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DOCTORAL THESIS

Development, Application and Limitations of Open Energy System Analysis Approaches for Sustainable Energy Transformations

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Summary

Energy system analysis and modelling have played a crucial role in energy system design since the 1960s, and both the methods and main objectives for them have evolved with time. In recent years, three main technical, economic and socio-political developments have influenced the field of energy system analysis. First, a transition to renewable energy sources, driven by concerns about climate change, requires new methods for modelling increasingly interconnected, sector-coupled and distributed energy systems. Second, the liberalisation of energy markets is changing power structures within the energy sector, enabling but also requiring new ways of knowledge creation and dissemination. Third, as part of a general development towards a new mode of open science, demands for transparency and reproducibility of methods and results are increasing.

The thesis addresses methods of energy system analysis, their development, application and limitations for the design of sustainable energy systems. The work is based on the proposition that collaboration is an essential part of Open Science. In the context of the outlined developments, the work aims to answer how software development can be performed openly and collaboratively and at the same time enable a transparent and reproducible application for renewable sector-coupled energy system analyses. Furthermore, the work probes the limits of quantitative techno-economic open energy system analysis approaches for successful sustainable energy transformations, by analysing the role of the important yet underrepresented sustainability strategy of sufficiency.

To address these questions, the thesis presents an open and collaborative energy system analysis approach, which is implemented in Python as the Open Energy Modelling Framework (oemof). In oemof, collaboration between researchers is governed by common development rules which are applied to all oemof-related projects. Furthermore, discussions about future developments as well as decision-making processes are openly organised on the collaboration platform GitHub. At the same time, oemof features a generic graph-based software concept which enables flexible modelling of sector-coupled energy systems using the bottom-up optimisation model generator oemof-solph. This library provides a rich set of components which allows for the modelling of unit-commitment, dispatch, investment and multi-period expansion problems within different levels of abstraction. To improve the transparency and use of oemof-solph, the software concept of facades is applied to an extension called oemof-tabular. This extension allows users to instantiate models from tabular data sources such as friction-less data packages or spreadsheet files and generate reproducible results.

Open energy system analysis approaches were applied in three studies presented within this thesis to analyse sustainable energy systems. In two studies, techno-economic optimisation approaches based on oemof-solph were applied, demonstrating the importance and the potential of techno-economic strategies to mitigate climate change. The first study investigated the flexbilisation of dispatchable heat pumps in renewable energy systems in Germany and shows the benefits of sector-coupled systems. Flexible heat pump operation is shown to contribute significantly to the reduction of short-term electricity storage, leading to cost reductions and lower resource consumption. The second study analysed the optimal expansion of renewable energy sources and electricity storage in Jordan. Compared to local resources such as oil shale, renewable energy sources offer a cost-efficient and environmentally friendly way to increase energy security with a significant CO_2 reduction potential. In the third study, a bottom-up simulation model of the German household heating sector was used in a transformation pathway scenario analysis. The analysis took not only consistency and efficiency but also sufficiency measures into account. Apart from the high relevance of a rapid expansion of renewable energy sources and efficiency improvements, the results highlight that the necessary CO_2 reductions to enable the 1.5°target of the Paris Agreement to be met are unlikely to be achieved in the German household sector without sufficiency.

The results in this thesis show that open software and collaborative development can be established to answer current research questions in the field of energy system analysis and sustainable energy system design. This implies that scientific progress in the field of energy system analysis is possible in compliance with the scientific standards of scrutiny and reproducibility. Nevertheless, social challenges for effective collaboration, limits to software-side solutions and qualitative aspects of uncertainty remain. In addition, energy system analysis is limited by the exclusion of some of the available sufficiency CO_2 mitigation measures. Therefore, future energy system analysis needs to take into consideration qualitative social dimensions of energy systems to support successful sustainable transformations.

Acknowledgements

> *"Patience is a form of wisdom. It demonstrates that we understand and accept the fact that sometimes things must unfold in their own time."*
>
> – John Kabat-Zinn, *Full Catastrophe Living*

In retrospect, the work on this thesis can best be described as a journey with some stops and detours. Therefore, this work is probably not like a straight line, but it definitely follows a common thread, as the thoughts and values reflected in it have accompanied me from the beginning. On this journey, I have been supported and inspired by many people who deserve recognition.

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The process of developing the concept of oemof, but also its implementation, was based on the work of many people and is still ongoing. It took countless tiring, sometimes frustrating discussions about things that in retrospect seem quite unimportant. It is therefore great to see how this process has turned out for the oemof community. Looking at this community, I would like to thank Uwe Krien for always defending and pushing the idea of community-based energy modelling and for continuing to work on this project with other people. Further thanks must go to: Cord Kaldemeyer for his enviable perseverance in software development, fruitful discussions and support in scientific work that goes beyond the scope of this thesis; Stephan Günther, on the one hand for his support in computer science, without which this work would not have been done, and on the other hand for his stimulating political discussions and company at openmod meetings; Clemens Wingenbach for inspiring and always helpful suggestions

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Part I - Introduction and Foundations

1

Introduction

1.1 Context & Rationale

Since *The Limits to Growth* was published by the Club of Rome in 1972 (Meadows and Club of Rome 1972), causes and effects of anthropogenic climate change have been discussed in science, politics and among the general public. Despite ongoing research and discussion, a broad consensus on man-made climate change and its severe consequences exists. This consensus was expressed by the Paris Agreement, signed by 197 states in 2015 within the United Nations Framework Convention on Climate Change. The agreement aims to keep global warming to within 2 °C above pre-industrial levels and to improve climate resilience (UN 2015, p. 3). In 2018, the importance of this agreement was underlined by a special report of the Intergovernmental Panel on Climate Change (IPCC), which showed that there are significant differences between the impacts of 1.5 and 2 °C warming (IPCC 2018). In addition, climate change is embedded in a network of coupled earth system processes whose regenerative capacities are reaching or already exceeding planetary boundaries (Rockström et al. 2009; Lade et al. 2020).

One of the main drivers for climate change is the consumption of fossil fuels in the energy sector. In 2010, greenhouse gas (GHG) emissions from this sector accounted for 35 % of the total global GHG emissions (Bruckner et al. 2014, p. 516). A central pillar of worldwide climate mitigation strategies is thus the development of sustainable energy systems. Globally available and cost effective renewable energy resources such as wind and solar energy are the backbone of these systems (IRENA 2019b, p. 30) leading to a transformation from centralised, controllable fossil fuel based systems to decentralised, renewable energy based systems with intermittent supply. This transformation process with the development of new system structures imposes several challenges for the scientific domain of energy system analysis (ESA), an interdisciplinary field which deals with the analysis and planning of an increasingly complex socio-techno-economic system.

The main purpose of ESA, as well as its practices and associated challenges, have evolved over time. Modelling is a central part of ESA and has been used in the planning of energy systems since the first half of the 20th century. Initial modelling efforts focused on transport and demand-side forecasting. As a result of the Arab oil embargo in 1973, low-cost and secure energy supply became increasingly relevant (Samouilidis 1980). In recent years, ESA has been carried out in the light of climate change and environmental considerations (Pfenninger et al. 2014, p. 75). With regard to the aforementioned energy system transformation, ESA is being used as a driver for transformation by making system dynamics comprehensible and identifying the limits of current practices and opportunities for change. However, ESA is also affected by the transition as it has to operate in an evolving system. Simultaneously, ESA processes are interlaced with other social and technological developments, such as the trend towards open science in all scientific disciplines, advances in computer science, and information technology and energy market liberalisation.

1.2 Research Questions

The combination of socio-technological developments and energy system transition processes creates a unique composition of challenges. First, calls for transparency and reproducibility, i.e. scientific standards, of methods and results are increasing. These calls are part of a general trend towards open science characterised by transparent, shared, accessible and collaboratively-developed knowledge (Vicente-Saez and Martinez-Fuentes 2018, p. 428). Second, the energy system transition requires simulation of renewable energy feed-in with high spatial and temporal resolution, representation of system flexibility, adequate grid modelling and an incorporation of different policy and regulatory frameworks in liberalised energy markets. Authors have argued that issues of transparency and energy system specific modelling challenges can be addressed at the same time (Bazilian et al. 2012, p. 152) and conclusive arguments such as higher productivity, efficiency and quality for open science are presented (OECD 2015, pp. 10f). In addition, there is a normative argument that methods and results from publicly-funded research should be available to the public (Pfenninger et al. 2018, p. 64). Although these arguments have led to a trend towards open energy modelling approaches in recent years (Lopion et al. 2018, p. 160), it is questioned whether open source tools are mature enough to be used (Groissböck 2019; Oberle and Elsland 2019) or whether energy research is lagging behind other scientific disciplines when it comes to opening up research (Pfenninger 2017). Finally, the field of ESA is criticised for focusing on techno-economic and quantitative methods (Sovacool et al. 2015, p. 96) as well as on technical solutions for climate change mitigation (Samadi et al. 2017, p. 129). Therefore, Pye et al. (2021, p. 4) point out that in light of climate change and the need for net-zero emissions systems, the space for demand-side mitigation options is limited and needs to be expanded.

Within the outlined context, the presented thesis aims to answer the following research questions:

1. *How can open scientific practices of collaborative software development and application in the field of energy system analysis be designed to meet scientific standards?*

2. *Can research, which meets these scientific standards, provide insights for relevant research questions and address challenges in the domain of energy system analysis?*

3. *What are the limitations of current techno-economic energy system analysis approaches for shaping sustainable energy systems?*

1.3 Structure of Thesis

This publication-based thesis is composed of three parts. The first part contains the Introduction and Chapter 2. Chapter 2 outlines three socio-economic transformations which impact the field of energy system analysis. It also provides conceptual and theoretical foundations for energy systems analysis, as well as methods and practices. Finally, Chapter 2 presents the idea of open modelling and summarises the state of research of open energy system analysis software to delineate the scope of this thesis.

The second part of the thesis encompasses Chapter 3 to 9 and contains the seven peer-reviewed publications listed in Table 1.1. The publication in Chapter 3 presents a structured review of energy system modelling challenges and provides a method to evaluate energy system modelling frameworks. The three publications in Chapters 4, 5, and 6 highlight how software development and application processes can be designed to meet scientific standards in the age of open science. These chapters thus relate to research question 1. Chapters 4 and 5 place emphasis on collaborative development and conceptual design. Chapter 6 focuses on the provision of transparent and reproducible modelling. In Chapters 7 and 8, the described methods and software are applied to the research questions related to renewable energy transitions and serve to answer research question 2 of this thesis.

Table 1.1: Overview of peer-reviewed publications in this thesis.

Chapter	Chapter Name / Publication Title	Journal
3	A qualitative evaluation approach for energy system modelling frameworks	Energy, Society and Sustainability
4	The Open Energy Modelling Framework (oemof) — A new approach to facilitate open science in energy system modelling	Energy Strategy Reviews
5	oemof.solph — A model generator for linear and mixed-integer linear optimisation of energy systems	Software Impacts
6	oemof.tabular — Introducing Data Packages for Reproducible Workflows in Energy System Modeling	Journal of Open Research Software
7	Effects of Decentral Heat Pump Operation on Electricity Storage Requirements in Germany	Energies
8	Analysis of cost-optimal renewable energy expansion for the near-term Jordanian electricity system	Sustainability
9	Why Renewables and Energy Efficiency are not Enough - The Relevance of Sufficiency in the Heating Sector for Limiting Global Warming to 1.5°	Technology Forecasting & Social Change

To address research question 3, the final publication in Chapter 9 applies an open source simulation model to analyse decarbonisation pathways in the German heating sector. In addition to renewable energy expansion, the role of different demand side CO_2 mitigation measures, including sufficiency, are investigated in this study.

The third part of this thesis consists of Chapter 10, which provides a synthesis of the individual publications by linking the methods and results as well as pointing out critical aspects, limitations, and areas for further research.

2

Theoretical and Conceptual Foundations

All chapters, including the publications included within this thesis are written from the perspective of Western industrialised countries. The context of this thesis with developments in the field of energy system analysis and modelling, energy market liberalisation, and a trend towards sustainable energy systems and open science can, however, be observed worldwide. All of the developments and trends are shaped by Western cultures, in particular by countries in Europe and North-America, which still dominate science, technological development and economic paradigms. The reader should keep in mind that general descriptions of social and techno-economic developments come from, and apply, to Western countries and will require further differentiation if transferred to countries of the global south.

2.1 Energy System Analysis

Energy systems are the object of investigation for the field of Energy System Analysis (ESA) and are often understood as techno-economic systems meeting an energy demand (Groscurth et al. 1995, p. 941). These systems can include power plants converting primary energy (e.g. natural gas) to electricity as well as electric vehicles converting electricity to mechanical energy. A more encompassing description in the Global Energy Assessment (GEA) considers all steps in the process chain on the supply side including extraction, conversion, and distribution, as well as process steps on the demand side to provide energy services (GEA 2012, p. 104). Similarly, Jaccard (2006) defines an energy system as “the combined processes of acquiring and using energy in a given society or economy” (p. 6).

As a scientific discipline, ESA serves to support decision making with regard to energy policy and the energy economy. One of the central goals of ESA is the provision of insights for the design of future energy systems by working from a holistic perspective

(Fichtner 2018). While the system boundaries can be defined on a global, national, regional or local level, the ESA perspective aims to take environmental, social, political and economic aspects into account.

For ESA, the system under study contains multiple nested and interdependent subsystems, which feature different degrees of complexity, as illustrated in Figure 2.1.

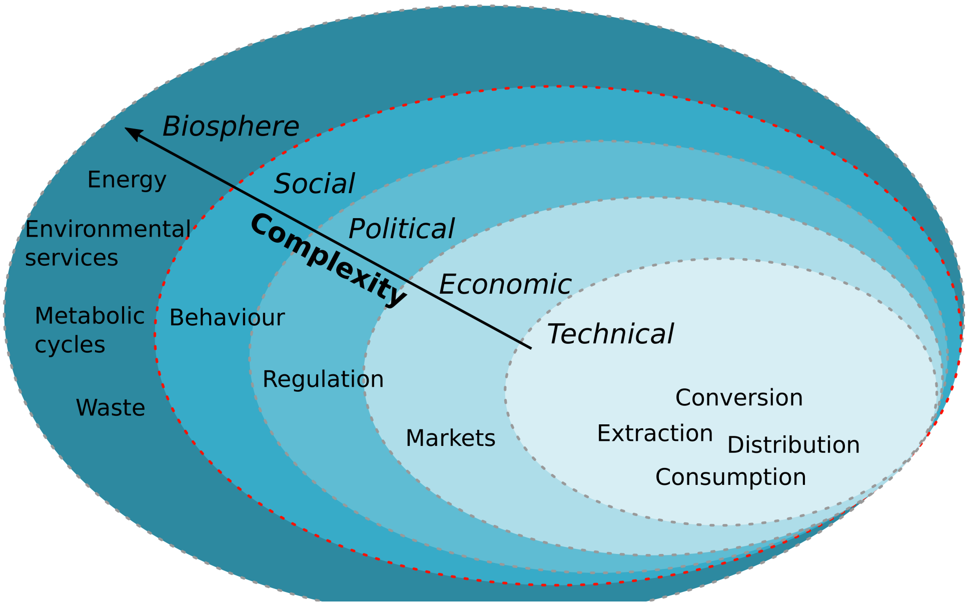

Figure 2.1: Illustration of socio-political-techno-economic energy system (red dotted line) embedded in the bio-geosphere. Source: Own Illustration inspired by Jaccard (2006).

The technical (physical) system is embedded in an economic system, which allows for the allocation of resources via markets or other mechanisms, such as central planning. These mechanisms are designed and determined by a political sphere via regulation, trade agreements and subsidy schemes. This techno-economic-political system is a sub-system of the social system as it exists through thoughts, preferences, attitudes and behaviours of individuals as well as cultural practices. The holistic view of an energy system with all its nested and interacting sub-systems is part of the bio-geosphere, which provides energy and environmental services and also assimilates waste and integrates end or side-products in different metabolic cycles. The degree of complexity of these systems increases from the technical level up to the biosphere. Pure technical systems can be rather complicated[1], but they generally do not exhibit characteristics of complex systems such as emergence, self-organisation or spontaneous order (Ladyman et al. 2013). Therefore, complexity in energy systems emerges to a large extent from socio-political-economic dimensions of the systems. As Bale et al. (2015) shows, energy systems feature characteristics of complex systems and “[...] understanding energy system change would benefit from the application of complexity science thinking and modelling” (p. 158).

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[1] For a discussion about complicated vs. complex see Forss et al. (2011, pp. 34-50).

Today, ESA is a multi-disciplinary field including economics, engineering, meteorology, geography, geology, computer science, as well as social and political sciences. However, most questions are focused on techno-economic aspects of the system guided by social-environmental-economic considerations, such as:

- What is the cost-optimal mix of technologies within a system?
- How can energy demands in a society be met with limited CO_2 emissions?
- Should markets be organised by nodal or zonal pricing?

To answer such questions, qualitative as well as quantitative methods are applied, with computational modelling playing a critical role.

2.2 Three Transformations

Before engaging with the role of modelling and its energy system specific characteristics in Section 2.3, it is important to understand that the field of ESA is interweaved within three ongoing transformation processes: First, there is the transformation from fossil fuel based systems to sustainable, renewable energy based systems due to climate change concerns (Section 2.2.1). Second, the process of energy sector liberalisation, which was introduced by a set of policy reforms, is changing the economic and power structure within the energy system in many countries around the world (Section 2.2.2). And thirdly, the scientific transformation, due to new information technologies, which are changing the way knowledge is created and disseminated (Section 2.2.3). While processes are taking place worldwide, they are more representative for industrialised countries, in particular countries in North-America and Europe. The goal here is not to provide a comprehensive and differentiated description of worldwide developments, but to work from the perspective of industrialised countries.

2.2.1 Energy System Transformation

To begin with, it is crucial to recognise that “energy transitions are complex, and irreducible to a single cause, factor, or blueprint” and that there is a “difficulty of defining and dating them” (Sovacool 2016, p. 211). Nevertheless, it seems evident that countries worldwide are transitioning from the use of fossil fuel based systems to renewable energy ones indicated by growing shares of renewable energy sources (IRENA 2019a, pp. 10-14).

The negative effects of fossil fuel emissions have been studied since the 1960s (George and Chass 1967). On a local level, the direct effects on human health of air pollution from particular matter can be observed. On a global level, greenhouse-gas emissions such as carbon dioxide (CO_2), nitrogen oxides (NO_x), or methane (CH_4) can be seen to be fuelling global warming. However, only since the 1990s increasing (public) awareness and concerns about the consequences of anthropogenic climate change have become the main driver for an energy transition towards sustainable energy systems. The unsustainable mode of current energy systems is not restricted to environmental effects. As Grubler (2012) points out, "current energy systems are simply unsustainable on all accounts of social, economic, and environmental criteria" (p. 8).

Therefore, shaping sustainable energy systems to minimise environmental impact and mitigate climate change is part of sustainable development balancing social, economic and environmental sustainability (Mensah 2019, p. 8). There are three main political strategies for sustainable development of systems: 1) sufficiency (behavioural change), 2) efficiency and 3) consistency (Huber 2000, p. 275). While the first strategy is a social one, the latter two are rather technology-focused. ESA is strongly dominated by quantitative methods and techno-economic sciences. As a consequence, their dominating paradigm can be described as quantitative-techno-economic and focus is put on the two technological strategies of efficiency and consistency for climate change mitigation (Sovacool et al. 2015; Sovacool 2014; Samadi et al. 2017). This is also reflected in policy agendas which concentrate on renewable energy sources (consistency) and technological advances for demand reduction (efficiency). For example, the EU 2030 climate and energy framework aims for a 55 % reduction of GHG emissions compared to 1990 levels, where the two central key elements are the increase of the renewable energy share up to 32 % and improvements of energy efficiency to at least -32.5 % (EUC 2020, p. 12). Therefore, energy system transformation is predominantly characterised by an energy demand reduction through technical measures and a transition towards renewable energy sources.

Renewable Energy Transition

In Germany, a country considered to be a front-runner with respect to the current energy transition movement, the period from 1998 to 2009 is identified as a crucial turning point for (renewable) energy transformation (Hake et al. 2015, p. 39). The passing of the Renewable Energy Act in Germany in 2000 provided a stable regulatory framework, which facilitated the diffusion of renewable energy technologies in the country (Quitzow et al. 2016, p. 164).

In recent years there has been growing evidence that, despite all challenges, 100% renewable electricity systems are technically feasible and economically viable (Brown et al. 2018a; Diesendorf and Elliston 2018; Hansen et al. 2019). However, expansion of renewable energy sources to replace fossil fuel technologies is not only a transition from one supply technology to another. Significant technological differences between fossil fuel based and intermittent renewable technologies means that more substantial changes are required within the system. To cope with volatile supply patterns of wind and photovoltaic (PV) technologies, additional system flexibility, such as the use of storage units, is needed. In addition, the decentralised characteristics of renewable energy systems necessitate the requirement for a different type of electricity grid infrastructure to that used for centralised fossil fuel based systems (Müller et al. 2019, p. 25). Finally, a limited supply of suitable renewable energy resources for heating and transportation require electrification of processes within these sectors. To integrate the vast amounts of intermittent renewable electricity supply, sector coupling of electricity, heat, and transport has been identified as an important cost effective measure (Brown et al. 2018c, p. 720).

2.2.2 Energy Sector Liberalisation

The expansion of renewable energy use in industrialised countries at the end of the 20th century coincided with a fundamental transformation on the economic side, namely energy sector liberalisation (Byrne and Mun 2003, pp. 50-51). The changing market structure is arguably important for understanding developments in the field of ESA for two reasons. First, modelling approaches for non-liberalised and liberalised markets differ and this has a significant impact on short-term planning models (Hobbs 1995; Kagiannas et al. 2004; Foley et al. 2010). Second, and equally important, the degree of accessibility and dissemination of knowledge has been impacted by liberalisation processes.

Before market liberalisation, many energy utilities were vertically integrated state-owned monopolies or private companies operating as monopolies (Byrne and Mun 2003, p. 50). Forces such as technological innovation, financial problems, economic, environmental and socio-political concerns affected the energy sector. In addition, an increasing neo-liberal policy agenda promoted liberalisation in sectors such as telecommunication, transport and energy (Clifton et al. 2006; Byrne and Mun 2003; Pollitt 2012). There is a common misconception that privatisation is a central aspect of liberalisation. However, countries have applied various models and applied different policy instruments resulting in a degree of diversity among liberalised energy sectors. Since the 1980s, the following elements have been part of worldwide energy sector liberalisation processes (Byrne and Mun (2003, p. 51) and Pollitt (2012, pp. 128-130)):

- Vertical unbundling of utilities by separating generation, transmission, distribution (and trading) to increase transparency, governance, and enable non-discriminatory access to transmission and distribution networks
- Horizontal unbundling to facilitate competition among state-owned as well as private utilities
- Creation of independent institutions for regulation
- Privatisation of state-owned assets, in many but not all cases
- Reduction of subsidies

Despite institutional reforms, market power in some countries, such as the United

States, still plays a crucial role, as Farrell (2021) shows. In addition, it is questioned to what degree promises of increased efficiency have materialised on a societal level (Byrne and Mun 2003, p. 62). According to Pollitt (2012, p. 135), more important than efficiency gains have been improved governance of monopoly utilities, a positive impact on competition and innovation, as well as increased quality of policy instruments for environmental emissions control. Nicolli and Vona (2019, p. 853) believe that liberalisation has a positive effect on renewable energy policies. However, Jegen and Wüstenhagen (2001, p. 54) pointed out that liberalisation itself does not achieve environmental goals in the electricity market and that additional (re-)regulation is required. Analysing the situation in Denmark, Meyer (1998) also shows that markets need regulation if environmental or social considerations are of high relevance. Indeed, the successful expansion of renewable energy sources in Germany, with a regulatory framework including subsidy schemes within a liberalised unbundled market, is a prime example of such (re)-regulation.

With regard to the evolution of energy system analysis and modelling, a particular set of properties and practices of the pre-liberalised energy sector must be understood. As Byrne and Mun (2003) summarise:

> Too often, important decisions regarding electricity supply were made by a closed circle of technical experts, government bureaucrats, and large corporate clients. Such a governance structure, coupled with the monopoly status of utilities, resulted in electricity industries developing into powerful organisations with their own political and economic agendas. In the absence of effective public supervision, moreover, electric utilities in many countries became a source of corruption, cronyism and pork-barrel politics rather than guardians of the public interest (pp. 50-51).

Energy system analysis and modelling has played a crucial role for energy system planning in non-liberalised energy sectors and many of the (optimisation) tools developed with public money at that time are still of high relevance today. Good examples of these include modelling tools originating in the 1970s, such as: MARKAL (Fishbone and Abilock 1981), developed within the Energy Technology Systems Analysis Program (ETSAP) of the International Energy Agency (IEA); MESSAGE (Schrattenholzer 1981) developed by the International Institute for Applied Sciences (IIASA); and WASP (IAEA 2001) developed for the International Atomic Energy Agency (IAEA). POLES (European Commission. Joint Research Centre. 2018), initially developed by the University of Grenoble, and the simulation model PRIMES (NTUA 2013), developed by the University of Athens in the 1990s are later examples.

The basic mathematical equations used in these tools have often been provided in scientific publications or software documentation. However, the accessibility of source code from publicly-funded modelling has been significantly limited. Moreover, and more fundamentally, full data-sets of conducted studies have also not been publicly available in most cases and were generally restricted to a subset of assumptions. As a consequence, data, methods and results of highly relevant studies cannot be scrutinised. This lack of transparency can also be related to the characteristics of the pre-liberalised energy sectors and has idiosyncratic consequences for the advancement in energy system modelling: Many open database and open source projects are re-discovering knowledge which has existed since the 1970s, but which has not been disseminated. Summarising, scientific scrutiny was not (fully) allowed for a long time in the field of energy system modelling.

2.2.3 Scientific Revolution

The comprehensive analysis and discussion of scientific history as well as its methods and practices is beyond the scope of this thesis. Nevertheless, it seems important to provide a basic conceptual background which frames the perspective within this thesis.

Historically, science is closely connected to socio-technological processes. Hence, it is important to note that science is not a static concept as practices, ethics and norms evolve with time. Bartling and Friesike (2014) describe science as “knowledge, creation and dissemination” (p. 4) and present a brief history of science. According to them, the history of science, can be divided into three main phases. The first pre-modern phase dates back to well-known philosophers such as Plato and Aristotle in Greece or Confucius and Laozi in China. The second phase is characterised by an institutionalisation and professionalisation of science, starting in the 17th century. With the possibility of printing, publishing scientific articles became the central part of knowledge dissemination. Due to the rapid increase in the number of professional researchers and the rate of increase in scientific advancement, this period is often described as the *(first) scientific revolution*. With the rise of modern information technologies, which has allowed not only for new ways of dissemination but also knowledge creation, science is currently undergoing the next transformation. Depending on the perspective and focus, this "new" mode of science is referred to as Science 2.0, Open Science or eScience. Despite the different names and concepts, all of them share the idea of a fundamentally different scientific mode. A central aspect of the new mode is the role of collaboration and crowd-sourcing for innovation (Bücheler and Sieg 2011). One important pre-condition for the successful exploitation of information technologies and collective intelligence is openness and diversity (Tacke 2011, pp. 41-42). Thus, throughout this thesis, the term *Open Science*, as well as its concept, will be used to describe the emerging mode of science.

Open Science

Open Science has gained momentum in recent years thanks to advances in information technology. New communication platforms, collaboration tools and reduced costs of (re-)distribution of information have been important driving factors for Open Science (see Bartling and Friesike (2014, pp. 8-9) and OECD (2015, pp. 8-9)). Practices associated with Open Science are open access to publications, open source software and hardware, open data, open review and open metrics, citizen science and open education (Herb 2012, pp. 11-38). Nevertheless, no common definition of Open Science exists. The definition of the OECD (2015) is directly linked to the process of digitisation: "Open science commonly refers to efforts to make the output of publicly funded research more widely accessible in digital format [...]" (p. 9). Bartling and Friesike (2014) highlight the social dimension and describe Open Science as a "scientific culture that is characterised by its openness" (p. 10). Similarly, Albagli et al. (2015, p. 9) state that Open Science can be best understood as a movement or process. Based on a comprehensive recent literature review, Vicente-Saez and Martinez-Fuentes (2018) conclude that "Open Science is transparent and accessible knowledge that is shared and developed through collaborative networks" (p. 434).

Open Science and Scientific Norms

Interestingly, many of the practices and characteristics which describe Open Science enable the scientific community to better serve their norms as described by Merton (1973). According to Merton, these norms, which characterise the ethos of modern science, are not given in a handbook of science. Instead they are expressed through what scientists believe they ought to do and what they think they are allowed to do. Merton (1973, pp. 268-278) breaks down the idea of the scientific ethos to the four norms of *communism, universalism, disinterestedness, and organised scepticism.* In this work he argues, that scientific findings are a social product and should be assigned to the scientific community.

Communism encompasses this idea of common ownership. Universalism refers to the idea that the value of scientific contributions is independent of the particulars of the person contributing. Disinterestedness describes the belief that scientists should seek for advances of knowledge independent of personal gain. Finally, scepticism is the belief that scientific claims should be sceptically scrutinised (Anderson et al. 2010, pp. 368-369).

According to Macfarlane and Cheng (2008, pp. 71-72), strong support for the norm of communism can be found among many scientists today. In Open Science, this is manifested in open licences for software and data, as well as in a new process of problem-solving, where professional researchers and citizens are invited to participate at different stages of the research process (Tacke 2011, p. 39). Citizen science even stretches the norm of universalism beyond the realm of professional scientists. This practice of openness can also facilitate the disinterestedness of institutions and researchers as claims for single ownership become increasingly futile. In addition, scepticism of research results and methods can be supported by increasing transparency as in the case of open source software, open peer-review or publishing pre-prints of scientific articles.

2.3 Energy System Modelling

2.3.1 Scenarios & Models

In the field of ESA, scenarios are closely linked to computational modelling and both are of high relevance to support policy decision making in designing future energy systems (Strachan et al. 2009; Dieckhoff and Grunwald 2016).

What is a Scenario?

Bradfield et al. (2005) state that the literature contains “different and at times contradictory definitions, characteristics, principles and methodological ideas about scenarios” (p. 795). In an attempt to resolve what has been referred to as “methodological chaos” (Bradfield et al. 2005, p. 796), over 405 publications were reviewed by Spaniol and Rowland (2019) to define the term scenario. The author found 77 differing definitions within the literature and summarises that a scenario is a future-oriented, plausibly possible, narrative description with an external context. Scenarios come in sets, which are systematically designed as a group of distinct alternatives (Spaniol and Rowland 2019, p. 8). Swart et al. (2004) states that in the field of sustainability science, which is closely linked to ESA, scenarios “may be thought of as coherent and plausible stories, told in words and numbers, about the possible co-evolutionary pathways of combined human and environmental systems” (p. 139). In the context of ESA, Dieckhoff et al. (2014, pp. 9-21) have developed important theoretical foundations and describe scenarios as coherent descriptions of possible futures based on the knowledge of the present. Additionally, the authors point out that scenarios are not predictions and that they do not imply a certain probability but are rather an extract of the possibility space. According to Dieckhoff (2015), scenarios in ESA are represented by quantitative elements, such as numerical data, framed by qualitative elements, such as narratives, story lines and derived assumptions. The quantitative part, often associated with modelling, is emphasised in the techno-economic field of ESA. However, the qualitative part is equally important for capturing crucial factors such as values and behaviour responsible for cultural shifts or institutional developments (Swart et al. 2004, p. 140). This is particularly relevant for the transition of complex socio-techno-economic energy systems.

Scenarios used in the ESA context allow for the exploration of possible future energy system trajectories by gaining insight into different energy system configurations, with regard to cost, technology developments, and environmental impacts. They are commissioned by companies from the energy industry, political stakeholders, and non-governmental institutions, and carried out by scientific institutions or consulting companies (Dieckhoff and Grunwald 2016, p. 7). Their application can, for example, be global (Bruckner et al. 2014), national (Pfluger 2018; Strachan et al. 2009) or local (Bohunovsky et al. 2011), and they can be used to focus on either specific sectors or the total energy system, covering short to long time horizons using a diverse set of methods (Paltsev 2017, pp. 2-5).

What is a Model?

According to Stachowiak (1973, pp. 129-133), models are representations of an original. The original can be definitions or a part of an imaginary world, i.e. symbolic, or part of the material world, i.e. physical structures. All models feature the three attributes of *reduction, representation and pragmatism.* Models *reduce*, as they only cover aspects of the original which are relevant for model developers or users. From a *pragmatic* viewpoint, they are representations of something and at the same time representations for someone or something, at a certain time and with a certain purpose.

For systems, Reddy (2011, p. 5) differentiates between empirical and structural models. Empirical models are based on collected data representing properties of the system (e.g. econometric models). Structural models apply mathematical relationships derived from theories about the physical nature of the system. However, both model types consist of four elements (Voigt 2016, p. 20):

- numerical assumptions for exogenous variables (input variables),
- numerical results for endogenous variables (output variables),
- mathematical equations, which establish relationships between the two above,
- and modelling parameters to adjust this relationship.

The Relationship between Models and Scenarios

Given the description of models above, a scenario can be understood to be a representation of a future original, i.e. a model. However the terms model and scenario are not interchangeable. While scenarios are by definition also models, models are not always scenarios, as the latter exclusively deal with future developments or possibilities.

Within the context of ESA and within this thesis, the term model refers to structural or empirical mathematical representations applied in connection with future oriented scenarios. Within scenarios, mathematical models are used to simulate the quantitative component.

2.3.2 Models, Model Generators and Modelling Frameworks

Models can be created with so-called model generators and/or modelling frameworks. The conceptual distinctions between models, model generators and frameworks and their implications are given below.

According to the definition of the Python package, Pyomo, models can be *concrete* or *abstract*. Abstract models have unspecified parameter values and may by used to specify a concrete model instance (Hart et al. 2012, pp. 14-15). Abstract models can be designed for a real world problem to create a set of concrete models with different parameters (e.g to simulate a set of scenarios). By this definition, abstract models are similar to model generators. Model generators (sometimes described as model frameworks), serve as tools which provide a predefined set of abstract technology and market descriptions based on a specific methodology and analytical approach, implemented with a specific mathematical approach. However, the construction of abstract models is based on an existing or future object, while model generators do not relate to any specific object at all. Model generators feature a higher level of abstraction than abstract models.

A central characteristic of models is the function to represent a physical and/or symbolic object. It is not possible to create an energy system model without a physical or symbolic energy system which has some sort of system boundaries, defined by a specific geographical and temporal scope. These system boundaries are not required for model generators. The *Atlantis* energy system example provided by the developers of the model generator OSeMOSYS (Howells et al. 2011) illustrates the problem of a missing representational object. To illustrate the usage of their model generator, a model was created which represents the artificial, i.e. symbolic, energy system.

In contrast to models and model generators (model frameworks), modelling frameworks[2] are related to a specific analytical approach or theory. Modelling frameworks are defined as tool-boxes with a diverse set of software libraries, which are required to model energy systems. Such a tool-box can include model generators, libraries to construct demand profiles or renewable energy supply profiles based on weather, and source code for pre- and post-processing data including visualisation software.

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[2] Note the slight, but important, difference between model framework and modelling framework.

The distinction between models and model generators is crucial for a sound comparison or classification of modelling tools, but generally ignored by authors in the energy system modelling field. Different authors state that their goal is to review energy system models. However, in many cases energy system models and energy system model generators are mixed. As an example, Savvidis et al. (2019, p. 503) incorrectly lists the PyPSA model generator (Brown et al. 2018b) together with the LIMES-EU model (Osorio et al. 2020) for comparison; the PyPSA-EU model would have been correct (Hörsch et al. 2018). This type of mixing can be found in different scientific reviews on modelling tool comparisons (Hall and Buckley 2016; Bhattacharyya and Timilsina 2010; Savvidis et al. 2019; Prina et al. 2020b). The lack of theoretical conceptualisation of models can lead to false conclusions about the usefulness of models, model generators and frameworks, which all come with inherent strengths and weaknesses. If compared with regard to a specific purpose, results can therefore be biased.

2.3.3 Energy System Modelling Tools

Energy system modelling tools cover a broad spectrum. Predictive or forecasting models are used in short-term planning by grid operators for electricity grid operation and by energy supply companies for operational optimisation of dispatch (unit commitment). In these companies, models are also used for investment decision support. Explorative models, in combination with scenario analysis provide a long-term perspective and are also used for investment planning. In addition, explorative models are applied for policy advice to assess social, environmental or economic impacts of energy system developments and analyse dynamics among energy and non-energy sectors. Depending on the purpose, modelling tools differ on a fundamental level with regard to their 1) analytical approach, 2) underlying methodology and 3) mathematical approach. These three characteristics have significant impact on the extent and detail of technology and market representation, the geographical and sectoral coverage, the spatial and temporal resolution, and the time horizon within models.

Analytically, **Top-Down** (aggregated) vs. **Bottom-up** (disaggregated) energy modelling approaches are differentiated with regard to technology and market representation (Nakata 2004). The extensive description of these two categories can be traced back to Grubb et al. (1993) who interestingly state that "top-down and bottom-up are very imprecise terms" (p. 435). This statement can also be considered to be true for the underlying methodologies described below.

The top-down approach is often described as the economic perspective, using aggregated economic indices to represent market dynamics of the whole economy. Within these macro-economic approaches, technologies are modelled as "black-boxes" in efficient markets resulting in a production frontier. Top-down models are closely linked to economic theories and traditions and are assumed to be consistent with cost minimisation of producers and utility maximisation of consumers. Due to their aggregated representation, these models are less suited to the representation of systems with high shares of intermittent renewable energy technologies. Bottom-up models, referred to by some as the engineering approach, are energy sector specific and provide explicate representation of existing and emerging demand and supply technologies, energy carriers and conversion processes. While these approaches allow for a better technology representation, they do not cover feedback to other parts of the economy. Generally top-down models are considered to be pessimistic with regard to efficiency gains on the end-use side, while bottom-up models are considered to be rather optimistic (Grubb et al. 1993, pp. 435-436). Hybrid approaches attempt to combine the advantages of the technological detail of bottom-up models and representation of the whole economy in top-down models. However, dimensional limitations pose hurdles for practical applications of hybrid models (Böhringer and Rutherford 2008).

Models can been developed by applying different methodologies that reflect theory about the agent behaviour within the modelled system. Three important distinctions can be made between **equilibrium, optimisation, and simulation** methodologies.

The first distinction is made between **optimisation models**, where total system costs are minimised, and market **equilibrium models** where prices and quantities equilibrate (Hedenus et al. 2013). For macro-economic analyses, computable general equilibrium (CGE) models, which cover multiple sectors of the economy, have been applied since the 1980s (Despotakis and Fisher 1988; Nordhaus and Yang 1996; Gabriel et al. 2001; Bohringer and Loschel 2006; Huppmann and Egging 2014; Babatunde et al. 2017). The behaviour of economic representative agents within these models follows a neoclassical, i.e optimising, rationale. Partial equilibrium (PE) models are a special case of equilibrium models, which only cover one sector. As CGE models are associated with neoclassical economics, where prices, output, and input are the result of supply and demand functions, which include production factors such as capital and labour, they are often used within top-down approaches. Despite their neoclassical foundation, a strength of CGE models is the possibility to model strategic behaviour, imperfect competition and non-market clearing (Dagoumas and Koltsaklis 2019, p. 1573). It is noteworthy that under certain assumptions, optimisation and equilibrium models yield the same results (Grubb et al. 1993; Hedenus et al. 2013). For example, PE models of the electricity sector can be formulated as a total welfare maximisation problem if assumptions on perfect competition and information are made.

(Design) **optimisation models** often follow the approach of specific partial equilibrium models. To determine an optimal set of technologies, total system cost is minimised leaving the demand and prices fixed (Herbst et al. 2012, p. 120). However, additional constraints such a maximal CO_2-emission limit can be added to these models. Also, bottom-up optimisation models can be applied by maximising the profit of a single utility under given costs and prices. Mathematical programming, plays an important role in formulating and solving these models. In some cases, CGE models can be solved by converting them into Mixed Integer Linear Programs (MILP) or Non-Linear Programs (NLP).

If used as a modelling classification, optimisation generally refers to the underlying rationale for decisions represented within the model. Therefore, an important distinction between optimisation and **simulation models** can be made with regard to the modellers role in designing future energy systems (Lund et al. 2017, pp. 7-10). For Connolly et al. (2010, p. 1063), a simulation tool simulates the operation of a given supply system. Note, that such simulation can also be carried out with optimisation methods if assumptions of markets functioning close to the neoclassical theory are justified. In design optimisation, an optimal configuration of an energy system is based on a set of constraints and a defined objective. With the simulation approach, important decisions relating to system design are made by the modeller, i.e. technology development within the system is driven by exogenous scenario assumptions and a set of rules which describe desired or observed system behaviour (Nakata 2004; Herbst et al. 2012). Simulation methods have been applied for ESA and include system dynamics (Ansell and Cayzer 2018; Gravelsins et al. 2018; Liu and Xiao 2018; Qudrat-Ullah 2013) or agent-based approaches.

Other methodologies to analyse and plan energy systems use input-output models (Ansell and Cayzer 2018; Liu et al. 2019; Zhang et al. 2019), or econometric models (Dagoumas and Barker 2010; Pretis 2020). These methodologies are based on empirical data and are often applied within top-down models, i.e. models of more than one economic sector. As both types depend on historical data, which represent a current picture of the economy, they are rather suitable for short-term and medium-term analysis, where the system under study does not undergo significant changes (Herbst et al. 2012, p. 114).

Finally, all of the described methodologies and approaches can be combined within modelling tools in different ways (Fragkos et al. 2017; Kahsay et al. 2019; Krook-Riekkola et al. 2017).

2.3.4 Energy System Modelling Challenges

The three transformations of market liberalisation, renewable energy transition and open science, described in Section 2.2, pose challenges for ESA and particularly modelling. These challenges have been analysed from different perspectives and categorised in the last decade. At this point, a summary of published scientific reviews on these challenges will be provided as one of the reviews is part of this thesis in Chapter 3.

One of the first attempts to review and categorise challenges for the domain of energy system modelling was undertaken by Pfenninger et al. (2014). To review the challenges, the authors distinguish model paradigms of: a) optimisation models, b) simulation models, c) power system and electricity market models and, d) qualitative and mixed scenarios. For these four paradigms, the corresponding challenges were identified: 1) resolving details in time and space 2) uncertainty and transparency, 3) complexity and optimisation across scales and 4) including the human dimension. While the authors argue that uncertainty and transparency are particularly relevant for simulation models, these two challenges are not unique to the simulation model paradigm. Transparency is an important characteristic for all scientific models. Likewise, uncertainty is not only a challenge for simulation models but also for power market models. However, in both cases the origin and the degree of uncertainty may differ. With a focus on energy modelling frameworks, Wiese et al. (2018) describe five main energy system challenges of: 1) complexity, 2) scientific standards, 3) utilisation, 4) interdisciplinary modelling and 5) uncertainty. Lopion et al. (2018) review current trends and challenges in energy system modelling and conclude that climate protection strategies in European countries has led to the development of many new models since 2000. Within this set of models, open source approaches are identified as a significant trend. In addition, complexity is named as a central challenge for renewable energy system modelling (Lopion et al. 2018). An analysis by Prina et al. (2020b) provides a classification for bottom-up energy system models and associated challenges, which are resolutions in time, space, techno-economic representation, and sector-coupling. In addition, they stress that transparency is a challenge which needs to be addressed.

All of the articles mentioned above, highlight the need for higher transparency and reproducibility, i.e. open modelling. In addition, the analysis of energy system modelling challenges is centred around problems of technical (supply-side) challenges, such as the complexity posed by increasing shares of renewable energy sources.

2.3.5 The Role of Social Sustainability Strategies

A focus on technical sustainability strategies to shape energy transitions has been identified as a problem by different authors. Sovacool et al. (2015) criticise that there is a “preponderance of quantitative perspectives, mapping a general tendency to propose technical solutions to social problems” (p. 96). Therefore, Sovacool et al. 2015, p. 95 recommend better collaboration between techno-economic (physical) and social sciences to design future energy systems. Similarly, Pfenninger et al. (2014, p. 79) state that one shortcoming of current modelling practices is a tendency for modellers to focus on technological and economic factors which lend themselves to modelling.

The exclusion of social sciences and a predominance of techno-economic methods may be reasons for the emphasis on technical strategies, i.e. consistency and efficiency measures, to the exclusion to social ones, i.e sufficiency. From the perspective of sustainable energy systems transitions, this exclusion can be criticised. An exclusive focus on consistency measures neglects the fact that energy use is an important factor in shaping the energy transition (Grubler 2012, p. 10). Moreover, in some cases, technology change cannot solve the problems. In the case of mobility, Jochem et al. (2016, p. 74) conclude that the external costs of internal combustion engine vehicles and electric vehicles do not differ significantly. Another aspect are rebound effects (Binswanger 2001) of efficiency measures which have been observed and analysed by numerous authors (Font Vivanco et al. 2016). These effects can account for up to 100 % of the initial efficiency savings (Stern 2020; Wei and Liu 2017).

As a result, authors argue that lifestyle changes may be indispensable to achieve ambitious public policy climate goals (Samadi et al. 2017; Trainer 2007). For example, complying with the 1.5°C goal of the Paris Agreement is becoming increasingly challenging due to shrinking carbon budgets. In this context, Pye et al. (2021) conclude that “this includes the need for radicalism in exploring solutions, including those not yet deemed politically palatable or salient [...]” (p. 228). These solutions may include different demand-side sufficiency mitigation measures which are currently underrepresented in ESA.

2.4 Open Energy System Modelling

Dieckhoff and Grunwald (2016) have analysed the role and usage of energy scenarios for energy policy advice and conclude that scenarios used for scientific consulting must be *scientifically valid, transparent and unbiased.* As shown in section 2.3, software tools, in particular models, are a critical part of energy scenarios. However, a large proportion of models applied by utilities, consultancies and public research institutes continue to be inscrutable ‘black boxes’. (Pfenninger et al. 2017, p. 211). As a consequence, scientists in the field of energy system modelling have criticised the lack of transparency and a lack of reproducibility of model-based results, and argue for open source and open data approaches aligned with sound scientific practices (DeCarolis et al. 2012; Pfenninger 2017; Pfenninger et al. 2018; Morrison 2018; DeCarolis et al. 2017; Cao et al. 2016; Hülk et al. 2018). Indeed, a trend in energy system modelling towards increasing transparency by applying open source and open data approaches can be observed in recent years (Lopion et al. 2018, p. 160). The first open source model, released in 2001, is Balmoral, which was designed to analyse the Danish and North European energy system (Ravn 2001). This marks the starting point for open source model development in the energy system modelling field. However, the development of open source tools did not pick up speed before around 2010. In spite of the trend, authors such as Oberle and Elsland (2019) ask whether open access models are able to assess today's energy scenarios. This question relates to the problem of knowledge creation within non-liberalised markets as described above. Tools developed since the 1970s which include closed data sets have a large lead compared to open initiatives starting from scratch. Nevertheless, it is arguable whether there is still a gap between closed and open tools.

2.4.1 The Open Modelling Process

According to the *Open Definition* of the Open Knowledge Foundation, "[o]pen means anyone can freely access, use, modify, and share for any purpose" (OKFN 2018). In line with this definition, the open modelling process has previously been described by us in the article "Opening the black box of energy modelling: Strategies and lessons learned" and it is illustrated in Figure 2.2. The core practices of open data, open source and open access are applied at different stages of the modelling process, which includes the interpretation of results.

