MODELING ENERGY SCENARIOS WITH POWER-FLOW CONSTRAINTS - Transparency, challenges and system adequacy

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(2) Cao, Karl-Kiên, Metzdorf, Johannes and Birbalta, Sinan (2018) *Incorporating Power Transmission Bottlenecks into Aggregated Energy System Models*. Sustainability, 10 (6). Multidisciplinary Digital Publishing Institute (MDPI). DOI: 10.3390/su10061916

(3) Cao, Karl-Kiên and Pregger, Thomas (2019) *Grid Expansion, Power-To-Gas and Solar Power Imports - Multi-Scenario Analysis of Large Infrastructure Options for the Decarbonization of the European Energy System*. ETG-Fachberichte (Energietechnische Gesellschaft im VDE). VDE Verlag. ETG Kongress 2019 - Das Gesamtsystem im Fokus der Energiewende, 08.-09.05.2019, Esslingen am Neckar

(4) Cao, Karl-Kiên, von Krbek, Kai, Wetzel, Manuel, Cebulla, Felix and Schreck, Sebastian (2019) *Classification and evaluation of concepts for improving the performance of applied energy system optimization models*. Energies, 12(24) (2019). Multidisciplinary Digital Publishing Institute (MDPI). DOI: 10.3390/en12244656

ABSTRACT

The understanding of how today's energy supply systems work and getting ideas of how a secure, affordable and sustainable energy supply can be achieved with respect to changing framework conditions in the future is an important aspect in the research field of energy systems analysis. Energy scenarios are such ideas of possible future energy systems, which are often designed and analyzed with models. The aim is to set the course today for an energy supply that is in line with the efforts to mitigate global warming. Publication 1 of this dissertation is devoted to the question of how to deal with the challenges that arise concerning the frequently observed insufficient traceability of corresponding scenario studies.

In such energy scenarios, electricity generation from renewable energy sources is crucial. However, it is not arbitrarily available and independent of location. Therefore, the transport of energy for spatially balancing of power demand and production is a key element for the transformation of today's energy system. However, optimization models that are frequently used in energy systems analysis are limited when trying to capture the implications of power transmission. Nevertheless, established methods of power-flow analysis could be used more for this purpose.

Bringing these two modeling worlds together by using approaches, such as model coupling and model integration, is therefore a major contribution of the research and studies associated with this dissertation. For this purpose, new instances of the energy system optimization model REMix have been developed. By using linear power-flow constraints to model electricity transport and grid expansion, the system adequacy of future energy systems can be examined in detail. For example, this concerns questions on the extent to which electricity transport has a complementary or competitive effect on the interaction with energy storage technologies or the coupling of energy sectors in European energy scenarios. The corresponding results (Publication 3) show that an expansion of cross-border transmission capacities is a robust and cost-efficient measure to ensure system adequacy across a broad spectrum of scenarios and parameter variations. However, this particularly holds true, if commonly used model resolutions on country level are applied.

Spatially higher resolved models, however, are necessary to find out how far the striking benefits of grid expansion also apply when explicitly considering transmission grid infrastructures. A scenario analysis focusing the German power system and using an integrated energy system optimization model confirms this finding, but also reveals that the need for energy storage is underestimated in macroeconomic studies due to insufficient model resolutions (Publication 2).

In order to be able to conduct further comprehensive investigations in the future, it is desirable to extend the geographical scope of approaches that integrate power flows, to also include sector coupling in the appropriate models and to carry out parameter variations for a large number of scenarios. In this context, computing times for solving the corresponding optimization problems represent a critical bottleneck to deal with. Therefore, with this dissertation, a systematic analysis of approaches for speeding-up of energy system optimization models is presented for the first time. The heuristics evaluated for this purpose show reductions of the total computing time up to a factor of ten while maintaining a sufficient degree of accuracy (Publication 4).

KURZFASSUNG

Ein wichtiger Forschungsschwerpunkt der Energiesystemanalyse ist es zu verstehen wie heutige Energieversorgungssysteme funktionieren und darauf aufbauend eine Vorstellung davon zu entwickeln, wie eine sichere, bezahlbare und nachhaltige Energieversorgung unter sich ändernden Rahmenbedingungen auch in der Zukunft bewerkstelligt werden kann. Energieszenarien sind solche Vorstellungen von möglichen zukünftigen Energieversorgungssystemen, welche oft mit Hilfe von Modellen entworfen und analysiert werden. Ziel ist es, damit bereits heute die Weichen für eine Energieversorgung zu stellen, welche im Einklang mit den Bestrebungen zur Begrenzung der Erderwärmung stehen. Der Frage, welche Herausforderungen sich hinsichtlich der oft schwierigen Nachvollziehbarkeit entsprechender Szenario-Studien ergeben, widmet sich Publikation 1 dieser Dissertationsschrift.

Eine bedeutende Rolle in solchen Energieszenarien spielt die Stromerzeugung aus erneuerbaren Energiequellen, welche allerdings nicht beliebig und ortsunabhängig stattfinden kann. Der Transport von Energie zum räumlichen Ausgleich von Endenergienachfrage und Stromerzeugung ist daher ein Schlüsselelement für die Transformation des heutigen Energiesystems. Insbesondere die häufig in der Energiesystemanalyse genutzten Optimierungsmodelle sind allerdings selten in der Lage diesen Energietransport hinreichend genau zu erfassen. Auf der anderen Seite existieren im Bereich der Stromnetzausbau- und -Betriebsplanung bereits Modellierungsinstrumente, die ebendies bewerkstelligen.

Ein wesentlicher Beitrag der mit dieser Dissertation verbundenen Arbeiten ist daher die Zusammenführung dieser beiden Modellierungswelten mittels Ansätzen zur Modellkopplung und Modellintegration. Die hierfür erstellten und weiterentwickelten Instanzen des Energiesystem-Optimierungsmodells REMix nutzen lineare Restriktionen zur Berücksichtigung von Leistungsflüssen, womit die Rolle des Stromtransports und Netzausbaus zur Sicherstellung der zukünftigen Energieversorgung detailliert untersucht werden kann. Dies betrifft beispielsweise Fragestellungen inwiefern der Stromtransport ergänzend oder konkurrierend auf Technologien zur Energiespeicherung oder bei verstärkter Kopplung von Energiesektoren in Szenarien der europäischen Energieversorgung wirkt. Die entsprechenden Ergebnisse (Publikation 3) zeigen, dass ein Ausbau von länderübergreifenden Grenzkuppelkapazitäten für eine Vielzahl von Szenarien und Parametervariationen als robuste und kosteneffiziente Maßnahme angesehen werden kann. Allerdings gilt dies vor allem unter Anwendung etablierter, länderscharfer Modellauflösungen.

Inwiefern die Vorteilhaftigkeit von Netzausbau auch bei einer expliziten Modellierung von Übertragungsnetzinfrastrukturen gilt, kann beispielsweise

mit Hilfe höherer räumlicher Auflösungen beantwortet werden. Eine erste auf das deutsche Stromversorgungssystem beschränkte Szenario-Analyse unter Anwendung eines integrierten Energiesystem-Optimierungsmodells bestätigt diese Aussage zwar, zeigt aber auch, dass der Bedarf an Energiespeichern in makroökonomischen Betrachtungen durch unzureichende Modellauflösungen unterschätzt wird (Publikation 2).

Um zukünftig umfassende und weitergehende Untersuchungen mittels integrierter Modellierung von Leistungsflüssen durchführen zu können, ist allerdings eine Erweiterung des geographischen Untersuchungsgebiets unter Einbeziehung der Sektorenkopplung und die Durchführung von Parametervariationen für eine Vielzahl an Szenarien empfehlenswert. Begrenzend wirkt sich hierbei allerdings die benötigte Rechenzeit zur Lösung der Optimierungsmodelle aus. Im Rahmen dieser Dissertation wird daher erstmalig eine systematische Analyse von Ansätzen zur Beschleunigung von Energiesystem-Optimierungsmodellen vorgelegt. Mit den hierfür evaluierten Heuristiken können unter Beibehaltung einer hinreichenden Modellgenauigkeit Reduktionen der Gesamtrechenzeit um bis zu Faktor zehn erreicht werden (Publikation 4).

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TABLE OF ABBREVIATIONS

DC	Direct Current
ESOM	Energy System Optimization Model
GTC	Grid Transfer Capability
HPC	High Performance Computing
HVAC	High Voltage Alternating Current (≥220 kV)
HVDC	High Voltage Direct Current
LP	Linear Program
MIP	Mixed-Integer Program
NTC	Net Transfer Capacity
OPF	Optimal Power-Flow
PTDF	Power Transfer Distribution Factors
REMix	Renewable Energy Mix for a sustainable energy supply
TYNDP	Ten Year Network Development Plan

1 INTRODUCTION

1.1 BACKGROUND AND MOTIVATION

1.1.1 SCENARIOS OF LARGE-SCALE ENERGY SYSTEMS

A scenario represents a possible and plausible future but does not claim to be a forecast. More precisely, a scenario provides a "[…] description of how the future may develop based on a coherent and internally consistent set of assumptions about key driving forces (e.g., rate of technological change, prices) and relationships" [1]. In this sense, scenarios are very useful to gain insights for the development of policies.

Energy scenarios in particular aim at providing such insights with regard to the energy system. In this context, energy systems include all aspects of power generation, consumption, and the cross-coupling of electricity supply, transport, heating and cooling while considering technologically required options. Moreover, large-scale energy systems are characterized by taking a macroscopic system view and capturing effects on extensive geographical scales. Understanding large-scale energy systems and especially transforming them in a way that desired targets are met–such as formulated in the Paris Agreement [2]–is accordingly a challenging task.

