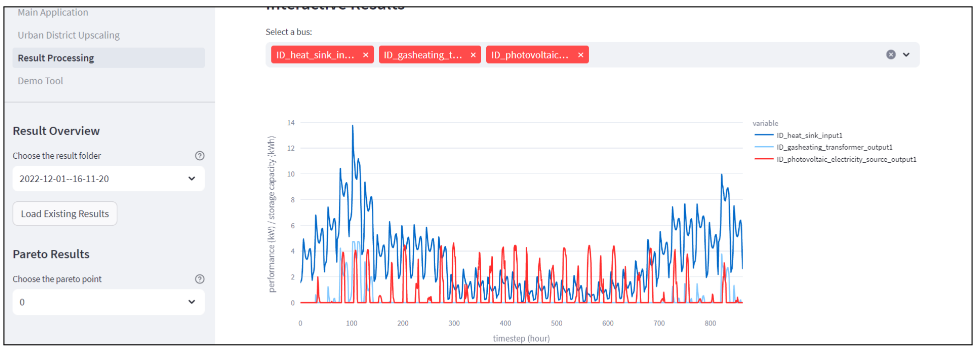

Figure F.5: Screenshot of automatically generated model results (time series plots). The result output is interactive, the user can select which plots are displayed and scale them as desired.

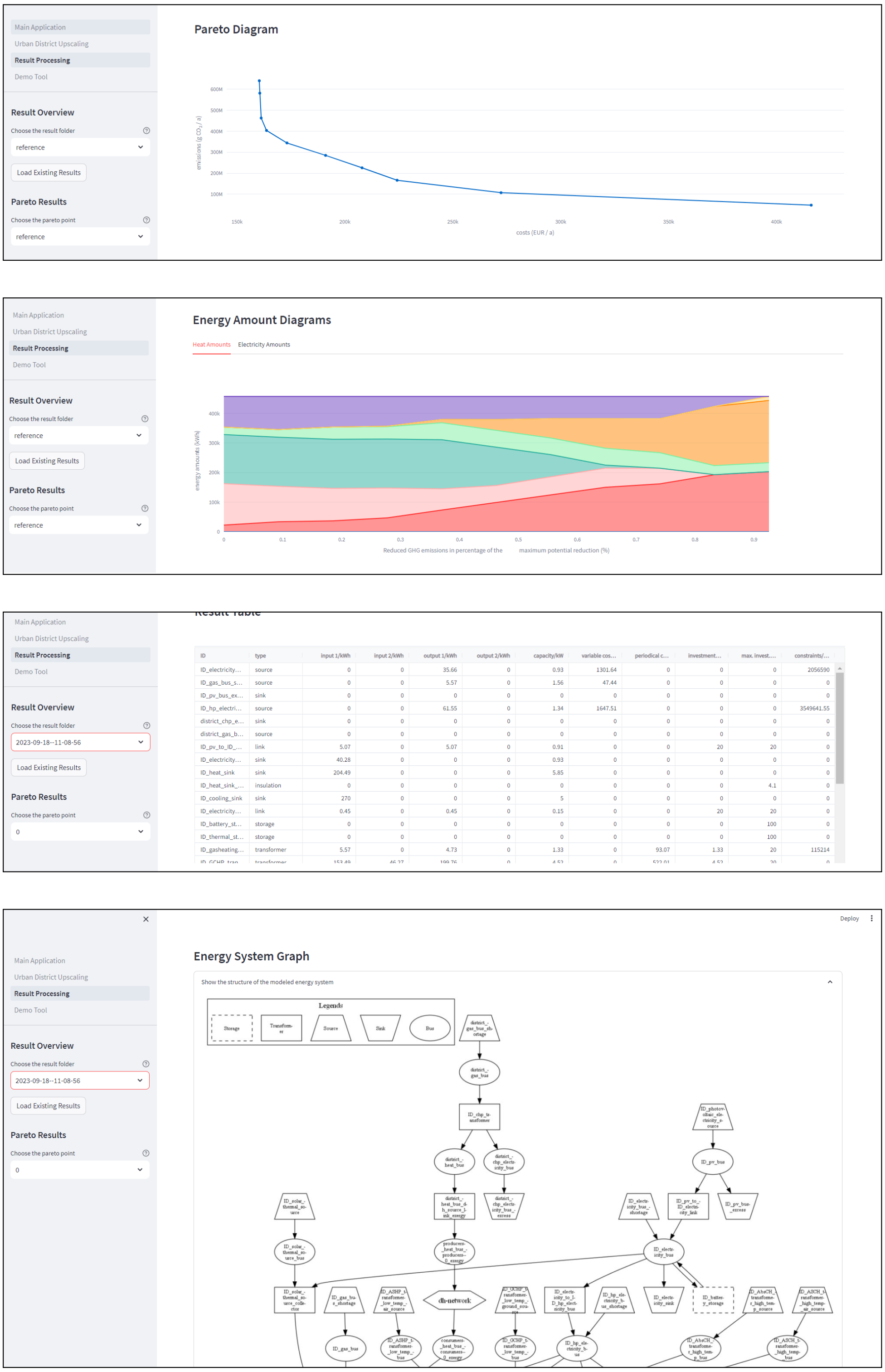

Figure F.6: Screenshots of various automatically generated model results. From top to bottom: (1) Pareto diagram, (2) energy amount diagram, (3) tabular summary and (4) system graph. The results outputs are interactive, users can select and deselect plot elements, and table elements can be filtered as desired.