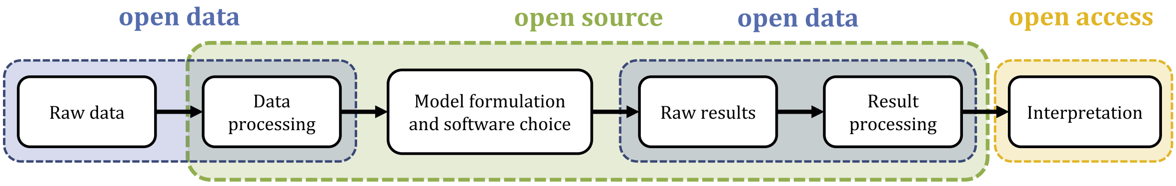


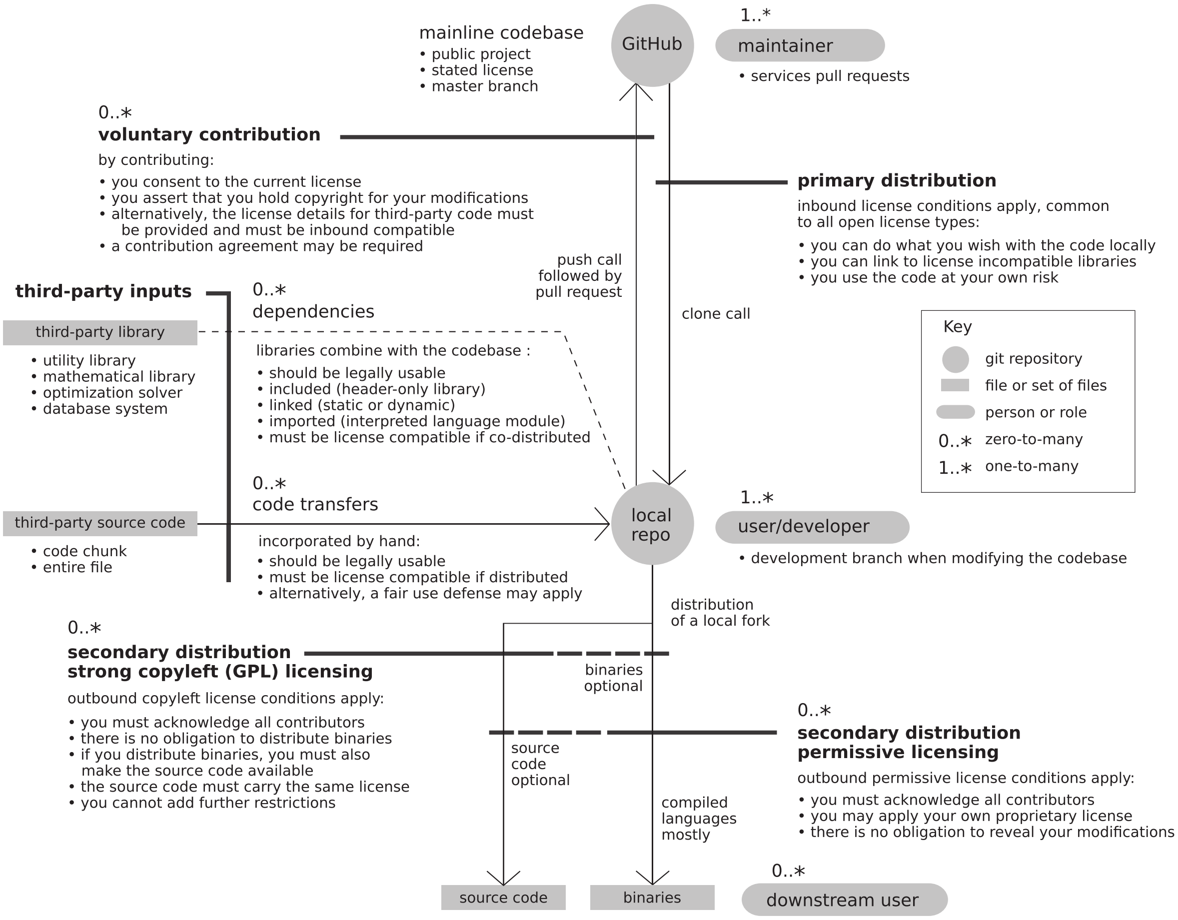
Figure 2.2: Schematic illustration of an idealised open modelling process based on Pfenninger et al. (2018, p. 64).

While the open modelling process looks straightforward, it faces several challenges. For scientists, there is additional work to be carried out, such as writing documentation and clearing source code or data. This can take a significant amount of time. If implemented poorly, data and source code may be accessible by other researchers but not comprehensible, and transparency and reproducibility may suffer. Another challenge for the implementation of the open modelling processes can be rooted within the scientific institutions which adhere to closed source and data policies due to business cases and unique selling points (Pfenninger et al. 2017, p. 211). Even when institutions are willing to be open, scientists may be confronted with path dependencies when closed source (proprietary) software has been used for a long time within the institution. Switching to open modelling will require time and knowledge, which may not be available due to financial resource restrictions. Lastly, the open modelling process is hampered when data from statistical offices or other sources is not available under open licenses and hence the distribution is limited (Pfenninger et al. 2018, p. 69).

Open Source

Open source is not limited to the provision of software source code. According to the Open Source Initiative, open source software must be free, allow for modification, redistribution under the same license, and should be non-discriminatory against persons or fields of endeavour (OSI 2007). Moreover, a key characteristic of open source is the practice and principle of collaboration (see Levine and Prietula (2013)).

With or without collaboration, the distribution of source code can be achieved by using platforms such as GitHub or Gitlab. These platforms leverage the usage version control system, such as *git*, by not only tracking changes but also allowing for the management of the whole project development including (external) contributions, bug reports and software documentation. A typical development and distribution architecture is shown in Figure 2.3.



mainline codebase
- public project
- stated license
- master branch

- services pull requests

by contributing:
- you consent to the current license
- you assert that you hold copyright for your modifications
- alternatively, the license details for third-party code must be provided and must be inbound compatible
- a contribution agreement may be required

inbound license conditions apply, common to all open license types:
- you can do what you wish with the code locally
- you can link to license incompatible libraries
- you use the code at your own risk

- utility library
- mathematical library
- optimization solver
- database system

libraries combine with the codebase :
- should be legally usable
- included (header-only library)
- linked (static or dynamic)
- imported (interpreted language module)
- must be license compatible if co-distributed

- code chunk
- entire file

incorporated by hand:
- should be legally usable
- must be license compatible if distributed
- alternatively, a fair use defense may apply

- development branch when modifying the codebase

outbound copyleft license conditions apply:
- you must acknowledge all contributors
- there is no obligation to distribute binaries
- if you distribute binaries, you must also make the source code available
- the source code must carry the same license
- you cannot add further restrictions

outbound permissive license conditions apply:
- you must acknowledge all contributors
- you may apply your own proprietary license
- there is no obligation to reveal your modifications

Figure 2.3: Open modelling development and distribution architecture based on GitHub. Source: (Morrison 2018, p. 58).

To understand and use this architecture successfully, operators need to have knowledge of suitable ways of using the underlying versioning software *git*. In-depth information on the efficient usage of git can be found in Westby (2015). The code-base is hosted on GitHub (or a similar platform) and maintained by one or more people. These people manage and review new code, which can be used to enter the software via so-called pull requests. Users and developers can clone (download) the repository to their local machine and use and/or make changes to the source code. In the majority of cases, the software depends on other third-party inputs (dependencies), which are also downloaded when a repository is cloned. From local repositories, secondary distribution of the software can take place in accordance with requirements of the license.

Open Data

To allow for reproducible research, raw, intermediate and result data should be (made) publicly available. Intermediate and result data can be indirectly provided if a reproducible workflow is followed and all processing software scripts are made available (Sandve et al. 2013). Ideally, it should be possible for every part of the intermediate and result data to be regenerated. With regard to result data, the generalised FAIR principles proposed by Wilkinson et al. (2016) are important for energy systems modellers. Making data findable, accessible, interoperable and reusable, i.e. FAIR, requires assigning unique identifiers, adequate meta data in a standardised format and appropriate licensing.

The data can be published with a unique digital object identifier (DOI) on platforms such as Zenodo (CERN and OpenAIRE 2013) or the Open Science Framework (COS 2020). Additionally, the Open Science Framework (OSF) enables data sets to be published while they are still under development and allows them to be integrated with associated pre-registrations and pre-prints. Within its Open Energy Database, the Open Energy Platform (OEP 2020) provides an automated way to retrieve and query data sets via an application programming interface (API). The ability to publish a scenario data set on such a platform is one of the preferable ways to achieve reproducibility without barriers. For the publication of (numerical) data, a standardised format can be used, which enables automated handling as well as allowing for it to be readable by humans. For this purpose, the Open Knowledge Foundation has developed specifications for so-called *frictionless datapackages* (OKFN 2019).

Version control systems for data, which are comparable to source code version control systems, such as *git*, do not yet exist for all data formats. For data tables such as Data Packages, one way to apply version control is to use the *daff* software, which allows for file comparison. In addition, the software generates summaries of file differences, which can be stored and used to reconstruct versions of a file (Fitzpatrick 2013).

In addition to general software tools and platforms such as *git*, the *OSF* or *zenodo*,there are dedicated open data projects in the energy system modelling field. For example, the *Open Power System Data* (OPSD) platform aims to make not only statistical power system data but also model results available in a FAIR way (Wiese et al. 2019). Another energy system data project *Hotmaps*, which is funded within the

EU Horizon 2020 research program, focuses on heating and cooling (Hotmaps 2019; Pezzutto et al. 2019). Both projects utilise frictionless Data Packages.

Licensing

Questions of (third-party) compatibility of software and intellectual property are important for model developers and users that want to use open source software and open data. Like proprietary software and data, openness requires licenses for software, data and content which differ with regard to possible purpose of use, modification and (re)-distribution. The legal aspects of open modelling are a highly relevant and large area of study. However, these issues are not treated in this thesis. Relevant information can be obtained from Morrison (2018) for a general overview and Hirth (2020) for data-related aspects.

2.4.2 Open Model Generator Landscape

This section provides an overview of current open energy system model generators. To create this list, 55 open source tools from the Open Energy Modelling Initiative website were analysed. Of these 55 tools, 22 do not focus on specific regions and can be considered to be model generators. Some of the remaining 23 tools can possibly be adapted to other geographical regions, but their purpose is not to serve as a generalised model generator. Additionally, model generators formerly under a closed license were added to the list, resulting in a list of 24 model generators. This list includes an open source version of the Integrated Assessment Model (IAM) MESSAGE with an additional modelling platform with connections to databases and different models which was released in 2018 (Huppmann et al. 2019), as well as the TIMES model released on GitHub under an open license in 2020.

Table 2.1 provides a list of open source model generators. The year specifies the time a tool was either labelled as an open source tool in academic literature or source code from the tool was made publicly available, e.g. via Github. All of the model generators listed in the table follow bottom-up approaches, with a large number of them applying an optimisation methodology applying mathematical programming approaches such as Linear or Mixed Integer Linear Programming (MILP). Therefore, algebraic modelling language designed for mathematical programming such as GAMS or libraries within high level programming languages such as pyomo (Hart et al. 2012) for Python and JuMP (Dunning et al. 2017) for Julia are widely used. It should be noted, that GAMS model generators can be considered a borderline case with regard to the categorisation of being open source, as modellers need a proprietary GAMS version to compute models, which can pose significant barriers with regard to re-usability.

Table 2.1: List of open source model model generators. Source: Own compilation based on data from OpenModInitiative (2021).

Name	Year	Meth	EX	OO	IO	UC	Model Software	Math
Temoa	2010	Opt	✓	✓	✓		Python/Pyomo	MILP
OSeMOSYS	2011	Opt	✓	✓	✓		GNU MathProg	LP
Urbs	2012	Opt		✓	✓	✓	Python/Pyomo	MILP
Mosaik	2013	Sim	-	-	-	-	Python	Agent
Calliope	2014	Opt		✓	✓	✓	Python/Pyomo	MILP
oemof-solph	2014	Opt		✓	✓	✓	Python/Pyomo	MILP
ficus	2015	Opt		✓	✓	✓	Python/Pyomo	MILP
OnSSET	2015	Opt	✓	✓	✓		Python	LP
PyPSA	2015	Opt		✓	✓	✓	Python/Pyomo	MILP
Switch	2015	Opt	✓	✓	✓		Python/Pyomo	LP
SAM	2016	Sim			✓		C++, WxWid.	indiv.
backbone	2017	Opt		✓	✓	✓	GAMS	MILP
ESO-X	2017	Opt	✓	✓	✓		GAMS	MILP
OMEGAlpes	2018	Opt		✓	✓		Python/PuLP	MILP
MESSAGEix	2018	Opt	✓	✓	✓		GAMS, Python	MILP
AnyMod	2019	Opt	✓	✓	✓	✓	Julia/JuMP	MILP
CapacityExpansion	2019	Opt	✓	✓	✓		Julia/JuMP	LP
EOLES_elec	2019	Opt		✓	✓		GAMS	LP
EnergyRt	2019	Opt	✓	✓	✓		GAMS	LP
OpenTUMFlex	2020	Opt		✓		✓	Python/Pyomo	MILP
POMATO	2020	Opt		✓		✓	Julia/JuMP	indiv.
PyLESA	2020	Sim		✓			Python	indiv.
Reopt	2020	Opt		✓	✓	✓	Julia/JuMP	MILP
TIMES	2020	Opt	✓	✓	✓		GAMS	MILP

EX: Expansion, OO: Operational Optimisation, IO: Investment Optimisation, UC: Unit Commitment, Math: Mathematical Approach, Meth: Underlying Methodology, Opt: Optimisation, Sim: Simulation.

With regard to the underlying software of model generators, a shift from Pyomo to JuMP can be observed. Pyomo was used in many model generators after 2010, before JuMP was developed. However, as Julia allows for the use of computational resources with high efficiency and user-friendliness at the same time (Bezanson et al. 2017), a significant number of the model generators developed since 2019 have been built on JuMP.

In most model generators, optimisation can be carried out for operation and/or investment of the system, but multi-period expansion (EX) optimisation and unit commitment (UC) functionality are mutually exclusive. This can partly be explained by the tools purpose. For example, POMATO is a power market model generator for short-term planning including a flow-based-market-coupling mechanism (Weinhold and Mieth 2020). This tool requires detailed operational modelling of energy supply technologies and market mechanisms but no investment or expansion modelling. For long-term and exploratory analysis, the level of technological detail is limited by computational resources. Thus, model generators such as OSeMOSYS (Howells et al. 2011) or CapacityExpansion (Kuepper et al. 2020) do not generally include UC functionalities. The only software which covers all four types of optimisation is the recently developed AnyMod model generator (Göke 2020). However, this does not mean that all functionalities will be used within a specific model instance as computational restrictions apply as well.

The purpose of the listed model generators ranges from power market operation and analysis of local energy systems to investigations of sector-coupled and internationally-connected energy systems. To illustrate the broad range of research questions addressed with open modelling tools, a collection of selected peer-reviewed literature is provided below.

Short-term / local and regional

For some model generators, such as OMEGAples or Mosaik, there is no scientific literature about there applications as they are not being used by academics but rather in applied energy system design by consultants on single power plants, at local or regional level. For example, OMEGAlpes has been designed for urban energy system optimisation to support decision making for energy district development (Pajot et al. 2019). The Mosaik toolbox is one of a few simulation software and was built to develop smart-grid control strategies based on agent-based scenario simulations of smaller energy (sub-)systems (Rohjans et al. 2013). For these tools, documentation of model and application will be found in (interal) reports or presentations instead of international scientific journals.

Nevertheless, peer-reviewed literature in energy system and economic related journals exists for local applications of model generators. From a local perspective, Zade et al. (2020) use OpenTUMFlex to analyse the flexibility potential of electrical vehicles in German and Californian energy markets. In addition, district heating systems have been analysed with oemof-solph models by applying MILP approaches (Wehkamp et al. 2020; Boysen et al. 2019). Similarly, Atabay (2017) applies a ficus based MILP model to design a distributed energy system of a factory.

In addition, scientific analysis have been carried out with a short-term planning focus. Two examples include a stochastic unit commitment and economic dispatch optimisation, which was carried out with a *backbone* model by Rasku et al. (2020) to analyse the effect of weather forecasts on power system planning, and an analysis of different strategies for predictive parameters in flow-based-market-coupled systems conducted by Schönheit et al. (2020).

Long-term / (inter)-national

More scientific literature exists on long-term and (inter)-national analyses than on local or regional and short-term applications. Morgenthaler et al. (2020) deploy the calliope model generator (Pfenninger and Pickering 2018) for an long-term analysis of cost-optimal layout and operation of distributed electrolysis sites in Europe. Hainsch et al. (2020) combine the AnyMod model with an OSeMOSYS model (GENeSYS-MOD) to model long-term energy system pathways to 2050 in EU which comply with the 1.5 °C target of the Paris Agreement.

Co-benefits of sector-coupled energy systems in Europe without a specific target year but with an international long-term perspective have been identified by Brown et al. (2018c) using the PyPSA-EUR model (Hörsch et al. 2018). The impact of renewable energy and transmission grid expansion on the European power market has been analysed by Schaber et al. (2012).

Eshraghi et al. (2018) analysed possible long-term developments of CO_2 emissions to 2040 in the US in the absence of a federal climate policy using Temoa. Long-term optimisation applications based on OSeMOSYS have also been applied for renewable energy system analysis in many non-Western countries, such as Tunisia (Dhakouani et al. 2017), Brasil (Moura et al. 2018) and India (Riva et al. 2019). Zhou et al. (2020) used a MESSAGEix-based IAM model for scenario analyses of decarbonisation pathways in Asia.

Several other publications detailing the application of PyPSA, OSeMOSYS, Urbs, and Calliope are listed on the corresponding project websites and show the high relevance of open source model generators for the analysis of current and future energy system.

2.5 Scope of Publications

This Section provides background information and a conceptual framework for topics covered (and not covered) within academic publications in Part 2 of this thesis.

Energy systems are affected by significant technological, economic and scientific changes, which have significant impact on the analysis of systems. On the one hand, system complexity is increasing due to energy system transformation and energy market liberalisation. On the other hand, a call for transparency and reproduciblity is made by many scientists in the field of ESA. This call is part of a general trend towards open science with crucial aspects of openness and collaboration. All of this is taking place in the light of climate change, which is prompting a search for solutions in line with global sustainable development.

With regard to open science, this thesis contributes to advances in collaborative open source model development (Chapter 4 and 5) and reproducible model-based research (Chapter 6). Other practices of Open licensing, Open Data, Open Metrics, and Open Review may be touched upon, but are not the focus of this thesis.

Theoretically, the work within this thesis is not restricted to a specific analytical modelling approach or methodology. However, the research was carried out using bottom-up optimisation (Chapter 7 and 8) and simulation approaches (Chapter 9). In addition, the thesis deals with publicly-funded energy modelling for policy advice and excludes tools developed by companies and utilities for internal use. Most of these publicly-funded models are used for strategic mid- to long-term energy system planning. Therefore, short-term planning models, particularly affected by energy market liberalisation, are not dealt with in depth.

Within this thesis, energy systems are understood as not only techno-economic systems, but also complex social ones. Hence, their analysis is a multidisciplinary field requiring different quantitative and qualitative methods. Energy system analysis tools, in particular computational models, support sustainable energy systems design but are no end in themselves. Therefore, a contribution to shaping sustainable energy systems is made by going beyond techno-economic optimisation approaches and addressing climate change mitigation new measures on the end-user side (Chapter 9).

Part II - Publications

3

A qualitative evaluation approach for energy system modelling frameworks[1]

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Energy, Sustainability
and Society

REVIEW Open Access

A qualitative evaluation approach for energy system modelling frameworks

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Abstract

Background: The research field of energy system analysis is faced with the challenge of increasingly complex systems and their sustainable transition. The challenges are not only on a technical level but also connected to societal aspects. Energy system modelling plays a decisive role in this field, and model properties define how useful it is in regard to the existing challenges. For energy system models, evaluation methods exist, but we argue that many decisions upon properties are rather made on the model generator or framework level. Thus, this paper presents a qualitative approach to evaluate frameworks in a transparent and structured way regarding their suitability to tackle energy system modelling challenges.

Methods: Current main challenges and framework properties that potentially contribute to tackle these challenges are derived from a literature review. The resulting contribution matrix and the described application procedure is then applied exemplarily in a case study in which the properties of the Open Energy Modelling Framework are checked for suitability to each challenge.

Results: We identified complexity (1), scientific standards (2), utilisation (3), interdisciplinary modelling (4), and uncertainty (5) as the main challenges. We suggest three major property categories of frameworks with regard to their capability to tackle the challenges: open-source philosophy (1), collaborative modelling (2), and structural properties (3). General findings of the detailed mapping of challenges and properties are that an open-source approach is a pre-condition for complying with scientific standards and that approaches to tackle the challenges complexity and uncertainty counteract each other. More research in the field of complexity reduction within energy system models is needed. Furthermore, while framework properties can support to address problems of result communication and interdisciplinary modelling, an important part can only be addressed by communication and organisational structures, thus, on a behavioural and social level.

Conclusions: We conclude that the relevance of energy system analysis tools needs to be reviewed critically. Their suitability for tackling the identified challenges deserves to be emphasised. The approach presented here is one contribution to improve current evaluation methods by adding this aspect.

Keywords: Energy system analysis, Model challenges, Open science, Open source, Energy modelling framework, Oemof

Background

Energy systems are subject to substantial structural change, mainly due to environmental reasons and concerns about supply security. One central driver for these changes is the increasing share of decentralised and intermittent generation units based on renewable energy. As energy constitutes one foundation of modern societies, modification within the generation, consumption, and distribution of energy affects a broad range of stakeholders. Ministries and likewise municipalities as well as economic and social interest groups are confronted with a constantly changing environment and high uncertainty regarding the future composition and design of increasingly complex energy systems.

Within the transformation process, model-based analyses have become indispensable for advice addressing a diverse set of questions. Among others, this includes grid

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control and planning, dispatch and unit commitment, expansion planning, and energy market design, as well as environmental and social analysis of highly integrated energy systems. Energy system modelling software has been heavily discussed, and in recent years, model-based results have been criticised for the black box character of internal model logic and underlying assumptions [1, 2]. As a result, more researchers have opened their software and data [3] which improves transparency, enables reproducibility, and allows other people to re-use or build upon existing tools. Thus, a rough division into a group of closed (*1st generation*) and a group of open (*2nd generation*) energy system models and frameworks can be identified [4].

The diverse research questions associated with the transformation of energy systems can obviously not be addressed by one single model or approach. This is underpinned by the large amount of existing models and their differentiation along social, technologic, and economic lines.

In the following, we distinguish between the three terms *model*, *model generator*, and *framework*. Models are concrete representations of real-world systems (e.g. with a specific regional focus and temporal resolution). Such a representation may consist of multiple hard- or soft-linked sub-models to answer clearly defined research questions. Models can be built from model generators that allow to build models with a certain analytical and mathematical approach (e.g. by the use of a pre-defined set of equations and represented technologies). Finally, a framework can be understood as a structured toolbox including sub-frameworks and model generators as well as specific models (e.g. wind feed-in models).

Although existing energy model and framework overviews are not comprehensive [3, 5], it is obvious that their number is growing. Multi-purpose model generators or frameworks such as MARKAL [6], TIMES [7], OSeMOSYS [8], PyPSA [9], or oemof [4] are important within the energy modelling community. In this context, it is crucial for users and developers to identify software that is fit for the intended purpose. Due to the nature of model generators and frameworks with their multi-purpose design and versatility, this task is not trivial. Hence, methods for quantitative as well as qualitative evaluation are important in terms of software selection. For this task, scientific model comparisons for specific models and model fact sheets as well as transparency checklists have been proposed (see section 'Background and motivation'). However, there is a lack of comprehensive evaluation of energy modelling software with regard to their suitability for tackling described modelling challenges.

In this paper, we propose a qualitative evaluation approach as a step towards model generator and framework evaluation. To illustrate its application, we apply the approach to a 2nd generation energy modelling tool. Within a case study, the Open Energy Modelling Framework (oemof) is evaluated regarding its capability to address present and future challenges in energy system modelling.

First, we give a short overview on existing evaluation approaches in the 'Background and motivation' section. Then, we describe the 'Method' section to derive our evaluation approach. Subsequently, the 'Challenges' section is discussed and summarised in combination with the 'Framework properties' section. This forms the basis for the presented evaluation approach, for which the 'Application procedure' section is described. In the next step, the approach is applied exemplarily in the 'Case study' section. Finally, we discuss the proposed approach and general findings of the challenge-property-matching in the 'Discussion' section. The 'Conclusions' section summarises the main findings.

Background and motivation

An evaluation of energy system modelling software can be undertaken by quantitative, qualitative, or mixed methods. Quantitative approaches may be used to evaluate performance in terms of run-time or computational traceability as well as accuracy of results. The US Energy Modelling Forum has conducted model comparisons since the 1980s by looking at the foci of models, their internal logic and representation, and their results (see e.g. [10, 11]). One example is the ongoing project *RegMex*, comparing simulation pathways of renewable energy systems [12]. In this context, standard test cases serve as a common basis for model comparisons. A mixed quantitative and qualitative approach is used in [13], where the evolution of a model is characterised by comparing different model versions. In that paper, specific input- and output-related metrics are defined to allow for quantitative comparison.

For analysing aspects that cannot be expressed in numbers, qualitative methods can be applied. Systematic reviews of models and presentations of classification schemes [14–17] fall into this category and are important for modellers, model users, and decision makers to identify the potential application scope of a model. Similarly, qualitative model comparison helps to understand the details of and differences between models that are designed to answer similar research questions. Another qualitative approach is presented in [18]. In order to increase transparency of energy scenario-based studies, a transparency checklist is proposed. In addition to enhanced transparency, this list may also provide a basis for model comparison. Besides reviews and comparisons, a presentation of consistent argumentation provides possibilities for analysing modelling software with respect to for example practicability or the degree of openness. To our knowledge, this kind of analysis has not been applied to energy system modelling software. In particular, an approach specifically designed for a qualitative assessment of model generators or frameworks does not exist.

We know that on the one hand, literature that identifies challenges for energy system modelling exists and on the other hand, model fact sheets characterise properties of models are available as well. However, a systematic mapping of how framework properties can serve as solutions to specific challenges is missing. An evaluation based on the relationship between challenges and framework properties could therefore facilitate progress in model tool development with regard to the actual research needs. Furthermore, an analysis focusing on model generators and frameworks is missing. The suggested approach builds upon fact sheets and checklists as well as on challenge classifications, but combines both and lifts it from model to framework level.

Method

First, a literature review is conducted to compile energy system modelling challenges. Each of the five derived challenges and respective underlying aspects are then discussed and reasoned. Subsequently, framework characteristics that have the potential to tackle the derived challenges are listed. These characteristics are mainly based on the Open Energy Platform framework factsheets [19], which describe the properties of existing frameworks. By means of existing reviews and own expert judgement, suitable properties are selected and summarised in the list of characteristics. Challenge aspects and property characteristics are summarised in a matrix which serves as a template for the suggested evaluation. In the next step, the application procedure is tested with a case study and subsequently adapted. We illustrate the application procedure of the suggested evaluation by including the case study in this paper.

Challenges

Overview

Other authors have characterised the field of energy system modelling and its models as opaque to outsiders [13, 15]. One reason for this may be the broad definition of the term *energy system model*. Depending on the research question, energy system models may range from detailed highly technical models of small sub-systems to large macro-economic models covering whole economies. Typical criteria for categorising models are top-down (macro-economic relationship of components) vs. bottom-up (technology specific) approaches, simulation vs. optimisation of the system, and partial equilibrium (e.g. considering only the power sector) vs. equilibrium (considering the whole economy) models [20]. For a comprehensive description of the model (generator) landscape as well as of model topology, we refer to existing reviews [14, 15, 21, 22]. We restrict our analysis to general challenges and their respective aspects in the field of energy system modelling. These challenges relate to steps in the modelling process as described by [23], ranging from the development of a mental model of an energy system to the application of the model including the communication of results.

Coming up with a classification scheme for energy modelling challenges can be compared to proposing a scheme for energy model classification with regard to the generality of the categories. In case of energy system models, various options for classification exist, though there are ‘few models—if any—that fit into one distinct category’ ([24], p.7). This is similarly true for categorisation of energy system modelling challenges. For our analysis, we propose the five major challenge categories *complexity, uncertainty, interdisciplinary modelling, scientific standards, and utilisation*, which are characterised by different relevant aspects, summarised in Table 1. Generally, the relevance of a challenge for specific software may vary as it is determined by the focus of the underlying research question. The subsequent sections provide a detailed description for each of the identified challenges.

Complexity

The challenge category *complexity* with its main aspects sector coupling, technical, temporal, or regional resolution, input data, and result processing is linked to the challenges in the *utilisation* category. There exists a continuous trade-off between modelling complex interactions

Table 1 Categorised energy system modelling challenges

Challenge	Aspects	Literature
Complexity	Increasing sector coupling, high technical, temporal and regional resolution required, extensive input data preprocessing, extensive result data processing	[20–22]
Uncertainty	Epistemic, aleatory, linguistic, decision, planning	[23, 31, 39]
Interdisciplinary modelling	Inclusion of the human dimension, energy-water-food nexus, common transdisciplinary understanding	[42, 44, 54]
Scientific standards	Transparency, repeatability, reproducibility, scrutiny, scientific progress	[57, 58, 64, 65, 68]
Utilisation	Usability, applicability, re-usability, result communication	[64, 72, 74, 77]

with the required level of detail and keeping the model or framework simple and comprehensible for the recipients of the results and for the modellers themselves.

Diversification, distributed generation, and stronger integration of energy sectors with versatile interdependencies are growing challenges for energy system modellers. Considering the power-heat-transport nexus, integrated models nowadays play a decisive role in providing insight into different flexibility options [25], using excess electricity economically [26], and for meeting climate goals [27]. While a high spatial and temporal resolution is required to consider varying weather conditions and cover different flexibility options, spatial and temporal coverage is also necessary for analysing the long-term development of an increasingly interconnected power system. For instance, Després et al. [20] conclude that long-term energy models would benefit from an improved representation of fluctuating renewable energy sources in the power sector. The growing requirement of flexibility particularly on the demand side (e.g. storage or demand side management) additionally increases modelling complexity in systems with high shares of renewables.

The increasing complexity of models is accompanied by a rising amount and complexity of input and result data. Data are crucial since its absence may hamper the development of new modelling techniques, as Krysiak and Weigt [28] argue in the case of demand side management modelling. Keirstead et al. [22] state that data availability is one challenge for (urban) energy system modelling. Acquiring or generating input data is not a trivial task, as it requires versatile software skills (e.g. geographic information systems, databases, reverse engineering) and may be linked to other sophisticated research areas (e.g. meteorology in the case of power production from wind turbines). Therefore, data processing to generate model input data is often not only one of the most time-consuming tasks of the whole modelling process but also adds to the complexity. Different kinds of input data from different sources need to be consistent, and their influence on the results have to be assessed adequately.

Regarding the output, models with high spatial, temporal, and technical resolution usually produce large amounts of result data that have to be analysed. Among other aspects, appropriate visualisation of multi-dimensional data (temporal, regional, unit-wise) is increasingly challenging with increasing dimensions of model complexity. Depending on the kind of application and question to be analysed, the processing of results may be a difficult and time-consuming task in itself. Even if the question to be analysed focuses on just one result parameter, the relation to other result parameters and the relation between varying input parameters and the result parameters of interest need to be checked thoroughly to grasp interdependencies.

Uncertainty

Uncertainty has already been identified as a challenge for energy system modelling decades ago [29]. Craig et al. [30] state that uncertainties in long-range energy forecasts are systematically underestimated. Uncertainty in terms of energy system modelling can be sub-classified into a number of aspects. Generally, literature has different scopes, approaches, and scientific backgrounds to classify uncertainty, resulting in different classification schemes [21, 23, 31]. Mirakyan and Guio miss a 'common agreement on typology of uncertainty' [23]. They propose a new framework that has a broader scope and a more detailed classification compared to uncertainties described by Pfenninger et al. [21] and Hunter et al. [31]. This framework for categorisation of uncertainty incorporates energy system modelling, decision making, and subsequent planning processes: (1) *linguistic uncertainty*, (2) *knowledge or epistemic uncertainty*, (3) *variability or aleatory uncertainty*, (4) *decision uncertainty*, (5) *planning procedural uncertainty*, and (6) *level of uncertainty*.

Even though not very often discussed in the context of energy modelling, the aspect of *linguistic uncertainty* (1) affects energy system planning and decision making based on model results. *Linguistic uncertainty* arises from natural language being vague and ambiguous, as meaning of words may change over time [32]. An illustrative example is the ambiguous use of the term *model*.

Knowledge or epistemic uncertainty (2) covers various levels of uncertainty related to context or framing, data, structure of a model, or framework, as well as technical and accumulated uncertainty that includes all other. Various examples for this type of uncertainty exist in literature, as this category covers a wide range. Assumed learning rates and consequently future costs (e.g. for renewable energy technologies) are decisive parameters for energy system models, as those often aim for minimal system costs. If not carefully chosen, biased results may lead to incorrect policy recommendations if they do not reflect the sensitivity of these assumptions [33]. Methods and key pitfalls of assessing future costs of energy technologies based on learning rates are an important topic among the research community [34, 35] that illustrates the importance of dealing with uncertainty related to assumptions and input data. Another problem related to uncertainty is associated with scenario development. Laugs and Moll show that most scenarios only represent a small bandwidth of possible pathways. This under-representation of extreme scenarios hampers the scientific discourses and 'skews the overall outlook on possible energy futures' [36].

Structural uncertainty has special importance for long-term planning models as these cannot be fully validated [37]. Although tackling structural uncertainty is tricky, one attempt is made by DeCarolis et al. [38], who explore the near-optimal decision space with their technique *modelling to generate alternatives* (MGA) [39].

Variability or aleatory uncertainty (3) refers to 'inherent variability manifested in natural and human systems' [23]. It can also be referred to as random or stochastic. The aspect *variability* can be addressed with established mathematical methods. For example, the open-source model generator TEMOA applies stochastic programming [31] to deal with variability uncertainty. For deterministic models, other options, such as scenario and sensitivity analysis or Monte Carlo simulations are available. However, sensitivity analysis or stochastic programming counteract the challenge of *complexity*, as these measures are computationally expensive. Even if such approaches are applied under the reasonable assumption of increasing computational resources, missing regulatory certainty in combination with disruptive events can hardly be tackled by existing technical methods. Hence, policy makers need to be aware that reliable policies and regulatory schemes are crucial for the degree of reliability that advice derived from energy modelling can offer in the future. Instead of handling these uncertainties as practical constraints, they have to be analysed additionally (e.g. influence of temporal and regional resolution on results). This is important, as growing complexity of the modelled systems requires reducing model complexity. In turn, structural uncertainties of these simplified models increase. Connected to this issue are open questions that directly link to *utilisation* (e.g. 'Is a model with unquantified structural uncertainties fit for a specific purpose?').

Decision uncertainty (4) stems from decision makers with a different understanding and judgement of objectives and appropriate solutions and strategies [23]. For example, risk perception or the way of presenting model results to decision makers may affect their decision [32]. Availability of resources in terms of information and time to process it affect decision making as well [23]. According to Wardekker et al. [40], uncertainty perception varies depending on the way information is provided. This relates *planning procedural uncertainty* to the aforementioned aspect *decision uncertainty*.

Interdisciplinary modelling

The development of energy system models is typically undertaken from an engineering or economic perspective. Jefferson [41] argues that emphasising equations and economic theories prevents researchers from focusing on complicated factors and their future implications. Furthermore, Wiese [42] states that twenty-first century challenges need to include other perspectives than least-cost optimisation. As stated above, differences are inevitable between ideal results of optimisation models with one single rational decision maker and real-world developments with a multitude of heterogeneous stakeholders [43]. In addition to an increased complexity, this is also a challenge from an interdisciplinary point of view since modellers need to integrate perspectives that are not captured by standard economic or engineering approaches. However, if energy research is not undertaken in an interdisciplinary way, researchers 'are not likely to grasp the problems, and thus the solutions to this challenging (energy) research space'([44], p.247).

It is common to utilise Integrated Assessment Models in climate change research [45]. Also for the energy field, Integrated Assessment Models like TIAM-WORLD exist [46].

Social and behavioural factors are important to assess the adoption of renewable technologies [47, 48] or the representation of consumers' real behaviour in energy models [49]. For example, social acceptance has a relevant impact on grid and wind power expansion [50, 51]. Heinrichs et al. [52] combine a survey, a macro-economic input-output model, and an energy system model to assess phase-outs of coal-fired power plants in Germany. They conclude that integrated assessment of energy systems provides more robust results.

Attempts exist to capture the human dimension in energy system modelling by applying social science methods. But considering the strong interconnectedness of energy systems and society, social sciences are rather under-represented in contemporary energy research [53].

Another requirement in interdisciplinary modelling results from the strong interdependencies between the energy, water, and food sector. Granit et al. [54] argue that an increased understanding of the water-energy-food nexus is necessary to achieve sustainable development goals. They present first attempts for integrated tools and state that further cooperation between the modelling disciplines is required.

To comprehend the dimension of challenges in interdisciplinary energy modelling, one has to consider that finding a coherent terminology and taxonomy within one field is already complex. This is referred to as *linguistic uncertainty* in the 'Uncertainty' section. Between different disciplines, a lack of understanding due to different terms impedes a common understanding of energy systems.

Scientific standards

Complying with *scientific standards* includes the aspects transparency, repeatability, reproducibility, and scrutiny. These principles ensure that science moves forward and can perform course corrections through independent verification [55]. Beyond that, these are also fundamental for the societal progress, which depends on return of knowledge that has been publicly funded. Repeatability or the sometimes used term replicability describes the ability to repeat an experiment and come to the same results. In contrast, reproducibility means that results can be repeated by a different researcher in a different computer environment [56]. Although definitions exist, these two terms are not always used with this clear distinction in literature.

Transparency of methods, code, and data lays the foundation for the other three aspects, as it is a precondition for building up on existing scientific work in the field of energy system modelling. However, Ince et al. [57] state that for computer science, transparency at all stages constitutes a basic condition for reproducibility. Even if this is fulfilled, reproducibility remains a challenging task due to hardware, software, and natural language related uncertainty. The common situation of constantly changing versions of energy system models and failure to describe these precisely when presenting results, adds another dimension to the reproducibility challenge [13]. As Pfenninger et al. [1] argue, full—meaning effective—transparency of energy system models is still hampered by different barriers. Specifically, the lack of open licences on the original sources of data is an obstacle for making model data publicly available. Moreover, a sparse or non-existing documentation of data makes it inconvenient for others to use these data.

To facilitate repeatable analysis, DeCarolis et al. [58] recommend five steps of best practices in energy economic optimisation model development. These steps, we argue, can and should be applied to every energy system model and to some extent to frameworks: (1) make source code publicly accessible, (2) make model data publicly accessible, (3) make transparency a design goal, (4) develop test systems for verification exercises, and (5) work towards interoperability among models. In fact, with today's information technology, it has never been easier to comply with these recommendations. However, regarding data, significant barriers still exist as explained above. In context of code, progress can be observed. Source code of different model generators has been made publicly accessible in recent years (e.g. Balmorel [59], OSeMOSYS [8], TEMOA [31], calliope [60], PyPSA [9]). Meanwhile, up to now, 25 open energy models and frameworks are registered on the website of the open energy modelling initiative [3]. Contrary to increasing model transparency, publishing solely aggregated results of energy system models is still a common procedure. For instance, a list of models used in the UK shows that input data and code of the majority of models are not open [15]. As almost any result can be generated by modifying decisive input data, variables, or code, the common practice makes repeatable results impossible. Attempts exist to overcome these problems. Regarding data, the *Dataverse* project is one example of technical support in linking associated data with the published article [61].

While point three on the list (transparency as a design principle) has already been discussed above as the foundation, the fourth point (verification exercises) refers to the aspect of scrutiny. The importance of scrutiny for energy system modelling is (in this paper) mainly discussed not only in a technical sense but also on the societal level. Point five on DeCarolis best practice checklist addresses applicability and re-usability which is discussed related to *utilisation.*

On the technical level, scrutiny refers to identifying inconsistencies or faults (so-called bugs). Every computer model is prone to bugs, whereas the probability of theses errors increases along with the complexity and size of the model. Detecting bugs is particularly vital in energy system modelling, as small errors may have great impact on the results. Johnson [62] highlights that peer-reviewed open-source software has significant advantages regarding bug detection. Besides this, Ndenga et al. [63] point out that the size of a community, i.e. users and developers, is one metric for bug reports.

On a social level, scrutiny refers to the detection of bias in model code and data. The possibility to scrutinise model results is essential for credibility [64], and the development of public trust in the modelling results, particularly as participation of society in the design of energy pathways, becomes increasingly important [65]. Methods for stakeholder participation in transition processes towards sustainability are available and applied [66] although simultaneously creating new challenges [67].

Being widely used for policy advice, the trade-off between being policy-relevant without being policy-prescriptive is vitally important for model-based research [68]. Though, Mai et al. ([64], p.9) conclude that, accidentally or purposefully, all models incorporate biases. Going one step further, Biewald et al. [69] argue that value-laden and ethical issues cannot and should not be avoided in model-based studies, but assumptions based on ethical opinions should be communicated transparently, which can increase policy relevance of these studies. Similarly, Edenhofer and Kowarsch [70] state that value-neutral scientific recommendations for public policy are not possible. As model-based research has to deal with normative-ethical aspects, they suggests a new culture in academia that defines the role of modellers as cartographers of solution spaces. Detecting value-laden assumptions is even more difficult than detecting bugs, as software tests fail at this. Hence, again transparency of source code and data is pivotal for energy model use in policy advice and essential for complying with quality standards [71].

Although all discussed aspects refer to all computational intensive sciences, Pfenninger et al. [1] argue that energy policy research is still lagging behind other fields in terms of complying with *scientific standards.*

Utilisation

The aspects of the challenge *framework and model utilisation* are linked to growing model complexity. In the modelling process, three main groups of persons are involved: (1) developers, (2) users, and (3) decision makers. It is noteworthy that in some cases, these groups may not be completely distinct, as developers and users might be identical. Regarding the user/decision maker interface, the user needs to be able to explain the model logic and its effects on results to recipients of the results. The aspects *usability* and *result communication* are associated with the user/decision maker interface. The other two main aspects identified with regard to *utilisation* are *applicability*, that can be understood as a problem of 'ease of use' at the developer-user interface, and *re-usability*, that can be understood as 'ease of adaptation' at the developer/developer interface.

As models only produce useful information if the recipients understand the causal relations to a certain degree, there remains a trade-off between the level of complexity and the general usability. Bale argues that '[m]odellers need to engage with their beneficiaries from the outset so that models are properly scoped and fit for purpose' ([72], p.157). Most notably, this is important as models are made for obtaining insight, not for generating numbers [73].

The struggle of finding a common language between developers, users, and recipients of their results has existed almost as long as the models themselves. In 1976, the Energy Modelling Forum was formed to 'foster better communication between the builders and users of energy models in energy planning and policy making' ([74], p. 449). Energy research is generally application-oriented, but stands out among other policy fields with externalities. Due to its vertical and horizontal complexity, entailed costs, and strong path dependency, energy models are indispensable for policy support [75]. However, the decision makers' idea of useful information may differ significantly from those of the users ([64], p.9). This is a crucial point, as '[a] model is not fit for purpose if it is developed without sufficient critique of the motives for producing the model' ([72], p.155). Therefore, the aspect *communication of results* is a crucial aspect of the modelling process. In particular, valuable information may not only be lost at the user/decision maker interface. To tackle this problem in operation research, the concept of *model assessors*, analysing, and evaluating models for decision makers has come-up a long time ago [76]. Additionally, Strachan et al. [77] propose further improvements, such as platform-based expert user groups for coordination and interdisciplinary external stakeholder review for energy system models.

Between developers and users, an easier and better understanding of framework or model mechanisms than at the developer/decision maker interface could be assumed. However, this seems not always to be the case. One example for differences in understanding models and results is the discussion about results from the NEMS model (see [78] and [79] for details). The usefulness of a framework increases if it can be applied to a diverse set of problems and by different researchers. Ideally, the expense of a developer for building up on an existing framework should be lower than the expense for building a new one from scratch.

In context of energy system modelling, it has been argued that '[s]ociety as a whole saves time and money if researchers avoid unnecessary duplication' ([1], p.212). Considering the rising number of open energy models and frameworks for similar purposes [3], it yet seems that developers tend to rather develop a new framework than use existing ones. A reason for this may be the increasing complexity and different software skills required for adapting models or frameworks. Consequently, being open does not seem to be sufficient in terms of usability, even if a deep modelling understanding exists. Thus, the aspect applicability is also connected to *scientific standards* as it is vital for the repeatability and, more importantly, to the reproducibility of results.

The problem of how results are communicated is a recurring point in literature. Communication of energy system modelling results fails, when recipients only see concrete numbers (e.g. total energy system cost) as an outcome, though models should primarily be seen as a tool for understanding mechanisms and getting insights [70, 73]. Strachan et al. [77] proposed approaches to reinvent the modeller/policy interface for overcoming this problem. The communication with a recipient of model results cannot be tackled directly, but a framework can contribute to improving result communication by structured output that includes effects of parameters, ranges of uncertainties, and relative differences between scenarios, instead of results reduced to individual figures. Furthermore, extended use of pre-prints and discussions about results and methods within the community before the actual publishing process can be one step into the right direction.

Framework properties

We categorise framework properties that can contribute to tackling the challenges described above in three major categories: (1) open-source philosophy, (2) collaborative development, and (3) structural properties. More detailed characteristics of these three properties are listed in Table 2 and described below.

Free and open-source philosophy

Calls to 'open up' energy system models are getting louder, according to Morrison [80] motivated by the need for improved public transparency and scientific

Table 2 Framework properties with respective characteristics that are decisive for tackling the challenges

Property	Characteristics
Free and open-source software philosophy	Open-source, documentation, version control, openness of data, code review
Collaborative development	Consistency of terminology, developer perspective spectrum, interdisciplinarity, testing procedures
Structural properties	Modularity of framework structure, object-oriented implementation, generic concept of energy system representation, data model

reproducibility. Free software, open-source, and open-data are basic conditions for transparency and allow for repeatability, reproducibility, and scrutiny [58]. However, publishing undocumented source code of complex models still presents a serious obstacle to others. Therefore, code review, version control, and thorough documentation are important elements for effective transparency [81].

With a standardised input/output data format, simultaneous publishing of model source code and the corresponding documentation (including data and meta-data) is possible. Cross-platform data structure provides a flexible user interface and can contribute to lowering the entry barrier for new users. If supported by a clear version-control workflow, this allows for the release of monolithic model versions including data and documentation. In that way, scientific model results are transparent and enable reproducibility.

Policy measures and planning processes based on the results of energy system models cannot be affected directly by the modeller. However, an open-source and open-data approach enables decision makers and planners to obtain a deeper understanding of model results considering details of model inputs. This may enhance communication between modellers, decision makers, and other stakeholders.

Collaborative development

Different important characteristics of frameworks originate from collaborative development. This kind of development is a new challenge within the field of energy system modelling. But if it is done, it can trigger a process of finding common definitions and a shared understanding of energy research-related problems.

With a collaborative concept, frameworks can contribute to a process of addressing linguistic uncertainty. Identifying common elements in energy system modelling can help to determine coherent terminologies. Here, experience from collaborative modelling is key for the necessary interface definitions of different existing models. Therefore, at least ambiguity is inherently tackled as developers have to agree on specific terms during the development process. A common terminology enables the different groups to communicate effectively.

In the process of collaborative development, multiple perspectives of developers with different backgrounds can decrease the risk of overlooking or omitting decisive features of energy systems. Developing a common understanding of interdisciplinary problems is not a trivial task, but a necessary basis for appropriate modelling. Here, collaborative development may play an important role in translating into interdisciplinary model development.

Additionally, a collaborative framework development and thus more people working with the code basis increases the probability of finding bugs [82]. This can also be integrated in a more structural way by standard test procedures before merging new developments into the master version. Test systems for verification exercises are one of the recommendations for repeatable analysis by DeCarolis et al. [58].

A collaborative framework development with developers from different backgrounds requires a high-quality documentation. This results in improved transparency for new developers and external users and thus supports scientific progress.

The experience developers collect in a collaborative development process, how to find common definitions etc., are a good foundation for collaborating in an even more interdisciplinary team. The resulting generic basis allows for an easy coupling of energy system model components with new model components of other research areas (e.g. components in water resource modelling, investment delays due to public acceptance, demand changes due to behaviour changes). This supports the interoperability of models, which is important for repeatable analysis [58]. The generic approach is part of the structural properties, which is explained in the following.

Structural properties

Structural properties of frameworks decide how flexible energy system models can be created, adapted, and linked. If essential structural properties are shared, hard- and soft-linking of applications based on the same framework can be performed even with different modelling approaches or with models using different regional and temporal resolutions. As Trutnevyte et al. [83] argue, this can be a key for energy system analysis.