In order to tackle this challenge, the use of models is a very common approach to draft technologically feasible energy system designs when developing and analyzing appropriate energy scenarios [3]. As this often involves the application of multiple models, which demand for interdisciplinary expert knowledge, the derivation of policy recommendations from scenario studies thus proves to be an extensive and complex undertaking.[1]

1.1.2 LOAD-BALANCING AND SYSTEM ADEQUACY

Especially when the transformation of power systems towards decarbonized energy supply across all energy consuming sectors is to be investigated with scenarios, two important aspects are frequently to be considered.

1. As low-emission energy supply strongly depends on power generation from renewable energy sources [4], dealing with accordingly fluctuating availabilities of power generation on temporal and spatial scale becomes essential. In particular, this concerns balancing the fluctuating power generation with also varying energy demand patterns. In order to ensure that power generation and consumption match, measures for adaption are required. This is what is often referred to as "load-balancing".

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[1] The interdisciplinary authored Publication 1 of this thesis discusses the corresponding challenges especially related to comprehensibility and traceability of model-based scenario studies.

2. Existing power systems are by far the most complex technical systems. According to Schwab [5], this is due to the diversity of system components and the interactions between these elements, which take place at high energy levels. Ensuring a reliable power supply is thus a central issue. In this sense, system reliability is dividable into two aspects. On the one hand, “system security” (short-term reliability), which is related to the response on disturbances. This means that the system operation should be robust against unexpected outages of individual components. On the other hand, a presumption for ensuring this is “system adequacy” (long-term reliability), which, according to Billinton [6], “[...] relates to the existence of sufficient facilities within the system to satisfy consumer load demand or system operational constraints”.

If energy scenarios are supposed to outline desired but feasible alternatives of the existing system in the long-term, especially aspects concerning “system adequacy” need to be considered. This applies even more to energy scenarios, where the power generation from fluctuating renewable resources is characterized by limited predictability.

Addressing system adequacy with modeling tools requires that energy system models have specific characteristics. In order to model the availability patterns of renewable energy resources, both the spatial and the temporal scale need to be resolved up to a certain degree. The resolution of both is directly related to temporal and spatial gradients that occur during electricity generation and consumption (e.g., of a wind turbine and an industry facility, respectively). Additionally, since energy systems consist of a broad variety of technological elements, a discretization of this dimension must also be considered. Especially scenario analyses that address the structure of the energy systems require models, which allow for technological differentiation. The corresponding aim is to find implementations of conceivable technologies for the composition of a future system. For this, so-called bottom-up models [7] (see section 1.2) are particularly suited.

1.1.3 ELECTRICITY TRANSMISSION

The capability to interconnect locations with suitable potentials for electricity generation from renewable resources with regions characterized by high energy consumption is a key element for providing (spatial) flexibility in decarbonized energy systems. Although spatial load-balancing of energy supply and consumption can be realized in different ways (e.g., by transport of chemical energy carriers), electricity transmission is a very effective way to quickly compensate spatial imbalances over large distances at comparably low transmission losses. Furthermore, electricity grids are the infrastructure that interconnects at least all system components of a power system. The question of how a probably new or existing system component can contribute to (secure) energy supply is therefore strongly related to the availability of an appropriate grid infrastructure. This makes modeling of both power flows and grid transfer capabilities essential for addressing system adequacy in energy scenarios.

1.2 MODELING APPROACHES

Approaches for modeling energy systems are often distinguished into two categories. On the one hand, top-down models have a clear macroeconomic focus (e.g., Computable General Equilibrium models) [8]. On the other hand, modeling approaches that allow for the consideration of a broad variety of energy conversion technologies are referred to as bottom-up models. As the capability for technological differentiation is a precondition for analyzing the role of technologies such as for electricity storage and transmission within the energy system, bottom-up models are widely used for this purpose.

Within the group of bottom-up models, further distinctions are made between simulation (e.g., Agent-based Modeling) and optimization approaches. While simulation approaches are useful to virtually replicate the operation of real technical and social systems, the strength of optimization is rather the possibility to model decision-making processes model-endogenously with respect to an objective function. This makes optimization models particularly attractive for decision support.

In the recent years, a number of scientific review articles were published that provide a more detailed view on aspects concerning modeling approaches in the context of energy systems analysis (e.g., by Zerrahn and Schill [9], Ringkjøb et al. [10] and Collins et al. [11]).

1.2.1 ENERGY SYSTEM OPTIMIZATION MODELS

Energy System Optimization Models (ESOMs) that are developed for systems analysis of energy scenarios often have a techno-economical focus. The reason for this is the initial motivation to investigate how (i.e., with which technologies) energy policy goals could be reached and at which costs (techno-economic feasibility studies).

In the context of developing transformation pathways for the decarbonization of the energy system, optimization models are commonly applied [12]. For example, to find system configurations that meet given targets, investments into available technologies are defined as variables of a mathematical optimization problem. By introducing variables for the activity of energy converters also the operation of such a system configuration can be optimized and thus tested for feasibility. Although there is a gradual trend towards multi-objective optimization approaches in order to provide holistic scenario assessments [13], most ESOMs are still minimizing monetary costs. The following shows a typical objective function of a system cost optimizing ESOM.

Objective function:

$$Minimize\colon \sum_{t\in\mathcal{T}} \sum_{n\in\mathcal{N}} \sum_{u\in\mathcal{U}} c(t,n,u)\cdot p(t,n,u)$$

EQUATION 1

p: variable of total power supply
c: specific costs
$\mathcal{T}$: set representing of time steps
$\mathcal{N}$: set of modeled regions
$\mathcal{U}$: set of technologies

Typical constraints of such an ESOM ensure load-balancing or limit the usage of a certain technology up to its nominated installed capacity [14]. Notably, due to the typically used power-balance constraint, ESOMs ensure system adequacy of the modeled systems by default[2]. Especially for analyses that emphasize possibilities of load-balancing, additional constraints are used to model temporal or spatial shifting of either power provision or consumption. For example, with regard to temporal flexibility, energy storage facilities are characterized by an additional storage balance equation. [3]

1.2.2 CONVENTIONAL POWER-FLOW MODELING APPROACHES

Power-flow analysis is an established instrument used in the context of operation and investment planning of electrical grids. Given that the nodal power balance (balanced power consumption and generation at each node) within an electrical network is known, an equation system needs to be solved to observe the resulting power flows (i.e., voltages) over transmission lines or cables.

In the case of a High Voltage Alternating Current (HVAC) power system the fundamental relationship between nodal power and voltage

$$\underline{S_n^*} = P_n - jQ_n = \underline{U_n^*} \sum_{n'}^{N} \underline{Y_{nn'}}\,\underline{U_{n'}} \qquad \forall n \in \mathcal{N}$$

EQUATION 2

$\underline{S_n^*}$: Conjugate complex of apparent power at node n
P_n: Active power at node n
Q_n: Reactive power at node n (j indicates imaginary part of $\underline{S_n^*}$)
$\underline{U_n^*}$: Conjugate complex of nodal voltage at node n
$\underline{Y_{nn'}}$: Complex nodal admittance matrix
$\underline{U_{n'}}$: Complex nodal voltage at node n'

results in a set of non-linear equations (AC power-flow equations) to be solved in an iterative manner (i.e., with the Newton-Raphson-Method [5]). However,

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[2] However, this only applies for the assumptions used and for the chosen model abstraction, so that the system adequacy of a real-word system can be violated, even if this is not the case for the modelled system.

[3] Formulations of a typical objective function, associated constraints, and a discussion of the effects on the matrix structure of a linear program are provided in Publication 4.

besides AC power-flow, further approaches for modeling power flows (see also 1.2.3) and methods required for solving the corresponding equation systems exist (e.g., fast decoupled power-flow or DC power-flow) [15].

Simply solving power-flow equations can be referred to as simulation approach. It is useable for the prediction of system states that result from events or measures during the operation of an electrical power grid (e.g., outage of a transmission line). By adding costs (e.g., for power production or transmission) the optimal exchange of power between the nodes can be determined in an optimization model that considers power-flow equations as constraints. The appropriate problem class is referred to as optimal power-flow (OPF) [16].

Another problem class that is investigated for a long time in the context of power-flow analysis is transmission expansion planning [17]. It represents an extension of OPF problems that allows for the identification of grid expansion measures, such as the construction of new transmission lines.

From an overall system's perspective traditional power-flow modeling approaches are characterized by their comparably high spatial resolution as they are supposed to model existing or candidates of real infrastructures combined with a high accuracy in terms of electrical properties that imply a need for the corresponding availability of electrical grid parameters. Opposed to that, these approaches neither emphasize a broad technological differentiation nor on solutions for a large set of temporally consecutive grid usage situations.

1.2.3 MODELING POWER FLOWS IN ENERGY SYSTEM OPTIMIZATION MODELS

Incorporating approaches for power-flow modeling into ESOMs usually results in models that are similar to OPF problems. In the simplest case, modeling of technologies that allow for spatial energy shifting is realized with an economic transshipment model[4] first described by Hitchcock [18][5]. Such models are originally applied to economic transport problems. They are characterized by flow variables that represent the exchange of a particular commodity between at least two discrete locations.

Applying the transshipment approach for power-flow modeling is sufficient as long as the spatial resolution is low. With regard to the spatial dimension in ESOMs, these models are typically designed to represent electricity markets or national states (i.e., regions) rather than dedicated substations or nodes within a transmission grid. Modeling electricity transmission in ESOMs therefore means that power flows are mostly represented in a spatially aggregated manner and restricted by capacity constraints. For example, in the case of the

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[4] also referred to as "transport model"

[5] This means that for conventional ESOMs, traditional power flow modeling approaches as introduced in 1.2.2 are not applied (or even not required, if the spatial resolution is comparably low).