A modular design—where each module has a certain degree of interdependence from the remaining part of the framework—increases applicability of a framework since new users can create applications based on the desired module without knowledge of the complete framework. A framework that is not restricted to a specific mathematical approach facilitates the integration of other modelling techniques. That could be for example agent-based models or methods to capture the human dimension which would thus support interdisciplinary modelling.

Overall, a generic basis in combination with a flexible programming language facilitates a modelling process for complex and changing systems. Generic classes facilitate the integration with other models.

An object-oriented approach generally provides a flexible interface for extensions. This supports the development of energy systems based on the same framework separately by different persons and to connect afterwards.

Platform-independent software increases the usability of a model. If a model is tested on the main operation systems (Windows, Linux, Mac OSX), the potential user target group is enlarged. Python is a common programming language for relatively new open frameworks and models [81]. It has the advantage that required Python versions, and packages can be installed in a specific environment on the machine of the user. This makes sure that the framework can be run with the working version independently from other Python installations on the user's machine. Such a high re-usability and adaptability could save other resources (e.g. time) in terms of parallel work, especially when it comes to long-term projects with a great extent of interfaces between groups and work packages. This is in line with the argumentation of increased productivity through collaborative burden-sharing ([1], p.212).

Despite abovementioned problems of existing approaches to tackle variability uncertainty (see the 'Uncertainty' section), variability uncertainty can partly be addressed with incorporated tools for sensitivity analysis. Methods to explore a large space of parameter variations (i.e. scenario or sensitivity analysis) can be built on top of framework-based models. This is easier if a modular and generic structure allows for it. However, one has to keep in mind that *uncertainty* cannot only be fully tackled by an energy system framework with current methods but also depends on the regulatory consistency. Additionally, the trade-off between complexity and uncertainty has to be balanced by modellers and model users and does not fully depend on framework properties.

Application procedure

The result of our review of energy system modelling challenges on the one hand and framework properties influencing the capability of frameworks to tackle these on the other hand is summarised in a matrix (Fig. 1.)

This derived matrix can be used to evaluate energy system modelling frameworks or model generators regarding their capability to cope with present energy system modelling challenges.

The evaluation we suggest is made along the proposed challenge-property-matrix in the following steps:

- Quantify the characteristics of the framework's properties in focus: no/not available (o) - partly (+) - strongly (++).
- Argue for each challenge: how does each characteristic partly/strongly address which aspect of the challenges?
- Quantify the contribution level for each characteristic-aspect pair: not addressed (o) - partly addressed (+) - strongly addressed (++). Each characteristic can contribute to tackling a challenge aspect with at most equal rating. For example, if characteristic *documentation* is only partly available, it can contribute at maximum partly to tackling challenges.

		Complexity				Uncertainty					Interdisciplinarity			Utilization				Scientific standards				
		sector coupling	resolution	input data	result processing	epistemic	aleatory	linguistic	decision	planning	human dimension	energy-water-food	common understanding	usability	applicability	re-usability	result communication	transparency	repeatability	reproducibility	scrutiny	scientific progress
Open-source philosophy	open source																					
	documentation																					
	version control																					
	openness of data																					
	code review																					
Collaborative development	consistency of terminology																					
	developer perspective spectrum																					
	interdisciplinarity																					
	testing procedures																					
Structural properties	modular																					
	object oriented																					
	generic concept																					
	data model																					

Fig. 1 Challenges (with aspects)—properties (with characteristics) matrix

- Check if the written argumentation supports the quantitative result.
- *Optional:* If the framework in focus has additional properties and/or characteristics relevant for the challenges, these might additionally be added to the matrix and evaluated with regard to their contribution in a second round.
- Summarise potential changes of the framework that would improve the contribution to the challenges.

In the following, the procedure is exemplarily applied to a case study.

Case study

First, oemof is shortly described with respect to the listed properties (Open Energy Modelling Framework). Then, as outlined in the section 'Application procedure,' oemof's characteristics are checked for each challenge, and their contribution in tackling the challenge is debated ('Evaluation' section). Finally, the resulting matrix summarises the findings ('Summary' section).

Open Energy Modelling Framework

The framework itself and the characteristics we refer to in this section are described in existing publications [4, 84] and the online documentation of the framework [85]. In the following, additional literature is referenced where necessary. The framework has been developed for the analysis of energy supply systems considering power and heat as well as (prospectively) mobility. It consists of different libraries with defined interfaces for their combination. Applications depict concrete energy system models constructed from oemof libraries. Inside comprehensive models, specific parts of such an application can be developed flexibly by combining oemof libraries with external libraries. The core concept of oemof is based on a network structure which describes the general topology of an energy system.

Available applications built within oemof (e.g. renpassG!S [86], reegis [87], HESYSOPT [88]) demonstrate that the modular approach of the framework allows the creation of applications with very different objectives. The general description, the toolbox character, and the flexibility concerning temporal and spatial resolution makes oemof a framework instead of a model. It is implemented in Python using several packages (e.g. for data analysis, optimisation) and can optionally be combined with a PostgreSQL/PostGIS database.

As a first step of the evaluation process, the characteristics are quantified in Fig. 2.

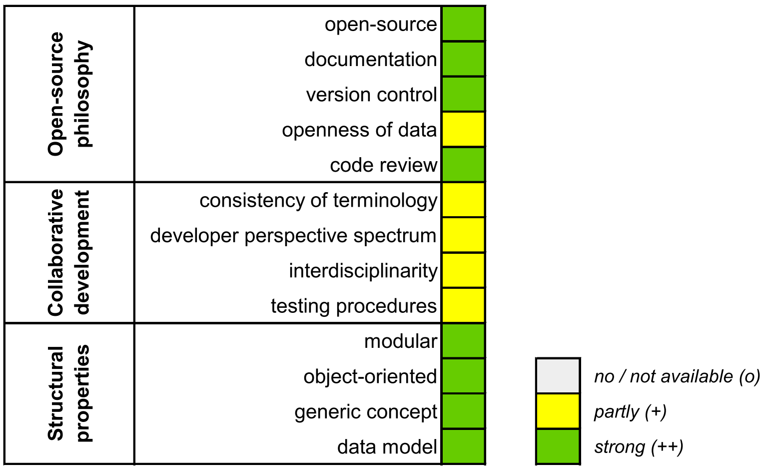
Evaluation

Complexity

Due to its structural properties, oemof allows to create flexible energy system models which can be adapted and linked. For example, modelling strongly integrated energy systems is straightforward, due to oemof's network structure. If, for instance, a specific sub-system should only appear in certain calculations, it can be connected and disconnected flexibly to a graph-based energy system representation with all its components depending on the requirements.

Additionally, generic classes can be used to easily integrate other models. This has, for instance, been tested with the PyPSA library [9]. Applications built in oemof have shown the integration of electricity, heat, and mobility as well as energy market simulation models [89] and power flow analyses [90].

The temporal and regional resolution are not fully addressed, as no specific methods are implemented within



Open-source philosophy	open-source	🟩
	documentation	🟩
	version control	🟩
	openness of data	🟨
	code review	🟩
Collaborative development	consistency of terminology	🟨
	developer perspective spectrum	🟨
	interdisciplinarity	🟨
	testing procedures	🟨
Structural properties	modular	🟩
	object-oriented	🟩
	generic concept	🟩
	data model	🟩

⬜ *no / not available (o)*
🟨 *partly (+)*
🟩 *strong (++)*

Fig. 2 oemof properties/characteristics the framework. Nevertheless, the problem of resolution is partly addressed. For example, the optimisation library *solph* provides time-step-flexible modelling with time-step-dependent weighting.

The object-oriented approach of oemof generally provides a flexible interface for extensions. Different applications based on oemof can be hard- or soft-linked even if using different regional or temporal resolution. Based on the underlying concept, incorporating new modelling methods is possible although not done yet (e.g agent-based models based on *core* components).

Moreover, the framework provides a complete toolkit for modelling highly integrated, renewable-energy-based systems. Thus, not only optimisation models can be built but also input data such as feed-in or demand time series may be generated on the basis of oemof functions. Especially, the feed-in libraries allow for a high spatial and temporal resolution.

Overall, the underlying generic basis in combination with a flexible programming language facilitates the modelling process for complex and changing systems.

Uncertainty

With its collaborative concept and a group of developers with different backgrounds, oemof contributes to a process of addressing linguistic uncertainty. *Epistemic uncertainty* related to *model structure uncertainty* is partly addressed by oemof as well due to the multiple perspectives of the developers. At the moment, the framework does not provide any functions tackling problems of *variability uncertainty*.

Interdisciplinary modelling

The provided framework does not directly address the aspect of taking down disciplinary walls between energy system modelling and other research disciplines. However, the concept allows to integrate other modelling techniques, i.e. approaches that suit interdisciplinary modelling.

Scientific standards

oemof is licenced under the GNU General Public License v3.0 and thus meets a basic standard in terms of transparency and allows for repeatability, reproducibility, and scrutiny. The developer group also aims at open-data, but that is not yet fully achieved.

Another element of effective transparency is the four levels of documentation: (1) comments inside the code explaining non-intuitive lines of code; (2) docstrings inside the source code describing how to use the various classes, methods, and functions; (3) higher level descriptions of possible interactions between different libraries or application-specific usage information; and (4) application examples especially useful to new users.

Transparency on application level is supported by a standardised input/output data format and functions for simultaneous publishing of model source code, data, and meta-data. The data structure is human-readable, spreadsheet-based, and thus cross-platform applicable, which can contribute to lowering the entry barrier for new users. The version-control workflow supports reproducibility of model results. Backward and forward compatibility is ensured as defined in the semantic versioning approach [91].

Regarding test procedures, there is a set of continuously extended tests (e.g. results, comparison of lp-files for mathematical models), which must be passed before merging into the development branch and thus also into the master branch. In addition, the oemof development uses (in addition to the tests) pull requests, which require review approvals of at least one more developer.

Utilisation

Beyond general challenges of utilisation outlined in ‘Framework properties’ above, oemof supports the energy system modelling community by providing a basis for model development that is highly reusable and adaptable. It can be applied on the main operation systems and is—with Python as the programming language—based on platform-independent software.

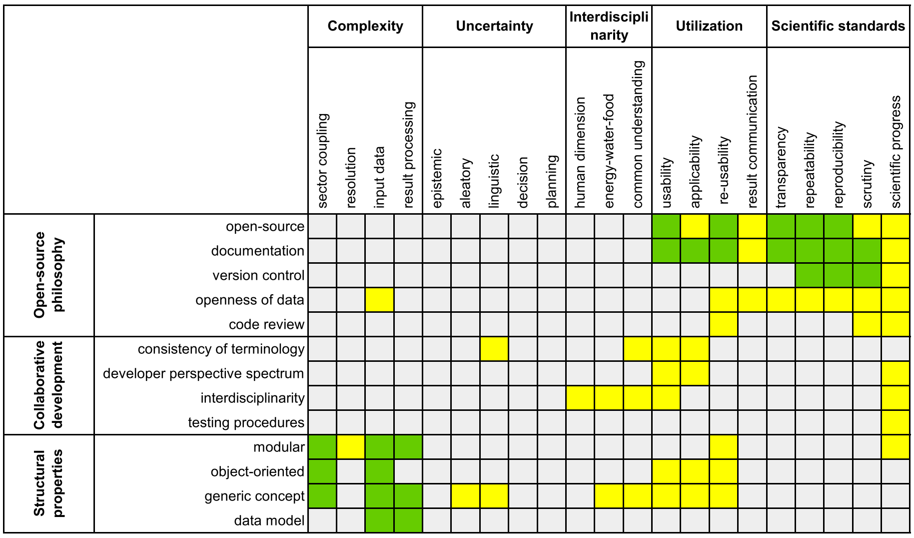
Also, the applicability of oemof models is improved by the underlying structure. Once this structure has been internalised by users and model developers, its usage and development is straightforward. The different layers of omeof are partly independent from each other, which enables new users to create applications without knowing all parts of the framework.

Moreover, the overall concept is consistent and the graph-based structure is in line with the code, data, and documentation. Thus, even complex cross-sectoral models or applications developed with another scientific scope can be understood quickly. Generally, a well-defined modelling workflow increases overall transparency. The problem of result communication is only addressed indirectly by structured output that enables graphs for relative scenario comparison. However, this could be improved by providing methods for stating uncertainty ranges and methods for example visualising how strong input parameter variations affect different output parameters.

Summary

Figure 3 summarises all challenges and properties with their specific contribution levels for the evaluated framework.

Important issues related to *complexity* are particularly addressed by oemof’s structural properties. Due to the generic code basis and the object oriented implementation, the modular framework allows modelling of



		Complexity				Uncertainty					Interdisciplinarity			Utilization				Scientific standards				
		sector coupling	resolution	input data	result processing	epistemic	aleatory	linguistic	decision	planning	human dimension	energy-water-food	common understanding	usability	applicability	re-usability	result communication	transparency	repeatability	reproducibility	scrutiny	scientific progress
Open-source philosophy	open-source													🟩	🟨	🟩	🟨	🟩	🟩	🟩	🟨	🟨
	documentation													🟩	🟩	🟩	🟨	🟩	🟩	🟩	🟩	🟨
	version control																		🟩	🟩	🟩	🟨
	openness of data			🟨												🟨	🟨	🟨	🟨	🟨	🟨	🟨
	code review															🟨					🟨	🟨
Collaborative development	consistency of terminology							🟨					🟨	🟨	🟨							
	developer perspective spectrum													🟨	🟨							🟨
	interdisciplinarity										🟨	🟨	🟨	🟨								🟨
	testing procedures																					🟨
Structural properties	modular	🟩	🟨	🟩	🟩											🟨						🟨
	object-oriented	🟩		🟩										🟨	🟨	🟨						
	generic concept	🟩		🟩	🟩		🟨	🟨				🟨	🟨	🟨	🟨	🟨						
	data model			🟩	🟩																	

Fig. 3 Visualisation of evaluation results. Derived from mapping challenges and their aspects with properties and their characteristics

integrated renewable energy systems, easy model linking as well as input and result processing.

Most aspects of *uncertainty* are not tackled by oemof, but the collaborative development and structural properties may reduce *linguistic* and *structural uncertainty*. Important aspects like *variability uncertainty* are not addressed. This may be improved in future versions.

As delineated in the 'Evaluation' section, oemof lays important foundations for *interdisciplinary modelling*, as the generic basis allows for modelling components that have their origin in other research areas. However, this has not been implemented in any oemof applications so far.

Being developed in an academic context, challenges related to *scientific standards* are addressed thoroughly with the free software and open-source philosophy. Collaborative framework development requires a high-quality documentation and improves transparency for new developers and external users. Moreover, potential bugs can be identified and fixed quickly, due to a growing community and direct feedback between users and developers. This level of addressing is underlined by being in compliance with the best practice recommendations of DeCarolis et al. [58].

Regarding challenges in terms of *utilisation*, oemof's philosophy constitutes an important precondition for tackling these. Effective transparency at all stages is crucial for communication of results, as well as for application building and re-usability of models. Similar to uncertainty, we find that frameworks could support tackling the aspects of the challenge *utilisation* to some extent. However, for example result communication, changes in debate culture would be required to fully make use of this provided support by energy modelling frameworks.

From the evaluation, we conclude that challenges related to *complexity* and *scientific standards* are strongly tackled. In contrast, *uncertainty* is not addressed at present, as major aspects of this challenge are not sufficiently considered. Regarding the challenges *utilisation* and *interdisciplinary modelling*, we argue that oemof captures these partially.

Discussion

This described evaluation approach provides a structured, hands-on procedure that comes with different disadvantages and advantages.

Due to the intensive analysis of framework properties required in the evaluation process, the addressees of this approach are rather developers or experienced users of the respective frameworks. This has been affirmed by the case study, which required specific experience which is difficult to derive from documentation only.

However, the general scheme can contribute to broadening the scope of a developer team applying it. The method of matching properties of a framework with challenges that need to be covered forces developers to think outside of the box of their own framework. Energy software development work is thus augmented by a societal perspective. Thus, it can be an assisting tool to relate one's own work to the energy system analysis field. Furthermore, it can assist in identifying potential improvements to increase the relevance of the framework. We argue that the evaluation approach may also be applied for framework comparisons, given that people with in-depth knowledge of the respective frameworks are involved.

Advantages of the proposed approach lie in its simplicity and flexibility. Modellers can reflect modelling tools in a structured way regarding the selected challenges and properties. For a framework comparison with a special focus, additional challenges or properties could be added to the matrix.

However, the step from the qualitative description of the properties to their evaluation, as well as the matching of the contribution level of the characteristics to the challenges could incorporate subjective bias and vagueness. The potential bias could be lowered by a review of the valuation step from argumentation to the filled matrix by modellers new to the framework in focus. In the presented version of the evaluation approach, no weighting exists. Thus, results cannot reflect the importance of an individual aspect or characteristic. This would be a potential improvement.

Beyond the specific case study and the evaluation approach itself, the detailed discussion of challenges and properties in this paper identifies general issues in energy system modelling. Some approaches for tackling challenges may counteract each other, such as complexity and uncertainty. To allow for rather sophisticated methods like stochastic programming, more research in the field of complexity reduction within energy system models is needed.

Furthermore, some challenges cannot be tackled solely by the framework approaches. Among these are problems of result communication and interdisciplinary modelling. We argue that these must be primarily addressed through changes in communication and organisational structures, thus, on a behavioural and social level. Additionally, we suggest to increase efforts in evaluating if a model is fit for purpose and what its results may reveal—or may not reveal—for each model application. Here, collaborative and interdisciplinary modelling can be a valuable method supporting this process.

Conclusions

Although different approaches for evaluating and comparing models have been proposed, systematic evaluations of frameworks are under-represented. This paper presents an evaluation method for energy system modelling frameworks regarding their capability to address present challenges in energy system modelling.

The application of our approach in a case study demonstrates its general capability to assess energy system modelling software in terms of present and future challenges. Advantages of the evaluation approach lie in its simplicity, flexibility, and transferability, whereas disadvantages are mostly due to potential subjectivity and bias.

In addition, the detailed mapping of challenges and framework properties reveals that an open-source approach is a fundamental condition for complying with scientific standards. Openness of a framework is also advantageous for its utilisation, meaning (re-)usability, and applicability. However, whether or not advantage can be taken from improved energy system modelling software is partly decided on social level. This is especially true for result communication and interdisciplinarity.

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Authors' contributions
SH and CK performed the qualitative analysis of the framework (case study) in close cooperation and intensive discussion and contributed to the design of the paper; FW originally initiated the paper and contributed to the design of the study, to the review of energy system modelling challenges, and to the properties and the methodology. GP contributed to the review of challenges, in particular the challenge of uncertainty; all authors engaged in the initial design of the analysis; FW conducted the restructuring of the paper and the revision of the evaluation approach. All authors read and approved the final manuscript.

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

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The Open Energy Modelling Framework (oemof) - A new approach to facilitate open science in energy system modelling[1]

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The Open Energy Modelling Framework (oemof) - A new approach to facilitate open science in energy system modelling[☆]

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ABSTRACT

Energy system models have become indispensable tools for planning future energy systems by providing insights into different development trajectories. However, sustainable systems with high shares of renewable energy are characterized by growing cross-sectoral interdependencies and decentralized structures. To capture important properties of increasingly complex energy systems, sophisticated and flexible modelling tools are needed. At the same time, open science is becoming increasingly important in energy system modelling. This paper presents the Open Energy Modelling Framework (oemof) as a novel approach to energy system modelling, representation and analysis. The framework provides a toolbox to construct comprehensive energy system models and has been published open source under a free licence. Through collaborative development based on open processes, the framework supports a maximum level of participation, transparency and open science principles in energy system modelling. Based on a generic graph-based description of energy systems, it is well-suited to flexibly model complex cross-sectoral systems and incorporate various modelling approaches. This makes the framework a multi-purpose modelling environment for modelling and analyzing different systems at scales ranging from urban to transnational.

1. Introduction

The global transition process towards more sustainable and low-carbon energy systems requires the development of alternative future trajectories for thorough scientific discussion. Using these, decision processes on different levels e.g. in transnational policy making or local energy planning can be supported. However, future energy systems imply a rising complexity in technical, economic and socioeconomic dimensions due to increasingly cross-sectoral and decentralized structures [1]. Insights into such complex systems can be gained by applying computer-based modelling approaches which create a quantitative basis for the above mentioned discussion and decision processes.

Depending on the specific investigation and research question, a variety of model types can be applied. Such model types include power flow models for electricity transmission network operation and planning, economic dispatch models for general capacity planning and unit commitment models for power plant utilization [2–5]. Applications range from large-scale transnational investigations using purely economic top-down equilibrium models to detailed technical local infrastructure planning using bottom-up models based on technology-specific data. Moreover, many models can be adapted to integrate different sectors such as electricity, heat and mobility to investigate cross-sectoral interdependencies.

Energy system models and derived results have often been heavily discussed among different stakeholders and been criticized for not opening their internal logic and underlying assumptions [6–8]. As a result, in the last decade more scientists have opened their models and data [9,10]. This process goes along with a general trend to open science in many other research fields. The rationale for open science includes improved efficiency, scrutiny and reproducibility of results, reusability of scientific work and increased transparency of all scientific processes [11]. As the European Commission has recently started to push open science in its research programs [12], the subject of openness has finally moved into the public spotlight.

This paper presents the Open Energy Modelling Framework (oemof) as a novel approach to foster open science in the field of energy

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[☆] This document is a collaborative effort.

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modelling and analysis. First, the idea of a single energy modelling framework is differentiated from other approaches to delineate the scientific contribution in Section 2. The underlying concept with its mathematical representation as well as the framework architecture and its implementation are outlined in Section 3. Building on this, the general process of application development is described in Section 4 along with a selection of existing applications. Finally, the general approach and its scientific contribution are summarized in Section 5.

2. Scientific contribution

To provide context, first a brief overview on relevant energy system modelling software is provided. Subsequently, the presented framework is compared to similar existing software and its unique features are outlined. For extensive reviews on this topic, please seeHall and Buckley [13], Connolly et al. [14] and Pfenninger et al. [1].

2.1. Overview of modelling landscape

In the following, we distinguish between the three terms *model*, *model generator* and *framework*. Models are concrete representations of real world systems (e.g. with a specific regional focus and temporal resolution). Such a representation may consist of multiple hard- or soft-linked sub-models to answer clearly-defined research questions. Models can be built using model generators that employ a certain analytical and mathematical approach (e.g. by the use of predefined set of equations, represented technologies). Finally, a framework can be understood as a structured toolbox including sub-frameworks and model generators as well as specific models (e.g. wind feed-in models). In addition this kind of a collection has other requirements for structures and processes that guide the development process.

With respect to open science principles, a rough division into a line of closed (1st *generation*) and open (*2nd generation*) models for energy system analysis can be derived.

The 1st *generation* models and model generators have a long tradition and are predominant in the academic energy system modelling field. Among the most widely used proprietary model generators is TIMES/MARKAL [15]. Models of this family have been used to answer research questions in the field of energy planning which is indicated by the high number of references in academic literature [13]. Similarly, MESSAGE is a prominent model generator that has been used for the IIASA global energy scenarios [16]. Besides this, the EnergyPLAN simulation model has been applied in various research projects to analyse sector integrated electricity, heat and transport systems [17].

The Balmorel model [18] can be seen as one of the first *2nd generation* energy system models. It has been designed for power and heat dispatch modelling with optional investment within the Baltic region and is written in GAMS. Another early project is the model generator OSeMOSYS [19] which is mainly used for long-term integrated assessment and energy planning. This project aims to facilitate modelling and education through a free software philosophy and a simple, easy-to-learn interface. Since then, various other projects with different purposes have been developed (e.g. urbs [20], PyPSA [21], calliope [22]). Their focus covers the full range from power flow simulation to long-term investment models. A list of open source models can be found on the website of the Openmod-Initiative [9]. While some of these projects are models for a specific region, others can be classified as model generators.

2.2. Comparison to other software

Since the list of available of modelling software is extensive, the framework is compared to similar existing tools. For this, major categories with single characteristics are introduced. These encompass the general suitability for *open science*, the technical *concept* and overall modelling *functionality*.

A requirement of *open science* is the free availability of the software itself. Freely available software is software that is available without additional cost. The usage of fee-based software creates barriers to reproducibility, since the experiment can only be repeated if the respective licence is procured. Moreover, an open licence enables users to distribute, understand and change the source code and thus enhances transparency since model assumptions and internal logic can be understood, changed and evaluated to determine their influence on the results. The issue of re-usability can also be addressed when software is published under an open licence since other developers can re-use any part of the software. Finally, collaborative software development allows for continuous improvements, enables an easier detection of bugs and makes it possible to discuss new features in a transparent manner. Collaborative development in this context refers to joint work on the software's code without mandatory institutional ties. This includes a common road map, discussion of new features and changes and in general a high level of communication among the developers. A central characteristic of this definition is the transparency of all associated processes.

The *concept* is defined by technical and structural characteristics. Implementing the software in a high-level language lowers barriers to usage and contribution. High-level programming languages are characterized by a strong abstraction from computer's hardware, are easier to use and understand, may include elements of natural language and make software development simpler. The more external libraries available for a language, the easier the implementation of various tasks in the modelling tool-chain. Further, interfaces to other languages can be used to extend capability. A generic data model enables a separation between the mere topological description and subsequent calculation (within an optimization, for example). Generic data models are data structures designed specifically to suit the representation of data of a particular problem rather than to store data of multiple different problems. Graph-based representation of energy systems, for instance, can be used to represent electricity systems as well as heating systems. Providing the option to define the level of accuracy flexibly is an added value of energy system modelling toolboxes. For example, it allows for user-defined precision in representation of time in modelling an energy system components by extending the libraries scope through user-defined components. Another aspect of the concept is designing it for multiple purposes. This extends the core functionality by other useful tools. An example would be an energy system modelling toolbox that includes tools for generating feed-in profiles of renewable energy sources.

Functionality, in this case, is defined by concrete modelling capabilities for model types such as economic dispatch, investment planning (also across multiple periods, called multi-period investment planning), power flow calculation and unit commitment. Furthermore, the general capability to model sector coupling problems is a prerequisite for modelling multi-sectoral energy systems such as electricity, heat and transport.

To compare the framework to other tools, Table 1 lists a selection of popular 1st and *2nd* generation of modelling frameworks and model generators. Though oemof shares certain characteristics with existing software, the collaborative development, the generic data model and multi-model toolbox (framework) differentiates oemof.

2.3. Unique framework features

A core feature of the framework is its *collaborative development* with the goal of *community building*. Many existing tools are not developed by a single institution. For example, researchers are encouraged to develop and improve the source code of MARKAL and other tools of the Energy Technology Systems Analysis Program (ETSAP) [26]. However, the review processes and decisions are not transparent and valuable information may be lost in case of rejection of input. In contrast, oemof strives for an open process to encourage future improvements. To align

Table 1
A comparison of features of selected software tools that are similar to oemof. Note that for *OSeMOSYS* multiple implementations in different languages exist.

	Open science		Concept					Functionality						Source
	Free of charge	Open licence	Collaborative development	High-level language	Generic data model	Flexible level of accuracy	Multi purpose toolbox	Economic dispatch	Multi period investment planning	Investment planning	Power flow	Unit commitment	Sector coupling	
WASP IV	✓							✓	✓	✓			✓	[23]
EnergyPlan v12	✓							✓		✓			✓	[17]
MARKAL/TIMES								✓	✓	✓			✓	[15]
MESSAGE-III								✓	✓	✓			✓	[16]
oemof v0.2	✓	✓	✓	✓	✓	✓	✓	✓		✓		✓	✓	[24]
urbs v0.7	✓	✓		✓				✓		✓		✓	✓	[20]
calliope v0.5.3	✓	✓		✓				✓		✓		✓	✓	[25]
PyPSA v0.12	✓	✓		✓		✓		✓		✓	✓	✓	✓	[21]
OSeMOSYS	✓	✓		(✓)				✓	✓	✓			✓	[19]

with open science principles the idea is to enable full transparency of the development process and not only the final source code. For that reason, the project follows a strict free software philosophy. In addition, processes are designed for community building, collaborative and transparent source code development.

Another unique feature is the *generic data model* which has emerged from the collaboration of various researchers with different research interests and backgrounds. This has led to the development of a framework with a common basis (Section 3.1) consisting of a layer-structured set of tools and sub-frameworks. A generic graph-based basis allows to differentiate between the topology of an energy system and its calculation based on a specific mathematical approach. The oemof framework may be seen as a domain specific language [27] that represents arbitrary energy systems as a graph. As a consequence, oemof can represent energy systems at a high abstraction level as well as a detailed single power plant.

Generally, the framework serves as a *multi-purpose toolbox* for energy system modelling and has been designed to integrate a growing set of toolboxes in future. Open source model generators like *calliope* Pfenninger and Keirstead [22] and the toolbox *OseMOSYS* Howells et al. [19] are designed to build specific models of one model family or type by the use of predefined sets of equations (e.g. bottom-up linear optimization based models). Furthermore, some of the existing projects, such as *PyPSA* [21], include several model generators for different purposes that may be combined. In contrast to other tools, oemof encompasses model generator methods to generate specific economic dispatch, investment and unit commitment models. Beyond this, it provides a structured set of tools to facilitate the modelling process. In its current state, this set includes an optimization library (model generator) as well as tools to simulate feed-in from renewable energy sources or local heat demand for a specific region.

In summary, the underlying concept, the software architecture, the free software philosophy and in particular the framing processes (e.g. open meetings, open code review, open web-conferences, open platforms and open pull-requests) enable collaborative development and participation. These combined features distinguish oemof from existing projects and constitute a basis for open science in the field of energy system modelling. Its academic value lies exactly in this difference in terms of open science.

3. Concept, architecture and implementation

To help in understanding the framework, its underlying concept, architecture and specific implementation are outlined here. First, a general mathematical representation of energy systems is proposed which serves as a base for higher level software architecture presented subsequently. Finally, the specific implementation is described and justified.

3.1. Underlying concept

The main feature of the framework is the separation of an energy system's topological description from its computation. The representation may serve as a foundation to run graph-based algorithms (to determine whether the graph is connected, for example) or to perform exploratory analyses. Subsequently parameters of the system (or subsystems) can be computed based on concrete modelling methods. Due to this property, oemof can incorporate other models and model generators with varying modelling approaches and different programming languages.

To achieve this, a generic concept which constitutes the foundation of all the oemof libraries has been developed. In this concept, an energy system is represented as a network consisting of nodes and edges connecting these. Nodes N are subdivided into buses B and components C. When representing an energy system, an additional constraint that buses are solely connected to components and vice versa is imposed.

Components are meant to represent actual producers, consumers or processes of the energy system while buses are meant to represent how these components are tied together. Edges are used to represent the inputs and outputs of a component.

An energy system that is represented in such a way can be mathematically described using concepts from graph theory by looking at it as a bipartite graph G. The mathematical formulation of this graph in its general form is given in equation (1). A more detailed description of this concept with its theoretical foundation has been published by Wingenbach et al. [28].

$$\begin{aligned} &G:=(N, E)\\ &N:=\{B, C\}\\ &E \subseteq B \times C \cup C \times B\\ &C^{+} \subseteq C\\ &C^{-} \subseteq C\\ &T \subseteq C \end{aligned} \tag{1}$$

Components can be subdivided further into sources C^{+}, sinks C^{-} and transformers T:

1. *Transformers* have inflows and outflows. For example, a gas turbine consumes gas from a gas bus and feeds electrical energy into an electricity bus. The relation between inflow and outflow can be specified in the form of parameters, for example by specifying the transfer function or an efficiency factor.
2. *Sinks* only have inflows but no outflows. Sinks can represent consumers of which households would be an example.
3. *Sources* have outflows but no inflows. For example, wind energy or photovoltaic plants but also commodities can be modelled as sources.

A similar, purely mathematical formulation of multi-commodity network flow optimization models for dynamic energy management has been illustrated by Zeng and Manfren [29]. Furthermore, related structures of energy systems can also be found in different energy models [15,19,30,31]. These publications demonstrate that using a graph is an intuitive way of representing an energy system. The main difference of our approach when compared to existing ones is the identification (and its object-oriented implementation) of a specific graph structure that may be used as a representation for all types of energy systems. Every calculation based on a specific model will be derived from this representation. A graphical representation of how to describe an arbitrary energy system using this network structure is shown schematically in Fig. 1.

Based on the described concept, oemof provides basic components which can be used directly while also facilitating the development of more specific components built upon the basic ones.

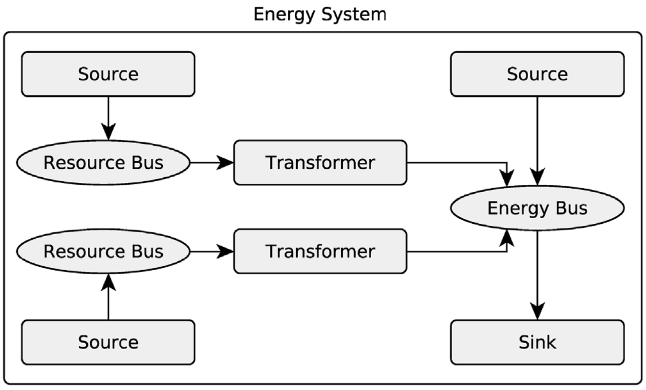

Fig. 1. Schematic illustration of an energy system represented as an oemof network.

3.2. *Mathematical description: the solph-library*

Currently, the solph-library can be used to create mixed-integer linear optimization problems from a pre-defined set of components. In order to model different elements of an energy system, several classes that may represent real-world objects such as power plants or consumers based on the described graph logic are provided. Every class has associated objective expression terms, optimization variables and constraints. Depending on the object attributes set by the user these associated terms will be added to the model.

The objective function for a specific model consists of different expressions depending on chosen components and their attributes. Hence, only a general description for main categories of distinct expression types is given in this section. Generally, total costs for the simulated time horizon T are minimized, whereas the expression term includes time-dependent terms for all variables w associated with an edge (s, e) (i.e. connecting a start node s and an end node e) and for all variables v associated with a node n. In addition, time-independent terms for node and edge weights may be added.

$$\begin{aligned} \text{min:}\ & \overbrace{\textstyle\sum_{t\in T}\left(\sum_{(s,e)\in E}\sum_{i\in I_1} c^{i}_{(s,e)}(t)\cdot w^{i}_{(s,e)}(t)\cdot\tau\right)}^{\text{t}-\text{ dependent expression for edge weights}}\\ &+\overbrace{\textstyle\sum_{(s,e)\in E}\sum_{i\in I_2} c^{i}_{(s,e)}\cdot w^{i}_{(s,e)}}^{\text{expression for edge weights}}\\ +\ & \overbrace{\textstyle\sum_{t\in T}\left(\sum_{n\in N}\sum_{i\in I_3} c^{i}_{n}(t)\cdot v^{i}_{n}(t)\cdot\tau\right)}^{\text{t}-\text{ dependent expression for node weights}}\\ &+\overbrace{\textstyle\sum_{n\in N}\sum_{i\in I_4} c^{i}_{n}\cdot v^{i}_{n}}^{\text{expression for node weights}} \end{aligned} \tag{2}$$

The parameter c may be interpreted as a specific cost and the time-increment τ is determined by the temporal resolution. Sets I_1 to I_4 stand for the possibility of multiple costs and weights for one edge or node. Domains D of variables w and v can either be positive reals, positive integers or binary, as a special sub-type of integer.

$$D = \{\mathbb{R}^{+}, \mathbb{Z}^{+}, \{0,1\}\} \tag{3}$$

Generally, all variables are bounded by lower and upper bounds which are set based on the class attributes of the modelled components.

$$0 \le w^{i}_{(s,e)}(t) \le \overline{w}^{i}_{(s,e)}(t) \qquad \forall\ i \in I_1, \forall\ (s, e) \in E, \forall\ t \in T \tag{4}$$

$$0 \le w^{i}_{(s,e)} \le \overline{w}^{i}_{(s,e)} \qquad \forall\ i \in I_2, \forall\ (s, e) \in E \tag{5}$$

$$0 \le v^{i}_{n}(t) \le \overline{v}^{i}_{n}(t), \qquad \forall\ i \in I_3, \forall\ n \in N, \forall\ t \in T \tag{6}$$

$$0 \le v^{i}_{n} \le \overline{v}^{i}_{n}, \qquad \forall\ i \in I_4, \forall\ n \in N \tag{7}$$

The library consists of a large set of constraints that are documented extensively in the latest online documentation of the software. In addition, the library is being continuously improved. Therefore, possible constraints are subject to changes and depend on the version of the library. For these two reasons the constraints are not outlined in detail. Instead, a general form of constraint which all specific component constraints must follow is given in equation (8).

$$\begin{aligned} &\sum_{k\in P_n}\sum_{j\in J_1} a^{j}_{(k,n)}\cdot w^{j}_{(k,n)} + \sum_{k\in S_n}\sum_{j\in J_2} a^{j}_{(n,k)}\cdot w^{j}_{(n,k)} + \sum_{j\in J_3} a^{j}_{n}\cdot v^{j}_{n} + M\\ &\quad \le 0 \qquad \forall\ n \in N \end{aligned} \tag{8}$$

The important characteristic of this constraint is the reduced possibility space of related variables inside one specific constraint. Defined from the perspective of a node n, only variables w and v associated with an edge from one of its predecessors P_n to node n, an edge from node n to one of its successors S_n, or the node itself may appear. In this context, the parameter a may be interpreted as an efficiency, for example. The

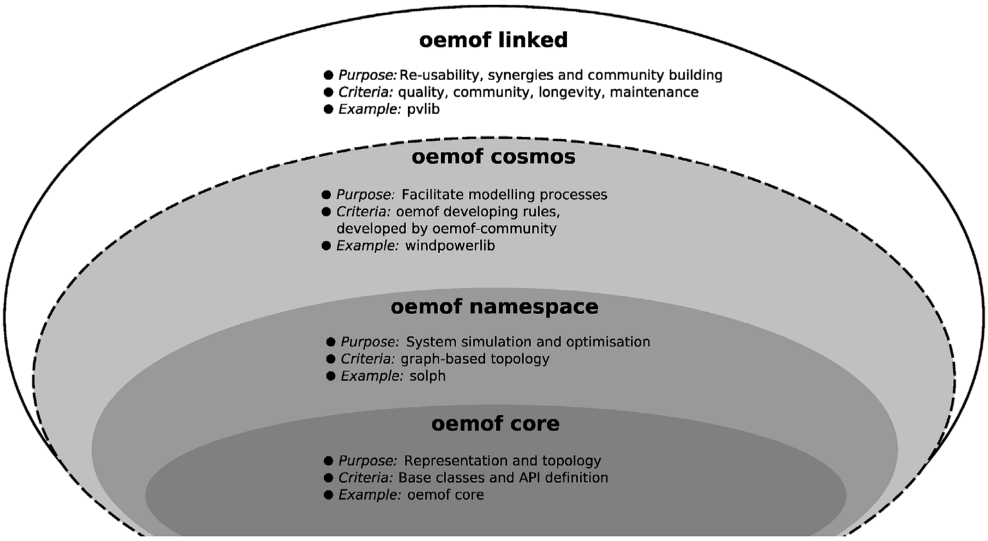

Fig. 2. Layer structure of the oemof project architecture.

sets J_1 to J_3 stand for the possibility of multiple parameters and weights for one edge or node.

3.3. Project architecture

The project tries to accommodate energy system modellers with a large set of functionalities they typically need. To achieve this, the project and its development process follow an architecture that groups the content of the framework into functional and organizational units. This architecture consists of the four layers depicted in Fig. 2. These four layers are used to categorize the libraries associated with the oemof project according to their dependencies and commonalities.

The framework itself and its underlying concept are implemented using an object-oriented approach in the high-level programming language Python and they are published under the GNU GPL3 licence. Python libraries are called packages; the main component of the framework is the oemof package. This package covers the first layer completely and the second layer partially. The layers beyond the first differentiate how closely libraries are associated with the oemof package and its developers in terms of organizational ties as well as technical dependencies.

1. At the *core* layer a generic graph structure is implemented via core classes. These classes are used to instantiate the objects comprising an energy system graph and define how an energy system is described. In addition, the basic application programming interface (API) is defined, through which the core objects and their properties representing the graph are accessed. The entire *core* layer is kept free from energy system-specific logic in order to accommodate a broad spectrum of modelling approaches. Additionally, it allows decoupling of the energy system's representation from how it is modelled. The intended use of the core objects in layers above the *core* layer is communicated via carefully chosen naming and explicit documentation.
2. The *namespace* layer contains associated libraries that share the same basic system formulations, i.e. libraries modelling energy systems as graphs described in terms of objects from the *core* layer. They depend on the basic API by either directly using *core* classes or adding functionality on top of them via inheritance. That way, different modelling approaches can be used on energy systems described in a uniform way, namely as energy system graphs consisting of instances of *core* classes or of classes inherited from them. Possible modelling methods can model energy systems with respect to cost, power-flow or any other kind of simulation or optimization goal. Currently the *oemof.solph* can be used to generate linear (mixed-integer) optimization problems from an energy system representation based on core objects. However, the graph structure is capable of accommodating other concepts such as evolutionary optimization or agent-based modelling.
3. The *oemof cosmos* layer contains libraries from the field of energy system modelling that are associated with oemof in an organizational way without sharing the basic API. These libraries, while still part of the oemof project, are not developed as part of the same package and may thus be used, reviewed and developed by third-party modellers and experts as well. However, as they are developed as part of the framework, they follow the common development rules (Section 3.5). As most modellers are not primarily programmers, sharing the same development, structure and documentation rules can help in learning how to use the libraries. One example of such a library is the windpowerlib [32], a library generating feed-in time series of wind energy turbines from meteorological data.
4. Open source does not necessarily lead to cooperation [10]. To facilitate cooperation, the *oemof linked* layer contains existing community libraries. These libraries are written in Python but do not necessarily share the same rules. However, in order to be considered associated, they should meet general standards for quality, code development, longevity, maintenance and community structure. One example of such a library is the pvlib [33], which is a library developed independently from oemof and which will be integrated into the framework via interfaces in the feedinlib. The process of developing these interfaces has already lead to code contributions towards pvlib, instead of the creation of a parallel, competing solution.

3.4. Implementation

The graph concept has been implemented at the *core* layer in the form of a class hierarchy which is sketched in Fig. 3. The root elements of this class hierarchy are *Node*, *Edge* and *EnergySystem*. *Node* is the abstract base class for *Bus* and *Component*, which are used to represent nodes in the bipartite graph representing the energy system. Further, components are subdivided into *Source*, *Sink* and *Transformer* classes depending on how they are connected to *Bus* objects. Objects of the class *Edge* represent the directed edge between two nodes, i.e. the connection between a *Bus* and a *Component* object. The class *EnergySystem* serves as a container for nodes and may hold additional information about the energy system.

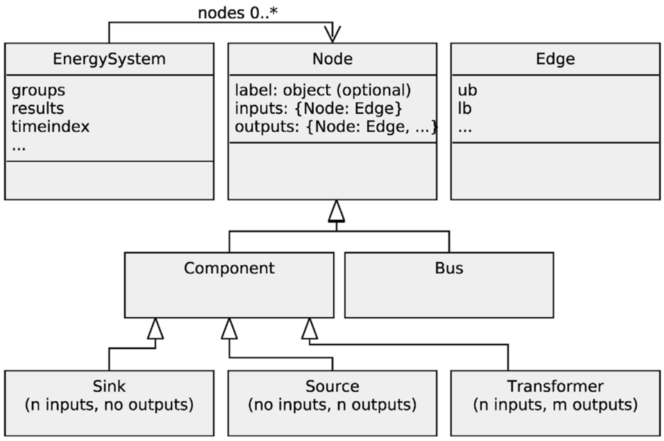

Fig. 3. UML class diagram of oemof core classes.

All basic energy system components such as energy demands, (renewable) energy sources and transformers between different energy buses can be modelled by means of these basic classes. Additional components that introduce new features can be added via inheritance. If sub-classing is not suitable, new classes can be created and used together with the core classes. As an example, the *solph* library introduces a storage class with different individual parameters.

A demonstration of separation of the description of the energy system from its computation can be seen through the introduction of the *Edge* class, which is separate from the *Node* class hierarchy. Objects of this class hold information about the flow between two nodes, such as maximum available transfer capacities of power line flows or whether the amount of a certain flow is fixed and if so, its value. As evidence of the generic flexibility, objects of this class are used in the *solph* library to build inter-temporal constraints for different kinds of energy system optimization problems such as combined heat and power modelling or unit commitment.

The *EnergySystem* class serves as a container for the aforementioned elements and provides the possibility of adding extra information such as grouping structures or optimization parameters. Additionally, it provides interfaces to save and restore the energy systems instance and to process results. This allows for an intuitive handling of energy systems by treating them as their own entity.

An implementation using the high level programming language Python has the advantage of a rich set of external libraries usable for scientific computing. Oemof itself makes heavy use of external modules for optimization problems (pyomo [34]) and data handling (pandas [35]).

3.5. Documentation, collaboration and testing

‘A critical part of any piece of software is the documentation’ has already been stated by Greenhall and Christie [36]. This is of particular importance for open source projects with many users and a changing developer base. With the objective of thorough documentation in all stages and formulation of general nomenclature, a documentation strategy on four different levels similar to that of Howells et al. [19] is followed:

1. *Comments inside the code* are used to explain non-intuitive lines of source code to new developers and interested users at the lowest level.
2. *Docstrings* located inside the source code describe the API, i.e. how to use the various classes, methods, and functions.
3. *Higher level descriptions* provide the user with additional information about the possible interactions between different libraries or application-specific usage information. These manuals are located inside the repository and are therefore shipped with the source code.
4. *Examples* provide an additional source of documentation that is particularly useful to new users and developers.

Keeping such detailed documentation consistent and up-to-date across continuous releases comes at the expense of a high maintenance effort. Nevertheless, it is of special importance; the oemof documentation is the place to find information on the formulas used within an oemof-based model. Up-to-date, consistent documentation that tracks changes in a timely fashion is essential if external users want to understand the internal logic of a model, especially in scientific applications. The upside is that documentation adhering to these principles acts as a citable source of information, reducing the amount of redundant information that must be sourced and digested in order to understand a model. This in turn increases transparency and comparability.

As oemof is an open-source community project, a common platform for collaboration is needed. Similar to Greenhall and Christie [36] as well as other open-source energy modelling projects, oemof uses GitHub for collaboration, code hosting and bug tracking, which allows for easy copying and forking of the project. To lower entry barriers for new developers, hierarchies for all processes are kept as flat as possible. We have found that this can create a sense of belonging for collaborating developers which increases participation. GitHub is based on the version control system *git* and code can be developed in parallel on different branches. In order to ensure an effective branching strategy and release management, a well-established git workflow model [37] is set as the standard for all developers. Contributions to the code base are managed through pull requests, which allow for an open review of potential changes. Further, code changes are checked for conflicts before being merged back into the development branch by the developer in charge of the affected library.

In order to test oemof's functionality in case of changes to multiple parts of the code base, *unit tests* are employed. During the testing process, all integrated application examples are run and the created results are checked against stored historical results. Only if all examples run without errors is a pull request merged back into the development branch. This procedure ensures the functionality even if major changes to the code base are applied from one release version to another.

4. Usage: applications

The framework is not designed to be a standalone executable. Instead, the oemof libraries are meant to be used in combination to build energy system models. In the following we will refer to such models as oemof-*applications*.

4.1. Application development

Applications can be developed by the use of one or more framework libraries depending on the scope and purpose. Fig. 4 illustrates an example process of building an application. Modelling can thus range from a few plain steps in a standalone Python executable to complex procedures bundled in a new Python library based on oemof. Due to the modular concept, specific functionalities of oemof libraries can be substituted easily depending on the modelling task. This provides a high degree of freedom for developers, which is particularly relevant in scientific working environments with spatially distributed contributors and fast evolving research questions.