ESOMs Eltramod [19] or DIME [20] these capacities are derived from net transfer capacities (NTCs). NTCs represent non-physical values to approximate the possible trade between bidding zones considering power generation schedules. Opposed to that, grid transfer capabilities (GTCs) define the maximal allowed power transmission taking into account technical operation limits of transmission lines [21]. Since GTCs reflect the physical transmission capability, they represent the quantity to be used to conduct transmission expansion planning with ESOMs.

However, modeling power flows in (roughly aggregated) electricity transmission lines with a transshipment approach is only sufficient if the magnitude and distribution of power flows can be fully controlled. Presuming the application of controllable power converters, this applies to High Voltage Direct Current (HVDC) transmission systems [6]. Nevertheless, today, the dominating electricity transmission technology is still HVAC transmission.

For modeling power flows in HVAC grids, simple capacity-constrained transshipment models are also applied, which is permissible as long as the modeled infrastructure is not fully resolved. In other words, especially in ESOMs that represent electricity markets, real HVAC transmission lines are modeled in an aggregated manner. Nevertheless, modeling HVAC transmission normally implies that the distribution of power flows cannot be arbitrarily determined. Compared to transshipment models this makes the introduction of additional constraints necessary.

The appropriate modeling approach that fully captures the physics of HVAC power flows (i.e., the consideration of active and reactive power flows) is the AC power-flow. However, accounting for AC power-flow constraints in ESOMs, results in non-linear optimization models and solving comparatively small instances of such ESOMs is already challenging. Therefore, often linear model formulations are sought. One way to achieve this is making permissible assumptions concerning voltage angle differences and the magnitude of nodal voltages and to neglect reactive power in HVAC grids. The non-linear AC power-flow constraints can be accordingly transformed into a linear equation system. The appropriate modeling techniques are referred to as DC power-flow [22] and summarize linear modeling approaches, where the distribution of active power flows is defined by distribution factors. These factors are determined exogenously of the ESOM either by a linearization of pre-executed AC power-flow simulations or based on electrical properties of the transmission lines[7].

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[6] For this reason, in the studies that are summarized in this thesis, power flows in HVDC infrastructures are modeled with the transshipment approach.

[7] The first method mentioned, referred to as PTDF method, is applied in the work associated with Publication 3, where the Power Transfer Distribution Factors (PTDFs) are derived from the spatial aggregation of distribution factors observed in several AC power flow simulations.

1.2.4 CAPACITY EXPANSION MODELING

When the composition of an energy system should be investigated with an ESOM, the corresponding model needs to support capacity expansion. In such cases, as mentioned in 1.2.1, investment decisions are part of the optimization. Such optimization problems are examined for several decades, initially in the context of generation expansion planning, where the optimal dimensioning and placement of power generation capacities is investigated [23].

With the increasing focus on energy scenarios that address high shares of renewable energy and the accompanied challenges regarding system adequacy, the technological focus of classical generation expansion planning problems is extended by technologies that provide both spatial and temporal flexibility for load-balancing. Hence, nowadays many ESOMs are combinations of models that allow generation, transmission, and storage expansion planning [24].

From an investor's perspective, decisions for investments into new infrastructures usually need to be discrete. This means that, for example, power plants cannot be realized with any nominated block size. Optimization problems that are suited for this purpose are mixed-integer programs (MIPs). However, for modeling of spatially aggregated large-scale energy systems that consist of great numbers of decentralized units (e.g., photovoltaics) often linear programs (LPs) are applied, where investment decisions are represented by continuous variables. The rationale behind is the fact that new capacities calculated at an aggregated level are several orders of magnitude larger than a discrete unit for power generation, storage or transmission. According to the findings of Cebulla and Fichter [25], the same justification shall also apply to normally discrete operation decisions within large-scale energy systems.

Concerning the treatment of planning horizons for expansion planning, different approaches are conceivable. In [24] the authors distinguish between static and dynamic methods where the first is commonly used for in-depth analysis of normative scenarios [26]. For explorative investigations of transformation pathways, however, the dynamic treatment of planning horizons is the more suitable approach.[8]

1.2.5 THE ENERGY SYSTEM OPTIMIZATION MODELING FRAMEWORK REMIX

In its initial implementation by Scholz [27] REMix (Renewable Energy Mix for a sustainable energy supply) focused on power system scenarios where power

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The PTDFs used in Publication 3 are therefore dependent on the operational state of the model. The latter variant of the DC power flow approach is the dominating method for modeling electricity transmission in Publication 2 and 4. It uses lines lengths and assumptions about the specific reactance of transmission lines to derive distribution factors, which are therefore static across the operation horizon of the model.

[8] In the model-based analyses of Publications 2 to 4 of this thesis, ESOMs are applied that are implemented as LPs. Capacities accounted for expansion planning are therefore modeled as continuous variables. Furthermore, the associated investment decisions are made based on static assumptions concerning annual capital expenditures of considered technologies.

supply is based on high penetrations with renewable energies. In this context, REMix was supposed for proving the sub-annual operational feasibility of energy scenarios that were developed based on consistent annual energy balances. For this reason, analyses with REMix mostly emphasized the optimization of hourly power system operation taking into account all kinds of renewable electricity supply.

Due to further model development in the last years, more recent instances of REMix are able to cover power supply for all energy consumption sectors and allow for capacity expansion of the associated technologies [28]. Applications range from long-term investigations of temporal flexibility requirements [29] over country specific decarbonization scenario studies [30,31] to mid-term analyses of system security [32].

Today, REMix allows the creation of ESOM instances that share similar source codes written in the algebraic modeling language GAMS but have different input parameters in terms of geographical scope, spatial resolution or analyzed time horizon. Hence, REMix is rather a model generator thanks to its modular structure combined with sub-version management.

An overview of all REMix modules applied in the context of this thesis is shown in Table 1. Also, the author's significant contributions to maintenance, development and data collection for the listed modules are indicated there. The latter is designated as "Input preparation" and includes the collection and documentation of raw data, and data processing for the creation of complete input data sets for a specific REMix application. Besides modules that provide basic functionalities for setting up an optimization model in GAMS and for input data treatment, these modules are mainly characterized by the representation of technology classes. Restrictions, which usually affect all technologies (e.g., politically motivated restrictions such as self-consumption quotas) are provided in a modular manner.

Although some modules of REMix are implemented as MIPs, the majority of applied ESOM instances created with REMix are LPs, where always the hourly dispatch of power plants and technologies for load-balancing is optimized seeking for minimal system costs. A commonly used term for such optimization problems is Economic Dispatch [33]. However, typical REMix instances are spatially resolved, which justifies the designation of such ESOMs as Multi-Regional Economic Dispatch models. In addition, capacity expansion is frequently applied to specific technologies (such as those for spatial and temporal load-balancing).

One particular contribution related to this thesis is the compilation of data sets that allow for analyses with spatially highly resolved ESOMs. The term spatially highly resolved means that compared to typical REMix applications, which usually optimize on country level, a regionalization is conducted necessary for modeling of power flows within the HVAC transmission grid. The corresponding model specifications allow for conducting OPF analysis with REMix [33].

In this regard, the dedicated specifications of the REMix models applied in this thesis are shown in Table 2.[9]

TABLE 1: OVERVIEW OF TECHNOLOGY SPECIFIC REMIX MODULES USED IN THE CONTEXT OF THIS THESIS AND AUTHROR'S CONTRIBUTIONS.

✓	yes
×	no
⦸	irrelevant

	Modelled technology (class)	Internal name	Electricity generation	Electricity consumption	Capacity expansion possible	Characteristic restrictions/properties	Contribution			
							(Co)-Maintenance	Documentation	New development	Input preparation
Electricity	Biomass-fired power plants	re_biomass	✓	×	✓	Limited annual fuel resources	✓	×	×	×
	Variable renewable energies	re_fluctuatingNoStor	✓	×	✓	Capacity expansion potentials and time series-based power generation potentials	✓	×	×	✓
	Conventional thermal power plants	convBase	✓	×	✓	Punishment costs for load cycling	✓	×	×	✓
	Concentrated solar power plants	re_csp	✓	×	✓	Time series-based heat generation potentials with heat storage	×	×	×	×
	Conventional power consumers	demand_electrical	×	✓	×	Time series-based power demand	✓	×	×	✓
	Electric vehicles	eCars_smpl	×	✓	×	Time series-based power demand with optional load shifting	×	×	×	✓
Renewable fuels	Electrolysis	hy_ElectrolyzerSimple	×	✓	✓	Power-to-hydrogen conversion	✓	✓	×	✓
	Hydrogen vehicles	hy_FixedAnnualDemand	×	×	×	Time series-based hydrogren demand	✓	✓	×	×
Heat	Electric boilers	heat_electricBoiler	×	✓	✓	Power-to-heat conversion	✓	×	×	×
	Gas boilers	heat_boiler	×	×	✓		×	×	×	×
	Combined heat and power plants	heat_chp_std	✓	×	✓	Co-generation of power and heat	×	×	×	×
	Heat pumps	heat_pump	×	✓	✓	Time series-based heat generation potentials	✓	×	×	×
	Heat consumers	heat_demand	×	×	×	Time series-based heat demand	×	×	×	×
Spatial load balancing	High voltage alternating current transmission	transport_ACExpansion / transport_ACAggregation	✓	✓	✓	Power transmission considering DC power-flow constraints, (spatial aggregation)	✓	✓	✓	✓
	High voltage direct current transmission	transport_DCSimple / transport_DCAggregation	✓	✓	✓	Power transmission using transport model, (spatial aggregation)	✓	✓	✓	✓
	Gas transmission	hy_NaturalGasNet	×	×	×	Unconstrained transmission, conversion losses for synthetic fuel production from hydrogen	✓	✓	×	×
Temporal load balancing	Demand side management	demandresponse_smpl	✓	✓	✓	Time series-based, temporally restricted load shifting potentials	×	×	×	×
	Hydro reservoir storage	re_reservoirHydro	✓	✓	✓	Time series-based power generation potentials with storage	×	×	×	✓
	Energy storage	storageStd	✓	✓	✓	Capacity expansion potentials	✓	×	×	✓
	Heat storage	heat_stoarge_std	×	×	✓		×	×	×	×
	Hydrogen storage	hy_Storage	×	×	✓	Capacity expansion potentials	✓	✓	×	✓
Global modeling constraints	Self-consumption quotas	domesticGenShare	⦸	⦸	⦸	Bounding of annual power generation per region with respect to annual power demand per region	×	×	×	⦸
	Fuels	fuelsAndACost	⦸	⦸	⦸	Fuel costs and/or limitation of annual availability	✓	×	×	⦸
	Emissions	pollutionAndACost	⦸	⦸	⦸	Emission costs and/or limitation of annual emissions	✓	×	×	⦸
	Firm capacity	firmCapacity	⦸	⦸	⦸	Bounding of total power generation capacity with respect to electrical peak load per region	✓	✓	✓	⦸
	Heuristc for temporal model decomposition	methods_rollingHorizon	⦸	⦸	⦸	Decomposition of sub-annual time horizon into time intervals to be solved as partial models	✓	✓	✓	⦸
Main		minCost_standart	⦸	⦸	⦸	Program control and objective function	✓	✓	×	⦸