Depending on the problem, input data can be created by means of libraries such as the *feedinlib* or *demandlib* library. A standardized result processing library (*outputlib*) provides all optimization results in convenient data structures that are ready for exports to different formats, detailed analyses and plotting. Although this feature might appear

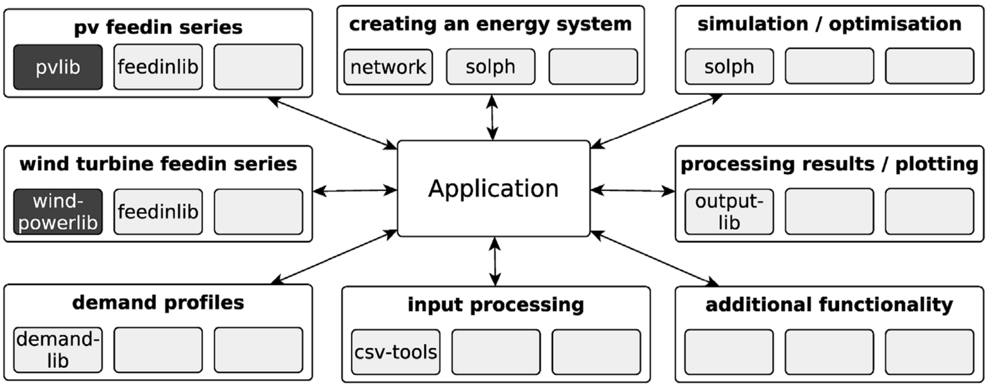

Fig. 4. Building an application based on libraries of the oemof cosmos and external libraries (dark grey).

trivial, it is one major advantage over other heterogeneous optimization tool-chains that require switching between tools e.g. GAMS for the modelling and a spreadsheet-based solution for result processing.

However, in considering the modelling workflow for the oemof namespace layer, all applications have some major steps in common and include all required data pre- and post-processing. First, an empty energy system object is created. This object acts as a container for the nodes and carries information such as the time resolution. The energy system object may also hold different variants of the system representing different scenarios. Additionally, methods to handle nodes are provided. The next step is the instantiation of nodes and flows of the modelled energy system which are added to the existing energy system instance (population of energy system). Subsequently, the results of the energy system can be computed by simulating or optimizing the system. Finally, results can be processed with the output library of oemof. The *oemof-outputlib* makes it easy to get different views of the results and plots based on a uniform output data format.

4.2. Example application workflow: system optimization

One common use case for a modelling process that utilizes different toolboxes is the optimization of energy systems. In this process the *solph* library can be used in combination with existing input and output data libraries. First, feed-in data for renewable power plants and electricity demand profiles can be generated within the *feedinlib* and *demandlib* libraries. Subsequently, the data are used as exogenous parameters within the *solph* library before the optimization results are processed within the *outputlib*.

The *solph* library allows the creation of mixed-integer linear models. As a common requirement, an energy system graph has to be created with classes from the *core* layer, respective *solph* subclasses from the *namespace* layer or a mix of both. The energy system serves as a container that holds all nodes and general information such as the temporal resolution of the optimization problem. Since an oemof optimization model inherits from a model of the *pyomo* package, the full functionality of this package can be leveraged. Depending on the experience and modelling task, three different ways exist to create an optimization problem based on an oemof energy system instance.

1. In the most common and easiest use case, the energy system describes a graph with flows on its edges by combining basic components and buses. The optimization model for this use case is automatically created by a logic that transfers the graph (connections between buses and components and their attributes) into respective constraints, e.g. commodity balance equations or inequalities for lower and upper flow bounds. When using this way of modelling, all models are derived by the object parametrisation and no mathematical definitions like sets, variables or parameters have to be implemented.
2. In the second use case, basic energy systems can be adapted by defining additional constraints on top of the aforementioned graph logic. Since this logic is consistent throughout, entry barriers for new users are lowered. As one example, an annual limit on a commodity flow can be implemented easily by a definition of (in) equations applied to a set of flows.
3. In the third use case, custom components can be added to a model. This is possible by subclassing from core components or by creating one's own components from scratch. As mentioned before, the full functionality of the *pyomo* package can be utilized to model complex internal relations of components with numerous constraints, specific sets and different variable domains. Such a component needs to provide input/output slots that may be connected with flows of graph.

All use cases can be applied separately or combined within one model. The model type itself, e.g. an economic dispatch, investment or unit commitment model, is determined by its parametrisation. This allows for maximum flexibility, as one can quickly change the model, from economic dispatch to investment, for example, by exchanging single components, say a storage with fixed capacity (parameter) by one with variable cost-determined capacity (decision variable), for example. In a similar way, complete sub-graphs can be exchanged quickly by connecting or disconnecting them from a main problem.

4.3. Existing applications

The framework has already been used to build comprehensive applications for different research projects (see Refs. [38–43]). In addition, oemof is also used actively in teaching by some institutions in order to gain insight into complex energy systems. An example for such a system modelled as an oemof application is illustrated in Fig. 5. In the following, selected oemof applications are described to illustrate the broad range of applications. These distinguish themselves by technologies considered, demand sectors modelled, regional representation, the time horizon of the analysis, the modelling methodology to represent technological characteristics and perhaps a market representation.

The renewable energy pathways simulation system (*renpassG!S*) [44] is a bottom-up fundamental Western European electricity market model. Future scenarios of the power plant dispatch and price formation in Germany and its interconnected neighbouring countries can be modelled based on operational and marginal costs and the assumption of an inelastic electricity demand. Based on *renpassG!S*, a spin-off model that is adapted to the requirements of the Middle East and North Africa

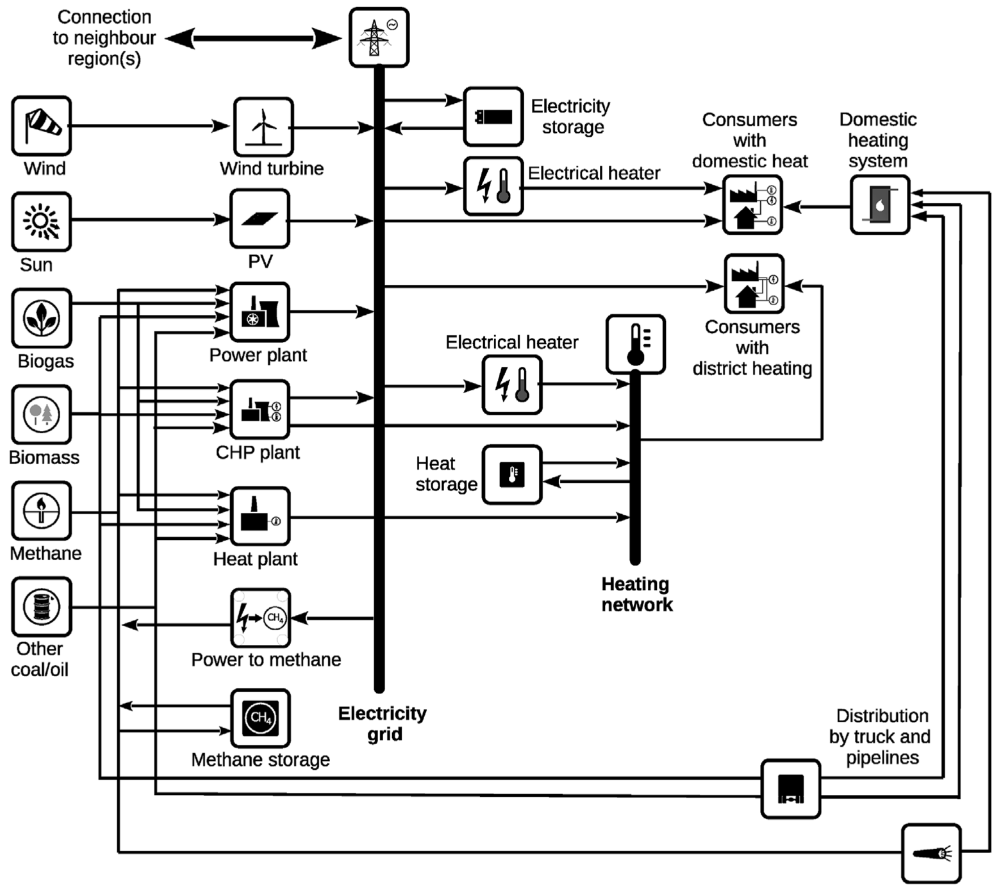

Fig. 5. Representation of a complex energy system within an oemof application.

(MENA) region was created. In this application the *solph* library was used with a restriction to purely linear equations. Both applications use a standardized interface to csv-files for the *solph* library that was created to simplify the usability for users with no programming experience.

The *openMod.sh* application is a flexible software tool that is strongly based on oemof's underlying concept [41]. This model has been applied in participative workshops for the development of regional climate protection scenarios. The combination of a graphical browser-based user interface combined with an open-source modelling approach enhances the modeller-decision-maker interface. The extension of the underlying concept to a database concept shows that this concept may not only be used for the computation of systems but also for their representation in a relational database. Due to the open licence and the high-level language, oemof applications can be set up on public servers with little effort and without legal barriers.

An example for the flexible extension of oemof at the application level is the Heating System Optimization Tool (*HESYSOPT*) [45]. In this application, detailed heating system components are modelled with mixed integer linear programming techniques that are based on oemof.solph functionalities. Using the underlying *pyomo* library *solph* provides an interface to add new components within the application. After a review, such components can be integrated into *solph* to be available for the entire community.

As a fourth example, *reegis*^{hp} [46] models heat and power systems on a local scale. The objective is to evaluate district heating and combined heat and power technologies in energy systems with a high share of renewable resources from an environmental and economical perspective. The local system is connected in terms of electricity to a national model based on the idea of the model *renpassG!S* [44] which is extended to include the heating sector. This application uses oemof's *windpowerlib*, *feedinlib* and *demandlib* to provide the input data for the model. Further, the *solph* library is used to create a large-scale linear model and a detailed mixed integer linear problem. This example demonstrates how models of different scale may be combined in one application.

These applications illustrate the flexibility of oemof and the extent of the potential user group, not only with regard to the content, but also concerning the level of involvement. It is possible to build a full-scale energy system model adapted to the user's needs by just employing existing functionalities. Moreover, different models can be combined and adapted with little effort to create tools for specific purposes. This enables users to answer challenging research questions within a single framework.

5. Conclusion

The paper presents the Open Energy Modelling Framework (oemof) as a contribution to the scientific modelling community. With a collaborative and open development process, it is designed for transparency and participation. Complementary to its technical features, the project constitutes a novelty in energy system modelling and aims to facilitate open science in this research field.

One central feature of oemof is the generic graph-based foundation which has been implemented using an object-oriented programming methods in the high-level language Python. The cross-institutional collaborative development of the framework has started a process towards this common and generic structure. This concept highlights the distinction between the description of an energy system with its components and subsequent computations based on combining an intuitive description with a specific mathematical approach. It lays the foundation for a universal representation of multi-sectoral energy systems at different scales. Another important feature is its strict open-source and non-proprietary philosophy. This philosophy, the underlying concept and the extensive documentation allow new developers to adapt or extend the framework easily and leverage features of other scientific Python libraries. With these properties, the project is suitable for new developers and users and thereby supports a continuous development process.

The framework has been successfully applied in different research projects at several institutions. Existing oemof applications include electricity market models, detailed technical unit commitment models for district heating systems and sector coupled regional energy system models. Energy systems ranging from distributed or urban ones up to a national scale may be modelled, making the framework a multi-purpose modelling environment for strategic energy analysis and planning.

Although it takes effort for new users to learn to build an oemof-based application, we think there are good reasons to choose oemof. Firstly, the flexibility in application development allows adjustments along with changing research objectives and may thus avoid lock-in effects. This seems to be particularly relevant for project-based research. Secondly, the community character of the oemof-project is another important factor. The possibility for active participation in development and decision processes allows users to be part of a community. We argue that this can create a sense of belonging, a value that goes beyond the technical features of the software.

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- Otto von Guericke University Magdeburg (OVGU)
- Reiner Lemoine Institut Berlin (RLI)

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5

oemof.solph — A model generator for linear and mixed-integer linear optimisation of energy systems[1]

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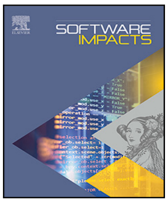

Original software publication

oemof.solph—A model generator for linear and mixed-integer linear optimisation of energy systems

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ABSTRACT

Energy system modelling is of high importance to investigate different scenarios in their technical, economical and environmental feasibility. The interplay of different technologies and energy flows in respective models can be represented as directed graphs in a generic but comprehensible formalism. However, additional effort is needed to create specific models and to derive an optimal sizing or operation of components. To tackle this problem, oemof.solph facilitates the formulation of (mixed-integer) linear programs from a generic object-oriented structure. Its structure allows to create models on different levels of detail by means of predefined components and an optional formulation of additional expressions and constraints. With its open and documented code base, extensive collection of examples and an active community it is useful across many levels, from simple applications to advanced modelling.

Code metadata

Current code version	v0.4.2dev0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2020-25
Permanent link to reproducible capsule	https://codeocean.com/capsule/8999562/tree/v1
Legal Code License	MIT
Code versioning system used	git
Software code languages, tools, and services used	Python (available for any OS)
Compilation requirements, operating environments & dependencies	blinker, dill, numpy, pandas, pyomo, networkx
If available Link to developer documentation/manual	https://oemof-solph.readthedocs.io
Support email for questions	contact@oemof.org

Software metadata

Current software version	v0.4.1 [1]
Permanent link to executables of this version	https://pypi.org/project/oemof.solph/
Permanent link to Reproducible Capsule	https://codeocean.com/capsule/8999562/tree/v1
Legal Code License	MIT
Software code languages, tools, and services used	Python (available for any OS)
Compilation requirements, operating environments & dependencies	blinker, dill, numpy, pandas, pyomo, networkx
If available Link to user manual — if formally published include a reference to the publication in the reference list	https://oemof-solph.readthedocs.io/en/stable/
Support email for questions	contact@oemof.org

The code (and data) in this article has been certified as Reproducible by Code Ocean: (https://codeocean.com/). More information on the Reproducibility Badge Initiative is available at https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals.

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1. About solph and oemof

The solph package [1] is part of the open energy modelling framework (oemof), which has been developed to model integrated energy systems [2]. Its basis is a graph structure consisting of buses and components connected by directed edges representing the flow of energy carriers and resources, their conversion and consumption. This structure allows to model different sectors of the energy system equivalently. Whereas the graph holds information on the topology and relationships between the nodes, solph converts this graph into an optimisation model.

It is implemented in Python based on the optimisation package pyomo [3]. In combination with the object-oriented graph based data model, modelling does neither require deep knowledge about mathematical optimisation nor an (algebraic) modelling language to implement linear (LP) and mixed-integer linear (MILP) problems. Instead, it can be undertaken by comprehensive domain-specific, in this case energy system, knowledge.

Within the workflow, different versions of an energy system model are built:

1. The oemof graph version is created.
2. The associated pyomo optimisation instance is constructed.
3. The model is passed to an external solver (for example using the LP file format).

The solver optimises for minimal costs that can be economic, environmental, technical or any other type of cost. Currently, users can create economic dispatch and unit commitment models with an additional investment optimisation. Due to the modular structure of the package, the API and underlying mathematical constraints of new components can be developed and reviewed individually. This allows to review, discuss, improve and add components in a collaborative process within the community and beyond. A comparison with other (linear) optimisation tools [4,5] has proven consistency of results.

2. Contribution to the scientific community

The research area of energy system analysis faces different challenges which lie in an increasing complexity, higher levels of uncertainty and more interdisciplinary properties of energy systems [6]. Moreover, the challenges of energy system modelling [7] have brought up the demand for suitable tools to better address scientific standards [8,9]. The latter were among the main drivers for the design of the oemof framework and the solph package, respectively [2]. Based on the previous experience with building energy system models, the initial development of oemof aimed to contribute to the scientific community through the following features:

Supporting reusability

A strong motivation to build oemof.solph is to avoid double-work. It is intended to relieve modellers from programming utility code and let them focus on their core task: modelling energy systems. To facilitate this, the source code has to be well tested and documented. Validation, including unit testing and usage within a community and many use cases, reduces the likeliness of bugs and creates a tested code base. Finally, a detailed documentation with many examples lowers the entry barrier for new users in the field of energy modelling. Therefore, oemof.solph is also suitable for projects and studies in which modelling is not the main focus or projects with a limited time budget. Beyond citations in scientific publications, usage itself remains almost invisible. However, a number of studies has been published, not only in scientific journals. Solph[1] is used by a number of other open source projects on GitHub [10,11]. Additionally, we get support questions from companies in the consulting and energy sector work with oemof.solph.

Building a developer community

Since the very beginning of oemof's development it was a strongly pursued goal to create a developer community that is open for members from various institutions. Such research groups value the existing code base as well as the possibility to discuss extensions in the community and to get a review for new components or additions to oemof.solph from other modellers. Since the beginning, new research groups from other institutions joined the developer team. For example, researchers of the projects Quarree100 [12] and EnAQ [13]. Both users at different levels and new developers, attend the oemof developer and user meetings that are held on a regular basis.

Supporting open science principles and transparency

Using solph it is possible to publish studies following Open Science and transparency rules. The permissive open source license facilitates users to build an open science tool chain. Models for the electricity sector [14–16] and for district heating grids [17] are show-casing how to implement a model chain incorporating open data from OpenStreetMap. Even without building a fully automatised tool chain, the permissive license of the oemof.solph's code facilitates to publish the model alongside with the data. This was done for a study about the validation of exit strategies for lignite and coal in Brandenburg [18].

Integrating a modelling toolbox

While oemof is meant to be a software cosmos, suitable for building model-chains and providing easy-to-use libraries and tools for energy system modelling, as of today, solph is the most recognised library of the framework. Thus, most studies citing oemof also use solph. However, there are also examples that use exclusively specific other oemof packages such as *demandlib* [19] for load curve generation [20], *TESPy* [21] for thermal engineering systems or the *windpowerlib* [22] for wind power feed-in calculation based on weather data.

3. Specific impact on research

The oemof.solph library is used for a wide variety of research questions. Its generic design allows to model energy systems in any possible combination of sectors. For the electricity sector, example publications discuss adding storage to existing supply [23,24] – in one case in addition to electrification of agricultural machines [25]. Others analyse the possible vulnerability for future energy systems [26], or optimise of the utilisation of pumped energy storage in Switzerland [27]. The possible integration of more renewable energy has been investigated for the case of Italy using both, a fixed model [28,29] and linear invest optimisation showing pathways to more renewable energies [30]. Other uses include the layout of a complete mini-grid [31–33], or providing the technical side of study social and ecological factors in energy system modelling [34–36]. For the heat sector, studies exist that determine the optimal size of heat and cold storage [37,38], check the use of district heating for demand side management [28], do a life cycle analysis [39], or increase the model accuracy using a pre-calculated fluctuating temperature supply [40]. Others use the solph for dispatch optimisation

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[1] Note that some dependencies still point to the oemof and not to the oemof-solph repository.

inside a non-linear size-optimisation heuristics for electricity and heat supply [41], or compare different mobility options [42].

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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6

oemof.tabular — Introducing Data Packages for Reproducible Workflows in Energy System Modeling[1]

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ABSTRACT

The paper describes how Data Packages can be used for creating reproducible workflows in energy system modeling. The presented concept has been implemented in the Python package *oemof.tabular*. The package is designed as an interface to instantiate energy system models from tabular data sources based on the *oemof.solph* library. To implement the data model, *oemof.tabular* extends the Open Energy Modelling Framework (oemof) by facada classes. The developed data model allows users to work with Data Packages and meta data information. The simplified tabular data structure can be used for large energy system models as well as in teaching environments leveraging functionalities of the already widely used *oemof.solph* library.

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1 INTRODUCTION

Analyses of future energy systems are based on tools for complex socio-techno-economic systems. The complexity of these systems increases due to the intermittent supply characteristics of renewable energies which require high temporal and spatial resolution modeling. Additionally, a higher interaction between sectors such as heat, power and transport leads to the need for comprehensive sector coupled approaches. At the same time, a trend towards open source energy (system) models can be observed in the energy system modeling research field [15], as models have been criticized for lack of transparency and reproducibility [17].

For energy system modelers, data handling including input collection, processing and result analysis is one of the most time-consuming tasks. Therefore, open source and open data modeling approaches are put forward as an argument for efficient use of resources [19]. Yet, there is no standardized or broadly used model-agnostic data container in the scientific field of energy system modeling to hold energy system related data. In most cases every software comes with its own logic relating to input-data and output-data of the model. In addition, the decision about how to create the required data sets from raw data sources and the post-processing of result data is often left to the user. Due to these two reasons, re-use of data and more importantly reproducibility of model results is a challenging task, even for experienced modelers.

To improve reproducibility of model results and re-usability of existing data, the following data model description has been developed. Energy system related data is stored in the Data Package format. The complete reproducible workflow from raw-data to final results is described for this data model. The data model has been implemented in the Python package *oemof.tabular* [7] which is based on the Open Energy Modeling Framework (oemof). However, the concept is not restricted to this package, but can be applied with other software as well.

2 BACKGROUND

Oemof is a powerful tool for the modeling of energy systems [8]. Functionalities range from large linear programming (sector coupled) market models [6, 23, 16] to detailed mixed integer heating system [2, 27] or battery models to assess the profitability of power plants in current and future market environments. The underlying concept and its generic implementation allows for this versatile application. It is based on a bipartite graph structure, where nodes are partitioned into buses and components. Most oemof components are of a rather abstract type. For example the `Transformer` class can be used to model different energy system components such as power plants (1 input, 1 output) as well as a heat pump (2 inputs, 1 output) or any other conversion process. To illustrate the concept, ***Figure 1*** shows a `Transformer` connected to different buses (1 input, 2 outputs) to model a combined heat and power (CHP) plant.

The usage of the Python API for this component in *oemof.solph* is shown in ***Figure 2***.

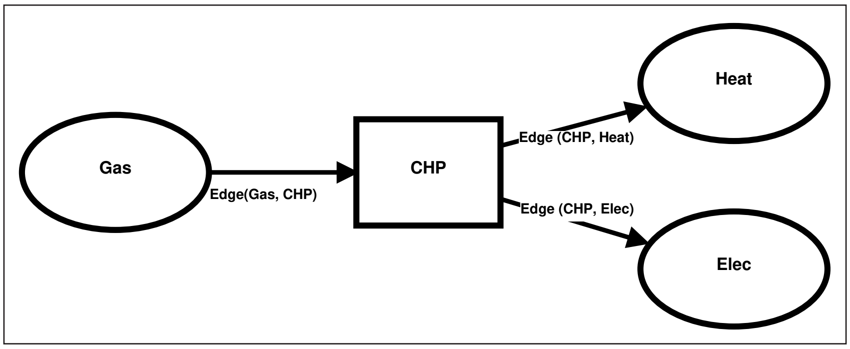

Figure 1 Illustration of a CHP plant model based on the *oemof.solph* `Transformer` class. Nodes are shown as ellipses/squares and edges between the nodes are depicted as arrows.

```
import oemof.solph

Transformer(
    label=’CHP’,
    inputs={
        Gas: Flow(variable_cost=0.6)},
    outputs={
        Elec: Flow(investment=Investment(ep_costs=50)),
        Heat: Flow(nominal_value=40)}
    conversion_factors={Elec: 0.4, Heat: 0.35})
```

Figure 2 Example of the *oemof.solph* Application Programming Interface (API) for a transformer component with one input and two outputs.

When building energy system models, data is often stored in a tabular data format, for example, CSV files, Excel files or relational databases. However, the design and implementation of a generic tabular data input processing tool for *oemof.solph* has proven to be difficult. One of the reasons is that tables are a flat and two dimensional data structure whereas *oemof.solph*'s API utilizes a high degree of nested objects and data structures. Mapping this nested approach onto flat tables is a non-trivial task.

3 FACADES

Facilitating the task outlined above is one of the functions *oemof.tabular* needs to accomplish. The package was developed in order to allow the user to create an oemof model via tabular data sources. This means that it must also enable her to specify *oemof.solph* components using such flat structures. In *oemof.tabular*, this is done by using the *façade design pattern* first introduced by Gamma et al. in 1994 [5]. The facade design pattern has two main purposes: 1. it provides a simple interface for users to access functionalities of a complex subsystem and 2. it loosens the coupling of consumers of the subsystem's interface with the components of the subsystem.

Therefore, facade classes have the following advantages when viewed in the context of *oemof.tabular*:

- Facades allow instantiation of models from two dimensional data sources as they provide a simplified interface to complex underlying structures.
- The simplified and thus restricted and less generic mathematical representation leads a more transparent modeling approach.
- The simplified interface is easy to use and integrate within the context of teaching and capacity building.
- It also allows building an interface for composed components which are constructed using multiple *oemof.solph* objects.
- Facades can be used with a different back-end, which allows the integration of other energy system modeling frameworks which may not even have to be written in the same programming language.

The implementation

A user of oemof and *oemof.solph* is expected to use instances of classes from a particular class hierarchy to build a model. Thus, facades are integrated into this class hierarchy as a mix-in class: a facade to a specific *oemof.solph* class is created by sub-classing it, mixing in the *Facade* class via cooperative multiple inheritance and then using the general facade methods to simplify the interface of the original *oemof.solph* class.

This allows for a two step approach to build complex components out of simple ones. One can first aggregate a complex subsystem using *composition*, without having to think about simplifying the interface of that system. Simplifying the interface can be done in a second step by creating a facade via *inheritance*.

The *oemof.tabular* package not only provides the facade infrastructure, but also implements a number of facades to regular simple *oemof.solph* components as well as complex compositions of *oemof.solph* components.

Since facades are integrated into *oemof.solph*'s class hierarchy, the classes of all *oemof.tabular* components are sub-classes of *oemof.solph* components, which means that they can freely be mixed with all their more generic parent class objects in a model. In addition, the data model is extendable and could be applied for various model generators, like for example PyPSA [13] or calliope [21]. However, currently the implementation for reading Data Packages is limited to *oemof.tabular* classes. The facade concept as used in *oemof.tabular* has also proved it's applicability by being transported to and used in the *oemof.thermal* [14] package.

The issue of transparency

Model generators such as *oemof.solph* can indeed simplify energy system modeling. However, it is noteworthy that this is a double-edged approach. Simplification for the user always comes with drawbacks as the complexity remains hidden from the user. Depending on the parameters provided, different sets of constraints are created. Nonetheless, resulting mathematical equations are not visible at any stage of the modeling process. Therefore, approaches like *OSeMOSYS* [11] can have a higher level of transparency than other object oriented model generators. As such models or model generators are implemented in a pure algebraic modeling language, every part of the model (variable definitions, constraints, etc.) is clearly and transparently detectable in the source code files. In the case of facades in *oemof.tabular*, mathematical relations of the models and their implementation are hidden by an additional layer of classes. However, since the *oemof.tabular* API is less generic and more restricted than the *oemof.solph* API, the additional layer may actually increase transparency compared to *oemof.solph* components by creating a clear link between input-parameters and the resulting mathematical model.

FACADE EXAMPLE: HYDRO RESERVOIR MODELING

To illustrate the facade concept, subsequently an *oemof.tabular* storage example is compared to the classical *oemof.solph* approach. The *oemof.solph* package provides a `GenericStorage` class to model different storages such as batteries, hot water storages or pumped hydro-electric storages. To model reservoir storages with an inflow and possible spillage, a set of connected *oemof.*

solph components is required. To simplify modeling, the `Reservoir` facade bundles these components and provides a high level API access to a more complex underlying model. ***Figure 3*** provides an illustration of the Reservoir facade.

The facade class itself is a subclass of the `GenericStorage`. However, to allow for a constant inflow into the storage, an additional `Source` object is created.

The reservoir is modeled as a storage with a constant inflow (x denote endogenous variables, c denote exogenous variables):

$$x^{level}(t) = x^{level}(t-1) \cdot (1 - c^{loss\_rate}(t)) + x^{profile}(t) - \frac{x^{flow,out}(t)}{c^{efficiency}(t)} \qquad \forall t \in T \quad (1)$$

$$x^{level}(0) = c^{initial\_storage\_level} \cdot c^{capacity} \quad (2)$$

The inflow is bounded by the exogenous inflow profile. Thus, if the inflow exceeds the maximum capacity of the storage, spillage is possible by setting $x^{profile}(t)$ to lower values.

$$0 \leq x^{profile}(t) \leq c^{profile}(t) \qquad \forall t \in T \quad (3)$$

The spillage of the reservoir is therefore defined by $c^{profile}(t) - x^{profile}(t)$. Additional constraints apply which have been omitted in the description but can be retrieved from the oemof documentation.

API comparison for the reservoir example

Subsequently, in ***Figure 4***, the Python code to instantiate this component is shown. In comparison to the *oemof.tabular* code, the required *oemof.solph* code differs significantly (see ***Figure 5***). First of all, more objects with a nested set of objects need to be instantiated (Flows, Sources). This nested structure allows for a very flexible modeling approach. However, it creates hurdles for writing a generic data interface to instantiate all these objects, due to the large set of possible combinations. In contrast, the flat structure of the facade arguments allows for a simple interface to tabular data. One additional difference which can be observed is the (energy) specific naming of attributes, for example efficiency, compared to outflow_conversion_factor. As the `Reservoir` class is a subclass of the `GenericStorage` class, some attributes

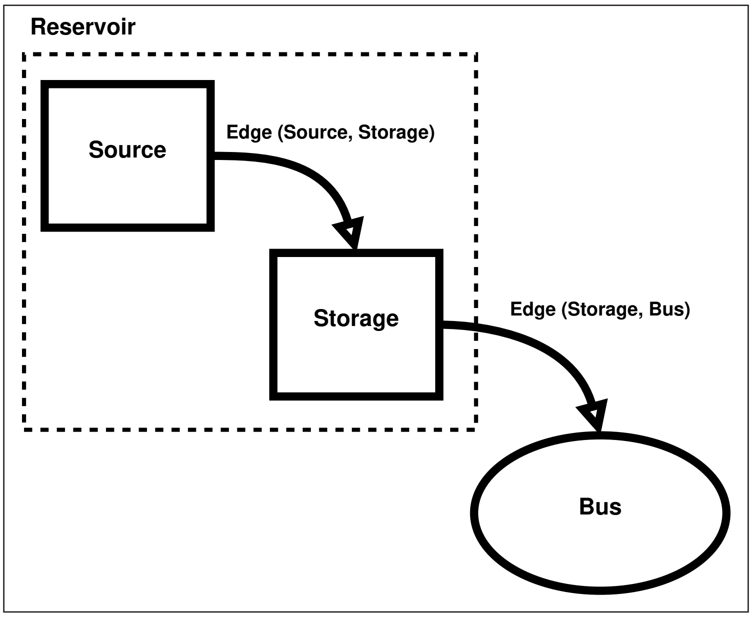

Figure 3 Illustration of a reservoir model in *oemof.tabular*.

```
from oemof.tabular.facades import Reservoir
from oemof.solph import Bus

bus = Bus("Bus")
rsv = Reservoir(
    label="rsv",
    bus=bus,
    carrier="water",
    tech="reservoir",
    storage_capacity=1000,
    capacity=50,
    profile=[1, 2, 6],
    initial_storage_level=0,
    efficiency=1)
```

Figure 4 API example for an *oemof.tabular* reservoir facade.

```
from oemof.solph import (components, Source, Bus, Flow)

bus = Bus("Bus")
rsv_solph = components.GenericStorage(
    label="rsv-solph",
    nominal_storage_capacity=1000,
    initial_storage_level=0,
    outflow_conversion_factor=1,
    outputs={bus: Flow(nominal_value=50)},
    inputs={})

inflow = Source(
    label="reservoir-inflow",
    outputs={rsv_solph: Flow(nominal_value=1, max=[1, 2, 6],
                                     fixed=False)})
```

Figure 5 API example for a simple *oemof.solph* reservoir model.

of the parent class are also available in the child class (`initial_storage_level`).

Even for comparably small systems, the example underlines the advantages of the approach.

4 DATA PACKAGES

A Data Package is, in its simplest form, not more than a valid JSON [4] file named "*datapackage.json*". The file contains meta data about data resources which can be specified inline in the same file. For more complex cases, data resources are stored in separate files inside the directory containing the "*datapackage.json*" file. The contents of the mentioned JSON file are standardized via the Data Package specification [22]. An example fragment of such a *datapackage.json* JSON file can be seen in ***Figure 7***. The Data Package has been extended by other standards, which further refine the format and contents of the meta data file and the resources to suit different application contexts. Examples of this are Fiscal Data Packages [25], meant to store fiscal data, as well as Tabular Data Packages [26], which refine the original Data Package [22] specification to handle table like data. The latter combines the advantages of databases and spreadsheets with the ubiquity and user-friendliness of CSV files. Tabular Data Packages allow storing type meta data and set primary keys as well as foreign keys across resources, i.e. different CSV files. They are more lightweight than databases and they are both, human readable and easily processable in almost any programming language. In recent years, different European projects in the field of energy system modeling have decided to opt for Data Packages to store model relevant data [18, 10]. Using Data Packages in the correct manner also allows to adhere to the FAIR principle of data handling proposed by Wilkonsen et al. 2016 [29].

In the context of *oemof.tabular*, Data Packages are used to hold information on the topology and parameters of an energy system model instance. At a minimum this includes all exogenous model variables and associated meta data. However, it may also include raw data and scripts for pre- and post processing. On top of the Tabular Data Package structure an structure an energy system specific logic is added, which adds minimal additional constraints on the format of Tabular Data Packages used to specify an *oemof.tabular* model, while still keeping them valid Tabular Data Packages according to the original specification. Therefore, *oemof.tabular* requires the following parts in a Tabular Data Package:

1. a directory named *data* containing at least one sub-folder called *elements*, which may optionally contain a directory called *sequences* and a directory called *geometries* and
2. a valid meta-data `.json` file for the Data Package.

The exemplary folder tree of such a Data Package is depicted in ***Figure 6***.

As stated above, data inside Data Packages is stored in so called resources, which, for a Tabular Data Package, are CSV files. The columns of such resources are referred to as *fields*. Therefore, field names of the resources are equivalent to parameters of the energy system elements and sequences. Connections between components and buses can be defined via foreign keys. These allow linking element fields to fields of other elements stored in other resources. To reference the *name* field of a resource with name *bus* a foreign key can be set within the JSON meta data file using the `forgeinKeys` key as shown in ***Figure 7***.

To distinguish elements and sequences, these two are stored in sub-directories of the data directory. In addition geometrical information can be stored under `data/geometries` in a `.geojson` format. To facilitate the process of creating, processing and calculating a Data Package, *oemof.tabular* offers several functionalities:

```
|-- datapackage
    |-- data
        |-- elements
            |-- demand.csv
            |-- generator.csv
            |-- storage.csv
            |-- bus.csv
        |-- sequences
            |-- volatile-profiles.csv
        |-- geometries
            |-- buses.geojson
    |-- scripts
    |-- datapackage.json
```

Figure 6 Example of an *oemof.tabular* Data Package folder tree.

```
...
"foreignKeys": [
  {
    "fields": "bus",
    "reference": {
      "fields": "name",
      "resource": "bus"
    }
  }
]
```

Figure 7 Setting foreign keys in the JSON meta data file for cross referencing connected components.

- `oemof.tabular.datapackage.building` contains functions to infer meta data, download raw data, read and write elements, sequences etc.
- `oemof.tabular.datapackage.processing` contains functions to process model results, which can be used in the `compute.py` script.
- `oemof.tabular.datapackage.aggregation` allows to aggregate time series to reduce model complexity.

5 REPRODUCIBLE WORKFLOWS

Reproducibility of results is a recurring point of discussions in the energy system modeling community [17, 20]. These discussions have mainly been centered around the availability of source code (open source) and data (open data). Historically, for many prominent models neither the source code nor all input data have been made available. Thanks to new open source developments [8, 11, 13, 21] this has partly changed in recent years (for example the open release of MESSAGEix [12]). However, not all barriers have been removed yet. Firstly, closed models are still being used for research purposes. Secondly, more subtle barriers exist even for open source models. For one of the first open source models, Balmoral [28], a GAMS software license is required, which constitutes a barrier to re-run computations. Another important issue is what can be described as the difference between *practical* and *theoretical* transparency. While for open source models with open data theoretical reproducibility should be possible, practical issues hamper such exercises. First of all, not all necessary information may be given by the respective authors. If provided, complexity of model environments with poor documentation can make any attempt time consuming. In these cases, reproducibility is hardly possible from a practical point of view, even for experienced researchers with domain-specific knowledge.

WORKFLOW DESCRIPTION

To improve reproducibilty of *oemof.tabular*-based research, a structure and workflow is proposed which is based on a the set of ten rules for reproducibility in computational research presented by Sandve et al. 2013 [24]:

1. For every result, keep track of how it was produced
2. Avoid manual data manipulation steps
3. Archive the exact versions of all external programs used
4. Version control all custom scripts
5. Record all intermediate results, when possible in standardized formats
6. For analyses that include randomness, note underlying random seeds
7. Always store raw data behind plots
8. Generate hierarchical analysis output, allowing layers of increasing detail to be inspected
9. Connect textual statements to underlying results
10. Provide public access to scripts, runs, and results

The starting point of this workflow is the folder structure shown in ***Figure 8***.

```
|-- repository
    |-- environment
        |--requirements.txt
            ...
    |-- raw-data
    |-- scenarios
        |--scenario1.toml
        |--scenario2.toml
         ...
    |-- scripts
        |--create-datapackages.py
        |--compute-datapackages.py
            ...
    |-- datapackages
        |-- scenario1
        |-- scenario2
    |-- results
        |--scenario1
            |--input
            |--output
         |-- scenario2
            ...
```

Figure 8 Folder structure for a repository suitable for reproducible workflows.

1. Everything in the `repository` is (if possible) generated by scripts, version controlled, and documented to keep track of every step in result production and avoid manual data manipulation (rule 1, 2). Obviously, the repository is made publicly available (rule 10).
2. The `raw-data` directory contains all input data required to build the input Data Packages for the model. Ideally, raw data sources come with meta data information and open licenses. Unfortunately not all data published comes with such information which hinders reproducibility of workflows. Raw data can also be bundled on remote persistent storages like Zenodo [1], which are suitable for FAIR data distribution.
3. The `scenarios` directory allows to specify different scenarios and describes them in a basic way. The TOML format provides an easy and, if necessary nested structure. In addition to a description, configuration settings for constructing the input Data Packages can be specified in these files. ***Figure 9*** provides an example for a scenario file in the TOML format. This file can be used in the scripts to build Data Packages. Note that the user-specific build-scripts will need to interpret keys and values. Therefore, scenario files in the TOML format do not follow a specific standardized structure, except using the TOML language.
4. The `scripts` directory contains code to construct input Data Packages for scenarios based on the configuration `.toml` files and the raw-data (rule 2). In addition, a script to compute the scenario(s) can be stored there. If possible, raw data can also be downloaded from persistent sources (for example Zenodo) using scripts. Finally, this directory would also contain code for post processing data and for result visualization (rule 7).
5. Results are stored in the `results` directory. One important part is the separation of input and output data. Input data contains model specific exogenous model variables (in this context, *oemof.tabular* Data Packages). The output data directory contains endogenous model variables. Altogether, this step acknowledges rule 5 and 10 of the ten rules.
6. The open license and environment definition in combination with a version control system such as *git* allows to reproduce results on different operating systems (rule 3, 4 and 10).

```
title = "Toy Scenario"
description = "Toy scenario for 3 Nodes"
name = "toy-scenario"

[scenario]
cost = "2030-high"
weather_year = 2011
year = 2030
pv_profiles = "ninja"
onshore_profiles = "emhires"
offshore_profiles = "emhires"

[buses]
electricity = ["DK", "NO", "SE"]
biomass = ["DK", "NO", "SE"]
```

Figure 9 Example *TOML* file with scenario specifications to build input Data Packages.

An example of this workflow has been published for a model-based analysis of the German electricity system [9]. The energy system model covers the German power system with its neighboring countries. Similarly, the workflow has been applied in an analysis for flexibilisation of heat pumps [6].

It should be noted that energy modelers also need to acknowledge energy modeling specific best practices such as proposed by Decarolis et al. [3].

6 CONCLUSION

This paper introduces the application of the facade concept and the usage of Data Packages for the Open Energy System Modeling Framework (oemof). The concept has been implemented in the Python package *oemof.tabular* which is designed as an interface to instantiate energy system models with the *oemof.solph* library from Tabular Data Packages. Using facades can (1) increase transparency by restricting generic components to energy specific components, (2) allow to build composed components and instantiate those from tabular data sources, (3) facilitate the application in teaching and capacity building environments and (4) allow for reproducible workflows. Additionally, the implementation based on the Data Package standard allows to store meta data of the model input data in a standardized way. To enable reproducibility of energy research results a workflow is proposed which is based on scientific literature.

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COMPETING INTERESTS

The authors have no competing interests to declare.

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Effects of Decentral Heat Pump Operation on Electricity Storage Requirements in Germany[1]

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Effects of Decentral Heat Pump Operation on Electricity Storage Requirements in Germany

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Abstract: Several studies show that heat pumps need to play a major role for space heating and hot water supply in highly decarbonised energy systems. The degree of elasticity of this additional electricity demand can have a significant impact on the electricity system. This paper investigates the effect of decentral heat pump flexibilisation through thermal energy storage units on electricity storage investment. The analysis is carried using an open source model for the German electricity system based on the Open Energy Modelling Framework (oemof). Results highlight the importance of flexible heat pump operation in 100% renewable energy systems and relate well to findings of other existing studies. Flexibilisation of heat pumps in the German energy system can reduce the need for electricity storage units significantly. While no impact was found for systems with a share below 80% renewable energy, investment in short term storage units is reduced by up to 42–62% in systems with shares of more than 80% renewable energy. In contrast, the impact on long term electricity storage investment was comparatively low in all modelled scenarios. Conducted sensitivity analyses show that both findings are rather insensitive with regard to the available biomass for electricity supply as well as to changes in the heat demand covered by heat pumps. Economically flexible heat pump operation has only a minor effect on system costs. However, the indirect replacement of battery with thermal energy storage units is environmentally beneficial due a lower resource consumption of minerals.

Keywords: energy system modelling; 100% renewable energy systems; open science; sector coupling; heat pump; flexibility options; thermal energy storage; electricity storage

1. Introduction

The goal of the 2015 Paris agreement [1] is to keep global warming well below two degrees compared to pre-industrial levels. In 2018, the special report of the Intergovernmental Panel on Climate Change (IPCC) [2] reaffirmed the importance of this goal by analysing pathways for a warming of 1.5°. Due to the remaining carbon budget, a drastic decarbonisation up 100% of all sectors until 2050 with even negative emissions after the year 2050 will be required to reach the 1.5° goal. In the electricity sector emissions are mainly reduced through a shift from fossil fuel based to renewable energy based supply. Within the heating sector, this solution is rather challenging as renewable resources are limited. Therefore, reducing energy consumption in the heating sector by insulating measures is on the top of the agenda. Nevertheless, a residual heat demand will have to be covered by renewable energies. District heating (DH) systems allow for better integration of renewable technologies compared to individual heating systems. However, the DH potential is also limited as systems require certain spatial heat demand densities for economic operation.

For individual heating solar thermal, biomass or electricity are left as the major options in Germany. Solar thermal energy has to cope with opposed seasonality of demand and supply. Hence, only small shares of solar thermal energy may be integrated in the heating sector without seasonal storage units.

Therefore, the economic potential of solar thermal supply in Germany is limited to around 60 $\mathrm{TWh_{th}}$ annually [3]. Energy production from sustainable biomass conflicts with nature conservation and food production. In addition, the heating sector and the transport sector (aviation and shipping) will compete with one another in carbon neutral societies due to the high value of transportable and storable energy (see discussions in References [4–7]). Finally, heat pumps are an energy efficient option to supply heat and reduce CO_2 emissions [8,9]. Due to the above mentioned reasons, the authors argue that "[. . .] heat pumps are deemed the most suitable individual heating solution in a 100% renewable energy system for the EU" [10], p. 1644. In various studies for highly decarbonised energy systems heat pumps and solar thermal collectors are the dominant energy sources [11–13]. Especially for individual heating systems this technology is often mentioned as the major option in Germany [14,15]. A broad roll-out of decentralised heat pumps moves decarbonisation challenges from the heating sector to the electricity system. A central question regarding the added electricity demand induced by heat pumps is their elasticity to match with intermittent renewable energy supply. Elasticity of heat demand may be increased by a thermal energy storage (TES) with a positive impact on the electricity system. The aim of this paper is to analyse the effect of decentral heat pump flexibilisation on electricity storage investment in renewable energy systems.

2. State of Art and Research Question

Bloess et al. [16] review power to heat technologies for renewable integration. The authors conclude that sector coupling comes with multiple benefits such as a reduced peak load, lower electricity storage needs, less renewable curtailment and more efficient power plant dispatch. For the mid-term perspective the Danish energy system in 2030 is optimised with the open source *Balmorel* model by Hedegaard and Münster [17]. Results suggest great importance of residential decentralised heat pumps for the integration of wind energy. However, only a minor effect of flexibilisation through TES is observed. At the European level, Brown et al. [11] analyse synergies of sector coupling in highly decarbonised energy systems with an open source investment model based on the Python package *PyPSA*. The heating scenario of this study shows a positive effect of long and short term thermal energy storage (TES) for integrating solar thermal heat as well as thermal energy from power to heat units. Heat pumps play a significant role for decentralised heat supply, that is, in areas with low density of heat demand where district heating is not a reasonable option. For the electricity-heat coupling long term storage units contribute significantly to integrating Wind and PV. However, no detailed analyses of HP flexibilisation in systems under different renewable energy penetration and different heat demands are provided in this study. Also, the power-to-energy ratios are fixed in this model. Hence, no statement on required optimal storage energy capacity can be given. An analysis for Germany in the European context is presented by Bernath et al. [18] to investigate the role of heat pumps for renewable energy integration using the optimisation tool *Enertile*. The closed source model includes district as well as decentral heating systems with heat pumps. Ruhnau et al. [19] analysed the effect of heat pumps on the economic value of wind with the open source market model *EMMA* for Germany. The modelled scenarios also include an analyses of interdependencies between different flexibility options that indicate lower electricity storage investment due to the existence of thermal storage capacities in scenarios with 30% wind energy supply. Fehrenbach et al. [20] optimised the residential German heating sector under varying levels of renewable energy expansion using a *TIMES* model. Unfortunately, model source code and data for this study are not publicly available. In addition, the overall optimisation approach does not allow to compare effects of inflexible and flexible operation. The impact of increased power-to-heat on the heat sector transformation in Germany is also analysed by Bloess [21] with a multi-period expansion model. This study models different levels of heat demand with and without power-to-heat and determines a major impact of power-to-heat on the electricity sector. The author concludes that thermal storage plays a greater role than short term electricity storage, although further verification is required. Many studies have investigated electrical storage requirements on the European and German level [22–25]. These studies solely focus on the electricity sector and do not analyse the interdependencies between flexibility options in the heat and electricity market.

The literature review shows that a number of relevant studies for sector coupling and heat pumps are available. Nonetheless, no open source modelling approach exists to analyse the effect of heat pump flexibilisation in settings with different renewable shares. Specifically the interdependencies with other flexibility options are not assessed in detail by a ceteris paribus approach. This paper investigates the interactions of flexibility options in an electricity-heat sector coupled system. In particular the impact of heat pump flexibilisation through TES in the decentral heating sector is analysed, regarding its influence on electricity storage investment and operation. The analysis is conducted based on an open source model for the German energy system including the neighbouring countries.

Subsequently, Section 3 provides a mathematical description of the model followed by an overview of modelled scenarios with their relevant input data in Section 4. Based on these two sections results are presented in Section 5. The last section provides a short summary followed by a critical appraisal of the study.

3. Method

Lund et al. [26] describe differences between two methodological positions: simulation vs. optimisation. In this paper a hybrid approach is chosen to analyse the effects of heat pump flexibilisation. While installed generation capacities and the transmission grid capacities are defined exogenously, storage and heat pump capacities are determined endogenously by optimisation. With this approach, effects of heat pump flexibilisation on electricity storage units can be assessed without interference of other system variables. The analysis is carried out with a linear programming optimisation model based on the Python package *oemof-tabular* which is part of oemof cosmos [27]. The source code of the package is available on GitHub [28] under the BSD 3-Clause license.

Figure 1 illustrates the graph based model of a power and heat coupled energy system with this software.

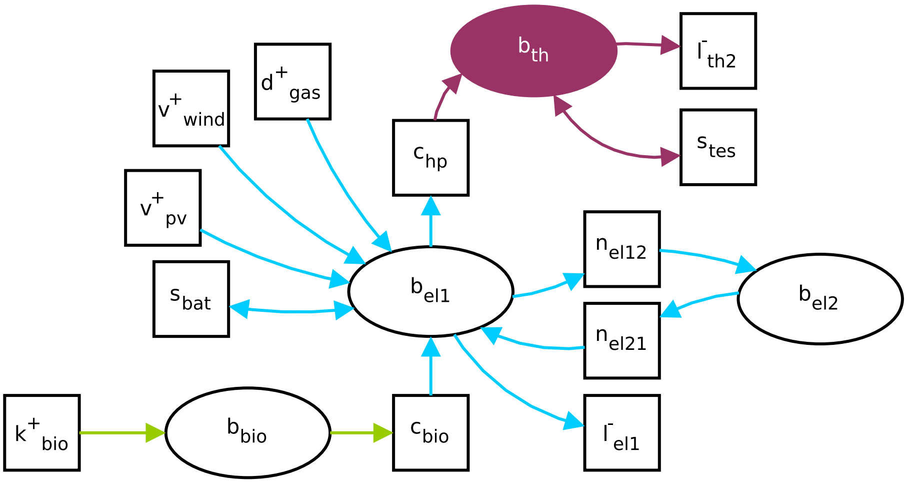


Figure 1. Illustration of a sector coupled energy system modelled based on oemof tabular. The energy system is modelled as a bi-partite graph with components (squares) and buses (ellipses). Electricity flows are coloured blue, biomass green and heat red.