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[9] A technology-oriented overview of the models applied in the context of this thesis is provided in the Appendix.

TABLE 2: MODEL SPECIFICATION OF THE REMIX MODELS APPLIED IN THE PUBLICATIONS SUMMARIZED IN THIS THESIS.

	Publication 2 & Publication 4	Publication 3
Model specification	Linear programming Minimization of total costs for system operation and expansion	
	"REMix Germany": Linear optimal power-flow and capacity expansion of lithium-ion batteries and grid transfer capacity	"REMix Europe" Multi-regional capacity expansion of power generators and technologies for temporal and spatial load-balancing
Scope of model application	Methodological development	Analysis of normative energy scenarios
Sectoral focus	Electricity	Electricity, heat, individual transport
Geographical focus	Germany	Europe and Northwest Africa
Spatial resolution (number of regions)	High-voltage (220 and 380 kV) substations (488)	European countries and Germany regionalized (58)
Analyzed normative scenario	2012, 2030	2030, 2050
Temporal resolution	8760 consecutive, hourly time steps	

1.3 CHALLENGES AND RESEARCH QUESTIONS

Pfenninger et al. [34] define four dedicated challenges related to energy system modeling:

1) Resolving details in time and space
2) Uncertainty and transparency
3) Complexity and optimization across scales
4) Capturing the human dimension

ESOMs in particular, are addressed by the very first of these challenges. It is directly related to the aspect of combining the capabilities of conventional energy system optimization and power-flow analyses in order to enable in-depth assessments regarding the contribution of power transmission to system adequacy in in low-carbon energy systems. However, this has several methodological and data-related challenges to harmonize the typical temporal, spatial and technological scales of the corresponding modeling approaches (see Table 3).

For example, on the ESOM side, modeling of many different technologies for power supply and conversion is state-of-the-art. As mentioned in 1.2.1, this capability is required to find system configurations that meet given targets (e.g., greenhouse gas mitigation). However, concerning the spatial dimension, the definition of more highly resolved regions[10] is necessary to take into account anticipated grid congestion, which significantly affects the energy system's ability to utilize renewable energy sources. On the other side, by considering all transmission lines of the transmission grid, the ability to discover grid congestion is already ensured in conventional power-flow analyses, but the technological origin of power feed-in at a dedicated substation is of little interest.

TABLE 3: TYPICAL MODEL SCALES OF ENERGY SYSTEM OPTIMIZATION MODELS AND POWER-FLOW ANALYSES

Modeling approach	Energy System Optimization Modeling	Power-Flow Analysis in HVAC grids
Spatial scale	Aggregated regions (|n|<100)	Buses within an electrical grid (|n|>>100)
Temporal scale	Time series (|t|=8760)	Snapshots (|t|<<8760)
Technological scale	Bottom-up modeling of a broad spectrum of technologies	Physical representation of network resources

Besides the technological variety and typical spatial resolutions, the way of treating the temporal scale is another major difference between traditional power-flow modeling approaches and ESOMs. Power-flow analysis in general is mostly based on a small number of temporal snapshots that represent, for example, worst case situations in terms of the network's utilization. Opposed to that, in order to prove operational feasibility, ESOMs are supposed to appropriately model the temporal dimension either by time series or by a reduced, but still large number of representative time slices.

To conclude, only bringing together both modeling approaches enables the identification of decarbonized energy systems that, from an overall system's perspective, provide the required spatial load-balancing capabilities to ensure system adequacy. Therefore, the particular challenges that arise from this claim are detailed in the following. In general, all of them can be traced back to the trade-off between two fundamental claims: (i) keeping an overall system's perspective and (ii) providing a sufficient level of detail for translating results into comprehensive recommendations for actions or applicable measures.

1.3.1 INCREASING RESOLUTIONS

First techno-economic feasibility studies were often conducted on an annual basis and on national or super-national level [35]. The underlying modeling approach can be denoted as the creation of consistent annual energy balances. As in the case of REMix, an extension of this approach obviously becomes necessary when the sub-annual fluctuating availability of renewable energy

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[10] Publication 2 of this thesis proposes a new method, which allows for automated determining of such region definitions.

sources cannot be neglected anymore. This applies to techno-economic feasibility studies with the objective of mitigating greenhouse gas emissions in the energy sector. As a consequence, today many ESOMs resolve the operational time horizon by hourly time series.

The techno-economic feasibility of energy systems that mainly rely on renewable power generation can be seen as the driving research question addressed up to this decade, which is currently followed by the next crucial topic - the implementation of such systems. Therefore, the point of ever-increasing model resolutions results from the trend of seeking for more concrete measures directly derivable from model-based analyses. It is thus related to the claim of providing a sufficient level of detail and applies to all of the characteristic dimensions of ESOMs. Consequently, established modeling approaches that often simplify these dimensions by aggregating technologies, time steps or regions are no more sufficient for finding answers related to the realization of infrastructures, especially if the corresponding error is not fully understood.

For example, insufficient temporal resolutions cause the same effect as energy storage– they smooth both power generation and demand profiles and accordingly lead to an underestimation of storage demand. In addition, for selecting an appropriate technology for the realization of a particular energy storage facility, the variety of technologies needs to be represented in a way that strengths and weaknesses can be modeled. In practical terms this means, that only temporal resolutions <1h are appropriate to capture the benefits from batteries that allow for rapid charging. But still, time horizons must be large enough (>3 months) to account for seasonal storage capabilities (e.g., of cavern storage).

The similar applies for the spatial dimension, where the identification of sites for building up the energy storage facility and the conceivable need for expanding a particular transmission line requires resolutions that at least enable modeling of these individual system elements (as done in traditional power-flow analyses). Nevertheless, typical ESOMs that account for power transmission strive for the coverage of large areas. In a European context, this is mainly due to two reasons: 1) the wide area synchronous grid, which also covers countries in North Africa and 2) the objective of creating an internal energy market without transmission congestions within the European Union. However, efforts to maintain the perspective of the overall system typically result in spatial resolutions on country level. Therefore, model-based scenario studies that additionally provide high spatial resolutions are rare although former issues such as data availability improved over the last years (e.g., SciGrid [36] or Open power system data [37]). Increasing the spatial dimension is especially challenging since the structure of the resulting mathematical optimization problems becomes rather complicated and so solvability deteriorates. This is, on the one hand, due to the characteristic of linking constraints[11]. On the other hand, also the translation into a continuous linear optimization problem (LP) must be critically questioned, whereas the more appropriate problem class –MIP - is even harder to be solved.

Accordingly, a pressing challenge is increasing the spatial resolution within ESOMs in a way that the ability to solve the mathematical optimization problems within manageable time spans is maintained. This becomes even more obvious because, according to Pfenninger et al. [34], most simplifications applied to current ESOMs already stem from the need to reduce computing times.

From this, the following research question to be addressed within this thesis is derived:

What are the impacts of integrating power flows in energy system optimization models and what are appropriate solution approaches?

1.3.2 EXTENSION OF SYSTEM BOUNDARIES

The need for approaches that allow for solving very large optimization models is also driven by the extension of boundaries of the systems to be modeled. Opposed to model resolutions, which refer to the extent of discretization within given boundaries, this trend enlarges the definition of what the overall system is. It especially applies to the technological dimension.

For example, while ESOMs such as REMix initially had a clear focus on the power sector, the extension of system boundaries is caused by taking into account the broad variety of technological solutions implied by coupling energy sectors and commodities. In addition, as scenario analyses are always associated with high uncertainties, proving of the robustness of the outcomes is more and more addressed by extensive parameter variations. This is also equivalent to an extension of system boundaries, namely those of the analyzed techno-economic scenario space. Finally, the basis of evaluation is broadened if energy systems are to be assessed based on sustainability criteria rather than on monetary costs.

One illustrative example in the context of electricity infrastructure planning is the increasing extent of the Ten Year Network Development Plan (TYNDP), which is regularly issued by the association of European Transmission Grid Operators [38]. In order to identify infrastructure projects, which contribute to the achievement of the EU’s climate and energy objectives, extensive model-based scenario analyses are part of the assessment framework.

The first issue of the TYNDP contains two scenarios with a 10-year foresight (“conservative” and “best estimate”) and one 15-year trend, whereas from a technological point of view only power generators and demand forecasts are

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[11] The role of linking constraints is discussed in detail in Publication 4.

focused. In its version from 2018, three scenarios (considering electricity and gas transmission infrastructure) are conducted with foresight up to 2040 and accompanied by variations of input data such as weather years. Moreover, the role of additional technologies such as prosumers, including demand response measures, electric vehicles and heat pumps is considered.