Mathematical Description

The underlying mathematical model of this graph structure is implemented in the *oemof-solph* package. In the following, mathematical description of all endogenous variables are denoted by x, while all exogenous variables are denoted by c.

The model is a combined dispatch and investment model with exogenously defined parameters for the electricity system and investment for electricity storage units and the decentral heating system (HP and TES). For the investment part of the model all dispatch constraints below apply as well. However, the upper bounds of the maximum capacity of HP, TES and electricity storage units (except PHS) are subject to optimisation. The objective function of the model minimises total operating and investment costs, as shown in Equation (1).

$$\begin{aligned}\text{min:} \sum_g \sum_t \overbrace{c_g^{mc} \cdot x_g^{flow}(t)}^{\text{operating cost}} + \\ \sum_h \overbrace{c_h^{capacity\_cost} \cdot x_h^{capacity}}^{\text{investment cost HP}} + \\ \sum_s \overbrace{c_s^{capacity\_cost} \cdot x_s^{capacity} + c_s^{energy\_cost} \cdot x_s^{storage\_capacity}}^{\text{investment cost storage}}.\end{aligned} \tag{1}$$

The marginal costs c_g^{mc} of a generator g are calculated based on carrier c_g^{cc} costs, variable operation and maintenance c_g^{vom} cost and CO$_2$ costs c_g^{co2} that are determined based on the carrier specific emission factor of the generator $e_g^{carrier}$ (Equation (2)).

$$c_g^{mc} = \frac{c_g^{cc}}{\eta_g} + c^{co2} \cdot e_g^{carrier} + c_g^{vom}. \tag{2}$$

The investment costs are defined as the annualised capacity costs including fixed operation and maintenance (fom) costs. For storage units, these costs are composed of an energy and a power component. For the TES, the power-energy-ratio is not fixed to determine the optimal TES sizing.

Energy balances and **commodity balances** are modelled with the set of Buses B. For buses all inputs $x_{i(b),b}^{flow}$ to a bus b must equal all its outputs $x_{b,o(b)}^{flow}$ (Equation (3)).

$$\sum_i x_{i(b),b}^{flow}(t) - \sum_o x_{b,o(b)}^{flow}(t) = 0 \qquad \forall t \in T, \forall b \in B. \tag{3}$$

Equation (4) shows the constraint for inelastic loads. For the set of all **loads** denoted with $l \in L$ the load x_l at time step t equals the exogenously defined profile value $c_l^{profile}$ multiplied by the total annual demand c_l^{demand}

$$x_l^{flow}(t) = c_l^{profile}(t) \cdot c_l^{demand} \qquad \forall t \in T, \forall l \in L. \tag{4}$$

Dispatchable units ($d \in D$) such as fossil fuel based power plants are limited by the defined capacity (Equation (5)). Marginal costs of the generators are calculated based on Equation (2) and added to the objective function.

$$x_d^{flow}(t) \leq c_d^{capacity} \qquad \forall t \in T, \forall d \in D. \tag{5}$$

Volatile renewable supply is modelled as must-run production. For all volatile components denoted with $v \in V$ the flow is fixed as described in Equation (6). The set of all volatile components includes all volatile sources.

$$x_v^{flow}(t) = c_v^{profile}(t) \cdot c_v^{capacity} \qquad \forall t \in T, \forall v \in V. \tag{6}$$

Biomass units and **Heat pumps** are modelled with a conversion process of one input and one output and a conversion factor shown in Equation (7).

$$x_{c,to}^{flow}(t) = c_c^{efficiency}(t) \cdot x_{c,from}^{flow}(t) \qquad \forall c \in C, \forall t \in T. \tag{7}$$

In the case of biomass plants the outflow is exogenously bounded by its nominal power rating as it is modelled for other dispatchable units. For the set of heat pumps $h \in H$ the flow is bounded by an optimisation variable $x_{h,to}^{capacity}$ shown in Equation (8).

$$x_{h,to}^{flow}(t) \leq x_{h,to}^{capacity} \qquad \forall h \in H, \forall t \in T. \tag{8}$$

In combination with the commodity components (Equation (9)), the biomass supply can be limited by the available biomass potential by setting an upper limit on the aggregated flow of the component. The variable $x^{flow}k$ represents inflows for a biomass commodity bus from which the conversion process is fed.

$$\sum_t x_k^{flow}(t) \leq c_k^{amount} \qquad \forall k \in K. \tag{9}$$

For **storage** units ($s \in S$), the mathematical representation includes the flow into and out of the storage as well as a filling level. The inter-temporal energy balance of the storage is given in (10). The loss rate for the storage can be obtained by a time constant $loss\_rate = 1 - \exp^{-\frac{1}{24 \cdot d}}$, where d denotes the time constant in days.

$$x_s^{level}(t) = x_s^{level}(t) \cdot (1 - c_s^{loss\_rate}) - \frac{x_{s,out}^{flow}}{c_s^{eta\_out}} + c_s^{eta\_in} \cdot x_{s,in}^{flow}(t) \qquad \forall t \in T, \forall s \in S. \tag{10}$$

For the storage technologies with investment, the out- and inflow $x_{s,*}^{flow}$ as well as the energy x_s^{level} is bounded by an optimisation variable (Equations (11) and (12)).

$$x_{s,in}^{flow}(t) \leq x_s^{capacity} \qquad \forall t \in T, \forall s \in S \tag{11}$$

$$x_s^{level}(t) \leq x_s^{storage\_capacity} \qquad \forall t \in T, \forall s \in S. \tag{12}$$

Hydro reservoirs are modelled as storage units with a constant inflow and possible spillage described in Equation (13).

$$x_r^{level}(t) = x_r^{level}(t-1) \cdot (1 - c_r^{loss\_rate}(t)) + x_r^{profile}(t) - \frac{x_{r,out}^{flow}(t)}{c^{efficiency}(t)} \qquad \forall t \in T, \forall r \in R. \tag{13}$$

The inflow is bounded by the exogenous inflow profile (Equation (14)). Thus, if the inflow exceeds the maximum capacity of the storage, spillage is possible by setting $x_r^{profile}(t)$ to lower values. The spillage of the reservoir is therefore defined by $c_r^{profile}(t) - x_r^{profile}(t)$.

$$0 \leq x_r^{profile}(t) \leq c_r^{profile}(t) \qquad \forall t \in T, \forall r \in R. \tag{14}$$

Transmission between the countries is modelled with a transshipment approach, as shown in Equation (15).

$$x_{from,n}^{flow}(t) = (1 - c_n^{loss}) \cdot x_{n,to}^{flow}(t) \qquad \forall n \in N, \forall t \in T. \tag{15}$$

CO_2-emission limit $\overline{L_{CO_2}}$ is set for all flows x_e^{flow} indexed by $e \in E$ with by Equation (16).

$$\sum_t \sum_e x_e^{flow}(t) \cdot c_e^{emission\_factor} \leq \overline{L_{CO_2}}. \tag{16}$$

4. Scenarios

Systems with different renewable energy shares of 60% in 2030 to 100% in 2050 have been implemented within the described model to analyse the impact of heat pump flexibilisation with TES in Germany. The scenarios are based on the TYNDP2018 for the years 2030 and 2040 and on the e-Highway scenario 100% RES [29]. The following section provides an overview about important scenario assumptions. The source code of the model including script for generating input data is publicly available on Github [30].

The model covers Germany with its electrical neighbours applying a spatial resolution of one node per country. A temporal resolution of one hour is chosen with a total time horizon of one year. The grid capacities are taken from the e-Highway and TYNDP2018 databases (s. Appendix B.3). For the neighbouring countries of Germany published data on installed capacities from the TYNDP2018 [31] as well as the e-Highway [29] project have been used. This data has also been used for commodity cost and operational expenditures. Adaptions have been made for Germany with regard to the installed capacities as well as the electricity and heat demand assumptions (Sections 4.1 and 4.2 below). With these adaptations the 2050 scenario represents the Green Late (GL) scenario of the RESCUE study for Germany [14].

4.1. Installed Capacities

Figure 2 shows the installed capacities in Germany and the respective renewable energy share for each scenario.

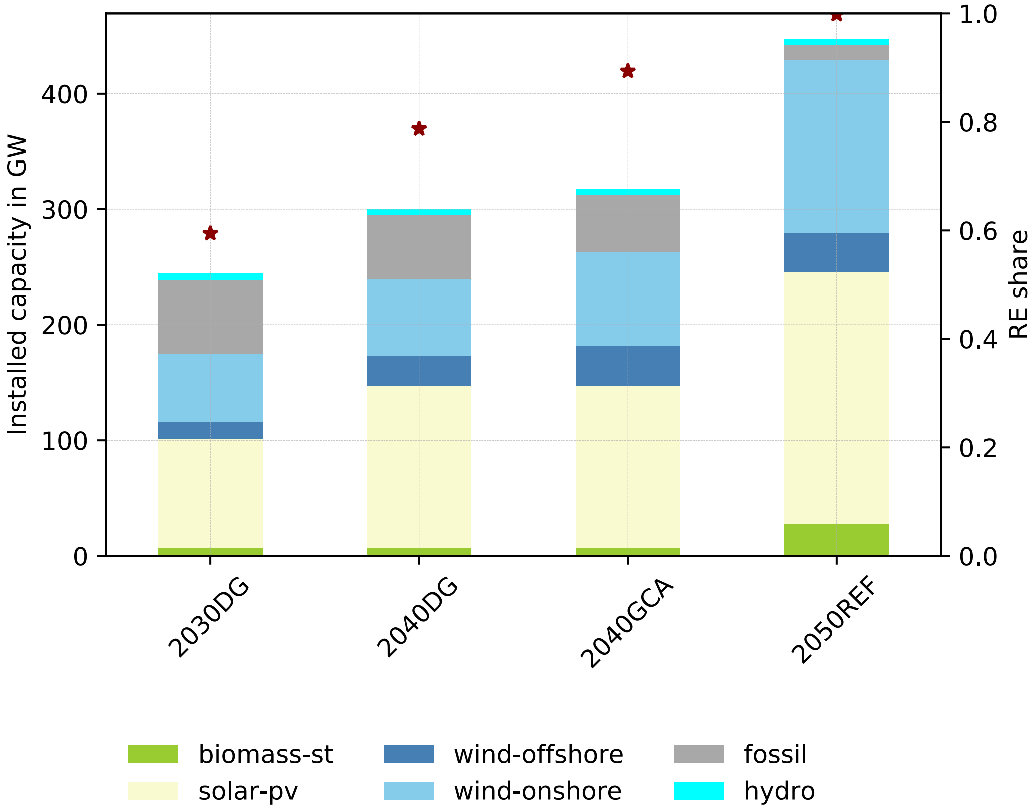


Figure 2. Installed generation capacities in Germany (DE) for all scenarios.

The *2030DG* scenario has the lowest installed capacities of renewable energies resulting in the lowest renewable energy share of around 60%. In 2040 the most progressive scenario is the *2040GCA* with a renewable share of approx. 88%. Compared to the *2040DG* this scenario has more wind onshore and offshore capacity installed. Also other European countries have a higher share of renewable energy in their energy mix. The *2050REF* scenario is based on the e-Highway 2050 100% RES (Europe) and the RESCUE 2050 GL scenario (Germany) and results in a scenario with 100% RE supply.

4.2. Demand

Assumptions regarding the electricity demand are a driving factor for the energy system. Values are associated with a high degree of uncertainty as the development of the future electricity demand strongly depends on demographic and economic development as well as implemented policy measures. The German goals regarding efficiency aim to reduce the conventional electricity demand (i.e., excluding electric vehicle, power-to-heat) by 10% until 2020 and 25% by 2050 compared to 2008 levels (403.8 TWh). Within the *Basis Szenario* of the German *BMWI Langfristszenarien* the conventional net electricity demand accounts for 417.2 TWh in 2050. The total gross electricity demand accounts for 612.4 TWh [32], p. 221. In the e-Highway 100% RES scenario the total gross demand is 665 TWh. Other studies suggest considerable higher electricity demand levels for 100% systems. For example, Reference [33], p. 9 model systems with a demand higher than 1000 TWh_{el} and over 200 TWh_{el} of excess energy in some scenarios. This shows the great range of possible future electricity demand levels. For the scenarios of this study the inelastic electrical demand (demand excluding heat pump consumption) has been based on scenarios for electrification of other transport and heat sectors according to the RESCUE [14] study to match with the installed generation mix. The demand calculations are shown in Table 1. For non-German countries, data from TYNDP2018 and the e-Highway project has been used. Normalised time series for electricity load profiles have been generated with the OPSD project data [34].

Table 1. Electricity demand values are based on the German efficiency goals. For the GS scenario it is assumed that a reduction of 25% and for GL 15% reduction is achieved.

	2030	**2040**	**2050**
Reduction (2008)	0.10	0.125	0.15
Electricity demand in TWh	485	471	458
Transportation (EVH) in TWh [14]	30	80	115
Demand in TWh_{el}	515	551	573
Distribution Loss [32], p. 221	0.11	0.09	0.07
Demand incl. losses in TWh_{el}	571	601	613
Heat covered by HP in TWh_{th} [14]	57	195	284

Total heat demand per year is based on the RESCUE scenarios, which describe CO_2 neutral energy systems in 2050. In the selected *GreenLate (GL)* scenario heat demand covered by heat pumps accounts for 57 TWh_{th} (2030), 195 TWh_{th} (2040) and 284 TWh_{th} (2050) [14]. Values for decentral heat production from heat pumps of the *RESCUE GL* scenarios are in the range of scenarios described in Hansen et al. [33]. Compared to [18] the additional electricity demand induced by decentral heat pumps is considerably higher in the RESCUE scenarios. To examine impacts of different heat demand levels a sensitivity analysis for the heat load is conducted. For the normalised heat profiles of hot water and space water heating another OPSD data set [35] has been used. The same data set has also been used to model the variable COP of the HP.

4.3. Investment Data

Pumped hydro storage (PHS) capacities have been set endogenously as their potential is strongly limited. For additional storage investment two different types of storage units are modelled.

One representing a short term storage option (lithium battery) and another representing a long-term storage (hydrogen storage) option. The parameters for the storage and heat pump investment are shown in Table 2.

Table 2. Data for the decentral heating system based on [11], data for the electricity storage based on [23,36,37]. Storage efficiency is shown as round trip efficiency.

	Investment Cost		**FOM**	**Lifetime**	**WACC**	**Efficiency**	**Storage Capacity**
	Euro/kW	**Euro/kWh**	**Euro/kW(h)a**	**Years**			***h***
HP	1400	-	49 (Value in Euro/kWa)	20	0.05	variable	-
TES	0	38.4	0.39	20	0.05	0.81	endogenous
Lithium 2050	35	187	10	20	0.05	0.92	6.5
Hydrogen 2050	1000	0.2	10	22.5	0.05	0.46	168

4.4. Renewable Generation

The solar PV and onshore wind profiles are based on the *renewables ninja* project [38,39]. Run of river profiles have been calculated with results of the Restore2050 project [40]. The total inflow provided in the data set has been split in proportion to the run of river and reservoir capacities in the scenarios. The weather year 2011 has been selected for all scenarios [11]. The full load hours of the volatile energy supply for different renewable technologies and each country are given in the appendix in Table A4.

The maximum biomass potential per country is derived from the *hotmaps* project [41] and is equal among all scenarios. The potential does not cover waste but only agriculture and forestry residues. For Germany the available potential has been adapted to values of the RESCUE study. With an electrical efficiency of 48.7 % for biomass to electricity conversion the potential in Germany is around 22 TWh_{el} (s. Appendix B).

5. Results

The following section presents the results of the modelled scenarios. First the optimal investment in storage units is presented. Results of the sensitivity analyses are described at the end of this section.

5.1. Heating System Investment

Figure 3 shows the results for the investment in the heating system. The interaction between electricity system and heat pump operation can already be identified in this figure. The main driver for the investment in TES is the heat demand. For the 2030 scenario with low heat demand covered by heat pumps and a lower share of renewable energy no investment in TES is chosen.

In all scenarios with renewable energy shares above 80% the installed energy capacity ranges from around 108 TWh to around 150 TWh. No additional investment into heat pumps above their lower bound of the heat peak-load demand is observed. The optimal sizing of TES for the covered heat demand of 284 TWh_{th} in 2050 is around 150 GWh. With the area for space heating of the GL scenario, this would amount for 0.5 L/m^2 water tank volume of the heated space area (6.37 Mrd m^2 in the GL scenario). The TES investment of 108 to 152 TWh_{th}) for all scenarios above 80% RE share is in the range of results determined by [20] (52–252 TWh_{th}).

For all scenarios the energy of the storage is in a range of 1.2–1.4 times the respective thermal peak load. Interestingly, this value is in line with current practices of storage sizing in (district) heating systems [42,43]. The power-to-heat ratio of the TES is significantly lower than the assumed values of 72 h of maximum installed capacity in MW_{th} by Reference [11]. The reason for this difference can be found in the low investment cost per MW_{th}. With low cost per MW_{th}, the optimal values shift to higher capacities even though only a marginal return on investment exists.

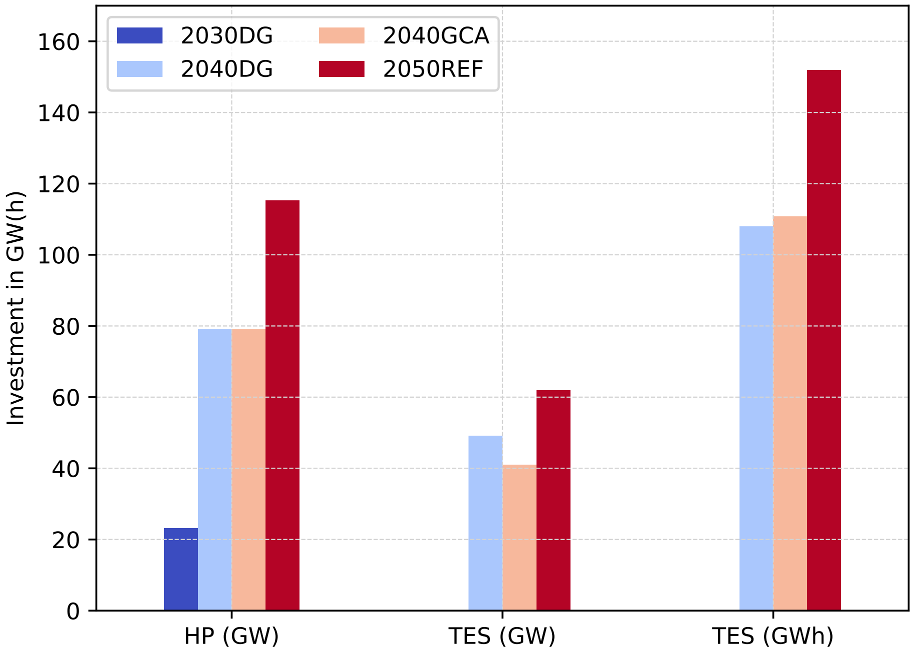


Figure 3. Investment in decentral heating system components for different scenarios. Units are given in GW and GWh.

5.2. Electricity Storage Investment

Figure 4 shows the investment in short-term (lithium) and long-term (hydrogen) storage units for the different scenarios. The investment increases with higher shares of renewable energy. For the *2030DG* system no additional storage besides PHS is required in Germany. Long term storage investment can only be observed in the 2050 scenario.

The results show that the effect of heat pump flexibilisation is significantly higher for short term storage units. Obviously, for the scenario where no TES is installed, no change in electricity storage capacity can be observed. Flexibilisation of HP by TES can reduce short-term storage investment by 3.3 GW (42%) up to 5 GW (61%) . For the long term storage, investment is only decreased by 0.37 GW (6.8%) in the 2050 scenario.

The reduction in short term electricity storage investment induced by heat pump flexibilisation matches with results from [19], where PHS investment can be reduced by around 5 GW in a scenario with 30% wind share. Results for the *2050REF* scenario (12.8 PHS and almost 11 GW lithium battery) are also comparable with 21 GW of short term storage requirement in 100% systems in Germany of [23]. However, a highly flexible heating sector can reduce additional investment by around 4.9 GW (44.5%). The authors of the “storage roadmap study” [25] highlight the great range of storage investment and their dependence on driving system variables like biomass potential and demand side management (DSM). In their study, DSM can reduce storage demand from 19.2 (no DSM) to 5.5 GW (max. DSM) for a system with around 88% RE-share in Germany, i.e., by around 71% in Germany [25], p. 88. The short-term storage requirements within these scenarios are also similar to the *2040GCA* scenario with 88% RE-share. For a 100% RE-system in Germany Müller et al. [37] identify a total storage investment of 13.7 GW (excluding PHS) with a majority of the investment found in hydrogen storage units. In contrast to this paper, their model includes an intra-country grid constraint. Grid bottlenecks can cause higher long-term storage investment to integrate (offshore) wind supply, which is indicated by investment in northern Germany. Due to the copper-plate approach in the presented model in this study, such bottlenecks can not be reflected.

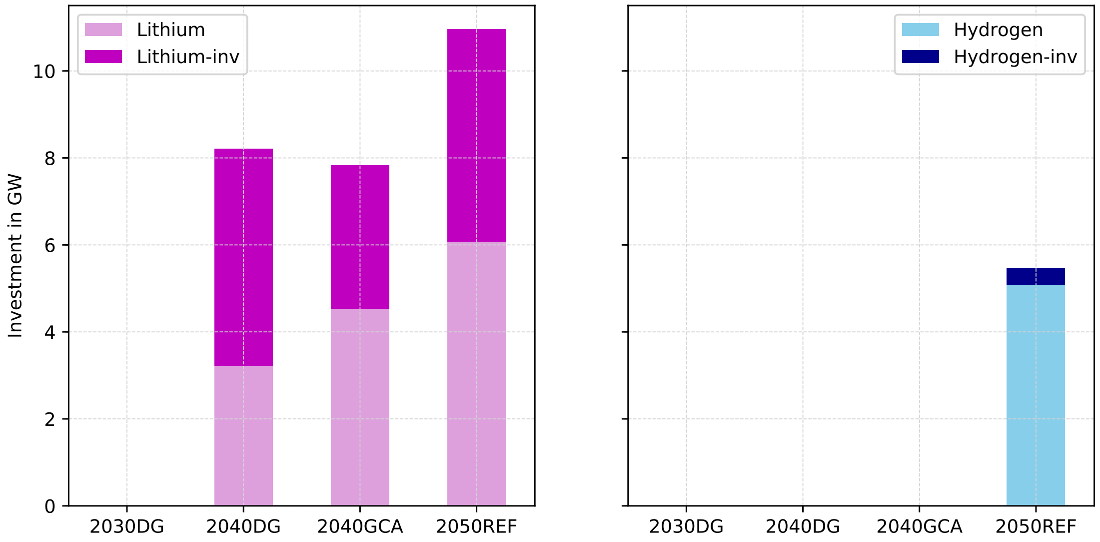


Figure 4. Investment in electricity storage units in GW with lithium on the left and hydrogen on the right side. The power has been chosen for better representation. Energy can be calculated based on the assumption of the maximum storage capacity in hours (6.5 h for lithium and 168 h for hydrogen). The absolute height of the bars represent investment without TES, that is, heat pump flexibilisation. Light dyed part represents electricity investment with HP flexibilisation. Therefore, dark coloured parts of the bars represent investment required due to inflexible heat pump operation.

5.3. System Costs

Table 3 lists the objective values for four scenarios. Economically, only small changes can be observed due to the flexibilisation. For the 2050 scenario the total costs are reduced by 0.52% in the case of elastic heat pump electricity demand compared to an inelastic demand. The lowest reduction with 0.27% takes place in the *2040DG* scenario.

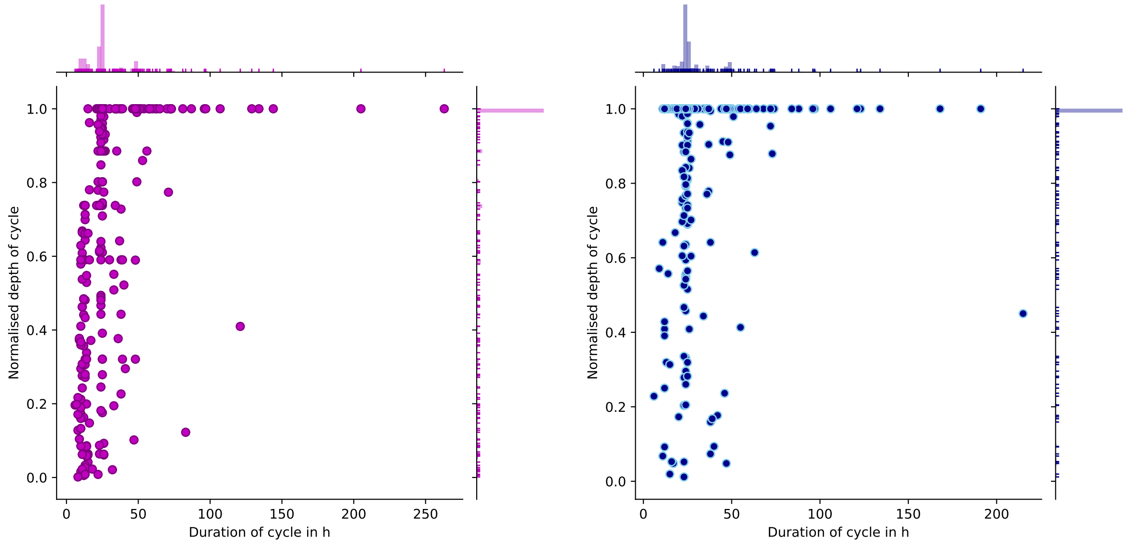
Table 3. Objective value for scenarios with (Flex) and without (No-Flex) flexibilisation. Deviation may occur due to rounding of values inside the table.

	No-Flex (bn Euro)	Flex (bn Euro)	Change (%)
2050REF	22.32	22.20	0.52
2040DG	41.49	41.38	0.27
2040GCA	26.80	26.71	0.34
2030DG	45.38	45.38	0.00

5.4. Storage Dynamics

Figure 5 presents a closer look on lithium battery (b) and the TES storage (b) cycles for the 2050 scenario. For cycle counting the Python package CyDeTs [44] has been used. The plot shows that the majority of cycle length are below the value of 72 h with a clear peak around 24 h and a smaller peak at around 10 h. The pattern of the electricity and the TES storage are similar. Note that this is not forced by the same underlying mathematical model approach as the ratio between storable energy and capacity of the TES, which has not been fixed inside the optimisation.

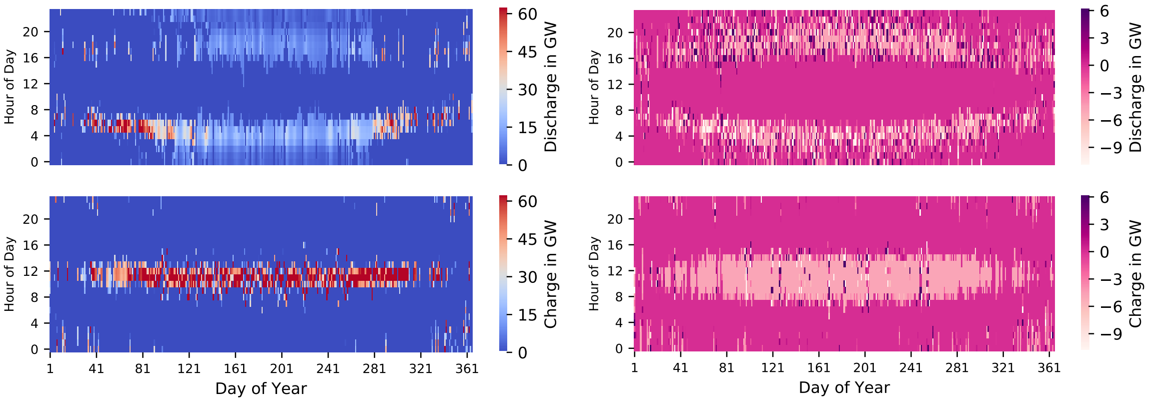
A majority of time, the storage units operate at full cycles (DoC of 1). Two different cycle length occur due to different operations in winter and summer time. In winter, shorter cycles are used to integrate PV peaks and shift energy a few hours towards the evening. In contrast, shifts in summer can be used to meet demand of longer periods of time during the night. The analysis of TES storage cycles shows that a fixed ratio of 72 h proofs as a reasonable assumption for systems with high shares of renewable energies. If a complexity reduction of models is required, results can also be used as an indication for temporal aggregation measures to reduce computational run times of large models. Here, aggregating data on a daily basis will reflect the basic pattern of storage dispatch as most cycles of the TES are included.



(**a**) 2050REF lithium battery (**b**) 2050REF TES

Figure 5. Storage cycles of lithium battery and TES for the 2050 scenario.

Figure 6 shows the temporal operation of TES during the year (a) and caused differences in storage charge and discharge for lithium storage units (b) due to heat pump operation with and without TES. The temporal impact on electricity storage operation can be analysed in Figure 6b. The plot reveals a clear seasonal and daily pattern. Charging is reduced during the summer months at noon, when PV generation peaks. In contrast, discharge is reduced in evening times. Charging and discharging of the storage is reduced to over 9 GW in some hours of the year. This pattern shows the PV integrating effect of TES by replacing electricity storage units. Due to the cycles of the TES, impact on long-term storage operation is significantly lower compared to short-term storage operation, which is reflected in the investment as well.



(**a**) TES operation (**b**) Change in electricity storage operation.

Figure 6. Temporal operation of TES during the year (**a**) and caused differences in storage charge and discharge for lithium storage units (**b**) due to heat pump operation with and without TES.

From Figure 6a, it can be seen that the daily effect also applies for TES operation. For TES charging is mainly taking place around noon. In this case low heat demand allows to charge storage units with

PV during the day. In the summer discharge is lower and distributed for a longer period of time. Whereas in the colder month, discharge is shorter with a higher rate. In the main heating period, the pattern changes and charging is done at night instead during the day.

5.5. Sensitivities

The dispatchable biomass potential has a major impact on (electricity) storage investment [25]. Therefore, a sensitivity analysis has been conducted for the 2050 scenario with regard to the biomass potential. As shown in Figure 7, an increasing biomass share reduces battery as well as hydrogen storage investment.

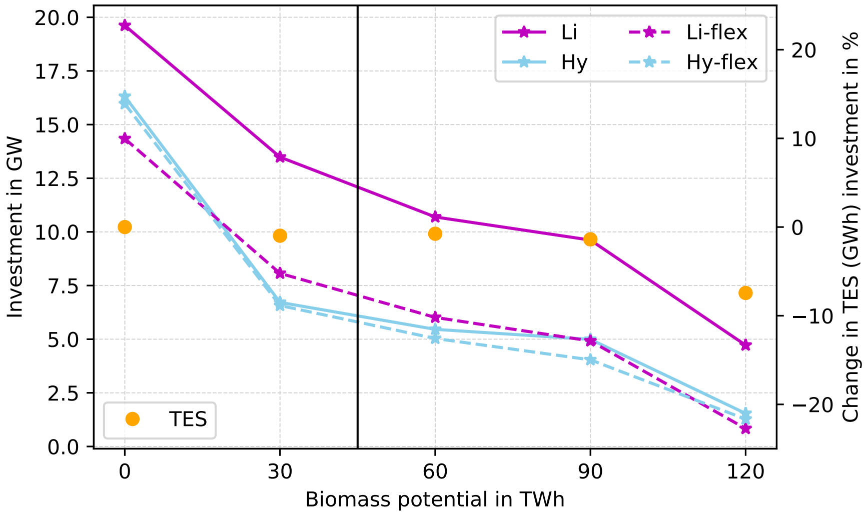


Figure 7. Sensitivity for installed storage capacities in GW in the 2050 scenario at different biomass potentials. Values for flexible heat pump operation are depicted as dashed lines. The *2050REF* scenario is indicated by the vertical line inside the figure.

At the same time, investment in TES is less sensitive with regard to the biomass potential. Without any biomass available, the hydrogen investment increases considerably by around 214% to 16 GW, while lithium increases to 19.6 GW by around 136% compared to the *2050REF* scenario. With a biomass potential of 120 TWh$_{th}$, investment decreases to 4.7 GW (lithium) and 1.5 GW (hydrogen). The effect of the HP flexibilisation is not effected substantially by the biomass potential. A reduction from 5.3 GW to 3 GW can be observed for the difference of flexible vs. in-flexible heat pump operation for short term storage units.

Figure 8 shows the results for the heat demand sensitivity. Clearly, electricity as well as TES investment increases with higher heat demand. While the TES investment changes linearly by about ±20%, electricity storage units show a non-linear increase. Storage investment rises by 62.5% from 11 to 17.8 GW for lithium and by 67% from 5.5 to 9.1 GW for hydrogen with a 30% higher heat demand.

Nevertheless, according to the biomass potential, reduction in electricity storage investment due to heat pump flexibilisation is not affected substantially at different heat demands. Compared to the reference case (4.9 GW), short term electricity storage investment increases to 5.9 GW in the case of 30% higher demand. Similary, investment decreases to 4 GW in the case of 30% lower heat demand.

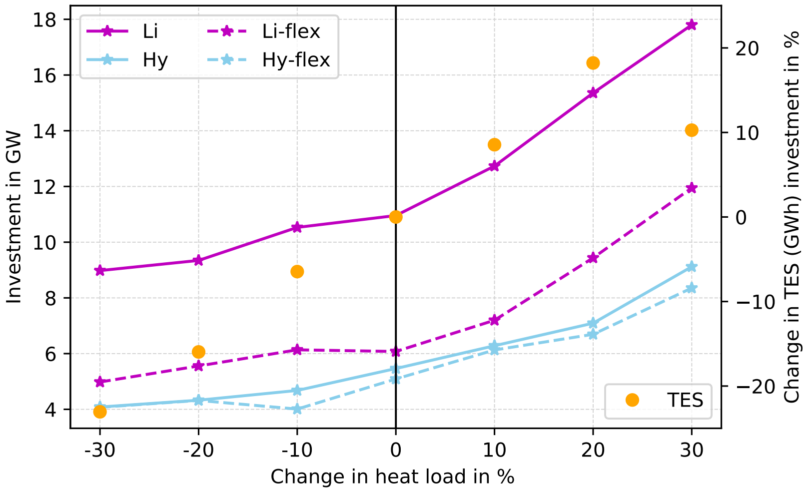


Figure 8. Sensitivity for installed storage capacities in GW in the 2050 scenario at different heat demand levels. Values for flexible heat pump operation are depicted as dashed lines. The *2050REF* scenario is indicated by the vertical line inside the figure.

6. Discussion

The presented results confirm the conclusions of Hedegaard and Münster [17], that the impact of heat pump flexibilisation is not relevant in systems with renewable energy shares below 80%. However, with higher RE shares, the importance of TES increases significantly. In addition, the conducted sensitivity analyses reveal the crucial role of available biomass potential for overall electricity storage investment. In particular long-term storage can by reduced more than half with the first 30 TWh of dispatchable biomass. Regardless, it has been shown that the flexibilisation of heat pumps is only slightly affected by the available biomass potential and therefore constitutes a robust option to reduce electricity storage requirements. Although the overall economic effect is small, indirect replacement of electricity storage investment by TES can be beneficial as less minerals like Cobalt, Lithium or Silver are required. Worldwide demand for Cobalt due to lithium batteries in 100% RE systems could exceed reserves even with high recycling rates and improvement in technologies. Similarly, lithium reserves may also be exceeded without high recycling rates [45], p. 446.

It is important to note that, due to the spatial resolution of the model, grid constraints inside countries are not modelled. Hence, storage investment might be required also in systems with less renewable penetration to ensure intact markets and avoid re-distpach. For example, the German grid development plan 2019 (German: “Netzentwicklungsplan”) models scenarios of the electricity system with a RE share of around 67–68% in Germany and installed battery capacities of 8 to 12.5 GW [46] for 2030. Therefore, further investigations should include a higher spatial resolution including grid constraints of the transmission grid inside countries. With such a resolution, heat pump flexibilisation may become relevant even at lower renewable energy penetration.

Another aspect for discussion is the 100% RE scenario setting for the year 2050. This setting constitutes a scenario with an highly integrated European electricity system. In particular, Norway with large hydro capacities plays a crucial role in this scenario. While several studies have shown the benefits of integrated systems solutions opposed to island solutions, it is by no means clear that such scenarios actually materialise. Therefore, other 100% scenarios within less integrated systems should be developed to examine a broader spectrum of possible solutions. Nevertheless, the overall results indicate robustness for systems above 80% RE share.

As shown by Reference [25], DSM is an important option for renewable energy integration and can reduce electricity storage demand. Further research should cover interactions between heat pump flexibilisation, electricity storage and (electrical) DSM. As most electrical DSM options and the TES work on short time scales, the question of their combined potential arises.

7. Conclusions

This paper presents an open source model for Germany to analyse the interaction between investment in electricity storage and thermal energy storage units for heat pump flexibilisation in decentral heating systems. Overall, the results relate well to existing studies and show that TESs can help to integrate renewable energies by reducing electricity storage investment. In energy systems with a share of more than 80% renewable energy share the investment in short-term storage units can be reduced up to 42–62% by TES. Except for the 100% scenario, no investment in long term energy storages were observed. With a reduction of 0.37 GW (6.8%) the impact in this setting was comparatively low. Generally, storage investment increases significantly with reduced available biomass for dispatchable electricity generation. However, sensitivity analyses show, that the results of heat pump flexibilisation are rather insensitive with regard to the available biomass for electricity supply as well as to changes in the heat demand covered by heat pumps.

Overall, the results reveal only moderate need in additional short-term storage investment in the medium run in Germany. In particular, long term storage units like hydrogen are not required before renewable energy shares approach 100% of the electricity supply. With less than 1% reduction in system cost, the economic effect of flexible heat pump operation was found to be low. However, the indirect replacement of batteries with thermal energy storage units is environmentally beneficial due to a lower resource consumption of minerals. Therefore, heat pump flexibilisation can play an important role for a resource efficient energy transition.

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Conflicts of Interest: The author declares no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

COP	Coefficient of Performance
FOM	Fixed Operation and Maintenance
HP	Heat Pump
IPCC	Intergovermental Panel on Climate Change
LP	Linear Programming
PHS	Pumped Hydro Storage
PV	Photovoltaic
RE	Renewable Energy
RoR	Run of River
TES	Thermal energy storage
TYNDP	Ten Year Network Development Plan
WACC	Weighted Average Cost of Capital

Appendix A. Model Symbols

Table A1. List of sets in the model.

Symbol	Description
C	Set of all conversion processes
D	Set of all dispatchable generators
H	Set of all heat pumps
K	Set of all commodities
L	Set of all loads
N	Set of all transmission lines
R	Set of all reservoir units
S	Set of all storage units
T	Set of all timesteps
V	Set of all volatile generators

Table A2. List of optimisation variables in the model.

Symbol	Description
$x^{flow}(t)$	Energy flow at timestep t
$x_{h,to}^{flow}(t)$	Heat flow to heat bus from heat pump h timestep t
$x_s^{level}(t)$	Storage (energy) level of storage s at timestep t
$x_{h,to}^{capacity}$	Thermal capacity of heat pump h
$x_s^{capacity}$	Capacity (power) of storage s
$x_s^{storage\_capacity}$	Storage capacity (energy) of storage s

Table A3. List of parameters in the model.

Symbol	Description
c_g^{mg}	Marginal cost of generator g
c_g^{cc}	Commodity cost of generator g
c_g^{vom}	Variable operational and maintenance cost of generator g
c_k^{amount}	Absolute amount of commodity k
$c^{loss\_rate}(t)$	Loss of storage energy per timestep t
$c^{profile}(t)$	Profile of generator, reservoir or load timestep t
$c^{capacity}$	Capacity of dispatchable or volatile generator d / v
c_n^{loss}	Loss on transmission line n
$c_e^{emission\_factor}$	Emission factor of carrier e
$c_c^{efficiency}(t)$	Efficiency of conversion process c at timestep t
$c_s^{eta_in}$	Charge efficiency of storage s
$c_s^{eta_out}$	Dis-charge efficiency of storage s

Appendix B. Scenario Assumptions

Appendix B.1. Residual Load

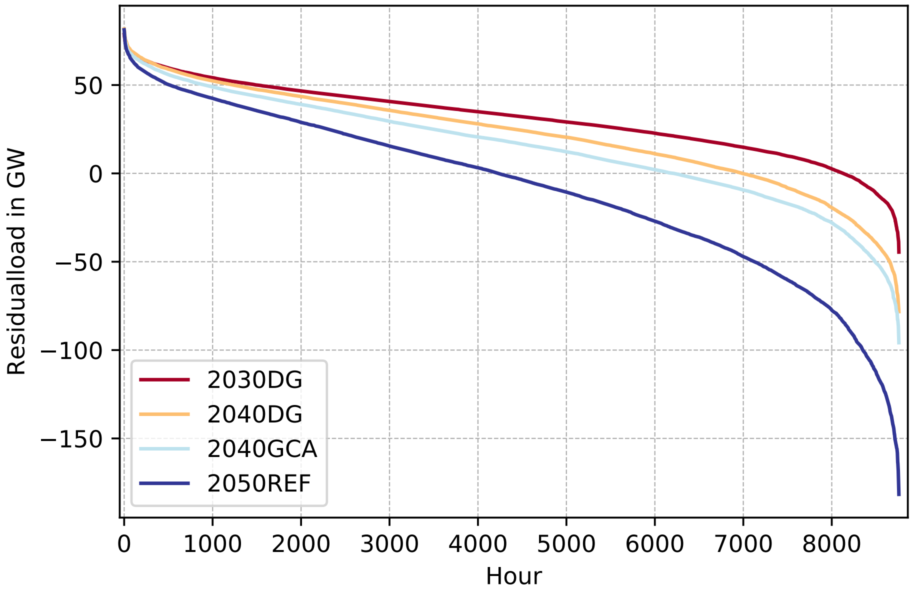


Figure A1. Electrical residual load in Germany within all main scenarios.

Appendix B.2. Renewable Energy and Biomass Potentials

Table A4. Full load hours of onshore, offshore, pv and run of river (RoR) supply.

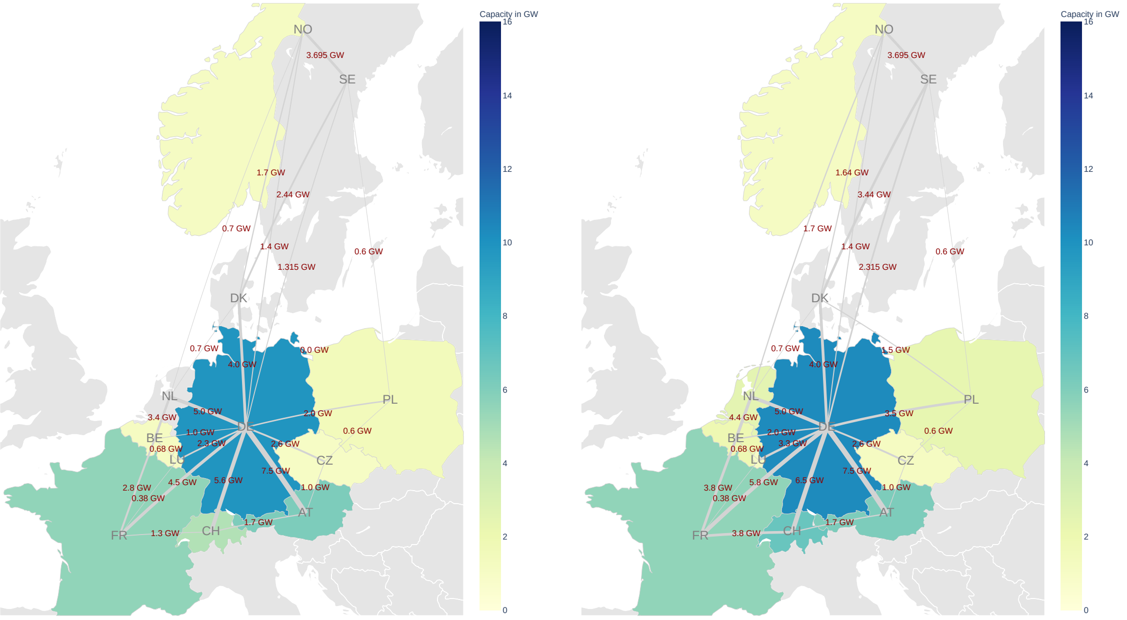
Country	Offshore	Onshore	PV	RoR
AT	-	1507	1291	3058
BE	3939	2406	1135	1335
CH	-	1354	1416	3832
CZ	-	1875	1226	1974
DE	3976	1951	1151	4043
DK	4224	2670	977	-
FR	3295	2040	1265	2722
LU	-	2917	1192	2644
NL	4025	1921	1095	1518
NO	4341	3562	811	2028
PL	3964	1834	1113	1493
SE	3792	2654	862	2161

Table A5. Biomass potential of agriculture and forest residue per country in 2050 based on the *hotmaps* project [41]. For consistency German potential for electricity has been adapted with regard to the RESCUE study assumptions.

	AT	BE	CH	CZ	DE	DK	FR	LU	NL	NO	PL	SE
Amount in TWh	23.61	8.08	0.0	32.78	45.05	13.56	149.56	0.61	2.81	0.0	71.36	86.75

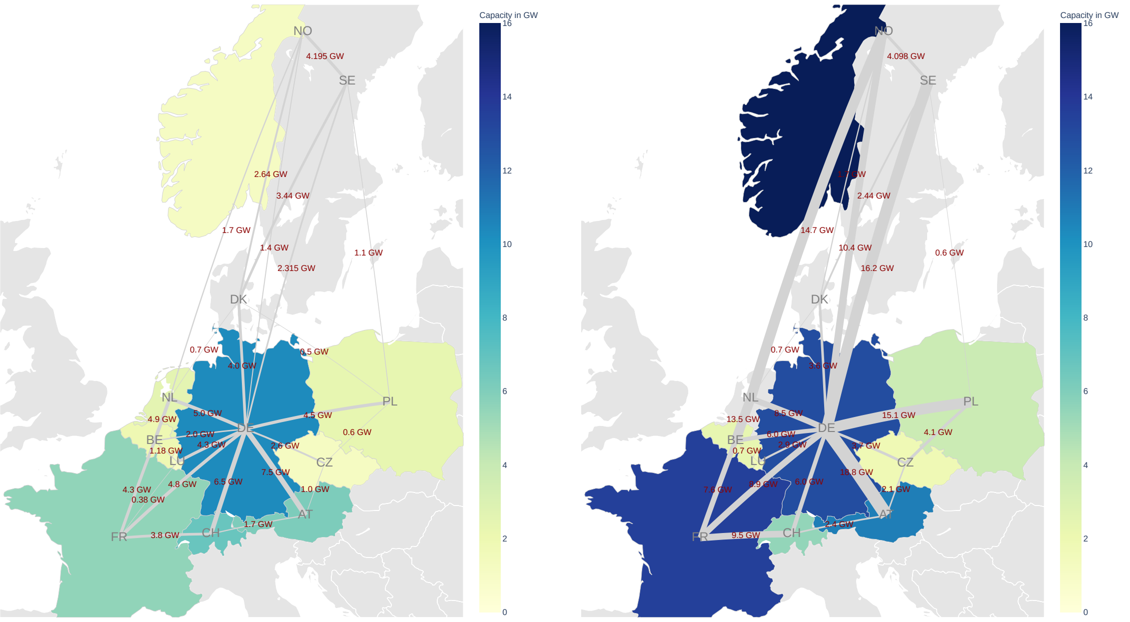
Appendix B.3. Grid Capacities

Figure A2 shows the installed the transmission capacities of the electricity system and pumped hydro storage capacities for all scenarios. As described above, the transmission system is modelled with a transshipment approach. The e-Highway 2050 in Figure A2d scenario includes major grid expansion to Scandinavian countries and the south east while the other scenarios only differ within a narrow range.