Particularly, these technologies are frequently discussed in the context of load-balancing and thus will have also an impact on future system adequacy. Furthermore, they also represent the need for cross-coupling of the power sector with its counterparts in heat and transport, as the majority of low-carbon energy conversion paths rely on electricity generation from renewable energy sources.

In this context, electricity transmission and thus the consideration of limited power flows in ESOMs play a crucial role in scenarios of future energy systems. This is due to fact that power transmission is the key technology for accessing remote power generation potentials from renewable sources at comparably low transmission losses.

Therefore, the related research question is:

What is the contribution of power transmission and grid expansion to ensure system adequacy in energy systems with low carbon emissions?

1.3.3 TRACEABILITY

Given that ESOMs tend to become larger and more complex due to both increasing resolutions and extending system boundaries, two derivative challenges arise. As mentioned above, the first concerns the computational effort that disproportionally increases with growing model sizes. The second challenge is related to the need for more data. This comes together with additional effort to be made with regard to processing and analyzing of large data sets and with stricter requirements concerning data quality.

Already existing studies conducted with simple ESOMs suffer from a lack of traceability. Reasons for this are manifold. Some aspects are related to practical issues such as incomplete documentation for different purposes and target groups or an insufficient use of state-of-the-art software engineering approaches for the model development and application by teams. However, more importantly, the general nature of scenarios hampers typical confidence-building towards modeling tools since traditional model validation techniques based on comparisons with reality are not applicable by ease. In other words, finding ways to measure states of large-scale energy systems by appropriate observables is already challenging but becomes even harder if the corresponding system states lie in the future. In addition, due to a lack of fully consistent and complete empirical input data, assumption making is always related to modeling energy scenarios. In particular, this in turn complicates documentation as also implicit assumptions are made unconscious.

However, for ensuring best scientific practice, experiments and thus model-based analysis need to be reproducible and accordingly traceable in the first place. In the context of energy scenarios of large-scale energy systems, this leads to the following research question:

How to make modeling of scenarios of large-scale energy systems traceable?

1.4 OBJECTIVES AND SCOPE

In order to address the three fundamental research questions of this thesis, the following overarching objectives are specified (Table 4):

TABLE 4: RESEARCH QUESTIONS AND RELATED OBJECTIVES

Research question	**Objective**	**Content-related focus**	**Methodological focus**
1) How to make modeling of scenarios of large-scale energy systems traceable?	a) Identification and discussion of reasons for lacking traceability of model-based energy scenario studies b) Development of criteria to better assess model-based energy scenario studies	☒	☐
2) What are the impacts of integrating power flows in energy system optimization models and what are appropriate solution approaches?	a) Implementation of methods for modeling power flows in large-scale energy systems b) Parameterization of a spatially highly resolved model c) Implementation of approaches to ensure solvability of the spatially highly resolved model d) Analysis of the impact of regionalization and model simplification by spatial aggregation e) Analysis of the impact on model results of different approaches for modeling power flows in ESOMs	☐	☒
3) What is the contribution of power transmission and grid expansion to ensure system adequacy in energy systems with low carbon emissions?	a) Definition of scenarios and parameterization of an ESOM that allows for power transmission and grid expansion among alternative technological options for load-balancing b) Analysis of the role of power transmission as load-balancing measure in order to ensure system adequacy	☒	☐

These objectives are to be met within particular framework conditions. In this sense, energy scenario analyses conducted in the context of this thesis always rely on the application of modeling tools (i.e., ESOMs with the objective to find compositions of energy infrastructure based on existing technologies). Therefore, the term energy scenario is rather to be understood in a techno-economic than in a socio-economic context.

As described in section 1.2.5, model development and application are conducted with REMix, which implies the creation of ESOMs formulated as LP. The content-related scope of this thesis concerns normative long-term scenarios for Germany and Europe for the years 2030 and 2050 taking into account CO_2 mitigation targets of up to 85% reduction compared to the emissions in the year 1990 in power generation.

2 PUBLICATIONS

In the following, the four publications summarized in this dissertation are enclosed. In order to provide a common characterization scheme and to show the relation to the central objectives of this thesis (section 1.4); each publication is introduced by a table where used methodologies, models and key outcomes are summarized. Furthermore, these tables provide general information such as access or the author's contribution to the associated scientific process (e.g., conducting the study and a writing a corresponding paper).

2.1 PUBLICATION 1

Status	**Published** in: Energy, Sustainability and Society 6 (1): Art.Nr.: 28 (2016)
Title	Raising awareness in model-based energy scenario studies - a transparency checklist
Co-Authors	Felix Cebulla, Jonathan J. Gómez. Vilchez, Babak Mousavi, Sigrid Prehofer
Publication year	2016
Access	https://doi.org/10.1186/s13705-016-0090-z ☒ Gold Open Access ☐ Green Open Access ☐ Closed access
Applied model	-
Specific objective	Compilation of criteria for the assessment of transparency in energy scenario studies that largely rely on the application of complex models
Thesis-overarching objectives	1.a) Identification and discussion of reasons for lacking traceability of model-based energy scenario studies 1.b) Development of criteria to better assess model-based energy scenario studies
Methodology	Qualitative expert interviews and expert validations
Key outcome	Transparency checklist to be used by authors and users of energy scenario studies

Cao *et al. Energy, Sustainability and Society*
DOI 10.1186/s13705-016-0090-z

Energy, Sustainability
and Society

ORIGINAL ARTICLE **Open Access**

Raising awareness in model-based energy scenario studies—a transparency checklist

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Abstract

Background: The focus of the paper is on scenario studies that examine energy systems. This type of studies is usually based on formal energy models, from which energy policy recommendations are derived. In order to be valuable for strategic decision-making, the comprehensibility of these complex scenario studies is necessary. We aim at highlighting and mitigating the problematic issue of lacking transparency in such model-based scenario studies.

Methods: In the first part of the paper, the important concept of transparency in the context of energy scenarios is introduced. In the second part, we develop transparency criteria based on expert judgement. The set of selected criteria is structured into 'General Information', 'Empirical Data', 'Assumptions', 'Modeling', 'Results', and 'Conclusions and Recommendations'. Based on these criteria, a transparency checklist is generated.

Results: The proposed transparency checklist is not intended to measure the quality of energy scenario studies, but to deliver a tool which enables authors of energy scenario studies to increase the level of transparency of their work. The checklist thus serves as a standardized communication protocol and offers guidance for interpreting these studies. A reduced and a full version of the checklist are provided. The former simply lists the transparency criteria and can be adopted by authors with ease; the latter provides details on each criterion. We also illustrate how the transparency checklist may be applied by means of examples.

Conclusions: We argue that transparency is a necessary condition for a reproducible and credible scenario study. Many energy scenario studies are at present characterized by an insufficient level of transparency. In essence, the checklist represents a synthesizing tool for improving their transparency. The target group of this work is experts, in their role of authors and/or readers of energy scenario studies. By applying the transparency checklist, the authors of energy scenario studies signal their commitment to a high degree of transparency, in consonance with scientific standards.

Keywords: Scenario analysis, Energy modeling, Transparency, Open access

Background

Model-based energy scenarios

Scenario analysis is becoming an increasingly recognized area of research. As a result, the number of scenario studies published in recent years has risen tremendously. In 2011, for example, the European Environment Agency (EEA) listed 263 scenario[1] studies [1]. Despite its limitations (e.g. availability bias[2]) [2], the scenario analysis is regarded as an adequate method to deal with what Lempert et al. [3] call 'deep uncertainty'. Furthermore, Wright and Goodwin [4] propose an approach on how to overcome some of these limitations. In the context of energy research, energy scenarios are considered to be a suitable and helpful means of depicting possible future pathways in an energy system. Basically, they have two main purposes: First, to offer orientation and contribute to discussions about energy futures [5]; second, to support strategic decision-making on energy issues. In this case,

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they can be seen as 'a useful tool to helping decision-makers in government and industry to prepare for the future and to develop long-term strategies in the energy sector' (p. 89) [6]. Attempts to classify scenarios have been made by other authors (see e.g. [7, 8]).

Due to the complex nature of energy systems, mostly energy scenario studies benefit from models[3] which may capture qualitative and quantitative aspects of the systems. We call these 'model-based energy scenario studies (ESS)'.

Challenges in dealing with model-based energy scenarios

The complexity of the present and future energy systems and their highly uncertain and dynamic nature evoke challenges for energy scenario analysis. The related questions most likely have to be tackled from an interdisciplinary perspective which consequently leads to the application of a broad diversity of methods and models, with their underlying assumptions. Thus, this represents a challenge for the readers[4] of the ESS. In our view, comprehensibility or intelligibility of a particular model-based ESS requires two conditions to be met for a reader:

First, the reader needs to have the technical expertise or skills to understand what has been done in the study. Energy scenarios in model-based ESS vary depending on their primary purpose (e.g. assessing mitigation possibilities [9]). Even if a single method is used to construct a model-based ESS, various modeling techniques may be employed by the authors of the study [7]. For example, a model resulting from applying a particular simulation method may encapsulate a series of scientific techniques such as Monte Carlo simulations and Kalman filtering. Often, model-based ESS are the result of adopting several methods. In addition, the results of model-based ESS may be used as input data for further model-based investigations regarding questions of future developments. Suffice to say here that the adaptation of different models and the abundance of ad hoc techniques from which results can be derived are a source of rich diversity in energy scenarios [1, 10].