(**a**) 2030DG (**b**) 2040DG

Figure A2. *Cont.*



(**c**) 2040GCA (**d**) 2050REF

Figure A2. Transmission and PHS storage capacities. Countries are dyed based on their installed PHS capacity in each scenario. The 2050 scenario is based on the *e-Highway2050* [29] 100% RES scenario. All other scenarios are based on the TYNDP2018 [31].

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Analysis of cost-optimal renewable energy expansion for the near-term Jordanian electricity system[1]

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Article

Analysis of Cost-Optimal Renewable Energy Expansion for the Near-Term Jordanian Electricity System

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Abstract: Jordan is affected by an ever changing environment in the midst of climate change, political challenges, a fast growing economy and socio-economic pressures. Among other countries in the Middle East and Northern Africa, Jordan is facing a number of electricity related challenges, such as a rising energy demand, high dependency on fossil fuel imports and management of local, fossil and renewable resources. The paper presents an analysis based on an open source optimisation modelling approach identifying a cost-optimal extension of the Jordanian electricity system with growing demand projections until 2030 utilising pumped hydro energy storage and determining the costs of different CO_2 mitigation pathways. The results highlight the large potential of renewable energy for the cost effective, environmentally friendly and energy independent development of the Jordanian electricity sector. A share of up to 50% renewable energy can be achieved with only a minor increase in levelised cost of electricity from 54.42 to 57.04 $/MWh. In particular, a combination of photovoltaic and pumped hydro storage proved to be a superior solution compared to the expansion of existing shale oil deployments due to high costs and CO_2 emissions. Aiming for a more than 50% renewable energy share within the electricity mix calls for substantial wind energy deployments. In a system with a renewable energy share of 90%, wind energy covers 45% of the demand.

Keywords: energy system modelling; open science; GHG mitigation; pumped hydro storage; scenario analysis

1. Introduction and Background

Jordan is, in the midst of global warming and socio-political pressures, at an energy crossroads. Despite being in the middle of several oil-rich countries in the Middle East, Jordan is struggling to increase energy independence, being reliant almost entirely on fossil fuel imports. Despite having substantial renewable energy resources to increase energy independence and reduce greenhouse gas emissions, the most recently published energy strategy for 2040 [1] is more than conservative regarding their aims to increase the renewable energy share. Prior to the Arab Spring, Jordan relied almost entirely on natural gas imports from Egypt for electricity generation, which were disrupted in 2013 [2]. To satisfy energy demands, Jordan consequently switched to a petroleum based system. The government introduced substantial fuel subsidies to meet the increased costs and make energy available and affordable for the population [3], resulting in major governmental debt.

Between 1960 to 2011, six regional conflicts had direct or indirect effects on the energy sector in Jordan, namely, the Six Day War, the Lebanese Civil War, the Iraq–Iran War, the First Gulf war, the invasion of Iraq and the Egyptian revolution [4]. More recently, Jordan has been facing additional

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challenges concerning the energy and water sectors, such as a low level of foreign investment and substantial population growth due mainly to migration from war stricken Syria [5,6]. Unfortunately, there is a lack of literature dealing with the roles of foreign policy and politics and energy security in the case of Jordan. This rapidly changing and highly uncertain environment underlines the necessity for highly flexible energy system analysis tools to swiftly adjust to new circumstances.

1.1. Electricity Supply and Demand

Regardless of being in the midst of several oil-rich countries, Jordan struggles to secure its own energy resources for improved energy independence. Only recently, local oil shale resources were exploited, and a minor share of locally extracted natural gas was introduced to the system [7]. Table 1 introduces the installed capacities of Jordan's electricity system as of 2018 and the near-term forecast for 2023. In 2011, 97% of Jordan's energy needs were covered by oil and gas, consuming 19% of the Jordanian gross domestic product (GDP) [8] and only 2% were covered by renewable energy sources [9]. More recent, figures show that 19% of the installed capacity is covered by renewable energy power plants with 10.7% of the electricity generation of 2018 being covered by renewable energy sources [7]. Within the National Energy Masterplan for 2007–2020 [10] a reduction of energy dependency from 82% to 40% in 2020 was envisioned, which was not achieved, as Jordan is still importing 94% of its oil and gas to meet energy needs [11]. In 2018, 15% of the total electrical power consumption was used for water pumping, 45% in the residential sector, 22% in the industrial sector, 15% for commercial purposes and 2% for street lighting [12]. However, Jordan holds large renewable energy potential [5].

Table 1. Installed capacities in MW of Jordan's electricity system in 2018 based on NEPCO data [7] and for 2023 based on [1] with planned projects and retirements of conventional units (CC: combined cycle gas turbine, GT: gas turbine, DE: diesel engine, ST: Steam turbine)

	CC	GT	ST	DE	Shale-ST	Wind	PV	Hydro
2018	2740	83	602	814	-	280.4	698.4	12
2023	2567	83	363	810	470	663	1144	12

In 2018 the Jordanian peak load amounted to 3205 MW, which meant a decrease by about 3.4% from 3320 MW in 2017 [7]. NEPCO (National Electric Power Company) expects an increase of 1.9% by 2019 and a further 3% increase annually between 2019 and 2040 [7,12]. This means an electricity demand increase from 20,143 GWh to 38,261 GWh in 2040. Omary et al. [13] analyse the peak power demand development in three scenarios. The business as usual scenario assumes that the demand for electrical energy will grow continuously according to the growth of the last decade, reaching 25.3 TWh in 2030. The upper scenario assumes a higher increase with 30.3 TWh in 2030. The lower peak demand development path assumes a much lower demand of 15.8 TWh. Earlier studies examining potential future energy systems for Jordan, such as [14], expected an electricity demand of 106 TWh in 2050. This is due to the demand development between 2007 and 2013, showing a steady growth of electricity loads with an actual increase in consumption of 6.8% on average per year in the mentioned time period [8,12,15]. This was predicted to resume with a projected growth rate of 7.4% annually between 2014 and 2020 within the Master Strategy for Energy in Jordan [10], leading to an overestimation of the current demand. However, the most recent study from the Jordanian University of Science and Technology from 2019 [16] estimates a higher demand of 82.4 TWh for 2050 partly because of an electrification of other sectors. The unexpected demand decrease between 2018 and 2019, however, lead to a halt in the development of renewable energy projects. Before 2018, Jordan was progressing with the installation of renewable energies, becoming a leader in the Middle East on renewable developments. However, Jordan suspended renewable auctions and licenses for projects of 1 MW as of January 2019, due to concerns related to grid capacities [17]. Even considering a strictly fossil fuel based system, the future rising demand needs to be addressed, giving more stress to the grid, invalidating the argument of lacking grid capacity. Additionally, Jordan cancelled the tender for the first planned electrical storage project for renewable energy in 2020, inter alia due to the uncertain financial situation because of the global pandemic.

1.2. Strategies and Targets

A number of energy strategies were developed in Jordan: among others, the most relevant are the Energy Strategy 2030, the Energy Sector Strategy 2015–2025, the National Renewable Energy Action Plan, the National Energy Efficiency Action Plan and the Climate Change policy. However, some aims and visions are contradictory and incompatible, and previously set targets and goals were revised and neglected. For example the National Master Strategy of the Energy Sector for 2007–2020 and the National Strategy for the Development of Renewable Energy Resources stated the aim of 10% electricity generation based on renewable energies (wind and solar) by 2020, increasing to 20% by 2025. However, the latest energy strategy released in 2019 for 2018–2030 [1] aims in the baseline scenario at 21% for 2030, which indicates no evolution of the previously developed strategy. The penetration of renewable energy (RE) in the primary energy supply is predicted to increase from 3% in 2017 to 5% in 2020, reaching 6% in 2025 with no further increase up to 2030 in the reference case scenario [1]. The most ambitious scenario, increased sustainability, aims at 11% renewable penetration rate in 2030. Still, the energy import dependency will be as high as 73% in this scenario and between 92–94% in the reference case and business as usual scenario. As a least cost solution the share of renewable energy will not exceed 2.6 GW by 2030 (38% of installed capacity) with respect to the 2.4 GW of existing permits, and 5.7 GW by 2050 (47% of installed capacity). Contrary to the previous energy strategy and annual reports, which included the development of a nuclear power plant with a capacity of 220 or 660 MW being operational by 2026 [7], the revised strategy [1] does not foresee the development of nuclear energy.

Regarding CO_2 emission reduction targets, the revised energy strategy [1] envisions a CO_2 reduction of 10% by 2030; however, it fails to name a reference year. This goes along with the Intended Nationally Determined Contribution (INDC)[18], which aims at reducing greenhouse gas (GHG) emissions by 14% until 2030, again lacking a reference year. The mentioned 14% will be unconditionally full-filled by the country's own means at a maximal 1.5% reduction compared to a business as usual scenario. In comparison, the European Union's (EU) target is a reduction by 40% in 2030 compared to 1990 levels, and carbon neutrality by 2050 [19]. The temporary freeze in new renewable energy projects puts even this unambitious target at risk.

1.3. Research Question

The situation in Jordan puts strong emphases on energy independence and energy security because of the political and economical difficulties in the region. The research questions in this paper deal with the techno-economic assessment of the mid-term feature (2030). Therefore, we present an open source model based on the Open Energy Modelling Framework (oemof) [20] for the Jordanian electricity system. With the model the following research questions will be answered: (1) What is the cost-optimal mix, based on the current system, to meet the future electricity demand? (2) How can the future electricity demand be met by renewable energies in combination with pumped hydro and battery storage? (3) What are the costs of different RE shares in the electricity system?

2. State of the Art

2.1. Future Scenarios

The most recent study depicting the current Jordanian electricity system, as of 2018, underlines the number of challenges Jordan is facing, especially considering the current and coming energy demands [13]. The study does not offer any scenarios where energy storage is utilised, but does emphasise and suggest that the use of renewable energy resources could play a major role in a carbon relieved and more energy independent Jordanian energy system for 2030. Another recent study on electricity generation for Jordan was conducted by the University of Jordan, identifying mainly different scenarios in the face of two main issues, which are economic reasoning and geopolitical uncertainties [21]. Using GAMS, the study identified Combined Cycle Gas Turbine (CCGT) units mainly fired by natural gas in combination with PV and wind as the optimal choices with 70%, 19% and 11% shares respectively in 2018, changing to 10%, 71% and 19% in 2035. Dawoud et al. [21] recommend providing integrated storage options, without introducing concrete possibilities. Researchers from the school of energy systems with LUT Unjversity, Finland, [22] conducted an in-depth analysis of energy security of a 100% renewable energy transition in Jordan by 2050, projecting renewable electricity generation to increase from 0.1 TWh in 2015 to 110.7 TWh in 2050, 92% being covered by solar energy. Therefore, levelised cost of electricity (LCOE) develop from 78 EUR/MWh in 2015 to 61 EUR/MWh in 2050. For the calculation of scenarios an expansion model with 5 year time periods and an hourly resolution within each year is applied. The study recognises the importance of energy storage within a renewable system, introducing battery storage from 2025 onwards, with an installed capacity of 1 GWh increasing to approximately 67 GWh in 2050. Additionally, a compressed air energy storage (CAES) is included in the system in 2030, with a capacity of 31 TWh in 2050. Another study by the Jordan University of Science and Technology from 2019 [16] established various scenarios using EnergyPlan and LEAP, with one being 100% renewable, while others integrated natural gas, oil shale and nuclear power. The 100% renewable scenario was introduced with a high share of concentrated solar power (CSP), 10.6 GW, wind power of 4.5 GW and 25 GW of PV to cover the predicted demand of 2050 (82.4 TWh respective 14,350 MW peak load), and introduced a 90 GWh storage system to meet dispatchability problems. Kiwan and Al-Garibeh [16] found that the 100% is also economically feasible, with cumulative expansion cost of the renewable system amounting to $60 Billion compared to $52 Billion for the conventional system.

Within the MENA-Select (Sustainable Electricity Trajectories) project, participatory scenarios for the future Jordanian energy system for 2050 were established with local stakeholders [14]. In the other participating countries, Tunesia and Morocco, 100% renewable energy scenarios were considered and investigated; however, Jordanian stakeholders did not explore this possibility. The lowest CO_2 emissions were achieved within the no imports scenarios, reliant heavily on wind and PV (15 GW, 25 GW) as well as CSP (20 GW) and oil and gas (5 GW and 4 GW). Here, the largest energy storage (batteries) was modelled, with a capacity of 18 GW and an energy capacity of 40 GWh. Although this scenario is by far the most expensive, it was ranked the most preferable by local stakeholders due to the increased energy independence. However, due to changing developments, these scenario are not suitable to give guidance for the near and mid-term future. In another consecutive study, IIASA (International Institute for Applied Systems Analysis), among others [23], identified that energy security is preferable for all stakeholders over environmental concerns, which might be why a 100% renewable option is not as relevant for Jordan as for other countries.

2.2. *Pumped Hydro Storage*

The possibility of a pumped hydro storage system for Jordan was analysed within the Renewable Energy and Energy Efficiency Program for Jordan [24,25]. Pumped hydro storage (PHS) can facilitate a smoother integration of renewable, volatile energy sources into the national electricity system, if geographical features are beneficial. In Jordan, out of ten water reservoirs, three were identified to hold potential for pumped storage plants, namely, Mujib, King Talal and Wadi Arab. Mentioned here is the need for further studies to investigate the energy storage demand within the energy system, to verify assumptions. The study, however, did not analyse the integration of a pumped hydro storage into the Jordanian electricity system. The current energy strategy [1] advises in the increased sustainability, minimum dependency and rational use of energy scenario, a PHS of 220 MW to be introduced by 2025, to avoid renewable energy curtailment. Furthermore, the strategy selects Mujib as the only cost effective option. Generally speaking, a number of studies have been conducted that have identified the benefits of hybrid pumped hydro and battery storage for renewable energy based power systems, e.g., most recently [26]. In the Jordanian context, a number of studies have analysed in detail the renewable energy potential, such as a study by the Tafila Technical University [27] revising the renewable situation in Jordan in 2005. Here, a strong case for pro renewable energy was made, regarding energy security, energy independence and potentially lowered costs due to less operation and maintenance, as well as the environmental benefits in contrast to conventional energy sources. A more recent study of 2019 [28] explored the possibility of a combination of wind and pumped hydro storage within the Jordanian energy system. The team from the Yarmouk University, the University of Jordan and Texas A&M University used a Matlab optimisation toolbox to find the cost-optimal solution, showing that a combined wind and hydro storage system is economically, environmentally and technically more efficient than conventional power generation with CO_2 emissions and conventional grid energy purchases being reduced by almost 25%.

2.3. Contribution

As the State of the Art section shows, several modelling and scenario efforts have been made around the future Jordanian energy system. However, there is not an open source energy system modelling approach for Jordan, nor have the defined research questions been addressed. To our knowledge, no studies analysed how the existing energy system can be extended by renewable energy sources in combination with pumped hydro and battery storage to meet the expected rising energy demand in Jordan. In fast changing environments, open source models with open data can be of great value to adapt in a short manner. Additionally, the presented open source model can be used to assess similar research questions for any other country. Therefore, the presented work not only contributes to the scientific debate on decarbonisation of energy systems for climate change mitigation in Jordan, but also builds an important bridge for capacity building and development cooperation for other countries. The tool can facilitate a discussion among different sectors, e.g., the water and energy sectors, to identify joint solutions for common problems.

3. Mathematical Model

The developed and applied model is a linear (mixed-integer) optimisation model for the Jordanian electricity system. It is based on the open source package oemof-tabular [29]. In the following, endogenous (optimisation) variables are shown in bold to differentiate between these and exogenous model variables. The model minimises total operational cost for the time horizon T and all units $u \in U$, and annualised investment cost of all units $i \in I$, along with storage investments of all storage $s \in S$ for the Jordanian electricity system. Elements of the sets for the scenarios are listed in the Appendix A. The respective objective function is given below in Equation (1). The implemented model as well as the input data are provided in the Supplementary Material.

$$\min : \overbrace{\sum_{t \in T} \sum_{u \in U} c_u^{opex} \mathbf{p}_{u,t}}^{\text{operational cost}} + \overbrace{\sum_{i \in I} c_i^{capex,p} \mathbf{p}_i^{nom}}^{\text{power inv. cost}} + \overbrace{\sum_{s \in S} c_s^{capex,e} \mathbf{e}_s^{nom}}^{\text{energy inv. cost}} \tag{1}$$

The operational costs are calculated based on the efficiency η_u of a unit u and its fuel cost c_u^{fuel} according to Equation (2). Annualised investment costs c^{capex} are calculated based on the lifetime n, weighted cost of capital (WACC) i and specific investment cost of a technology $CAPEX$, along with the fixed operation and maintenance cost FOM in Equation (3). The scenario specific values for this study are found in Table 2 in the next section.

Table 2. Scenario assumptions for the year 2030. Renewable energy profiles (FLH) have been calculated based on renewables.ninja [30,31]. For calculation of annualised investment, weighted cost of capital (WACC) 5% was applied in all scenarios.

	η_u (-)	FOM (%/c^{capex})	CAPEX ($/kW)	c_u^{fuel} ($/MWh$_{th}$)	FLH (h)	Lifetime (Years)
Wind	1	3	1182 [32]	-	2050	20
PV	1	2	750 [32]	-	1912	20
CCGT	0.48 [1]	3.5	800 [1]	20.5	-	30
GT	0.33 [1]	3.5	550 [1]	20.5	-	30
ST	0.38 [1]	3.5	1300 [1]	20.5	-	30
DE	0.33 [1]	3.5		20.5	-	30
Oil shale ST	0.32 [1]	3	3720 [16]	25.2	-	30
Battery (power)	0.86[33]	3	306 [33]	-	-	10
PHS (power)	0.80[33]	1.5	1500 [34]	-	-	60
	(-)	(%/CAPEX)	($/kWh)	($/kWh$_{th}$)	(h)	
Battery (energy)	1	0	285 [33]	-	-	10

$$c^{opex_u} = \frac{c_u^{fuel}}{\eta_u} \tag{2}$$

$$c^{capex} = CAPEX \cdot \frac{(\mathrm{i} \cdot (1+\mathrm{i})^n)}{((1+\mathrm{i})^n - 1)} \cdot (1 + FOM) \tag{3}$$

Demand must equal the sum of supply of all producing units, as described in Equation (4). Note that in the case of the storage units, p can also take negative values when the storage is charging.

$$\sum_{u \in U} \mathbf{p}_{u,t} = d_t + \mathbf{p}_t^{excess} \qquad \forall t \in T \tag{4}$$

For all investment units, the supply is limited by the installed nominal power $\mathbf{p}_i^{nom}$ described in Equation (5).

$$0 \leq \mathbf{p}_{i,t} \leq \mathbf{p}_i^{nom} \qquad \forall i \in I, t \in T \tag{5}$$

$$\underline{p}_i \leq \mathbf{p}_i^{nom} \leq \overline{p}_i \qquad \forall i \in I \tag{6}$$

The energy storage balance in Equation (7) is applied for all modelled storage types. The balance includes standing losses η^{loss} as well as charge and discharge efficiencies $\eta^{in/out}$.

$$\mathbf{e}_{s,t} = \mathbf{e}_{s,t-1} \cdot \eta_s^{loss} - \frac{\mathbf{p}_{s,t}^{out}}{\eta_s^{out}} + \mathbf{p}_{s,t}^{in} \cdot \eta_s^{in} \qquad \forall s \in S, t \in T \tag{7}$$

Additionally, the power of the storage is limited by the optimised nominal power shown in Equation (8).

$$-\mathbf{p}_s^{nom} \leq \mathbf{p}_{s,t} \leq \mathbf{p}_s^{nom} \qquad \forall s \in S, t \in T \tag{8}$$

For all RE technologies, i.e., PV and wind, the power output is determined by Equation (9) where $c_t^{profile}$ is the time-dependent normalised generation profile of the unit $i \in I$. The profile data can be obtained from measurements, calculated from re-analysis weather data or directly obtained from databases such as renewables.ninja [30,31].

$$\mathbf{p}_{i,t} = c_{i,t}^{profile} \mathbf{p}_i^{nom} \qquad \forall i \in I, t \in T \tag{9}$$

Analogously to Equations (5) and (6), the energy storage level and its maximum investment level are bounded as shown in Equations (10) and (11).

$$e_s^{min} \cdot \mathbf{e}_s^{nom} \leq \mathbf{e}_{s,t} \leq \mathbf{e}_s^{nom} \qquad \forall s \in S, t \in T \tag{10}$$

$$0 \leq \mathbf{e}_s^{nom} \leq \overline{e}_s \qquad \forall s \in S \tag{11}$$

For all conventional units $c \in C$, upper and lower limits for the total energy supply over the time horizon T can be bounded with Equations (12) and (13).

$$\sum_{t \in T} \mathbf{p}_{c,t} \geq \underline{E}_c \qquad \forall c \in C \tag{12}$$

$$\sum_{t \in T} \mathbf{p}_{c,t} \leq \overline{E}_c \qquad \forall c \in C \tag{13}$$

To model RE penetration within the system by an exogenously defined RE share an additional constraint is introduced. The renewable energy share is defined by Equation (14) by the share of conventional technologies $c \in C$.

$$\sum_{t \in T} \sum_{c \in C} x_c^{flow}(t) \leq (1 - RE^{share}) \cdot c_l^{amount} \tag{14}$$

4. Scenario Assumptions

Within this study four different scenarios are modelled to analyse the future Jordanian electricity system. Based on NEPCO forecast, the demand for all scenarios is 28 TWh [7].

The **BASE scenario**, considering the existing power park of 2023 shown in Table 1, is a lower bound to the capacity expansion. The **CONT scenario** includes fossil fuel contracts for minimum gas consumption as well as operational constraints for the existing shale-oil power plant. The operation of the shale-oil unit is exogenous, set to 7500 h full load hours. For natural gas, 24 $\mathrm{TWh_{th}}$ annual gas consumption is set in the model. All other assumptions are the same as in the BASE scenario. As the energy independence in Jordan plays an important role, an **AUT scenario**, wherein only local resources can be utilised, has been added. Finally, the **GRE scenario** is an unconstrained electricity mix optimisation (greenfield planning approach). Therefore lower bounds on the investment of units were set; all costs and technical parameters were the same as in the BASE scenario. For all scenario setups, different shares of RE are modelled with Equation (14).

Costs and Technology Parameter

Table 2 summarises the cost and technology assumptions for all scenarios. For battery storage units a power to energy ratio of 1/6 was used; for PHS a ratio of 1/10 has been used in all scenarios. The PHS potential in this paper was derived from the work of [17]. According to the study, three (Mujib, Wadi Arab and King Talal) out of ten dams operated by the Jordan Valley authority are suitable for PHS installations. For these dams only an upper reservoir needs to constructed. Due to geological limitations, the aggregated PHS potential is restricted to 3750 MWh. Cost estimations for these PHS storage units are based on reference [34].

5. Results

5.1. Cost-Optimal Mix

The results of the scenarios for the cost-optimal mix are presented in Figures 1 and 2. The CONT and BASE scenarios result in a similar technology mix with RE shares of around 33%. Compared to the current power park, almost no additional investment in conventional units is required to meet the future demand. Instead, PV is expanded by capacity of 4.27 GW while wind capacity is not expanded for the cost-optimal mix. The GRE scenario shows that without current restrictions, the optimal mix consists of 3.74 GW of CCGT followed by 4.47 GW of PV and 0.99 GW of GT. The only scenario where storage units are installed is the AUT scenario. With 375 MW the PHS potential is fully exploited, and an additional 1.28 GW of battery storage is installed. The RE share of above 60% is significantly higher compared to the other scenarios. In addition to substantial PV capacity of 6.78 GW, wind capacity of 3.58 GW and oil shale capacity of 2.88 GW of are installed.

Except for the AUT scenario with 10.27 $\mathrm{TWh_{el}}$ of shale oil based supply, most electricity is still supplied by conventional units in the cost-optimal mix. For the cost-optimal case with no constraints on the RE share, 16.41 TWh is supplied by CCGT in the BASE scenario. With the contracts applied, the oil shale unit supplies 3.53 TWh, which causes a drop in the CCGT supply to 14.01 TWh. In both cases, around 8.16 TWh is produced by PV units. Notably, emissions of the cost-optimal AUT scenario (9.42 million t), with a RE share of above 60%, are similar to the CONT scenario (9.62 million t) with a RE share of about 30%, as emission factors of shale oil are higher and efficiency is lower compared to CCGT units. Emissions within the BASE and GRE scenarios are lower with 7.93 and 8.27 million t respectively.

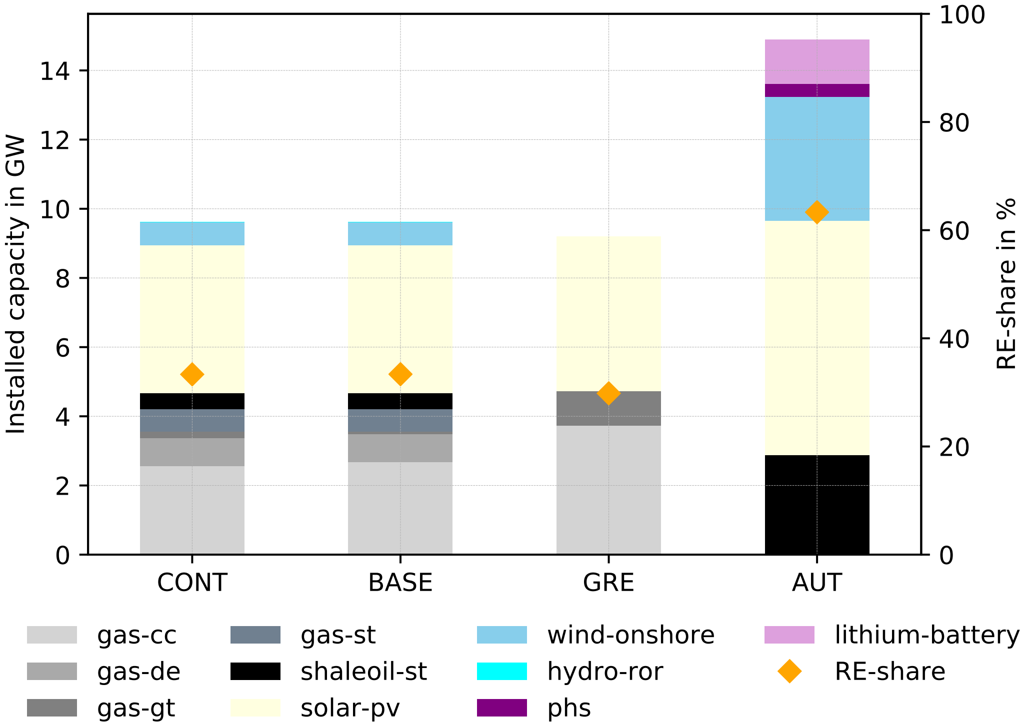


Figure 1. Installed capacities in the four scenarios and the cost-optimal case in GW (left axis) and renewable energy (RE) share in percent (right axis).

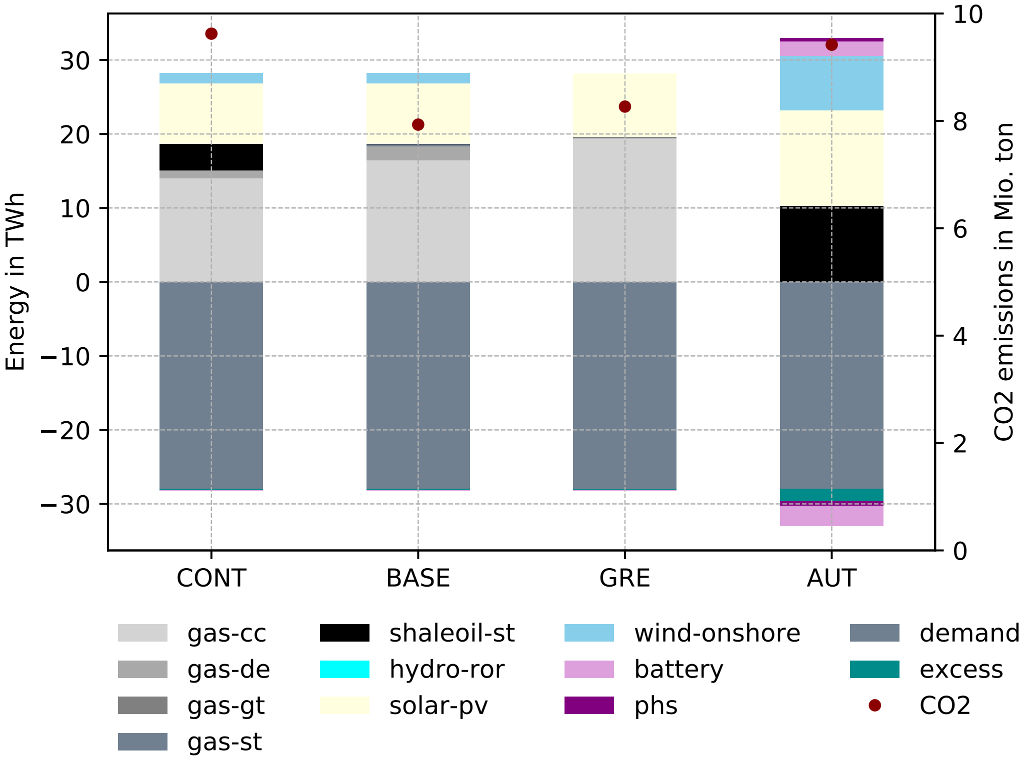


Figure 2. Supply and demand in the four scenarios and the cost-optimal case in TWh (left axis) and CO_2 emissions in million ton (right axis).

5.2. Varying Renewable Energy Shares

Figure 3 shows the installed capacities for 2030 for all scenarios with different RE shares. Detailed data are provided in the Appendix A. As described above, the cost-optimal mix in all scenarios already features a RE share 30% or above. Due to the lower bound on the gas consumption in the CONT scenario, higher shares of RE are not feasible within this setup. Compared to the status quo (2023), results show a significant increase in PV followed by wind investment in the BASE scenario to meet the increased demand of 28 TWh. In addition, minor investment in CCGT was chosen in the BASE scenario up to a RE share of 50%. This shows that due to the differences in marginal cost, additional CCGT investment is preferred instead of dispatching the shale-oil unit. PHS storage investment becomes relevant for RE shares of above 40% and the potential is fully exploited at shares above 50%. For up to 70% RE share, no additional storage than PHS is required to integrate the RE. Above 80% RE, investment in battery storage starts to increase significantly with over 3.15 GW installed capacity in the BASE-90 scenario and 3.82 GW in the AUT scenario.

Compared to the BASE scenario, a similar pattern with regard to installed capacities under different RE shares can be observed within the GRE scenario. However, in particular for shares above 80% RE, total conventional capacities are lower. Despite higher investment in shale oil, PV plays a bigger role than wind within the AUT scenario. In BASE-90 9.95 GW PV and 8.99 GW wind are installed compared to 10.89 GW PV and 6.93 GW in the AUT-90 case.

The energy supply, energy demand and corresponding CO_2 emissions are shown in Figure 4. For higher shares of RE, wind energy becomes more relevant and the need for additional battery storages increases significantly. In addition, limited (long) term storage options and missing transmissions to neighbouring countries cause high curtailment. In the BASE-90 scenario, over 35% of the RE production is curtailed. Due to higher storage capacities, curtailment is lower in the AUT scenarios.

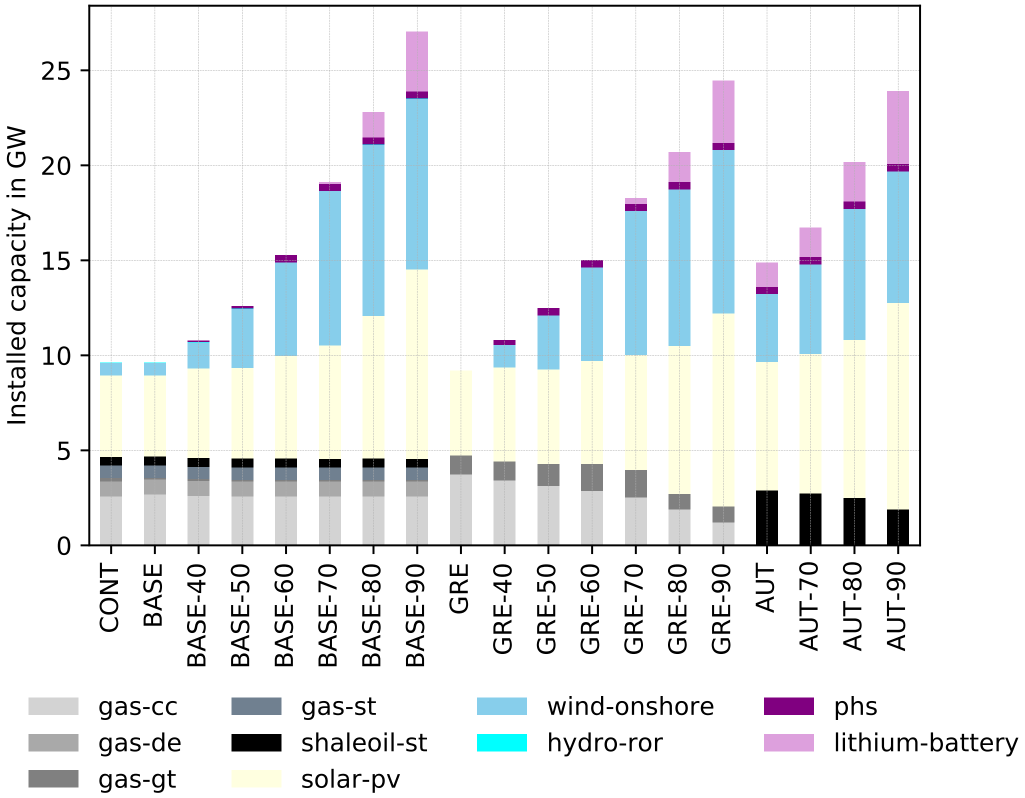


Figure 3. Installed capacities for all scenarios and varying renewable energy shares.

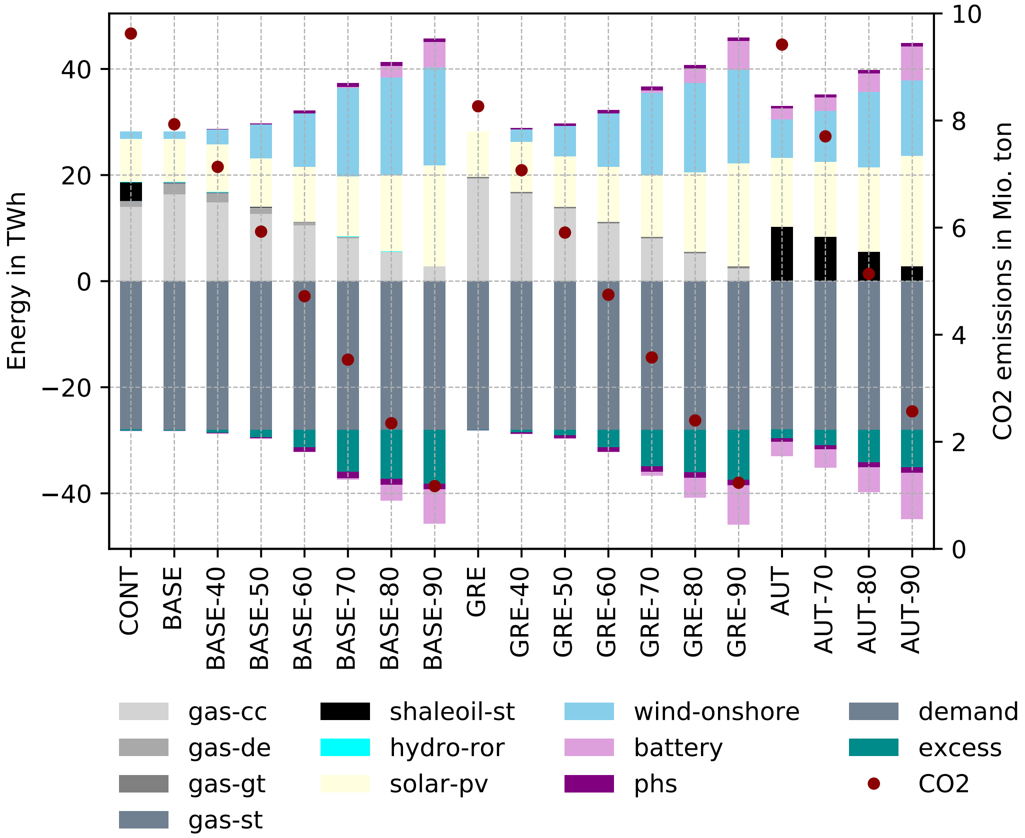


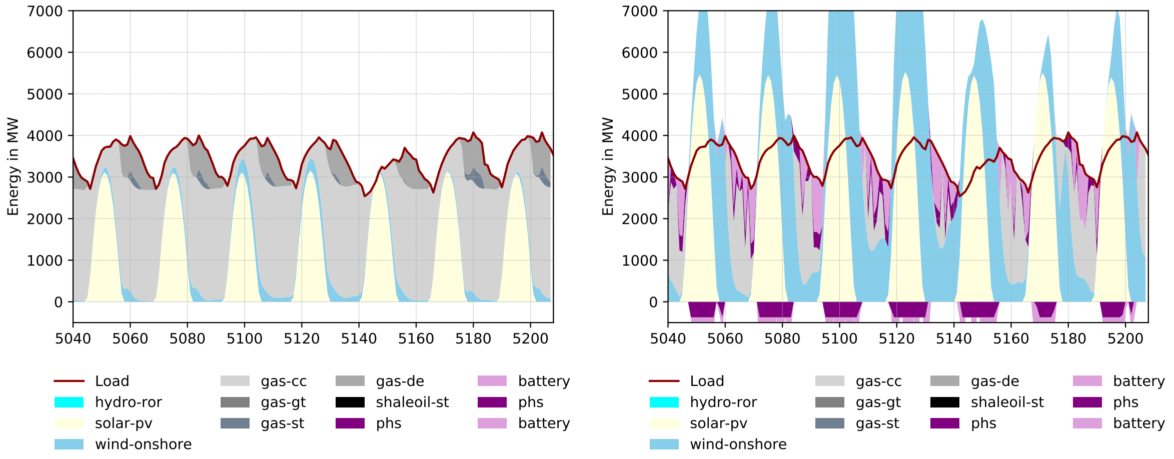
Figure 4. Supply/demand (left axis) and CO_2 emissions (right axis) for all scenarios.

With these results, three different stages within the system can be identified for the BASE scenarios: (1) low shares for up to 50% RE where PV supply is dominating; (2) medium share of RE between 60% and 80% where wind is higher than PV; and (3) high shares of above 80% where PV is equal to or more prevalent than wind. This shows the energy system's dynamic. PV has lower single technology cost of electricity and integrates well until a certain level of RE penetration is reached. After this point, the system value of wind starts to increase because it can supply electricity when PV is not available. Despite excellent solar resources and low cost, up to about 50% of the electricity supply comes from wind for scenarios of 90% RE share. A similar pattern can be identified within the GRE scenario. In contrast, the AUT scenarios feature higher storage capacities and therefore also in all cases higher PV supply than wind.

A major difference between the CONT and the BASE scenarios is the resulting level of CO_2 emissions. Due to the shale-oil unit, emissions are significantly higher for the CONT scenario.

5.3. System Operation

Figure 5 shows the dispatch of units for the BASE-40 and BASE-80 scenario. Within the system displayed in Figure 5a, mainly PV supply is consumed during the day while in the evening peaks and during the night CCGT and GT units are providing electricity. Storage operation is not required to integrate the RE. In contrast, Figure 5b shows the electricity system with a 80% RE supply. Here, consequences of increased RE supply can be observed. Storage operation increases notably, integrating wind and solar supply during the day and shifting this electricity to the evening peak. In addition, the high excess of RE during the day is also clearly visible.



(**a**) BASE-40 (**b**) BASE-80

Figure 5. Dispatch of supply and demand in a week of the year for two different RE shares within the BASE scenario.

For the same scenarios, the aggregated state of charge of the PHS units is shown in the heat map plot in Figure 6. The PV integrating pattern with fully charged storage units during the day and empty storage units in the morning is visible. It can be observed that the storage is operated more intensively in the case with higher share of RE. During the summer months, the storage is fully charged during the whole day in the BASE-40 scenario, whereas this can not be observed in the BASE-80 scenario.

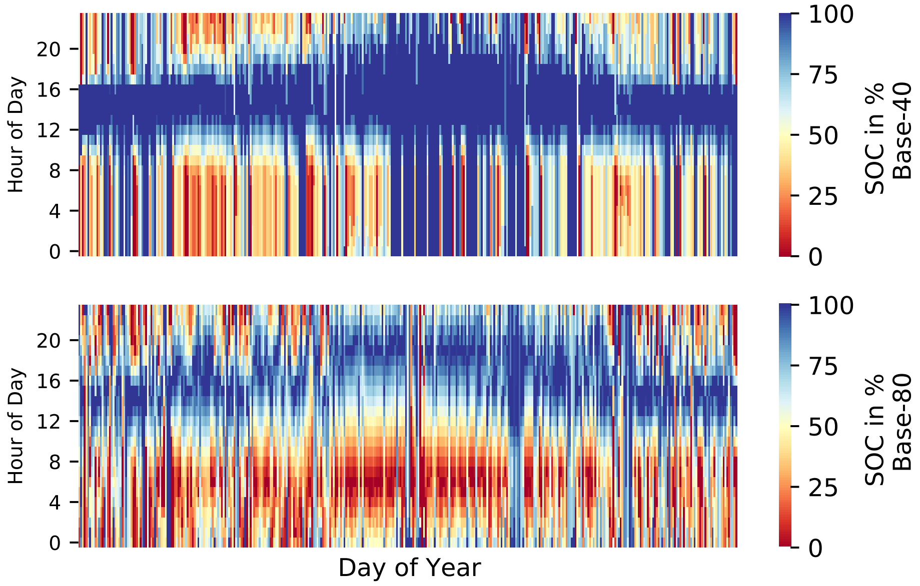


Figure 6. Aggregated SOC of pumped hydro storage (PHS) of BASE-40 (top) and BASE-80 (bottom) scenario.

5.4. Costs

Figure 7 shows the levelised cost of electricity (LCOE) for varying RE shares. LCOE has been calculated by dividing the total annualised investments and operational costs by the electricity demand covered. Note that for renewable energy systems, additional costs occur for integrating the intermittent electricity into the system, as discussed in [35].

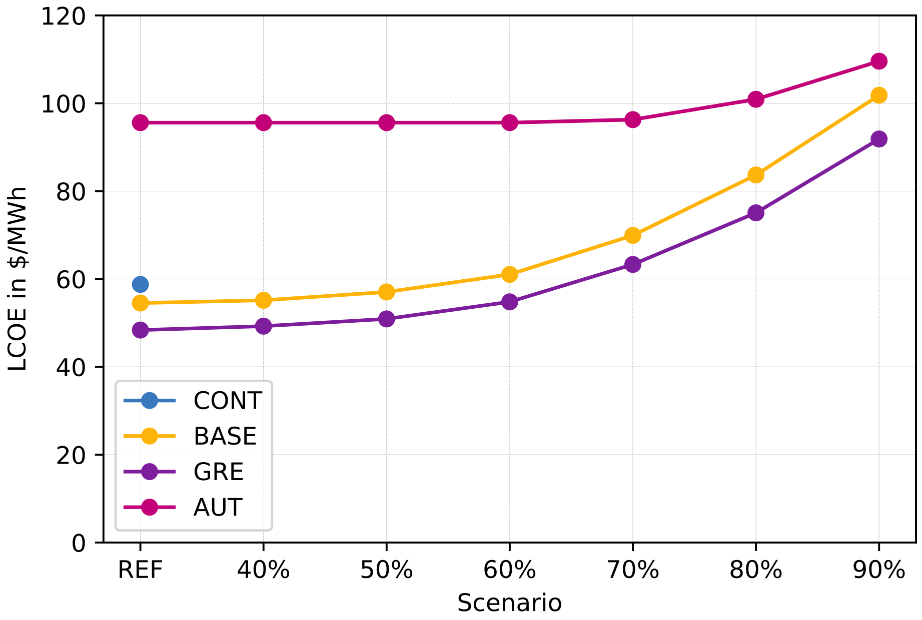


Figure 7. LCOE for different scenarios and RE shares.

Clearly, the AUT scenario comes with the highest cost, as autarchy has a high price. However, as it already features a RE share of above 60% in the cost-optimal mix, the increase in cost towards a 90% RE share setup is rather low in relative terms. The second highest cost for the cost-optimal case can be found within the CONT scenario with oil shale supply. The green field planning scenario GRE highlights that a combination of CCGT and RE is more cost efficient. The LCOE of the BASE and GRE setup do not differ significantly. With regard to rising RE shares, it can be observed that up to 50% RE can be achieved with a very small increase in LCOE from 54.52 to 57.04 $/MWh in the BASE scenario. For a RE share of up to 90%, LCOE increases almost to values twice as high as that in the cost-optimal case. The effects of higher storage requirements and thus additional investment costs and high excess electricity with curtailment can be reasons for these figures.

While PV has the lowest LCOE as a single piece of technology, the majority of the investment costs in scenarios with high shares of RE are caused by wind energy deployments and battery storage. The distribution of investment costs depicted in Figure A1 in the Appendix A shows that a combination of technologies within a system that strives for high RE shares has a different value compared to a single technology solution.

6. Discussion

The disruption of natural gas supply in 2011 caused by the Arab spring proved the unreliability and instability of the Jordanian energy system. Ever since, the country has failed to increase energy independence. With abundant renewable energy resources, a combination of PHS and RE energy and efficient CCGT units is the most cost effective way for gaining increased energy independence and simultaneously reducing GHG emissions.

6.1. Comparison with Other Studies

The presented results indicate a high share of RE within a cost-optimal energy system to meet the increased energy demand in Jordan by 2030 compared to what is envisioned within existing strategies, such as in references [1,7,18]. The herein determined cost-optimal energy mix includes a share of above 30% of RE by 2030, in all scenarios. In addition, the presented study also identified a greater role of wind energy and PHS for the Jordanian electricity system, contrary to [13], which underlined the importance of RE, while neglecting PHS utilisation though. Compared to [21], analysing the cost-optimal energy mix combining CCGT with PV and wind (10%, 71% and 19% in 2035), the calculated results indicate a lower share of PV—29.2% within cost-optimal mix of BASE scenario.

The integration of PHS is vital to a system with high renewable energy shares. The necessity of PHS and long-term battery storage to increase the share of RE and increase energy independence is recognised by [22] and [21]. The authors of [22] aim for 100% renewable energy supply by 2050, integrating 1 GWh of battery storage in 2025 up to 67 GWh in 2050; in this study 0.69 GWh PHS is necessary within the BASE scenario, with a RE share of 40%, and only with a share of above 70% RE does the battery storage become necessary. A RE share of 90% within the BASE scenario makes 3750 GWh PHS storage necessary. Along with [1], PHS is identified as an option to avoid or limit curtailment of renewable energies.

Supporting [27], the results clearly show reduced CO_2 emissions within the cost-optimal setting, which includes in all scenarios 30% or more RE and the high potential of further reductions due to the high potential of renewable energies within Jordan. Additionally, [28] proposed the combination of wind and PHS to be economically, environmentally and technically more efficient than conventional power generation in regard to CO_2 emissions. This is supported in this study.

As analysed within [4], a diversification of energy generation can have beneficial effects on the energy security of Jordan. According to this analysis, most relevant measures are continuing the decrease of imported energy through the utilisation of domestic energy resources such as oil shale and renewable sources (wind and PV). While this is certainly true for wind and PV, shale oil is environmentally and economically not recommendable, as shown within the here presented analysis. Instead, under the assumption of a growing electricity demand, PHS in combination with PV and wind energy can provide a secure, environmentally beneficial and cost effective energy supply.

Results show that shares of up to 50% RE share can be achieved by a slight increase in LCOE. Due to required storage investment and curtailment of RE, there is a high increase of LCOE for shares of up to 90%. However, it is important to note that an integrated electricity system of countries in the MENA region could reduce system costs significantly, as shown by [36]. Such integration will also help to reduce curtailment. Similarly, smart sector integration of the water and electricity sector is another option to increase RE penetration in the Jordanian energy system. Jordan, as one of the water-scarcest countries on the planet [37], has a high energy demand for the water sector, which is likely to increase in the coming years due to increased need for water pumping because of lowered water levels as well as the need for desalination of water as an additional source of fresh water.