Due to the increasing importance of ESS and the expanding computing possibilities, the total number of available energy models has grown considerably. These models vary significantly in terms of structure and application which leads to greater complexity in understanding and interpreting model-based ESS. Thus, navigating through this type of study becomes a challenging task. The heterogeneity of applied energy models and corresponding model-based energy scenarios demands specific technical skills for the adequate assessment of such (often complex) interdisciplinary studies. This represents not only a key barrier to the comprehensibility of a particular study but it also makes the comparability of the study more difficult. Over time, a number of studies (e.g. [11–16]) have presented numerous classifications of energy models which provide insight into the differences and similarities between the models to facilitate the understanding of ESS.

The second requirement for the comprehensibility of model-based energy scenario studies is transparency. Arguably, transparency is even more important than technical skills, for it is a basic requirement of any research. Transparency is a key concept of scientific work and is particularly relevant for studies looking to the future [17]. Transparency is a necessary but insufficient condition for a reproducible and valuable scenario study. In ESS transparency means that the necessary information to comprehend, and perhaps reproduce, the model results is adequately communicated by the authors of the study. Bossel [18] uses the concepts of 'black box', 'glass box' and 'grey box' to highlight 'different possibilities for simulating system behavior' (p. 19). These ideas can be related to different degrees of transparency, to be chosen by the modeler to characterize a certain system (e.g. energy) in a model-based study. In this manner, the black box represents a low level of transparency, and the glass box a high level of transparency. We argue that the employment of the latter is desirable in scientific work because it allows reproducibility. In addition, Weßner and Schüll [19] consider the provision of background information about a study, for example, if it is financed by a third party, to be important to ensure scientific integrity.

Considering one important part of ESS, a concrete example of the need for transparency is the communication of assumptions[5] (for further explanations see 'Methods' and 'Results and discussion' section). Ideally, the ESS author[6] would fully articulate all the assumptions, thereby facilitating that the reader understands how a particular model-based scenario study has been constructed. In practice, when a large model or a set of large models is used, there is a trade-off between completeness and succinctness and only the main assumptions can be communicated exhaustively in the model documentation. In extreme cases, critical assumptions are made implicitly, unnecessarily obscuring the modeling exercise. In the worst case, such an approach may be a deliberate strategy to attach objectivity to ideology [20]. It can be concluded that providing comprehensibility for ESS appears to be a challenging issue since the selection of information to be communicated needs to take into account various aspects.

Aim and outline

This paper addresses and attempts to mitigate opacity in model-based ESS. In particular, we adopt the view that comprehensibility is necessary, if ESS are intended to successfully fulfil their purpose of adding value to strategic decision-making. To do this effectively, there is a need to fully assess the essential content of an ESS. But many of the existing studies are not sufficiently comprehensible for a complete external evaluation of the quality and usefulness of such studies. Since readers do have different questions and educational backgrounds, there is a need for comprehensibility on several communication levels (inter alia proposed in [21]). In the best case, a wide spectrum of addressees such as experts, decision-makers and the public is enabled to build their own opinions based on the outcome of ESS.

However, even the minimum requirement, which is for us full traceability of ESS for experts, often cannot be met [5]. In general, two kinds of required comprehensibility can be distinguished in this context: First, model comprehensibility, which aims at ensuring comparability and reproducibility by experts. The second one is study-results comprehensibility which enables the interpretation of ESS outcomes also for non-experts. If results comprehensibility cannot be sufficiently provided, it is an obvious precondition that at least experts who work in the field of energy scenario construction and application need to be able to fully retrace the work of other experts in order to explain it to the remaining addressees.

We claim to tackle this issue by highlighting the important role of transparency. Therefore, we aim to provide an additional approach for practical use cases where a glass box model is difficult to be achieved. Its purpose is to ensure leastways the provision of necessary information for expert judgement for both model comprehensibility and also results comprehensibility. For this reason, the target group of our work's outcome is limited to experts, in their role of authors and/or readers of ESS.

The next subsection provides a review of existing scientific work that addresses quality criteria in model-based studies with guidelines of good practice. Furthermore, the applied methodology for the determination of the transparency criteria for model-based scenario studies is explained in the 'Methods' section. 'Results and discussion' section introduces the ESS transparency checklist where the identified criteria are collected and discusses several of its key points. Finally, in the 'Conclusions' section, a further collection of transparency criteria for addressees other than experts is suggested.

Literature review

The issue of insufficient comprehensibility in scenario studies is not new and the contributions of previous work to address it have been made. For example, a recent study of the International Risk Governance Council [22] provides a comprehensive methodological review on energy scenario and modeling techniques. The work emphasizes a clear (i.e. transparent) communication of the scenario and model outcome, especially in terms of possible uncertainties and biases. Although [22] delivers novel insights with regard to shortcomings of energy scenario methods, it provides little guidance on the possible ways of ensuring transparency in model-based ESS. In this section, two main bodies of literature are examined; one dealing more generally with model comprehensibility; the other, with existing tools for model documentation and transparency.

In general, there are several approaches to tackle the need for comprehensibility in model-based ESS. One is the use of standards which mainly refers to requirements for documentation and data handling. Standards enable the reader of ESS to find a common understanding of the whole modeling process. Examples which strive for the standardization of applied models, data sets or assumptions are calls for research projects in the context of the German *Energiewende* [23] as well as requirements of methodologies [24] and planning tools for policy advice in the USA [25].

Open source and access approaches for both model code and the related data are another way of dealing with the previously described challenges. The concept incorporates advantages such as improved reproducibility of results or distributed peer reviewing, which partially eliminates shortcomings regarding the comprehensibility of energy scenarios. While the idea of open source and access is claimed to be essential for transparent research and reproducibility [26, 27], the matter has not been fully established in model-based energy scenario analysis yet. Nevertheless, open access policy is a requirement for funding grants in some research fields, such as the Public Access Plan of the US Department of Energy (DOE) [28]. The plan demands that all DOE-granted publications have to be uploaded to a public repository, while for the related data, a data management plan has to be provided.

The issue of model documentation in scientific work is notably addressed in the field of ecology. Benz et al. [29] introduce ECOBAS, a standardized model documentation system that facilitates the model creation, documentation and exchange in the field of ecology and environmental sciences. ECOBAS is designed to overcome the difficulties in writing model documentation and applying the documentation to any model language. Schmolke et al. [30] and Grimm et al. [31] propose 'transparent and comprehensive ecological modeling evaluation' (TRACE), a tool for planning, performing and documenting good modeling practice. The authors aim to establish expectations of what modelers should clearly communicate when presenting their model (e.g. clear model description and sensitivity analysis of the model output). The purpose of a TRACE-based document is to provide convincing evidence that a model is thoroughly designed, correctly implemented, well-tested, understood and appropriately applied for its intended purpose.

In the context of model-based research in the social sciences, Rahmandad and Sterman [32] provide reporting guidelines to facilitate model reproducibility. They distinguish between a 'minimum' and a 'preferred' reporting requirement. For computer-simulation models, they further differentiate between a 'model' and a 'simulation' reporting requirement. Two types of simulation methods are commonly used: agent-based modeling (ABM) and system dynamics (SD). For studies using ABM, Grimm et al. [33] suggest a framework via the Overview, Design concepts, and Details (ODD) protocol and provide examples of how to apply it. The ODD can be understood as a communication tool to enable ABM replication. Later, the authors assess the critical points raised against ODD and offer an updated and improved version of the protocol [34]. Concerning the SD approach, Rahmandad and Sterman [32] illustrate how to implement their reporting guidelines using an innovation diffusion model. In principle, the SD modeling approach is suitable for a high level of model transparency. However, although the qualitative visualization of an SD model is common practice, this is not always the case for the model code. Efforts to enhance the documentation of such models are made by e.g. [35].

In the context of policy analysis, Gass et al. [36] propose a hierarchical approach for producing and organizing documentation of complex models. It recommends four major documentation levels: (1) rote operation of the model, (2) model use, (3) model maintenance and (4) model assessment. Another documentation framework, especially designed for energy system models, is published by Dodds et al. [37]. The focus of the work lies on the challenges due to the increasing complexity which is affected by the ongoing development of often applied optimization models. Although the proposed design metrics are influenced by the structure of optimization models, the presented approach incorporates a way of dealing with the evolution of different model types and thus their input and output data as well.

In essence, the literature shows that standards enable comprehensibility through the harmonization of regulations, frameworks and documentations, whereas open source approaches provide comprehensibility through transparency. However, on the one hand, standards, such as ECOBAS or ODD, are often specifically designed for a certain field of research (ECOBAS: ecology and environmental sciences) or model type (ODD: agent-based models). In this sense, we think that they are an adequate way to tackle what we call model comprehensibility, but do not provide full result comprehensibility. On the other hand, we consider open source approaches to be an extreme case of transparency that does not automatically facilitate the comprehensibility of studies for policy advice. For instance, in order to benefit from full open source, substantial investment in familiarization with the source is required. Thus, depending on the background knowledge of an ESS user, open source may also compromise the comprehensibility of a study due to information overload. The latter can be tackled through different levels of details (for a broader discussion of this issue, see section 'Results and discussion'). Our contribution to the current state of research therefore addresses a synthesis of standardization and increasing, but balanced, transparency in energy scenario studies (including result and model comprehensibility), if these are to be seen as the result of reproducible, scientific research.