6.2. Limitations of the Study

The study applied an open source investment model to analyse the future Jordanian electricity system. However, results need to be read in light of the modelling limitations. First of all, it is important to note that no transmission to neighbouring countries and Jordan's grid has been modelled. While the former can help to provide a solution with lower cost, due to reduced excess and lesser storage requirements, as discussed above, the latter can actually counteract these effects. In particular, curtailment and storage dispatch can be higher to keep the system balanced within the country on the distribution and transmission grid levels. Hence, storage units may be cost efficient within scenarios of shares below 40% RE.

Another important point is the cost-optimal dispatch based on perfect competition, where the existing contracts with independent power producers (IPP) need to be considered. While gas contracts have been integrated, additional contracts may exist that do not allow for a reduction of conventional power plant operation, and therefore limit RE expansion.

6.3. The Value of Open Source Tools

The context-specific boundaries, such as existing contracts, power plant characteristics and grid constraints, are important factors when modelling an electricity system. However, that information is not always available for scientists. In addition, political and economic dynamics can change fundamental assumptions, such as price and demand developments, in a short period of time. Therefore, open source approaches are of high value for further investigations. In addition to changes of basic assumptions and input data of this study, the model can be improved or extended. Among others, the applied Open Energy Modelling Framework (oemof) [20,29] provides the opportunity for detailed power plant modelling with minimum up and down times, part load efficiencies and linear optimal power flow grid modelling. Such functionalities could be integrated inside the developed model as well. The same holds for the PV and wind profiles, as [16] states, the exact renewable profiles which are technically feasible in Jordan have not been quantified yet.

7. Conclusions

The paper presents an analysis based on an open source optimisation modelling approach of the Jordanian electricity system in 2030. Results highlight and confirm the great potential of renewable energy for cost effective, environmentally friendly and more energy independent development in Jordan. Up to 50% renewable energy within the electricity system can be achieved with only a slight increase of levelised cost of electricity from 54.52 to 57.04 $/MWh. In particular, photovoltaic installations in combination with pumped hydro storage, as a low cost storage technology, seem to be a superior solution compared to the expansion of shale oil deployments due to high costs and CO_2 emissions. For higher shares of renewable energy, wind energy can play an important role, making up above 45% of the renewable energy supply in a 90% renewable energy based system.

However, high shares of renewable energy within the electricity mix require the analysis of long term storage options and grid expansion to neighbouring countries to avoid high costs as well as extensive curtailment of renewable energy. In addition, the water–energy sector cooperation using flexible desalination can be an important step to integrate renewable produced electricity and attenuate water stress at the same time. Within the transformation process, fossil fuel contracts pose a challenge, as they may hamper renewable energy expansion and increase integration cost. Modelling the scenario with existing long term gas contracts shows that renewable energy shares above 33% cannot be achieved, even under a growing electricity demand, by 2030. Therefore, strategic planning with a long term perspective is important for the Jordanian electricity system.

Supplementary Materials: The following are available online at https://github.com/znes/oemof-jordan/releases/tag/paper

Author Contributions: Conceptualization, S.H.; methodology, S.H.; software, S.H.; validation, S.H. and F.D. and A.A.; formal analysis, S.H.; investigation, S.H. and F.D.; resources, S.H. and A.A; data curation, S.H. and F.D. and A.A.; writing—original draft preparation, S.H. and F.D. and A.A.; writing—review and editing, S.H. and F.D.; visualization, S.H.; supervision, S.H.; project administration, S.H.; funding acquisition: S.H. and F.D.; All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CAES	Compressed Air Energy Storage
CC	Combined Cycle
DE	Diesel Engine
FOM	Fixed operation and maintenance
GAMS	General Algebraic Modelling System
GDP	Gross Domestic Product
GHG	Green house gas
IIASA	International Institute of Applied Systems Analysis
INDC	Intended Nationally Determined Contribution
LEAP	Low Emission Analysis Plattform
LCOE	Levelised Cost of Electricity
MENA	Middle East and Northern Africa
NEPCO	National Electric Power Company
GT	Gas Turbine
PV	Photovoltaic
oemof	Open Energy System Modelling Framework
RE	Renewable Energy
ST	Steam Turbine
WACC	Weighted average cost of capital

Appendix A. Results

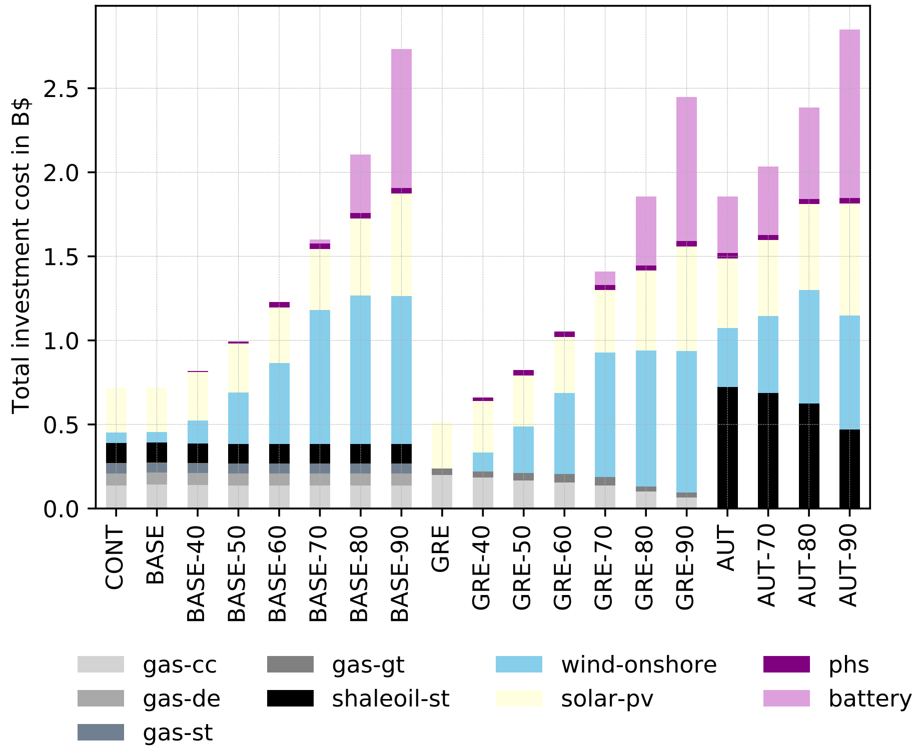

Figure A1. Annualised investment cost within all scenarios in Billion US $.

Table A1. LCOE in US $/MWh

	REF	**40%**	**50%**	**60%**	**70%**	**80%**	**90%**
CONT	58.76	-	-	-	-	-	-
BASE	54.52	55.15	57.04	61.04	69.92	83.68	101.83
GRE	48.37	49.26	50.91	54.79	63.31	75.06	91.87
AUT	95.59	95.59	95.59	95.59	96.28	100.91	109.58

Table A2. Annualised investment cost in million US $.

	Gas-cc	**Gas-de**	**Gas-st**	**Gas-gt**	**Shaleoil-st**	**Wind-Onshore**	**Solar-pv**	**phs**	**Battery**
CONT	138.27	70.9	55.67	7.02	118.09	64.77	261.93	0.00	0.00
BASE	144	70.9	55.67	3.07	118.09	64.77	262.27	0.00	0.00
BASE-40	140.08	70.9	55.67	3.07	118.09	135.65	288.44	5.56	0.00
BASE-50	138.27	70.9	55.67	3.07	118.09	303.45	293.54	10.43	0.00
BASE-60	138.27	70.9	55.67	3.07	118.09	479.53	332.55	30.16	0.00
BASE-70	138.27	70.9	55.67	3.07	118.09	795.27	365.10	30.16	21.22
BASE-80	138.27	70.9	55.67	3.07	118.09	881.53	460.03	30.16	346.41
BASE-90	138.27	70.9	55.67	3.07	118.09	878.64	610.81	30.16	826.25
GRE	201.19	0	0	36.84	0.00	0.00	274.11	0.00	0.00
GRE-40	184.21	0	0	37.23	0.00	113.16	304.40	19.88	0.00
GRE-50	167.89	0	0	43.4	0.00	277.35	304.91	30.16	0.00
GRE-60	154.26	0	0	52.39	0.00	480.34	333.36	30.16	0.00
GRE-70	136.23	0	0	53.36	0.00	738.83	372.42	30.16	77.48
GRE-80	102.57	0	0	29.37	0.00	807.10	477.83	30.16	410.32
GRE-90	64.84	0	0	31.69	0.00	841.63	622.36	30.16	855.80
AUT	-	-	-	-	724.27	349.56	416.02	30.16	335.34
AUT-70	-	-	-	-	686.15	460.42	451.38	30.16	406.25
AUT-80	-	-	-	-	626.15	673.96	511.25	30.16	543.04
AUT-90	-	-	-	-	471.19	676.66	668.73	30.16	1001.05

Table A3. Installed capacities in MW.

	Gas-cc	**Gas-de**	**Gas-gt**	**Gas-st**	**Shaleoil-st**	**Solar-pv**	**Wind-Onshore**	**Hydro-ror**	**phs**	**Battery**
CONT	2567	810	189	636	470	4267	663	12	0	0
BASE	2673	810	83	636	470	4272	663	12	0	0
BASE-40	2600	810	83	636	470	4698	1388	12	69	0
BASE-50	2567	810	83	636	470	4781	3106	12	129	0
BASE-60	2567	810	83	636	470	5417	4908	12	375	0
BASE-70	2567	810	83	636	470	5947	8140	12	375	80
BASE-80	2567	810	83	636	470	7494	9023	12	375	1320
BASE-90	2567	810	83	636	470	9950	8993	12	375	3150
GRE	3735	0	994	0	0	4465	0	0	0	0
GRE-40	3420	0	1005	0	0	4958	1158	0	247	0
GRE-50	3117	0	1172	0	0	4967	2839	0	375	0
GRE-60	2863	0	1414	0	0	5430	4916	0	375	0
GRE-70	2529	0	1440	0	0	6066	7562	0	375	295
GRE-80	1904	0	793	0	0	7784	8261	0	375	1564
GRE-90	1203	0	855	0	0	10,138	8615	0	375	3263
AUT	0	0	0	0	2882	6777	3578	0	375	1278
AUT-70	0	0	0	0	2730	7353	4712	0	375	1548
AUT-80	0	0	0	0	2492	8328	6898	0	375	2070
AUT-90	0	0	0	0	1875	10,893	6926	0	375	3816

Table A4. Energy supply and demand in TWh.

	Gas-cc	Gas-de	Gas-gt	Gas-st	Shaleoil-st	Hydro-ror	Solar-pv	Wind-Onshore	Battery	phs	Demand	Excess	phs-cos	Battery-cos
CONT	14.01	1.07	0.00	0.06	3.53	0.02	8.16	1.36	0.00	0.00	−28.0	−0.21	0.00	0.00
BASE	16.41	1.94	0.01	0.29	0.01	0.02	8.17	1.36	0.00	0.00	−28.0	−0.21	0.00	0.00
BASE-40	14.85	1.71	0.00	0.23	0.01	0.02	8.99	2.85	0.00	0.05	−28.0	−0.63	−0.08	0.00
BASE-50	12.73	1.13	0.00	0.13	0.00	0.02	9.14	6.37	0.00	0.14	−28.0	−1.45	−0.23	0.00
BASE-60	10.55	0.61	0.00	0.04	0.00	0.02	10.36	10.06	0.00	0.56	−28.0	−3.33	−0.88	0.00
BASE-70	8.05	0.33	0.00	0.02	0.00	0.02	11.37	16.69	0.15	0.72	−28.0	−7.99	−1.15	−0.21
BASE-80	5.58	0.02	0.00	0.00	0.00	0.02	14.33	18.50	2.18	0.69	−28.0	−9.30	−1.07	−2.95
BASE-90	2.80	0.00	0.00	0.00	0.00	0.02	19.03	18.44	4.80	0.63	−28.0	−10.25	−0.98	−6.49
GRE	19.44	0.00	0.20	0.00	0.00	0.00	8.54	0.00	0.00	0.00	−28.0	−0.19	0.00	0.00
GRE-40	16.60	0.00	0.20	0.00	0.00	0.00	9.48	2.38	0.00	0.20	−28.0	−0.55	−0.31	0.00
GRE-50	13.77	0.00	0.23	0.00	0.00	0.00	9.50	5.82	0.00	0.38	−28.0	−1.10	−0.60	0.00
GRE-60	10.90	0.00	0.30	0.00	0.00	0.00	10.38	10.08	0.00	0.57	−28.0	−3.35	−0.89	0.00
GRE-70	8.10	0.00	0.30	0.00	0.00	0.00	11.60	15.51	0.50	0.67	−28.0	−6.93	−1.06	−0.69
GRE-80	5.32	0.00	0.28	0.00	0.00	0.00	14.89	16.94	2.68	0.65	−28.0	−8.05	−1.03	−3.68
GRE-90	2.47	0.00	0.33	0.00	0.00	0.00	19.39	17.66	5.42	0.61	−28.0	−9.49	−0.98	−7.41
AUT	0.00	0.00	0.00	0.00	10.27	0.00	12.96	7.34	2.00	0.42	−28.0	−1.62	−0.66	−2.70
AUT-70	0.00	0.00	0.00	0.00	8.40	0.00	14.06	9.66	2.53	0.50	−28.0	−2.95	−0.78	−3.42
AUT-80	0.00	0.00	0.00	0.00	5.60	0.00	15.93	14.14	3.48	0.59	−28.0	−6.11	−0.92	−4.71
AUT-90	0.00	0.00	0.00	0.00	2.80	0.00	20.83	14.20	6.40	0.60	−28.0	−7.14	−0.96	−8.73

Appendix A.1. Mathematical Symbols

Table A5. Sets used in the model description and values of these sets used within the applied scenarios.

Symbol	Index	Description	Elements of Sets in Scenarios	Unit
T	t	Timesteps	{1...8760}	h
R	r	Renewable units	{Wind, PV}	MW
C	c	Conventional units	{CCGT, GT, ST, DE, Oil-shale ST}	MW
S	s	Storage units	{Battery, PHS}	MW, MWh
I	i	Investment units	Scenario dependet	-
U	u	All supply units ($R \cup C \cup S$)	-	-

Table A6. Optimisation variables used in the model description.

Symbol	Description
$\mathbf{p}_t$	Power output at timestep t
$\mathbf{p}^{nom}$	Upper limit of power output
$\mathbf{e}_{s,t}$	Storage level of storage s at timestep
$\mathbf{e}_s^{nom}$	Upper limit of storage output
$\mathbf{p}_t^{excess}$	Excess variable

Table A7. Exogenous model variables used in the model description.

Symbol	Description
$\overline{p}_i$	Upper power investment limit of unit i
$\underline{p}_i$	Lower power investment limit of unit i
$\overline{e}_s$	Upper energy investment limit of storage s
d_t	Electricity demand at timestep t
η_s^{loss}	Standing loss of storage s
η_s^{in}	Charge efficiency of storage s
η_s^{out}	Discharge efficiency of storage s
c_u^{opex}	Operational expenditure of unit u
$c_i^{capex,p}$	(Annualised) power expenditure of unit i
$c_s^{capex,e}$	(Annualised) energy capital expenditure of storage s
$c_r^{profile}$	Generation profile of renewable energy unit r
e_c	Emission factor of power output of unit c

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Why renewables and energy efficiency are not enough - the relevance of sufficiency in the heating sector for limiting global warming to 1.5°[1]

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Why renewables and energy efficiency are not enough - the relevance of sufficiency in the heating sector for limiting global warming to 1.5 °C.

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ABSTRACT

The decarbonisation of the German heating sector is challenging but necessary when aiming to limit global warming to 1.5 °C. Therefore, a fast reduction of the energy demand side and an increase of renewable energy on the supply side is required. However, related efficiency (energetic modernisation) and consistency (renewable energy) measures are limited through their potential, expansion speed, resources and acceptance. Sufficiency as an underrepresented measure has a high potential for heat demand reductions and can thus also relax pressure on the supply side. Nevertheless, sufficiency measures in the heating sector have not been investigated thoroughly. In this study we present scenarios for the German heating sector including efficiency, consistency and sufficiency measures and analyse their compliance with limiting global warming to 1.5 °C. The results of the model-based analysis show that efficiency measures and renewable energy in combination with heat pump expansion are not sufficient. Sufficiency measures, such as a reduced living space, have a high CO_2-emission reduction potential and must be considered as one important pillar for a successful heat sector transformation.

1. Introduction

In 2015, the Paris-Agreement has been ratified by 189 countries (Nations, 2019). Its goal is to keep the increase of global average temperature well below 2 °C. The importance of "well-below", i.e. limiting global warming to 1.5 °C, has been pointed out in the special report of the Intergovernmental Panel of Climate Change (IPCC) (IPCC, 2018). To limit global warming to 1.5 °C, cumulative emissions have to stay below 420 to 570 Gt CO_2 (probability of 66 %) (IPCC, 2018). Germany, which is part of the Paris Agreement, follows two main strategies in the energy sector to reduce CO_2-emissions: 1) *consistency* on the supply-side, for example replacing fossil by renewable sources and 2) *Efficiency* on the demand and supply side, i.e. improving the input/output ratio of processes and applications (Bundesumweltministerium, 2016). However, it is argued that efficiency alone is not sufficient to reduce energy demands in absolute terms as rebound effects can significantly decrease the effect of efficiency measures (Greening et al., 2000; Saunders, 2013; Shove, 2018; Sorrell et al., 2009). Also, the scenarios of the IPCC (2018) show, that relying solely on such technical measures would require negative emissions in the second half of the century, which need to equal 29 times of current global CO_2-emissions. This highlights the importance of additional climate change mitigation measures on the demand side (Creutzig et al., 2018; Mundaca et al., 2019). Similarly, authors argue that *consistency* and *efficiency* strategies alone may not be enough to comply with climate goals (Samadi et al., 2017; Zell-Ziegler and Förster, 2018). Another, complementary measures are so called *sufficiency* measures (Princen, 2003). Sufficiency aims at an actual reduction of consumption, e.g. through changes in consumer behaviour, which ultimately leads to a decreased energy demand (Brischke and Thomas, 2014). The concept of energy sufficiency leading to absolute energy demand reduction has gained attention in the scientific discussion in different areas (Grubler et al., 2018; Rohde and Bee, 2009). Energy scenarios, which are based on quantitative models, are an important source offering energy and policy advice (Le Gallic et al., 2017). Samadi et al. (2017) find that the inclusion of sufficiency in energy scenarios is both possible and useful. However, the potential contribution of sufficiency is not explored well enough in energy scenarios (Zell-Ziegler and Förster, 2018). One illustrative example of the shortcomings of efficiency and consistency without sufficiency can be found in the German housing sector. Although energetic standards and renewable heat supply increases, neither emissions, nor the demand have shown a significant decline in recent years (Agora, 2016; BMWi, 2020a; Umweltbundesamt, 2018a). One dominating factor of the rising energy demand in household consumption is the increasing size of living space (Lorek and

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Spangenberg, 2019). From 1995 to 2018 the average living space per capita in Germany has risen by 25.6% (own calculations based on development of population (Destatis, 2020a) and living space (Destatis, 2020b)).

Sufficiency measures for heat demand in the residential sector aim to reduce the heat service demand either by changing the living space towards a smaller living space per person or by changing the service demand within the living space by reducing the hot water and space heating temperature. The resulting reduction in heating demand consequently reduces the CO_2-emissions, corresponding to the amount and CO_2-intensity of the respective energy source saved.

The contribution of sufficiency measures to the reduction of heat demand related to the development of the building stock and thus to the reduction of CO_2-emission reduction, cannot be determined exactly, as the demand reduction is a result of sufficiency and efficiency measures. In order to investigate the effect nevertheless, we have examined four scenarios that differ by the sufficiency measures and keep the consistency / efficiency contribution constant. By comparison of those scenarios, the effect of sufficiency measures can be estimated.

Sufficiency measures have hardly been taken into account in scenarios of the heating sector so far, although according to Fischer et al. (2016) sufficiency measures have a great potential for reducing heat consumption when assessing them one by one. This study therefore investigates the potential of sufficiency measures in combination with other heating measures for residential buildings for their contribution to meeting a carbon budget that limits global warming to 1.5 °C.

In this paper, we analyse how a combination of consistency, efficiency and sufficiency measures in the German housing heat sector can lead to compliance with the carbon budget that limits global warming to 1.5 °C. For this purpose, we (1) derive a carbon budget that corresponds to limiting global warming to 1.5 °C for the German housing heat sector, (2) analyse the future development of heat demand in Germany until 2050 for different scenarios based on assumptions concerning new buildings and energetic restoration in combination with a reduction of living space, and (3) provide a supply side scenario as well as (4) quantify emissions of the different scenarios. The paper is structured as followed: Section 2 describes the method for deriving the carbon budget and the bottom-up simulation model. Section 3 explains the base data and introduces assumptions for the scenarios and describes the differences. The results of our analysis are presented in section 4. Based on the method and results, Section 5 discusses shortcomings and strengths of the chosen approach and gives examples of specific policy measures for a reduction of living space. Finally, section 6 presents a conclusion and policy implications of our findings.

2. Methods

The methods calculating the carbon budget as well as the demand and supply side of German residential heating sector are described in this section.

2.1. *A carbon budget for the German heat sector*

Global as well as German CO_2-emissions of 2017 are the basis for the budget calculation (IPCC, 2018; Umweltbundesamt, 2020b). The worldwide budget provided by the IPCC only includes CO_2-emissions and not CO_2-equivalent emissions, which also holds true for the German values and for our calculation.

Global budget

For carbon budget calculations we choose the 1.5 °C scenarios with a 66 % probability proposed by the IPCC (2018). Depending on the reference temperature the remaining budget amounts to 420 Gt CO_2 until 2100 using the global mean air temperature and to 570 Gt CO_2 with the global mean surface temperature. For our estimation, we apply the average of 495 Gt CO_2. The current global emissions amount to 42 ± 3 Gt CO_2 (IPCC, 2018) which means that with unchanged emissions, this budget would deplete in less than 12 years.

Allocation of the German budget

For further analysis, the global budget needs to be allocated to the national level. Different carbon budget allocation methods are summarised and discussed by van den Berg et al. (2019). These are 1) equal cumulative per capita emissions, 2) contraction and convergence, 3) grandfathering and 4) greenhouse development rights and ability to pay. Allocation methods differ concerning their social and political impacts due to their underlying equity principles reflected in the degree of sovereignty and equity among countries. In this paper, we consider the per capita distribution which represents a lower bound for the budget, the grandfathering distribution (upper bound), and contraction and convergence distribution (middle). The different approaches lead to considerable distribution differences. The per capita method distributes emissions based on avergae population shares. It is considered adequate under equity aspects and corresponds to the lower bound of our three budgets for Germany (van den Berg et al., 2019). Consequently, countries with currently high specific CO_2-emissions have to reduce these significantly faster than countries with low CO_2-emissions. In contrast, the grandfathering method demands equally fast reductions from all countries regardless of their current emissions and allocates the budget proportionally to current emission shares favouring developed countries. Finally, the contraction and convergence method represents an intermediate course. Here, until 2035, current emissions are highly relevant, but these converge to equal per capita emissions until 2035. Developing economies with currently low emission levels are given the possibility to increase emission levels in the next fifteen years. Although there is no international common political agreement on budget allocation, Denmark has already adopted the per capitamethod to develop policies in accordance with this budget (Klimaraadet, 2019). For Germany no such decision exist. However, groups like the German Advisory Council on the Environment (SRU, 2020) and the German Federal Constitutional Court (Bundesverfassungsgericht, 2021) refer to the per capita allocation approach.

Space heating emission budget

An allocated national carbon budget needs to be distributed to different sectors. Such distribution of the budget to sectors depends on political decisions associated with the ability of sectors to reduce emissions. We base our distribution on the scenario study from the Federal Environment Agency (UBA). The UBA study RESCUE (Purr et al., 2019) aims at a reduction of at least 95% greenhouse gas emissions in 2050 compared to 1990. Table 1 shows the contribution of the energy and the building sector in this study as well as the total reduction compared to 1990 within the most ambitious scenario *GreenSupreme*. The comparison of contributions to carbon emission reduction shows that the building sector contributes less to the reduction than the electricity sector and more than the overall reduction of all sectors.

Germany's contribution goals (Bundesumweltministerium, 2016) show a similar pattern. The building sector is ranked average in reduction contribution when comparing current sector emissions for 2018 and the goal for 2030 (Umweltbundesamt, 2020a). The energy sector is considered to contribute more than average since its costs for reduction are lower and its ability to reduce emissions is higher compared to the

Table 1

Sectoral contributions of the energy sector and the building sector and the overall reduction compared to 1990 values in the *GreenSupreme* scenario of Purr et al. (2019)

	Energy	Buildings	Total
2030	-79 %	-66 %	-69 %
2040	-93 %	-88 %	-88 %
2050	-100 %	-100 %	-97 %

heat sector. Runkel (2018), which provides a broad literature review of different decarbonisation studies, comes to the same conclusion. The energy sector (especially electricity) can be decarbonised faster than the heating sector whereas the transport-, agriculture- and industry-sector are slowest. For this study, we therefore derive a CO$_2$ budget for the space heating sector proportional to its historic emissions in relation to the total German CO$_2$-emissions.

2.2. Model overview

Scenarios in this study are computed with a techno-economic bottom-up simulation model for the residential heating sector in Germany. The developed model covers the annual development of the building stock (demand side) and the supply from 2020 to 2050. Figure 1 provides an overview of the model.

The starting point of the simulation is the year 2019, which represents the the status-quo of the average living space of the residential sector and the related heat demand and supply. The future development of the total living space depends on the population and the average living space per person. Both factors are exogenous model variables. The related heat demand depends on hot-water-demand, building condition, outdoor temperature and related heating behaviour. The building-condition are influenced by restoration rates and depth of restoration which are also exogenous model variables. The outside temperature and heating behaviour cannot be changed in the model and and are fixed with adjusted data from Loga et al. (2015). The development of the building-stock (endogenous) within the period under consideration is influenced by these mentioned factors. The supply mainly follows the data of the Federal Ministry of Economics and Technology (BMWi, 2020b), the Working Group on Renewable Energies (AGEE-Stat, 2020) and Federal Environmental Agency (UBA, 2020). Thereby the development of renewable energies and heat pumps depends on the potentials (exogenous), the expansion rates (exogenous) as well as further installation restrictions. For the latter the heat demand is split into three different categories according to their specific heat demand. This allows to restrict the installation of e.g. solar thermal energy for buildings with high specific heat demand with high temperature levels. Further, it enables to apply cover ratios and differentiated efficiencies for technologies such as heat pumps that are applied within these three categories. Beside the expansion of renewable energies and heat pumps the model also covers the fade-out of fossil fuels (exogenous and endogenous). The CO$_2$-emissions are composed by direct and indirect CO$_2$-emissions. Direct emissions result from energy sources used for heating plants and indirect emissions are caused due to the electricity demand for e.g. heat pumps and the electricity mix. Further details regarding the model can be found in the supplementary material.

2.2.1. Demand side - Building stock

The annual heat demand is derived from a detailed stock model of buildings and their respective energy demand. A detailed description of the data generation for the current status (2019) is provided in the supplementary material. Below, we outline the general structure of the model and introduce the relevant input data. The structure of the buildings classes as well as their data are based on Loga et al. (2015). One of the central units is the *energy supply* which is the energy content (TWh) of the energy carriers required to provide the *final heat demand*. The *energy supply* includes losses during conversion and distribution of energy (for example heat losses in district heating and/or within buildings) and the final consumption by end users.

Building classes

In the model, all residential homes are clustered into building-classes based on a detailed analysis of the current building stock in Germany conducted by Loga et al. (2015). Two characteristic values are considered: 1) the year of construction and 2) the building type (e.g. single-family or apartment houses). In total, this results in forty different building-classes. These building classes are not affected by an increase or decrease in average living space but the number of buildings can change.

Definition of living space

The living space refers to the living area in buildings and does not cover further usable areas. Moreover, only buildings with more living space than effective areas are counted. Other living arrangements like dormitories are included and counted as apartment buildings.

Energetic restoration

Following the structure of Loga et al. (2015), we distinguish between three categories regarding the restoration state: (1) *unrenovated*, (2) *standard*, and (3) the *ambitious restoration*. The *standard* restoration corresponds to current energy saving regulations (german:

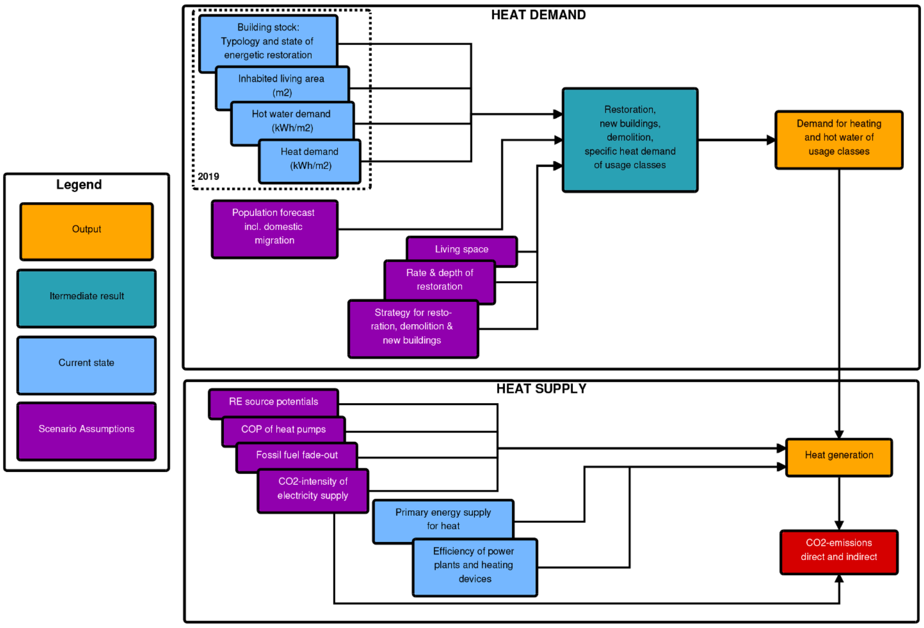


Fig. 1. Schematic illustration of the model and its supply/demand input data, scenario parameter and output.

Energieeinsparverordnung (EnEV), and since 2020 Gebäudeenergiengesetz (GEG)) and results in a reduced heat demand in the range of 59-129 kWh/m^2 depending on the type of house.The *ambitious restoration* corresponds to the so-called passive house standard and results in a reduced heat demand of 14-57 kWh/m^2. The specific measures and their effects are based on the detailed analysis of Loga et al. (2015, p.26-31). Combining the forty building-classes from above with the three restoration states leads to houndred twenty different building categories. Figure 2 provides an overview of the building-classes with their respective share of living space and their restoration state in 2019.

2.3. Supply side

The supply side model distributes the available potential of low-emission technologies to the respective heat demand. Main input parameters are the timeline for the fossil fuel based heating fade-out described in section 3 and the heat supply mix of renewable energies and heat pumps deployment. An overview of the 2019 energy mix and future supply assumptions is provided in Table 3 in the supplementary material.

3. Scenarios and future development

3.1. Shared assumptions

Parameters, which influence the heat sector but are not within the scope of the heat energy sector or policy measures of the building sector are equal for all scenarios. These are primarily the demographic development and the specific emissions of electricity which are described in the following.

Population

The demographic development has significant influence on the living space and therefore on the heat demand. In 2019, Germany had 83 million inhabitants (Destatis, 2020a). For 2050, 30 different forecast variants of the German Federal Statistical Office result in a range of 70.5-86.7 million inhabitants depending on different assumptions on birth rate, mortality and migration (Bundesamt). For all scenarios, we apply the arithmetic mean of all variants, which is 80.3 million in 2050.

Table 2

Overview of demand side scenario data. The restoration depth level I indicates *standard* and level II *ambitious* restoration.

	Year	Trend	Efficiency	Sufficiency	Combined
Living space (m^2)	2019	45.4	45.4	45.4	45.4
	2030	47.9	47.9	40.9	40.9
	2050	52.5	52.5	32.6	32.6
Restoration rate (%)	2019	1	1	1	1
	2030	1	2	1	2
	2050	1	2	1	2
Restoration depth level I/II (%)	2019	94/6	94/6	94/6	94/6
	2030	94/6	32/68	94/6	32/68
	2050	94/6	18/82	94/6	18/82
Demolition rate (%)	2019	0.05	0.05	0.05	0.05
	2030	$\geq$ 0.05	$\geq$ 0.1	$\geq$ 0	$\geq$ 0.05
	2050	$\geq$ 0.05	$\geq$ 0.1	$\geq$ 0	$\geq$ 0.05
Construction rate (%)	2019	0.6	0.6	0.6	0.6
	2030	$\geq$ 0.6	$\geq$ 1.2	0	$\geq$ 0.6
	2050	$\geq$ 0.6	$\geq$ 1.2	0	$\geq$ 0.6
Average hot water demand (kWh/m_2)	2019	10.7	10.7	10.7	10.7
	2030	11.1	11.4	10.0	10.2
	2050	11.8	13.6	10.0	10.8

Emissions of the electricity sector

Due to an expected increase in the electrification rate of the heat supply (Agora, 2016), the specific electricity sector emissions have a significant impact on total emissions of the heat supply. As described in section 2.1, the electricity sector is expected to reduce emissions faster than all other sectors. Following the most ambitious scenario *Green-Supreme* from Purr et al. (2019), we assume a CO_2-neutral electricity supply in 2050. The reduction path for specific emissions from electricity starts at 435 kg CO_2/MWh_{el} in 2019, decreasing to 160 kg CO_2/MWh_{el} in 2030 and 53 kg CO_2/MWh_{el} in 2040 for the respective scenarios *Trend, Efficiency, Sufficiency and Combined*, which are described in the following. In this pathway, scenario specific assumptions on electrified heating demands are not considered.

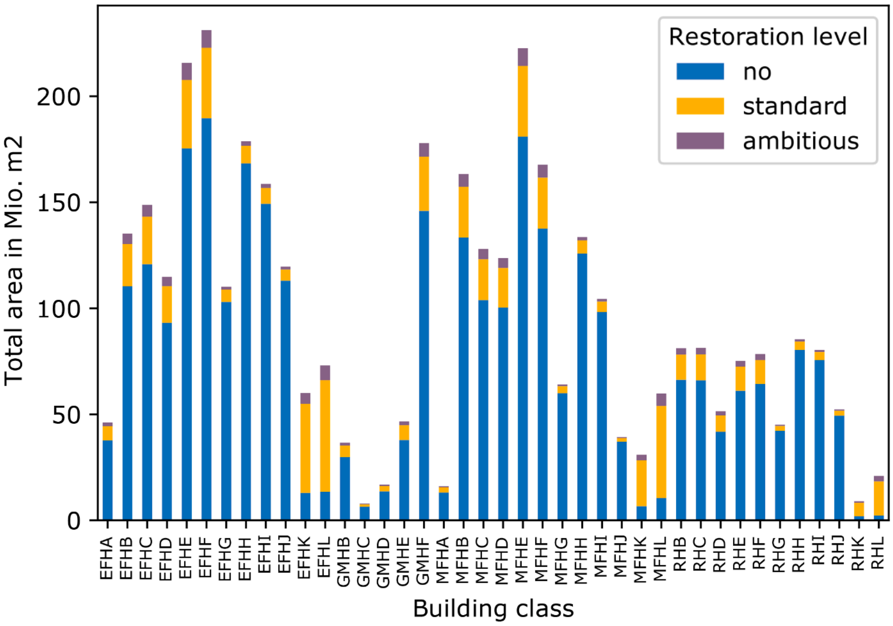


Fig. 2. Total living space per building class and restoration level in 2019 in Germany. Data based on Destatis (2019a); Jochum et al. (2015); Loga et al. (2015)

Table 3
Overview of supply side scenario parameter for starting year 2019, 2030 and 2050. Data in SEC column are used in *Sufficiency, Efficiency* and *Combined* scenario.

Energy supply	2019	2030 (Trend)	2050 (Trend)	2030 (SEC)	2050 (SEC)
Natural gas	266	194.6+	64.9+	0+	0+
Heating oil	126	-	-	-	-
Coal	19	8	-	-	-
Electric heater	24	-	-	-	-
Total conventional	435	202.6+	0+	0+	0+
Biomass	91.2	104.1	104.1	91.2	0
Other	12.6	12.6	12.6	12.6	12.6
Waste heat	-	-	-	3.0	8.3
Solar thermal	8.5	12.0	18.5	26.8	60
Geo thermal	0.6	2.1	3.4	8.9	24
Heat pump	14.7	25.2	44.3	41.2 +	950+
Total renewable	127.6	156	182.9	183.7	1054.9
Total	562	358.6	182.9+	183.7+	1054.9+

3.2. Scenarios

We investigate four main scenarios: *Trend, Efficiency, Sufficiency* and *Combined*. Each scenario comes with two different supply pathways, the *trend pathway* and the *progressive pathway*.

Within all scenarios, the following input parameters vary on the demand side:

- Average living space per person (m^2)
- Energetic restoration rate and depth of restoration
- Rate of construction
- Hot water demand

On the supply side, the following input parameters vary:

- Timeline of fossil fuel fade-out and electric heaters
- Potential of renewable energies
- Expansion rates of renewable energies and heat pumps

Table 2 and Table 3 provide a detailed overview of all scenario parameters for the demand and supply side.

Trend scenario

This scenario extrapolates recent developments in the heating sector. The rate of energetic restoration stays at the current rate of 1 % (Singhal and Stede, 2019). For the depth of restoration, we apply a split of 6% (*ambitious*) and 94 % (*standard*) based on Jochum et al. (2015). These rates are assumed to stay at the same level until 2050. The average living space per person follows the assumptions of the GreenEe scenario (Purr et al. , 2019). The average living space has increased in the past and amounts to 45.4 m^2/person in 2019 (own calculation based on Destatis (2020a,b); Purr et al. (2019)). According to Purr et al. (2019) it is assumed to increas to an average of 49-56 m^2/person in 2050. We use the average value of 52.5 m^2 for the *Trend* scenario. Demolition and construction take place continuing historic trends: Between 2010 to 2018, on average 0,05% living space of the building stock was demolished each year (Destatis, 2019b, p.22). In the same period the growth rate of living space in new buildings was on average 0.6%. (Destatis, 2019a). In case of energetic restoration, the specific hot water demand (kWh/m^2) in the vast majority increases due the correction factor, which takes the behaviour into account (Loga et al., 2015). Currently, the specific hot water demand in Germany for the different building-classes ranges from 6.3 to 17.6 kWh/m^2, in case of one and two family buildings between 6.3 and 14.2 kWh/m^2 and in case of apartment buildings between 9.6 to 17.6 kWh/m^2(non-renovated). In the *Trend* scenario, the specific hot water demand depends only on restoration level and building class. Regarding the supply side, a fade-out of fossil fuels with a linear trend is applied (oil until 2030, coal until 2038 and natural gas until 2060). Due to a lower efficiency of electric heater units compared to heat pumps we assume a fade-out until 2030. The development of renewable energies follows the trend of the last ten years except for biomass. Due to growing concern about biomass scarcity, we assume a slower increase following the trend between 2014 and 2019 until 2030 and a constant annual potential until 2050. The analysis of historic trends are based on data from AGEE-Stat (2020) and are further described in the supplementary material.

The described development of heat-supply does not necessarily cover the heat demand of the investigated scenarios. In this case, the gap can be filled with natural gas or with heat pump units. Within the *Trend* scenario, natural gas is used, while within all other scenarios additional heat pumps are assumed to fill the gap.

Efficiency scenario

In this scenario, the rate for energetic restoration is significantly higher, but demolition and living space per person are the same as in the *Trend* scenario. In accordance with the German government targets, we assume a doubling of the energetic restoration rate from currently 1 to 2 % p.a. (Bundesregierung, 2020). From 2019 to 2030 we apply a linear increase from 1 to 2 % p.a. and a constant rate of 2 % each year between 2030 and 2050. Regarding the depth of restoration we assume an increase of the *ambitious* share. In 2030 the share of *standard* restoration decreases to 32%, while the *ambitious* share increases to 68%. In 2050 only 18% of the restoration correspond to the *standard* and respectively 82% to the *ambitious* level. Between the years we applied a linear interpolation. These rates are in accordance with the *ambitious* scenario of Jochum et al. (2015). Rates for demolition are doubled compared to the *Trend* scenario to allow for an increased renewal of the building stock. As in the *Trend* scenario, the specific hot water demand depends on the restoration level it is higher than in the *Trend* scenario. Compared to the *Trend* scenario, the fade-out of oil, coal, gas and electric heaters is achieved earlier (natural gas until 2030, and the remaining units until 2026. The reduction is based on a linear reduction). The pathway for the progressive supply scenario is based on literature regarding potentials and expansion ratios described in section 2.3. As all technologies are mature, a back-casting approach with a linear increase is used to determine values before 2050 for the annual calculations. Biomass is an exception as the amount of heat is kept constant until 2030 and then declines until 2050. In 2050 the remaining Biomass is based on the amount of landfill gas and biogenic waste (namely ”Other”). The expansion rate for heat pumps is set to an annual increase of 17 %. In case of gap between supply and demand this will be filled additional marked heat pumps and for comparability also with additional natural gas.

Sufficiency scenario

In contrast to the *Trend* and the *Efficiency* scenario, the average living space per person decreases in the *Sufficiency* scenario. Fischer et al. (2016) state, that the living space can decline to 40 m^2/person in 2030 if appropriate measures are taken. For deriving an ambitious but still attainable target for our scenario, it is worth looking at current real-life examples of reduced living space. One example is the residential project Kalkbreite in Zurich. Their integrated concept of shared facilities and options of moving between differently sized flats within the project resulted in an average living space of 32.6 m^2 per person, including common areas (Kalkbreite, 2014). Within the *Sufficiency* scenario, this value is reached in 2050 by applying a linear interpolation from 45.4 m^2 in 2019 to 2050. This leads to a value of 40.8 m^2/person in 2030, being slightly higher as in the assumed living space per person in Fischer et al. (2016). For Germany, the per capita living space in the year 1990 amounted to 35 m^2 (Stieß et al., 2019). Restoration depth and rate are the same as in the *Trend* scenario. Demolition and construction are kept to a minimum, thus demolition only takes place in case of dilapidation and new construction in case of additional needed living space. In contrast to the *Efficiency* scenario, the *Sufficiency* scenario consequently reduces the resource intensity. For hot water demand, we also assume sufficiency measures to be applied. Purr et al. (2019) assume a reduction by 10 % until 2030 due to more showering instead of bathing, shorter showers, and a reduction of average hot water temperature by 2 °C. We follow this assumption until 2030 and assume that it will further decrease to 20 % until 2050. As a result, the hot water demand in 2050 is only slightly lower than in 2019, but around 20 % lower than in the *Efficiency* scenario. The assumptions of the supply-side, i.e. fade-out of fossil fuels, potentials of renewable energy are the same as in the *Efficiency* scenario.

Combined scenario

The *Combined* scenario combines the measures of the *Efficiency* and *Sufficiency* scenario. As shown in Table 2, energetic restoration rate and depth as well as living space of the *Efficiency* and the *Sufficiency* scenario are combined here. For new construction and demolition, the strategy from the *Trend* scenario is chosen, because it characterises the middle path between the *Efficiency* (strong renewal of the building stock) and *Sufficiency* strategy (reduce absolute energy service demand and resource intensity). Regarding hot water demand, the efficiency reduction potential by energetic restoration as well as the reduction by behavioural change are applied. The supply side assumptions are the same as in the *Efficiency* and the *Sufficiency* scenario.

4. Results

In the following section, we first present the results for a carbon budget for the heating sector. Subsequently, cumulative emissions within all scenarios are outlined. Finally, the supply and demand structure, as well as the temporal development, are explored in detail.

4.1. *Carbon budget for the German heat sector*

Based on the methods described in section 2.1, the German budget ranges from 5,385 to 9,257 Mio. ton CO_2 (see Table 4).

The resulting budgets from 2020 for space heating and hot water demand of households in Germany range from 747.5 to 1505.4 Mio.ton CO_2 (see Table 5). This includes direct as well as indirect emissions.

4.2. *Cumulative emissions*

Figure 3 shows the cumulative CO_2-emissions for each scenario and the different carbon budgets. Two different pathways are shown for each scenario. In the *hp+* pathway, heat pump instalments are expanded to meet the remaining demand, which cannot be covered by renewable energy sources or the scenario's pre-defined heat pump expansion rate. In contrast, within the *gas+* scenario, natural gas is used to fill this gap.

The results show that without further measures (i.e. *Trend* scenario), cumulative emissions exceed the budgets regardless of their allocation method. Furthermore the results show that expanding natural gas (gp+) instead of heat pumps (hp+) increases the CO_2-emissions significantly. Without sufficiency measures the CO_2-emissions exceed even the carbon budget with grandfathering distribution. In addition, cumulative emissions in all scenarios exceed the *per capita* budget, which is considered to be the most preferable under fairness aspects. Even the most ambitious scenario (*Combined* scenario with heat pump pathway) results in cumulative CO_2-emissions of about 848 Mio. tons. Out of these, 728 Mio. tons are caused by fossil fuels and 120 Mio. tons by heat pumps. The latter depends on the renewable energy mix of the electricity sector and would consequently increase with a lower share of renewable energies in the electricity mix.

Table 4
German CO_2 budget for three different allocation methods. Own calculation based on World population (Nations, 2019), German population (Destatis, 2020a), World emissions 2017 (IPCC, 2018), German emissions 2017 (Umweltbundesamt, 2020b), Share for the Contraction & convergence method (Gignac and Matthews, 2015)

	Share (%)	**CO_2 budget (Mio. t)**
Equal per capita	1.09	5,385
Contraction & convergence	1.50	7,425
Grandfathering	1.87	9,251

Table 5
CO_2 budget for Germany 2018 and for 2020 reduced by 2018/2019 emissions. Breakdown proportionally to 2018 emission share for space heating, own calculation based on data from Umweltbundesamt (2020b) and Umweltbundesamt (2018b). The data for space heating and hot water include direct and indirect emissions and are temperature adjusted.

	Germany	Space heating	Hot water	Sum
Emissions 2015 (Mio t)	795.8	128.8	26.4	155.2
Share 2015 (%)	100	16.2	3.3	19.5
Budget from 2018				
per capita (Mio t)	5,385			*1050.2*
Contraction & convergence (Mio t)	7425			*1448.1*
grandfathering (Mio t)	9271.3			*1808.1*
Budget from 2020				
per capita (Mio t)				*747.5*
Contraction & convergence (Mio t)				*1145.3*
grandfathering (Mio t)				*1505.4*

The two different pathways (hp+ and gas+) show that extending the application of natural gas instead of heat pumps makes a decisive difference in every scenario. In the *Combined* scenario CO_2-emissions can be reduced by around 34 % compared to a gas+ pathway. This may lead to a conflict between the carbon budget and techno-economic aspects. Furthermore, the results show, that a lower demand has a decreasing impact on CO_2-emissions with a gas+ pathway. In case of the *Combined* scenario CO_2-emissions decrease by 405 Mio. tons compared to the *Efficiency* scenario. Within the three reduction scenarios, emissions almost stop increasing (less than 5 % of the CO_2-emissions in 2020) between 2035 (*Combined* scenario and hp+) and 2041 (*Efficiency* scenario and gas+). Notably, this supply-side effect is caused by the fade-out of fossil fuels, decreasing specific CO_2-emissions of electrical energy, and hence lower CO_2-emissions of heat pumps. Consequently, all efforts made after these years have a minor contribution to the budget. These results point to the importance of CO_2-neutrality in the heating sector 10 to 15 years before 2050.

Interestingly, cumulative emissions of three reduction scenarios are in a small range of 848 to 923 Mio. tons CO_2 for the hp+ pathway. For the gas+ pathway, emissions are in a wider range of 1,283 to 1,689 Mio. ton CO_2. However, it is crucial to understand the economic, technical, ecological and social implications of different measures in each scenario that lead to these results. These issues will be addressed in the following sections.

4.3. *Heat demand and building stock development*

Although the heat demand decreases within all scenarios, final levels differ significantly as shown in Figure 4. The highest final heat demand of 441 TWh/a in 2050 can be observed in the *Trend* scenario. Additional reduction measures in the *Efficiency* and *Sufficiency* scenario lead to a final heat demand of 326 TWh/a and 258 TWh/a respectively in 2050. Their combination, namely the *Combined* scenario, leads to a further reduction resulting in 136 TWh/a in 2050.

The total reduction is mainly caused by the reduced area of total living space (sufficiency measure) as well as the effort of energetic modernisation (efficiency measure), which is achieved through restoration or replacement of old buildings by new ones. The increased living space in the *Trend* and *Efficiency* scenario requires more new buildings

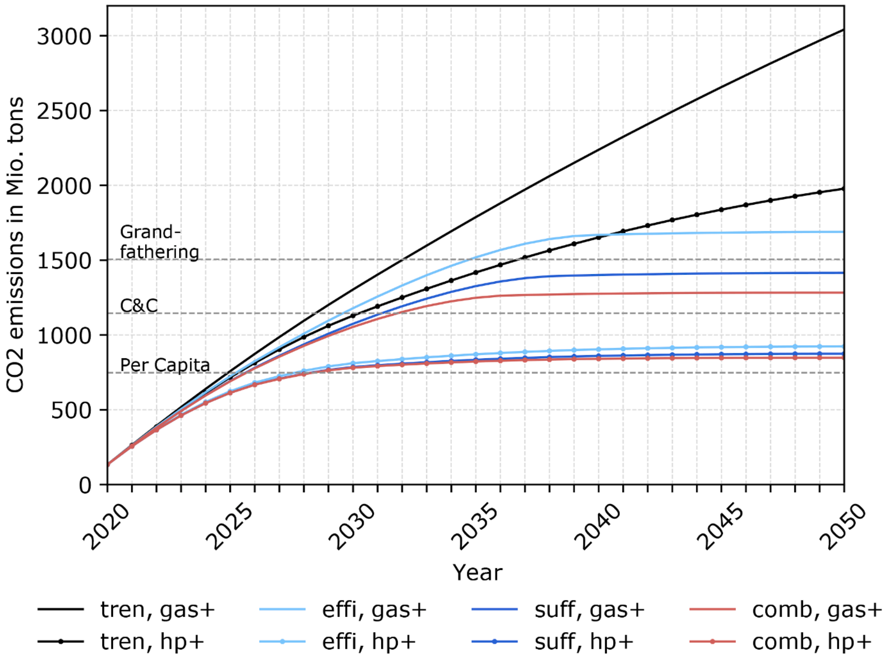


Fig. 3. Resulting cumulative emissions of the four scenarios (lines) facing the three different total budgets (dashed lines) derived for the German housing heating sector.

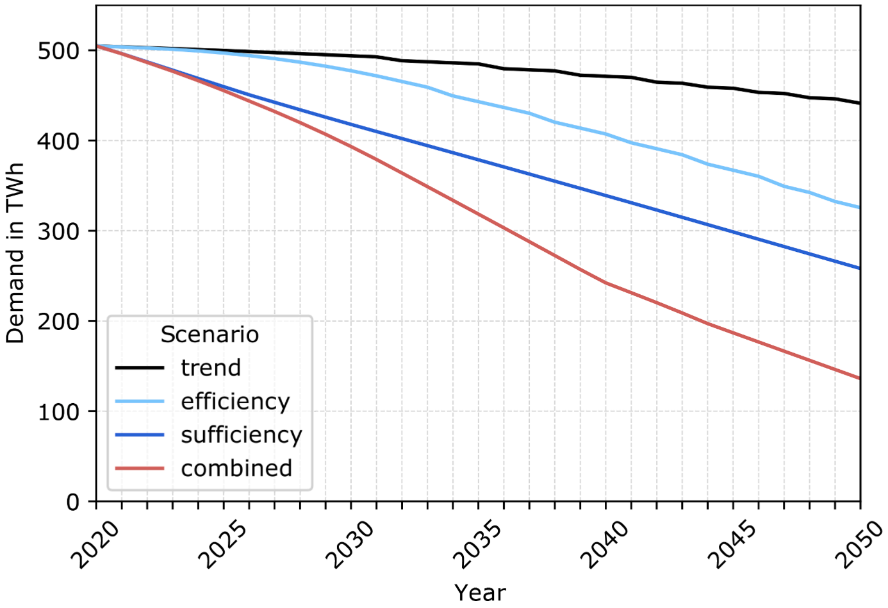


Fig. 4. Resulting yearly German housing heat demand for the four main scenarios.

than the two other scenarios. Therefore, scenarios differ significantly with regard to the building stock. In the *Trend* scenario an area of 1,839 Mio. m^2 has to be modernised. In the *Efficiency* scenario modernised living space amounts to 2,695 Mio. m^2. The *Combined* scenario with the lowest emissions requires 2,667 Mio. m^2 of modernised living space. The *Sufficiency* scenario stands out with the lowest amount of modernised living space of only 1301 Mio. m^2.

An early reduction of living space in the *Sufficiency* and *Combined* scenario leads to a significant faster decrease of the heat demand compared to the other scenarios due to the reduction of living space and corresponding faster energetic modernisation of the building stock.

The effect of the energetic modernisation is being revealed by comparing *Trend* and *Efficiency* scenario, respectively the *Sufficiency* and *Combined* scenario. In comparison with the living space reduction (see Figure 4) the effect occurs later due to the small increase of restoration rates. Overall, reductions of living space, new buildings and additional restorations after 2035 have a minor impact. This result implies that a fully restored building stock and a reduction of average living space down to 32.6 m^2 is not necessary to limit global warming to 1.5 °C, if a progressive pathway is pursued. Instead, a fast implementation of the measures has a significant impact on the the CO_2-emissions.

The hot water demand plays a minor role within the scenarios. It slightly increases from 40.6 TWh (2019) to 50 TWh in the *Trend* and to 54 TWh in the *Efficiency* scenario. Within the *Sufficiency* and in the *Combined* scenario hot water demand declines to 27 TWh and 28 TWh, respectively.

4.4. Heat supply

The heat supply mix for each scenario and every year are shown in Figure 5.

In the *Trend* scenario, the majority of heat is supplied by natural gas. In contrast, within the other three scenarios heat pumps provide the majority of the heat. The absolute level of renewable energy supply is similar in all scenarios. However, in the *Trend* scenario, the renewable energy supply is mainly provided with biomass. In contrast, biomass is reduced strongly in the other three scenarios and solar thermal and geothermal energy increases. For these three scenarios, the heat pump supply differs clearly in 2050 and around the year 2030. Therefore, we provide an analysis of the heat pump supply below.

Figure 6 shows the resulting heat pump electricity consumption and heat supply in the *Combined* scenario.

The annual expansion rate of heat pumps varies between 272 % and -7 % in 2020 to 2035 (average 22.5 %) and lasts until 2031, where the average annual growth amounts to 24.8 TWh/a. Compared to the *Efficiency* scenario this is 8.5 TWh/a less. This seems to be very ambitious since the required annual expansion correspond to 178 % of the total heat supplied by heat pumps in 2019. Moreover the highest expansions arise in the earliest years, which require a fast increase of production and installation capacities. In 2031 more than 71 % of the heat demand is covered by heat pumps, which corresponds to 267 TWh supplied heat. After 2031 the heat supplied by heat pumps decreases strongly - until 2050 by 83 %. This is caused by the decreasing heat demand and an increase of renewable energies. In addition to high expansion rates, heat pumps have to be applied in building-classes with the highest specific heat demand which is not desirable from an economic perspective as these buildings require high heat transfers and installations of floor-heating (Jochum et al., 2017).

On the electricity side, the highest consumption occurs in 2031 with up to over 65 TWh/a. Still this is 22 TWh/a less than in the *Efficiency* scenario, but for example more than 29 TWh/a within the scenario C of the German Grid Development Plan, which even cover all sectors (NEP, 2019).

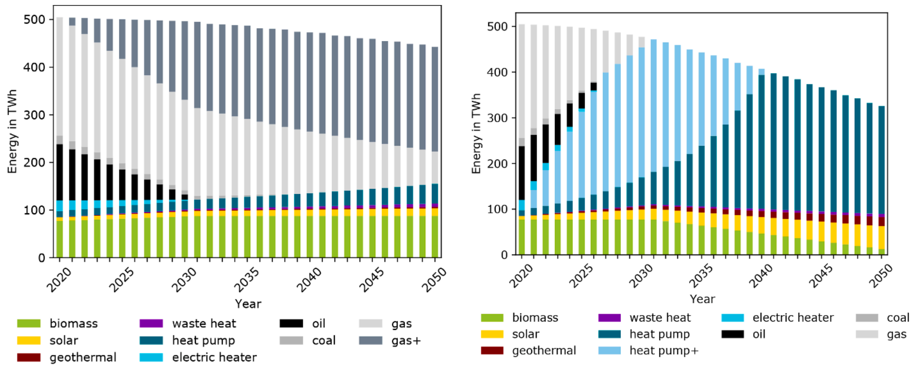
4.5. Further emission reductions

Since none of the modelled scenarios stays within the per capita carbon budget, we investigate the effect of further CO_2 reduction measures. We analyse the impact of six measures, five on the demand side and one on the supply side, as well as the combination of the demand-side measures and a combination all of these six measures.

1. Hot water reduction (demand): linear decrease from 2020 to 2030 to -20 %.
2. Higher restoration depth (demand): Linear increase of the ambitious share up to 100 % in 2030.
3. Higher restoration rate (demand): 3 % in 2030.
4. Space heating temperature reduction (demand): Reduction of average room temperature by 2 °C.
5. Earlier living space reduction (demand): Reduced average living space already reached ten years earlier compared to the Sufficiency and the Combined scenario.
6. Earlier renewable energy (supply): The renewable potential exploited to the maximum 2030 instead of 2050, constant until 2050.

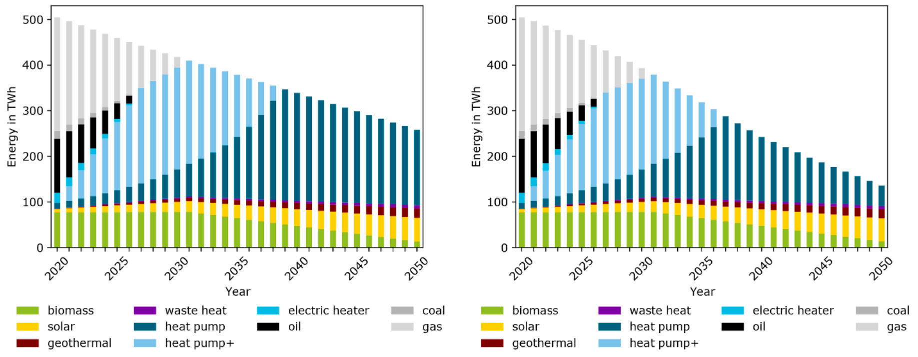
In Figure 7, the emission reduction of these measures in comparison to the *Combined* scenario is visualised. All measures result in a reduction of the CO_2-emissions, and a reduced power demand for heat pumps (2030).

An increased restoration depth and a further hot water demand reduction have the lowest impact, with both less than 2.2 % reduction of emissions. A higher restoration rate of 3 % has a slightly higher impact by reducing the CO_2-emissions by 1.1 % and the electricity demand for



(a) Trend scenario

(b) Efficiency scenario



(c) Sufficiency scenario

(d) Combined scenario

Fig. 5. Heat supply structure and temporal development within different scenarios.

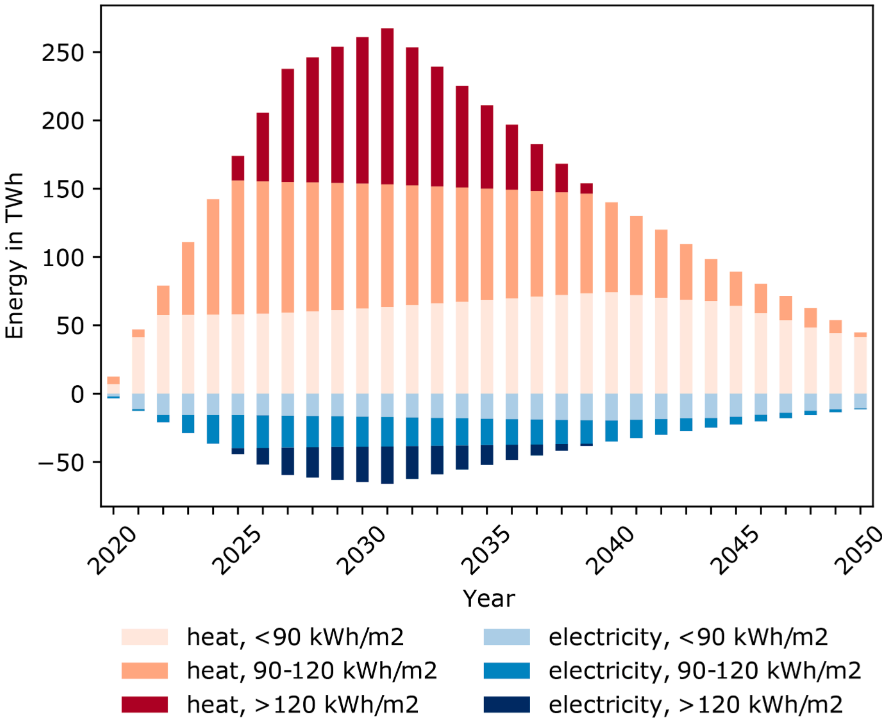


Fig. 6. Heat supplied by heat pumps in the *Combined* scenario in case of un-restricting expansion of heat pumps. The reddish bars (positive) show the final heat demand covered by heat pumps for the different classes of energetic restoration levels. The bluish bars (negative) display the electricity required to supply the respective heat.

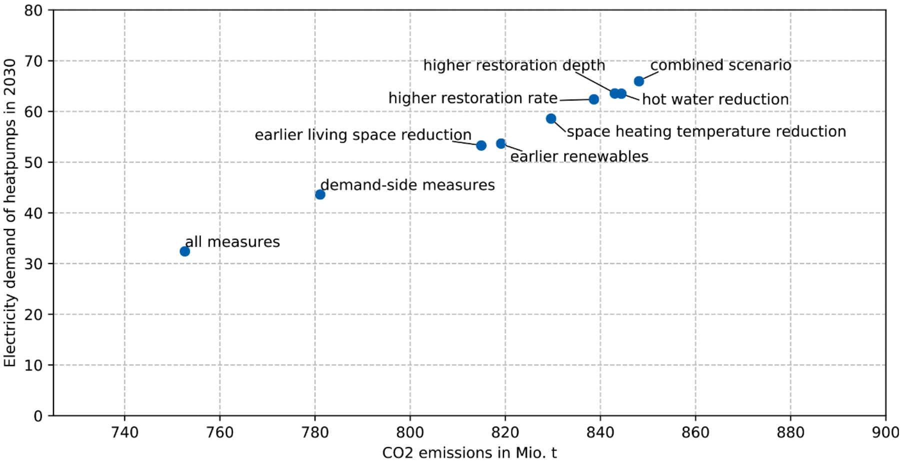


Fig. 7. Cumulative CO_2-emissions until 2050 and heat pump electricity demand in 2030 for additional selected measures.

heat pumps by 5.4 %. The decrease in space heating temperature by 2 °C contributes a reduction of 2.2% and relaxes the heat pump electricity demand by 11.2%. The most effective of the investigated measures are an earlier reduction of the living space and faster renewable expansion with an emission reduction of 3.9 % and 3.4 % respectively and a reduction of the electricity demand of 19 %. This clearly emphasises the importance of early and fast action of emission reduction targeting both - the demand as well as the supply side.

All of the described measures combine the advantage of lowering emissions and the benefit of lowering heat pump electricity demand during the transition around the year 2030 by either reducing the absolute demand or replacing heat pump supply with renewable energy. Though, none of the investigated measures alone is adequate to push emissions below the *per capita* budget of 750 Mio. tons. Only their combination yields emissions close to this value (753 Mio. tons). Further, the combination of all measures reduces the electricity demand by 51 %.

5. Discussion

We show that, staying within the derived heating sector carbon budget with a per capita allocation, cannot be achieved within any of the modelled scenarios. However, a carbon budget close to the per capita distribution can be achieved by a fast fade-out of fossil fuels in combination with fast renewable energy and heat pump expansion as well as fast heat demand reductions. Without a massive expansion of heat pumps, that might go well beyond technical feasibility, only the scenarios with applied sufficiency measures allow to stay within the carbon budget in accordance with the grandfathering allocation. The technical limitation is indicated by our scenario assumptions. Efficiency and consistency measures have been extended to an ambitious level. This is underlined by expansion as well as restoration rates that are both higher than the trend of last years. The successful transition of the residential German heating sector within the carbon budget limiting global warming to 1.5 °C holds challenges on the technical as well as on the policy and social level. These are further discussed in the following section.

5.1. Technical challenges and sufficiency as a social solution

Restoration rates are challenged by restricted economic resources and capacities within the building industry. In addition, toady's insulation materials are also criticised from a sustainability perspective. As these challenges exist, sufficiency can help on multiple levels. With a reduced living space, less buildings need to be rehabilitated and less new buildings have to be build. This can free capacities for the remaining building stock to be rehabilitated in the required time and consumes less materials. Further, reduced living space leads to additional head demand reductions.

High expansion of heat pumps are challenging but necessary for reducing CO_2-emissions. Expansion causes a significant additional electricity demand peaking the the 2030's which puts additional pressure on the electricity system transformation to provide electricity with low or zero CO_2-emissions. In addition, the grid infrastructure also needs to be capable of dealing with further loads in the low voltage grid (Rippel et al., 2019).

Another problem with regard to the transformation and heat pumps is revealed by our results. Built heat pump units up to 2030 are not required 20 years later (2050) when the building stock transition (restoration etc.) is completed. This transition constitutes a problem which needs to be investigated in depth. Beside the positive effect of the demand reduction possible solution might be the expansion of biomass usage until 2035/2040 to bridge the gap. If biomass is available for this purpose must be analysed in an integrated investigation with other sectors.

Again, sufficiency as a social solution can help rendering the transition successful as scenarios with sufficiency measures require the least amount heat pumps.

5.2. Policy challenges

5.2.1. Sufficiency policy

The reduction of living space demonstrates its effectiveness within our study. To counteract current developments of increased living space, policies and social innovations must be investigated and implemented. Despite their high climate protection impact sufficiency measures are underrepresented within the scientific and policy discussion.

Dubois et al. (2019) states that voluntary measures are not sufficient, but households need a regulatory framework supporting their behavioural changes. Analyses have investigated exemplary measures and their estimated effects in the areas of living, transport and nutrition (see Fischer et al. (2016)). Nevertheless, further research is required regarding political measures for sufficiency, including their respective effects on behaviour and as a consequences energy demand. This research need does not only include the heating sector but all sectors.

5.2.2. Carbon neutrality vs. carbon budget goals

Our findings are linked to a more general political challenge. Current policies in Germany and other countries focus on specific target years for CO_2-neutrality instead of a carbon budget approach. Based on our analysis, the target year for CO_2-neutrality is located in the the 2030's (for example, in the *Combined* scenario in 2035). In contrast, when CO_2-neutrality is reached in 2045, which is the new target year in Germany, following a linear reduction, the CO_2-emissions would even be higher than the carbon budget with a grandfathering distribution. Therefore, the target year approach may lead to policies falling short of the political goals. Thus we show that the current German goals in regards to the domestic heating sector do not comply with the Paris Agreement.

5.3. Model limitations

Energy system modelling can be undertaken with simulation and/or optimisation methods; both have their advantages (Lund et al., 2017). Although an optimisation approach would provided solutions from a cost-optimal point of view, certain characteristics of the approach deterred us from applying it. First of all, when combining efficiency, consistency and sufficiency measures, behavioural changes such as living in reduced space or heating less have no cost from a monetary perspective and would therefore be chosen first by a cost-minimising model. Secondly, multiple near-optimal solutions with various combinations of technologies may exist. In contrast, the simulation approach illustrates differences between efficiency and sufficiency strategies and the general difficulty to remain within the carbon budget.

The model can be improved by linking it to an electricity system model and/or increasing the temporal as well as the regional resolution of the model. This would provide more accurate values for specific CO_2-emissions associated with the electricity consumption of heat pumps. However, a more detailed model would introduce additional mathematical constraints and therefore deliver results even more challenging with regard to the carbon budget. Hence, improvements which help to understand dynamics and effects better, are not likely to change the general message of our findings.

6. Conclusion and policy implications

Our results reveal the challenges regarding a household heating sector transformation and the urgency for political action. Relying on technical measures of renewable energy expansion and energetic restoration are not sufficient to limit global warming to 1.5 °C. The reasons are the limited renewable energy potential in the heating sector and infeasible rates of restoration as well as heat pump expansion that would be necessary to keep the emissions within the budget. Therefore, sufficiency measures are important to add to the policy agenda. It is surprising to see that these measure do not play a role in current policy making, although they come with a huge climate protection potential. At the same time these measures come with additional environmental benefits due to an overall lower resource consumption for restoration and new buildings. Based on the presented results, we provide the following policy recommendations.

Policy recommendations

- Foster and accelerate technical measures on the demand and supply side. This includes accelerating heat pump expansion. In particular in buildings with a heating demand of less than 120 kWh/m^2. Renewable energy sources, particularly solar and geo-thermal, have to be promoted. In addition, increasing restoration rates have to be established.
- Plan faster fade-out of fossil fuels, which comply with the carbon budget.
- Complement these measures by sufficiency measures to stop and even convert the process of increasing living space per person. Since a fast change is required, measures should be placed on a structure level by policy regulations and incentives.
- Push the renewable energy expansion in the electricity sector as the decarbonisation of the heat supply strongly depends on clean electricity.
- Establish transition thinking and a transition culture. While a CO_2-neutral heating sector in 2050 is comparatively easy to achieve, main challenges are posed by the transition phase.
- Replace CO_2-neutrality goals by carbon budget goals to derive political agendas and regulations.

CRediT authorship contribution statement

Luisa Cordroch: Conceptualization, Methodology, Formal analysis, Investigation, Data curation, Writing – original draft, Writing – review & editing. **Simon Hilpert:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing, Visualization. **Frauke Wiese:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing.

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Supplementary material

Supplementary material associated with this article can be found, in the online version, at 10.1016/j.techfore.2021.121313

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Part III - Connecting the Dots

10

Synthesis

Energy system analysis (ESA) approaches are indispensable for shaping sustainable energy systems. Chapter 2 shows that, in the light of climate change, the domain of ESA is affected by energy system transformation, energy market liberalisation, and a profound scientific transformation. The challenges in the field of ESA, caused by these three transformations, have been reviewed and categorised in Chapter 3.2 into five important groups: *(1) complexity, (2) scientific standards, (3) utilisation, (4) interdisciplinary modelling, and (5) uncertainty.* It is clear, that a single thesis, piece of software or approach can not resolve all aspects associated with these five challenges, as endeavours from the whole scientific community are required. The presented work, with its development and application of open ESA approaches, is part of this collective effort. It aims to address the challenges categorised as different dimensions and highlighted in green in Table 10.1.

Table 10.1: Categorised energy system modelling challenges based on the publication in Chapter 3 (Wiese et al. 2018).

Challenge	**Dimensions**
Complicacy[a]	increasing sector coupling, high technical, temporal and regional resolution required, extensive input data preprocessing, extensive result data processing
Uncertainty	epistemic, aleatory, linguistic, decision, planning
Interdisciplinary Modelling	inclusion of the human dimension, energy-water-food nexus, common transdisciplinary understanding
Scientific Standards	transparency, repeatability, reproducibility, scrutiny, scientific progress
Utilisation	usability, applicability, re-usability, result communication

[a] The challenge has been renamed from complexity to complicacy.

In this chapter, important contributions from the publications in Part 2 are summarised and critically evaluated to show how challenges have been addressed, which open issues remain, and where future research is required.

10.1 Terminological Ambiguity

It is important to start this first section of the synthesis with a short discussion about language as it has become evident that the language we use shapes how we think about the world (Boroditsky 2012). Therefore, scientists need to be clear about their language to be able to grasp a problem and correctly frame an answer.

Complex or Complicated?

Energy systems are often described as complex. Their complex character is rooted in social, political, economical and technical dimensions as described in Chapter 2. Therefore, from a broader perspective, all challenges listed in Table 10.1 are in one way or the other associated with complexity. However, in the literature on energy system modelling challenges, the term complexity often refers to the technical dimension of the system which means the increasingly distributed and less controllable, i.e. volatile, supply units as well as more interdependent elements beyond sectoral boundaries. The perspective is taken by Pfenninger et al. (2014, p. 79), who associate complexity with a problem of scale, i.e. trying to model (technical) systems with higher temporal and spatial granularity and a greater geographical scope at the same time. Similar conceptualisations can be found in reviews of energy system modelling software by Prina et al. (2020b) and Lopion et al. (2018). Complexity, in this technical sense, is also used in studies trying to address problems of scale, e.g trying to reduce the number of time-steps with acceptable losses in accuracy (Ludig et al. 2011; Frew and Jacobson 2016; Nahmmacher et al. 2016). However, complexity as described by authors such as (Bale et al. 2015), is not a quantitative characteristic of scale. Therefore, the problem of scale is not so much a challenge of complexity even though it clearly poses a challenge for modelling.

In summary, all of the challenges listed in Table 10.1 are rooted within the complex character of energy systems. Hence, it seems reasonable to use a term which is better suited to represent the quantitative complicated nature of the challenge often referred to as complexity. The correct terminology can help to acknowledge existing complexity in all, but particularly in social, political and economic dimensions and allows for appropriate coping strategies to be found. As Bale et al. (2015, p. 157) point out, this includes understanding challenges at the interface of technology and behaviour.

Apples and Oranges

Ambiguous terminology, associated with linguistic uncertainty, is closely linked to decision and planning uncertainty as misconceptions can cause incorrect interpretations of model-based analyses.[1]

To reduce decision and planning uncertainty, energy system modelling software has been reviewed by different authors to identify weak spots and help modellers as well as decision makers to select the appropriate tools. However, any imprecision with regard to terminology can lead to comparing "apples with oranges" within these reviews, which is part of the linguistic uncertainty described in Chapter 3 *A qualitative evaluation approach for energy system modelling frameworks.* This work fills a conceptual gap related to the unclear terminology of modelling software, which in turn causes problems for the scientific comparison of modelling tools. The conceptual distinction between the terms *model, model generator* and *framework* is presented in Chapter 4 to delineate oemof's approach from existing modelling tools. Terminological ambiguity with regard to these three terms and their underlying concepts can be found in a series of general energy system modelling reviews (Hall and Buckley 2016; Bhattacharyya and Timilsina 2010; Savvidis et al. 2019; Prina et al. 2020b) but also within reviews dealing explicitly with open source tools, such as Groissböck (2019) and Oberle and Elsland (2019). Within this thesis, it is argued that the fundamental differences between models, model generators and frameworks play an important role and must be recognised in scientific reviews of modelling software. The argumentation is provided in Section 2.3.2, where models are described as concrete representations of real-world systems with a specific regional focus and temporal resolution, which can be built using model generators. In contrast, modelling frameworks are defined as structured tool-boxes including sub-frameworks and model generators, as well as specific models.

While some authors may prefer other terms, they should always keep in mind the different concepts behind them and explicitly describe the applied terminology.

10.2 Development and Application

A major part of this thesis is the development of the Open Energy Modelling Framework (oemof) described in Chapter 4.

The framework has been collaboratively developed, designed and implemented for flexible, transparent and reproducible modelling of sustainable energy systems at different levels of abstraction (international, national, local, power-plant level). To achieve this, a generic graph-based concept has been developed, which allows for the separation of the topological description of the system (What are the system boundaries? What elements exist? How are the elements connected?) from its mathematical computation (optimisation, simulation, etc.). Based on this generic concept, a Mixed Integer Linear Programming (MILP) bottom-up model generator oemof-solph (Chapter 5) has been

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[1] This is for example reflected in the discussion about the IEA annual energy outlook (AEO). Gilbert and Sovacool (2016), criticised the authors of the AEO for underestimating renewable energy generation. In a response, Daniels and Namovicz (2016) answer that the critics misconstrue the AEO projections as forecasts leading to incorrect and misleading results.

implemented, which allows users to model economic dispatch, investment optimisation and unit commitment problems. The library also includes DC-approximation based on the linear optimal power flow (LOPF) method[2].

Facilitating Transparency and Reproducibility

Open, i.e. transparent and reproducible, modelling of sector-coupled renewable energy based systems with high technical detail was a central motivation for the development of oemof.

Open source code is an important prerequisite for transparency, which in turn is the foundation for reproducibility. This requires extensive user and developer documentation as well as transparent discussions about past and future developments of the software. All of these points have been considered in the development of oemof and have been implemented as described in Chapter 4. However, open source code and good documentation makes software accessible but not necessarily comprehensible. Good software design plays a crucial role in enabling transparency and reproducibility. The difference between open accessibility and comprehensibility is part of the problem described as practical versus theoretical in Chapter 6. Practical transparency refers to the idea that the software and method must be comprehensible in a reasonable amount of time. Considering this idea, the goal of oemof-solph to represent energy systems of different abstraction levels comes with a drawback. Internally, the software requires sophisticated functionalities to handle many interdependencies of possible system and component configurations. For the user, this internal logic is hidden (practically) within the software due to its complicated structure. This can lead to a gap between user assumptions about the functioning of a model and its actual resulting mathematical representation.

In acknowledgement of this problem, oemof-tabular, described in Chapter 6, has been developed. Oemof-tabular addresses issues of practical transparency and utilisation which were lacking in the model generator oemof-solph. These issues include the applicability, usability and re-usability of modelling software, which are associated with different roles (users, developers) in the modelling process, as described in Chapter 3. In the context of frameworks or model generators, users of the software are at the same time developers of a model. Applicability is then defined as the ease with which model developers can use a model generator or framework to build a model. Usability is the ease with which a sensitivity analysis can be conducted or different scenarios can be computed with a model, (possibly) created by another model developer. Re-usability can be understood as the ease with which a model or parts of the underlying framework can be adapted.

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[2] The future version of oemof-solph will additionally include a Multi-Period-Expansion model generator which has been contributed by external developers (Kochems 2022).

The oemof-tabular library applies the software concept of facades to reduce barriers on the user side and allows for the population of models with input data from tabular data such as friction-less Data Packages or spreadsheets (usability). Data Packages have been applied by other researchers in different energy open data projects for the distribution of data, as described in Section 2.4, but not as an input data format for models. The tabular input-data structure simplifies model creation (applicability) and enhances model (re-)usability. The facade concept with an interface limiting user options also helps to reduce the likelihood of false model and result interpretations. Better software utilisation of oemof-tabular improves the application of oemof in teaching and capacity building environments.

To allow for reproducible applications of the software, a workflow concept has been published along with the software, which can also be applied for other model generators (see Chapter 6).

The extension of oemof-tabular described within this thesis has not only been applied to research questions within this thesis, but has also been used by other developers to create a heat-specific oemof library, *oemof-thermal*. This library improves detailed technical modelling of sector-coupled energy systems and has, for example, been applied to assess storage options for cooling systems (Köhler et al. 2019) and CHP based heating systems (Wolf et al. 2019).

Collaborative Development

As described in Chapter 2, a trend towards Open Science changes scientific practices fundamentally. Open Science can be described as the new emerging mode of science were transparency and collaboratively developed knowledge is widely shared and accessible (Vicente-Saez and Martinez-Fuentes 2018, p. 434). In the field of ESA, DeCarolis et al. (2020) advocate greater distribution and collaboration in open modelling approaches.

Facilitating collaboration has been a goal for the design of the Open Energy Modelling Framework, described in Chapter 4 *The Open Energy Modelling Framework (oemof) — A new approach to facilitate open science in energy system modelling.* The modelling framework is not a loose connection of tools; they are all embedded within a conceptual framework implemented with common coding and development rules, documentation, meetings and decision making processes. Development of the software and bug reporting is transparently discussed on the collaboration platform. This collaborative concept of oemof is unique to the energy system modelling community. Most other modelling tools are developed by a few developers affiliated with one or two institutions. Many of these tools, such as PyPSA, calliope or OSeMOSYS, use forums for questions and allow external contributions via GitHub. However, they are not designed and organised as collaborative community projects. Nevertheless, the open source code of these software tools also offers the possibility of community-supported development structures emerging from them. This can be seen, for example, in the *PyPSA-meets-Africa* initiative, which is supported by a large number of scientific institutions (PyPSA-Africa 2022).

A major advantage of a collaborating community is knowledge preservation and dissemination. Today, science heavily depends on project-based funding with the consequence of limited work contracts for researchers. The resulting volatility in staff can cause the loss of knowledge within institutions and eventually even kill open source projects. In contrast, the community structure of oemof allows for the longevity of the project without being bound to one institution or work contract of users or developers.

The collaboration within the framework is based on the work and creativity of many scientists with diverse backgrounds. The evolution of different tools from these activities and their application highlights the effectiveness of collaboration and practical usability. This includes the bottom-up model generator library oemof-solph and the extension for oemof-tabular, which have been described in Chapter 5 and 6. Furthermore, the modelling framework includes data-driven approaches for demand profile calculations applied by Kouhia et al. (2019), a thermodynamic structural tool for thermal engineering developed by Witte and Tuschy (2020), data processing software for analysing storage operation (Witte and Kaldemeyer 2019) used in Chapter 7, and a tool to generate renewable energy supply time series based on re-analysis weather data (Krien et al. 2019).

Analysis of Sustainable Energy System Transformation

In this thesis, three different sustainable energy systems have been analysed. In two of them, a bottom-up optimisation approach applying oemof-tabular was followed. In the first system, the effects of decentralised heat pump flexibility in the German heat and electricity system were analysed with energy supply containing up to 100% renewable sources. In the second system, renewable energy expansion in Jordan was assessed under economic and environmental criteria. In the third analysis, a bottom-up simulation spreadsheet model was applied expanding beyond consistency and efficiency by including sufficiency. All three publications show the applicability of the open analysis approaches to relevant research questions of sector-coupled renewable energy systems.

The first publication in Chapter 7, *Effects of Decentral Heat Pump Operation on Electricity Storage Requirements in Germany*, applies a hybrid optimisation-simulation approach and shows that a flexible heat-pump operation in Germany can significantly reduce storage requirements. In particular, short-term storage units, in this case batteries, can be reduced by 42 to 65 % compared to the inflexible operation of heat pumps. An impact on long-term (hydrogen) storage units was only found for a 100% renewable system with a reduction of around 6.8%. Moreover, results agree with those from previous studies showing that only moderate investment in short-term storage is required and long-term storage is only required for shares of renewable energies approaching 100%.

The work presented in Chapter 8, *Analysis of cost-optimal renewable energy expansion for the near-term Jordanian electricity system*, focuses on storage modelling and optimised investment of renewable energy expansion, and highlights the cost-effective potential of CO_2-emission reduction in Jordan. For this study, an adaptable spreadsheet interface was developed and applied. The results show that when aiming for high energy independence, a combination of PV and wind with batteries and natural gas imports is economically preferable to the domestic shale-oil resource. Moreover, this solution is also environmentally superior due to the lower emissions compared to other analysed scenarios. Within the context of political and economic volatility experienced in Jordan, the benefits of open approaches which provide high adaptability and a re-usability potential is apparent as model-based study results can become outdated within a short period of time. This context makes open models which can be easily adapted and re-used of great importance for countries which would otherwise continue to depend on external knowledge and closed or poorly-documented models.

Apart from this thesis (peer-reviewed) literature on oemof-solph applications exists, which indicates that collaboratively developed software can deliver novel results and provide answers to relevant research questions of sector-coupled energy systems. The range of applications covers national to local energy systems. On a national level Maruf (2021) applies the model generator to analyse 100 % renewable sector-coupled energy systems in Germany. In addition, Arnhold et al. (2017) use the tool for the analysis of the energy and transportation sector in Germany. A multi-objective optimisation with high temporal and spatial resolution has been carried out for the Italian energy system by Prina et al. (2020a). On a local level, district heating systems have been modelled with a micro-economic revenue optimisation (Boysen et al. 2019; Wehkamp et al. 2020; Röder et al. 2021; Kersten et al. 2021). On a regional level, models for increasing transparency and participation, such as the Stakeholder Empowerment Tool (StEmp) (RLI 2018) and similarly an open model for the State of Schleswig-Holstein (openmod.sh) (Wingenbach et al. 2017) have been developed and applied. Finally, rural energy system designs in Nigeria have been optimised (Juanpera et al. 2020).

In addition to the described application of oemof-solph, a first attempt to expand purely techno-economic modelling approaches is provided in Chapter 9 of this thesis. The scenario analysis with an open source and bottom-up spreadsheet simulation model is technically less detailed with an aggregated representation of supply technologies and an annual resolution compared to the other two applications in Chapter 7 and 8. Regardless, it enables the generation of valuable insights into the transformation of the heating sector and the required policy measures by investigating a blind spot in the field of scenario analysis and techno-economic modelling, namely social solutions for social problems. Specifically, the role of sufficiency as a complement to efficiency and consistency measures in the German household heating sector transformation was analysed. Based on a scenario analysis, the following findings are presented: Current energy policies are not sufficient to comply with the 1.5 °C target. Even with highly ambitious restoration rates, staying within the limits of a 1.5 °C carbon-budget based on a fair international allocation, i.e. a per capita distribution, can not be achieved. Reasons for this are the limited renewable energy potentials in the heating sector in combination with restricted restoration rates in the building industry. With regard to the future use of biomass, it is clear that the amount of sustainably-produced biomass is limited. At the same time, there is strong competition for the use of biomass among energy-related industries, as it is a direct substitute for fossil fuels. For these two reasons, the scenarios in Chapter 9 assume that biomass in the heating sector decreases (linearly) from 2030 to 2050. However, the future use and process chains of biomass are not yet foreseeable. Using Lund et al.'s (2022) multiple technology conversion approach, biomass can thus, under certain circumstances, also play a role as a primary energy source in the heating sector after 2030. Nevertheless, the central conclusions of the presented analysis in Chapter 9 remain unaffected, since the cumulative emissions occur for the most part in the period before 2030: Consistency and efficiency strategies alone are not in themselves sufficient to meet the 1.5 °C target. Therefore, complementary sufficiency strategies should be developed and implemented to enable a sustainable transformation of the heating sector.

10.3 Limitations and Further Research

A critical evaluation of the presented work reveals some limitations which not only apply to oemof and its applications but can be generalised for many open modelling software projects.

Path dependency: The Programming Language

The modelling framework is implemented in the high-level programming language Python, which provides a set of various libraries, making it a general-purpose programming language (Nosrati 2011; Srinath 2017). The characteristics of Python as an open source and easy-to-use language for numerous available operating systems makes it a solid choice for a modelling framework such as oemof. However, as a dynamically typed language, it has one central disadvantage, which is the slow speed and comparatively large usage of computational resources. This problem is particularly relevant for model generators. Most model generators use algebraic modelling libraries such as Pyomo (Python) or JuMP (Julia). These separate problem creation and solving, which is carried out by external libraries. Therefore, the issues with respect to computational resources are not always about how difficult problems are to solve (e.g. non-linear mixed-integer programs) but the level of resources required to build the model, pass it to the solver and load back results. In recent years, a trend towards the use of the Julia modelling library JuMP can be observed in bottom-up model generator development. One reason is that model creation and transfer to the solver is significantly faster with JuMP than libraries such as Pyomo (Dunning et al. 2017, p. 310). This advantage is of high relevance for many energy system models based on Linear Programming which are comparatively easy to solve due to simple mathematical equations, but very large due to the high regional and temporal resolution. On the other hand, the advantage is less relevant for problems which are hard to solve, such as non-linear (mixed) integer optimisation issues of power-plants, but are smaller in size. Therefore, it may make sense for strategic reasons to concentrate resources for future oemof-solph developments on components and functionalities required for smaller local or regional energy systems with high technical detail.

Data Packages as a Model Input Format?

Data Packages provide a good way to distribute data under the FAIR data principles, which have been proposed by Wilkinson et al. (2016). However, when used as model input data, practicability can be hampered by the structure and requirements of Data Packages. First, data is located in different files and not combined in one file with multiple tables, as in spreadsheets. Second, meta-data needs to be provided in a correct format which matches with file names, column names and content type within the columns (e.g. numeric, string, etc.). Experience shows that creating these coherent Data Packages for multiple scenarios is prone to errors. As working with Data Packages and meta-data is not yet common for many modellers, debugging errors caused by invalid Data Package structure or syntax errors in the meta data file can take up a substantial amount of time. This is one reason why for the Jordanian energy system model described in Chapter 8, a spreadsheet interface was applied instead of Data Packages.

Requirements for valid Data Packages are designed to ensure consistent and re-usable data sets. However, in the case of model-specific input data, the question arises as to whether this data has to be directly re-usable and distributable. In most cases, the collected and prepared raw data, as well as processed result data, will be of greater interest for others. At these stages of the modelling process, Data Packages can be of great value. Data Packages containing cleaned raw data in a FAIR format can be converted with open-source scripts to create model-specific input data. Future developments on the software side, including automatised checking of Data Package validity and user-friendly error handling, may reduce the aforementioned hurdles.

Notwithstanding, the developed library oemof-tabular based on the facade concept with a tabular data structure is a useful extension to omeof-solph as it provides the possibility of spreadsheet applications, which have proven to simplify model creation and (re-)usability significantly.

Challenges and the Next Steps in Collaboration

Collaboration does not come with advantages by default. Internal discussions and associated decision-making processes can take up a significant amount of time and can slow development. Without these community processes, software may be developed significantly faster by individuals or small heterogeneous teams sharing similar objectives and ideas. Therefore, community projects need to carefully think about communication, roles, and decision making processes. As O'Reilly (1999) points out, for open source software development, "one of the areas of study is where the ideal boundary ought to be between a core product controlled by a single individual or small team and the input of the user community" (p. 37). To cope with this challenge, within the *oemof-cosmos* (see Chapter 4), different libraries were developed and maintained by independent developer teams.

Beyond this general challenge of collaboration, another point needs to be addressed in the future by the oemof community as well as other modellers to leverage open modelling approaches. Not only does software need to be developed in collaboration, but diverse teams working together on full research project life cycles are needed (DeCarolis et al. 2020, p. 2). An example of such an approach is the open energy outlook for the US (OEO 2021). In the case of oemof, tools and new model features have been developed in collaboration. However, the oemof community has not yet been able to work collaboratively on scenario development, data-set creation or the carrying out of studies with a common research agenda. Therefore, further effort should be put into networking with other open modelling projects and initiatives. This includes building stronger links to data projects such as SzenarienDB (Reder et al. 2020) or OPSD (Wiese et al. 2019). Moreover, building communities of practice similar to the OSeMOSYS project (Gardumi et al. 2018) will be important for the continuity of the project and the whole open modelling community.

The Limits of Software Solutions

In addition to transparency and reproducibility, the quality of research needs to be given to facilitate scientific progress. Huebner et al. (2021) proposes a tool which covers the three aspects of transparency, reproducibility and quality (TREQ). Source code publishing and (FAIR) data distribution are foundations for TREQ. However, pre-registration of analyses to avoid poor study design or manipulation, reporting guidelines to provide sufficient and relevant information, and pre-prints to address long delay times are also necessary (Huebner et al. 2021). The work presented in Chapters 4 and 6 provides necessary conditions for complying with scientific standards in energy research. However, sufficient conditions can not just be implemented with the software as they are part of complex social processes in the scientific community. Therefore, as with the challenges of uncertainties rooted in non-quantifiable sources (see below), further research is required on how TREQ can be supported on a practical level. This means, how researchers can be enabled to apply proposed workflows, best practices and tools to deliver high quality research. In addition to the domain-specific knowledge and competencies, scientists require additional skills in open scientific practices. Therefore, these new skills need to be part of (public) education in academic study programs. Moreover, applying these skills requires infrastructure and is time-consuming, which must be acknowledged by funding agencies who support open science ESA. With a new mode of science on the rise, these points are the next to be addressed.

Quantitative and Qualitative Aspects of Uncertainty

Uncertainty has been and remains a significant challenge for modellers. For many of them, uncertainty relates to the stochastic nature of processes. This type of uncertainty is not addressed within this thesis but should be considered for further improvement of the Open Energy Modelling Framework. Quantitative approaches, such as stochastic programming, to tackle aleatory uncertainty could be integrated within the developed framework and its existing libraries. The Pyomo package used for oemof-solph offers stochastic programming functionalities (Watson et al. 2012), which could be exploited. Another option is the quantitative method of modelling to generate alternatives (MGA), which was first proposed by Brill et al. (1982) and applied by DeCarolis et al. (2016) as well as Berntsen and Trutnevyte (2017) within the energy system context.

With regard to modelling, only a fraction of the uncertainties stem from stochastic processes within complex systems (aleatory) and can be tackled with quantitative modelling techniques such as stochastic programming. A large number of uncertainties are non-quantifiable (Sluijs et al. 2005). As described in Chapter 3, important sources of uncertainty are the missing knowledge about the (future) world (epistemic), its symbolic conceptualisation (linguistic), and interpretation (decision, planning). Methods which are capable of dealing with these qualitative aspects need to be applied within ESA to tackle uncertainty on a broader level. An example for these methods is the Numerical Unit Spread Assessment Pedigree (NUSAP) system proposed by Funtowicz and Ravetz (1990) and applied in energy research by e.g. Pye et al. (2018). Further research is required to assess how the application of qualitative methods can be supported within the ESA domain, which means overcoming the reduced techno-economic conception of energy systems and the resulting techno-economic quantitative modelling paradigm.

Returning to the Problem of Climate Change

There is an undeniably important human dimension to energy systems (Aronson and Stern 1984), which means that “energy transitions will be complex socio-technological transformations that require major changes for many communities” (Miller et al. 2013, p. 144). Hence, as described above, many limitations and challenges are associated with qualitative aspects and the complex social processes of energy systems. Many authors have identified and criticised the techno-economic and quantitative methodological focus of the physical science–dominated research field of ESA and recommend the inclusion of insights from the social sciences in energy system analysis and modelling (Pfenninger et al. 2014; Trutnevyte et al. 2019; Jefferson 2014; Sovacool et al. 2015). The fostering of interdisciplinary modelling and the inclusion of new perspectives are important future steps for the ESA domain.

However, with respect to modelling, it should be made clear that the problem of climate change will not be solved by complicated quantitative or qualitative models alone, appropriate policies are also required. As Roelfsema et al. (2020) show, currently-existing policies in many countries are insufficient to achieve the pledged contributions to CO_2 reduction. Despite technological advances, such as significant cost reductions in renewable energy technologies, and methodological advances in ESA with increasingly detailed models, environmental crises are worsening. Therefore, it is necessary to expand thinking not only beyond purely techno-economic quantitative methods but also beyond their corresponding sustainability strategies, such as renewable energy expansion and energy efficiency. The IPCC special report (2018) identified that changes in behaviour, such as the use of different consumption patterns or alternative modes of transport, are crucial aspects for effective climate change mitigation. The support of regulatory frameworks and the analysis of behavioural, cultural, and individual changes to identify appropriate policy options for incentives are nevertheless underrepresented in ESA.

In this thesis, a first attempt has been made to represent sufficiency measures, in addition to consistency and efficiency, in open ESA approaches. As the results show, sufficiency can play a crucial role with regard to sustainable energy transitions. This work thereby supports the findings of the IPCC, which highlight that behavioural demand-response options can simultaneously support multiple sustainable development goals (IPCC 2018, p. 157). While the results in Chapter 9 demonstrate the need for sufficiency and illustrate its theoretical potential to transform the heating sector, this does not mean that this potential can be achieved in the required time. It is important to note that the context of sufficiency involves complex social dynamics and long-established cultural practices that make sufficiency a multidimensional challenge. As Spangenberg and Lorek (2019) conclude, sufficiency strategies "need to take account of individual (skills, habits, values, attitudes), social (cultural conventions, social norms), and material/formal institutional factors (infrastructure, technologies, legislative and administrative settings) and their dynamics" (p. 1076). Therefore, the successful implementation of sufficiency strategies requires different, possibly new, policies and mechanisms as well as also more time than that required for the implementation of purely technical solutions.

Despite or even because of the challenges of lifting sufficiency potentials, this thesis closes with the more fundamental hypothesis that the development of sustainable energy systems, which takes into account the planetary boundaries, cannot dispense with sufficiency strategies and their consideration in open energy system analysis approaches. Therefore, sufficiency modelling needs further exploration to investigate its demand-side climate change mitigation potential, and support is required in the implementation of appropriate policy measures.

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