Methods

Conceptual framework

In order to clarify the meaning of frequently used terms within the following text sections, Fig. 1 shows the data and information flow within a model-based ESS. Its purpose is to consistently put the key terms 'Empirical data', 'Assumptions', 'Model exercise', 'Results' and 'Conclusions and recommendations' into a context representing the background for the construction and discussion of transparency criteria. Thus, the conceptual framework follows the typical steps of conducting a model-based ESS: collection and preparation of empirical data for the model-based data processing, assumption-making, model application and preparation of model outputs as well as deriving comprehensive conclusions and recommendations. As depicted in Fig. 1, empirical data can be divided into primary input data which is imported to the model directly and secondary input data which needs pre-processing before being imported. The model exercise contains at least one model (here called 'model A'). However, in some cases, a combination of two models or more is applied (for simplicity, we depicted a combination of only two models via a linkage stream). Similar to input data, outputs are divided into primary and secondary data. Further, this figure illustrates that assumptions can be made for the model as well as optionally for the pre-processing, post-processing, additional applied model(s) and linkage(s) between models. Results represent the last step of the model exercise. They are given based on the model output data. Finally, conclusions and recommendations are made based on the whole chain from the empirical data to the results (indicated by the solid arrow in Fig. 1).

Construction of transparency criteria

With the aim of increasing the transparency of ESS, we collected criteria on information needed to understand the fundamental contents of an ESS, initially adopting the perspective of an ESS user. The applied methodology can be seen as an alternating combination of two established approaches: qualitative expert interviews [38] and expert validations. Applying the conceptual framework

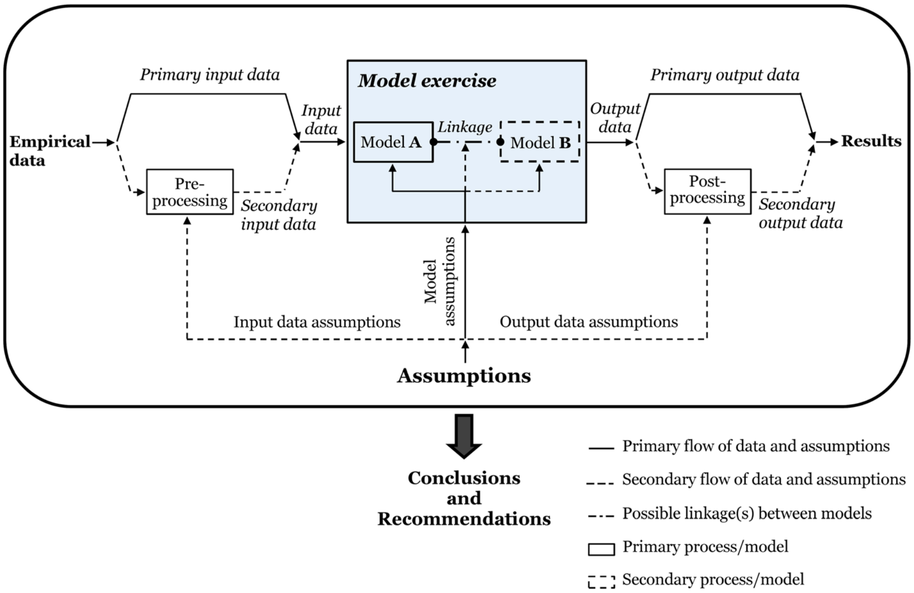


Fig. 1 Information flow and data processing in model-based Energy Scenario Studies (ESS)

above introduced, we set up a first collection of transparency criteria. It is based on the results of an ESS assessment workshop conducted by members of the Helmholtz School on Energy Scenarios [39]. In individual preparation for this workshop, specific questions[7] on two explicit ESS [40, 41] had to be answered. As all of the participants of this workshop are ESS authors as well as users, the initial compilation of transparency criteria represents the first round of the expert validations.

Meeting the identified transparency criteria means creating a complete and comprehensible overview of the underlying work and premises of an ESS. We found that this information needs to be provided in a format that can be easily used. Standard protocols or rather strict guidelines can help to list and describe assumptions as well as to transparently communicate the functional links between these and the model results. However, formulating such an instrument in a way that is too constricted bears the risk of high entry barriers and prohibits transferability over a wide range of model-based ESS. We therefore concluded that a simple as well as flexible tool is essential and intentionally propose the format of a checklist.

Thus, we subsequently rearranged the first collection of transparency criteria for ESS and extended it by frequently asked questions (FAQ). The first version of the checklist represented the template for individual interviews and discussions with three German post-doc researchers, one expert working with energy system modeling and two experts in the field of energy scenario assessment and scientific policy advice. Hence, the listing was updated by the feedback of these selected experts. For the second expert validation round especially, the perspective of ESS authors was emphasized. The idea of a transparency checklist for ESS was presented during the second workshop of the openmod initiative [26], attended by 35 researchers from European research institutions who are experienced in the field of energy system modeling. The presented version of the checklist was again evaluated and updated with respect to the feedback of the openmod workshop. Considering the outcome of our literature research, we finally added study examples to each transparency criterion and conducted final expert interviews. This time, one post-doc social scientist and one post-doc energy system modeler were asked to suggest improvements to the checklist.

In the following sections, we call the final product of this construction process the 'ESS transparency checklist'.

Limitations of the construction approach

Individual expert interviews are a well-established methodology in social science [42]. In addition, the expert validation has similarities to DELPHI approaches [43]. Hence, it provides the evaluation of a broad set of opinions on an interdisciplinary research topic and subsequently complements the individual expert interviews. It represents therefore an appropriate way to avoid expert dilemma and to gain an intersubjective collection of transparency criteria as far as possible [44]. However, only a limited number of experts were involved in the checklist compilation. Also, it should be noted that the energy modelers obviously dominated the selection of respondents. Thus, the checklist cannot claim to reflect a representative range of opinions in the scientific community dealing with ESS.

Moreover, the provision of a checklist template allows on the one hand a comfortable way to compare the outcome of the interviews and to extend it with additional viewpoints. But, on the other hand, as an existing guideline, it also restricts the spectrum of conceivable criteria to be discussed. Consequently, possible improvements to the construction methodology could be achieved by extending it by both further approaches such as constellation analysis [45] as well as a broader and more balanced selection of involved experts.

Results and discussion

The ESS transparency checklist can be seen as an overlay communication protocol between ESS authors and users which is not intended to automatically assess the quality of ESS and their content (data, model or assumptions), but at least to enable readers to assess these points for other addressees or their own work.

From the point of view of an ESS author, the collection of transparency criteria results in a checklist containing questions which are frequently asked by modeling experts trying to understand an ESS done by other experts. In this context, a checklist gives unexperienced ESS authors a summary of important aspects that need to be considered, especially for performing a scenario-based analysis used for deriving recommendations for decision-makers.

From the user's perspective, the ESS transparency checklist is a catalogue of FAQ related to a section of the appropriate ESS document or report. Consequently, adding the proposed checklist to an energy scenario study means in a broader sense providing effective access to individually relevant and structured information to the user by an additional table of contents. The experienced reader benefits from this representation format of transparency criteria because time-consuming searching through the document for specific information can be avoided.

The ESS transparency checklist and its application

We distinguish between two versions of the transparency checklist (see section 'Appendix'). The *full version*, provided at the end of this manuscript, can be seen as the checklist's manual which clarifies in detail what is meant by the various criteria. This is realized in three ways: by asking relevant expert questions, by using simple made-up examples and by referencing an existing study that meets the particular criteria. Although we consider the ESS transparency checklist to be, in principle, applicable to any model-based scenario study, the examples provided are, given our focus, pertinent to energy scenarios.

The second version of the transparency checklist is the *reduced version*. This version is intended for application to a particular ESS (cf. Table 1). As an additional table of contents, this reduced version only consists of the transparency criteria and a second table column. In the latter, an ESS author only has to enter the specific page numbers of the study, on which a certain transparency criterion is supposed to be fulfilled. However, the extent to which any criterion is met depends on the ESS authors' assessment. With the checklists' primary purpose to raise awareness for transparency, we intentionally chose this open way of dealing with the transparency criteria to keep the cost of its application low. Thus, ESS authors can use the reduced version of the checklist at ease and add it to any document without the need of

Table 1 The reduced version of the ESS transparency checklist to be used as an additional table of contents

Criterion	Page number
General information	
1. Author, institution	
2. Aim and funding	
3. Key term definitions	
Empirical data	
4. Sources	
5. Pre-processing	
Assumptions	
6. Identification of uncertain factors	
7. Uncertainty consideration	
8. Storyline construction	
9. Assumptions for data modification	
Model exercise	
10. Model fact sheet	
11. Model specific properties	
12. Model interaction	
13. Model documentation	
14. Output data access	
15. Model validation	
Results	
16. Post-processing	
17. Sensitivity analyses	
18. Robustness analyses	
Conclusions and recommendations	
19. Results-recommendation relationship	
20. Uncertainty communication	

changing the structure or content of the ESS it should be applied to.

Discussion of transparency criteria—the full version

In the following, we discuss the several categories of the ESS transparency checklist in more detail. It is mainly conceived for practitioners to facilitate full application of the checklist (see section 'Appendix').

This should be enabled by additional columns for a further description of the criteria. So, the column 'transparency question' contains one or more exemplary expert questions which can be assigned to a transparency criterion. The column 'examples and further description' shows simple examples for formulations that would contribute to fulfilling the transparency criterion. Finally, the column 'applied study' gives a concrete example of existing ESS where providing transparency is done from our point of view.

General information

The first part of the ESS transparency checklist targets basic background information required for the interpretation and classification of a study. Apart from giving information about the ESS author(s) and the institution(s), one key point is the communication of the objectives (e.g. overarching research question) and the funding of the study [46]. Another point that affects the interpretation of a study is the use of key terms, which usually depend on the professional background of the ESS authors. Often, similar terms are used which have very different meanings or definitions. Thus, we propose by providing a glossary describing those terms to avoid potential misunderstandings and misinterpretation of the study's outcomes ('Key term definitions').

Input data preparation

The main part of the ESS transparency checklist deals with the model exercise which, in a more simplified way, could be described as data processing with a model. Thus, the checklist's categories coming along with the model exercise ('Empirical data', 'Assumptions', 'Results and conclusions') include topics such as data sources, data selection, data processing or the interpretation of data.

As well as distinguishing several types of data like inputs and outputs, the ESS transparency checklist also stresses a distinction between data influenced by assumptions and data that is gained from the past. The category Empirical data therefore asks how the latter is treated. This kind of data is also known as primary data and includes data from statistical surveys (e.g. databases of the International Energy Agency [47]) or measurements of physical quantities (e.g. technical datasheets). According to the three levels of transparency [18], listing the sources of the empirical data and pointing out the modifications that are applied corresponds to providing the 'opaque box'. Thus, full transparency goes a step further and means also enabling access to the used primary data as it is described by [48] for the treatment of fundamental electricity data.

'Pre-processing' of data is often done to unify the given data from different sources or to adapt it to the requirements of the modeling environment. Due to a lack of appropriate empirical data, this also commonly goes along with the formulation of assumptions ('Assumptions for data modification'). A typical example is the spatial unification of technical characteristics and costs, which means that known regional differences of these parameters are ignored or considered to be negligible. Since such assumptions seem to be quite irrelevant in regard to the overarching objective of the study, they are often rarely documented. However, assumptions are an indispensable part of an ESS and therefore play a crucial role for the input and output data preparation as well as for the application of different model types (cf. Fig. 1). The knowledge about these assumptions is thus a precondition for ensuring complete reproducibility of the modeling exercise.

Assumptions communication

Besides the assumptions for data modification, estimations about the future developments also cannot be made without assumptions. The ESS transparency checklist emphasizes this issue with the following criteria for assumptions communication which are based on the three typical steps of a scenario construction process:

First, the necessity of the model exercise to rely on assumptions leads to intrinsic uncertainties within the study's conclusions and derived recommendations. In principal, two fundamentally different types of uncertainty exist. On the one hand, input data is associated with possible ranges of values and therefore may affect the outcome of ESS (data uncertainty). On the other hand, the model approach itself might include undetectable inaccuracies intrinsically (model uncertainty). The latter might also be interpreted as an error due to abstractions of the real world in order to create a simplified model. In this sense, Brock and Durlauf [49] give the example of economic actors which cannot fulfil the assumptions regarding rational behavior in macroeconomics (i.e. *homo oeconomicus*). A broader definition of uncertainty is given by Walker et al. [50] who describe uncertainty as 'any departure from the unachievable ideal of complete determinism' (p. 8). Trutnevyte et al. [51] point out that different dimensions of uncertainty (e.g. input data uncertainty, unawareness or unpredictability of events) lead to an infinite amount of robust scenarios. Therefore, the decisions about which uncertain developments are included and excluded in an ESS play a major role for the interpretation of its outcomes. The transparency criterion 'Identification of uncertain developments' addresses the associated requirement to communicate those uncertainties which are explicitly assessed in the study.

For the derivation of model inputs, usually, a range of future developments can be identified which is addressed by bandwidths of qualitative or quantitative values. In terms of quantitative values, it is a good practice in scenario studies to deal with them by performing parameter variations on input data. However, the number of practicable model runs is limited, and the number of assumptions can become quite large. Hence, parameter variations cannot be done for all quantitative values, and also qualitative assumptions are not covered by this approach.

There are qualitative assumptions which are considered only indirectly in a study, e.g. if a very high share of electric vehicles is assumed, this goes along with lifestyle changes, although those are not stated explicitly in the study. Still, qualitative assumptions like lifestyle changes can also find direct access in ESS by translating them into quantitative values for model input. But even in this translation process, it goes along with assumptions which do not necessarily have to be explicit. Therefore, the meaning of specific assumptions on the study's outcome is only comprehensible if it is complemented by the information in which way the corresponding uncertainties are treated in the study. Thus, the second aspect of assumption communication is about how the main uncertainties are considered ('uncertainty consideration'). This includes statements whether the bandwidth for certain numerical values which go into the model are justified by applying approaches such as own estimations, literature research or expert workshops. Even the explicit information that instead of a bandwidth, only a single, numerical value is chosen arbitrarily can contribute to an increase of transparency.

Third, to combine the involved assumptions to an applicable model framework, a storyline is usually constructed ('storyline construction'). 'Storyline-based scenarios are expressed as qualitative narratives that in length may range from brief titles to very long and detailed descriptions' (p. 26) [52]. For the users of model-based ESS, it is of interest what the storylines are about, how they were constructed and which normative assumptions[8] are included there as they are used to determine the relevant ranges for numerical assumptions.

Modeling

A critical aspect regarding transparency is the balance between enabling access to all relevant information and information overload. The easiest way of tackling this issue is to provide information on different levels of detail. In the case of listing all assumptions, this can be realized by selecting the crucial or new ones for the main document of the study while referring to an extra document which contains the complete list of assumptions.

Balanced information sharing is especially important when it comes to the description of the modeling itself. Thus, to be transparent and nevertheless avoid overstraining the user, we suggest different levels of detail for the model documentation beginning with a factsheet. The model factsheet lists basic information which is useful for comparing similar models. This includes the model category, its temporal resolution or its geographical and sectoral focus. As an example for model classification, we propose Fig. 2 given at the end of the full version of the ESS transparency checklist.

Another criterion on the ESS transparency checklist targets 'model-specific properties' which aims at providing a critical assessment regarding explicitly what the model can show and what it cannot show. Concerning the aforementioned risk of information overload, we suggest listing here only key aspects such as new equations or modules implemented. The 'model documentation' further refers to a more detailed information level of the process of modeling. This entails a description of how the perception of a real world problem is translated into a quantitative abstract model using mathematics (predominantly equations). It may also touch upon issues such as the range of application of the model and the feasibility of implementing the policies examined in the model. A separate document (following e.g. the TRACE guidelines [31]) may be used in this case, thereby mitigating the impact of information overload. Providing a structured and user-friendly documentation can be a challenging task as its users might have different expectations about the content. These can range from tutorials for out-of-the-box model application to concrete source code implementation details for further model development. In addition, usually model source code evolves continuously which demands maintaining also the documentation. In this regard, Dodds et al. [37] propose an approach called model archaeology to especially incorporate the effect of different model versions on the documentation in a structured way. While open source represents the most detailed information level in this context, it can be stressed that even limited access to the models' source codes contributes to an increase in transparency of a certain ESS.

As mentioned above, the model itself represents a source of uncertainty. It is state of the art to perform validation tests to tackle this issue. But as models applied for energy scenario studies cover whole systems and usually assess possible future developments, classical experimental validation techniques are rarely applicable on these models. However, several approaches exist to check the model's outcome. They range from simple structural validity tests (e.g. plausibility checks) to more sophisticated methods like empirical validity tests (e.g. back testing of the system's historical behavior) [18]. For a better external assessment of the model quality, the ESS transparency checklist therefore also lists the criterion 'model validation' where the applied methods can be documented.

Moreover, typical experts' questions aim at distinguishing inputs and outputs. Therefore, independent of what happens within a specific model, a clear labeling of the inputs and outputs of the model is required. This information becomes especially important if more than one model is involved in an ESS. In order to be able to assess whether a result is already predetermined by assumptions going into the model exercise, it is necessary to show by which input parameters an output value could be affected. Consequently, the transparency criterion 'model interaction' emphasizes the data exchange of a model with its environment. This environment can either be other applied models or in the simplest case the inputs and outputs of the whole model exercise.

To illustrate this model interaction in terms of transparent information exchange, various approaches exist. Standardized model documentation protocols, such as ODD or TRACE (see section 'Literature review') propose simple tables and class diagrams using Unified Modeling Language (UML) [53] for the documentation of model variables. However, we think that these methods are also applicable to show model interaction. The ODD protocol [33] suggests flow charts or pseudo-code for the transparent process overview and interactions between models. In addition, also a kind of interaction matrix could be provided. For instance, a listing of all inputs and outputs involved in the model exercise represents the matrix's rows, whereas each individual model of the model exercise is represented by a column. Finally, by checking the appropriate cells of the 'interaction matrix', the model interaction could be indicated.

Model output and results

Besides the required knowledge about the origin of certain data, we take the view that on a more detailed information level, also all numerical values generated within the study need to be accessible. The associated criterion 'output data access' is strongly connected to the transparency criteria regarding the results communicated in a study. But, since the raw model outputs are usually post-processed for the presentation of the study's outcome, we explicitly distinguish it from the 'Results' which represent information in a more condensed way. Although the usual purpose of these data modifications is the reduction in the complexity of the results (e.g. for answering the overarching research question), even assumptions can play a role at this point of the model exercise. In the simplest case, applying mathematical aggregation functions such as summation does not affect the meaning of the results (e.g. summing up the CO_2 emissions of administrative regions to obtain the number of total CO_2 emissions of a state). But, in contrast to this, data interpretation is another source for output data modification. ESS authors need to be aware that even if such data modifications are not intended, implicit assumptions such as individual opinions can affect the data interpretation and accordingly the results of the model exercise itself. Consequently, stating adaptations applied to the output data, the transparency criterion 'post-processing' aims at raising awareness on the ESS authors' side.

In order to assess the discussed types of uncertainty (see section 'Assumptions communication'), different methods exist. The most prominent examples are sensitivity and robustness analyses. While the former investigates the effect of input parameter variations on the results within the *same model*, the latter employs *different models* to validate the outcome of a specific ESS.

In the case of sensitivity analyses, Hamby [54] reviews alternative approaches. He shows that the use of sensitivity analysis techniques provides valuable insights with regard to the correlation of specific input parameters with the model output and also enables the elimination of certain input data due to its insignificance on the results.

Weisberg [55] defines a robustness analysis as 'an indispensable procedure in the arsenal of theorists studying complex phenomena' (p. 742), which examines 'a group of similar, but distinct, models for a robust behaviour' (p. 737), searching for 'predictions common to several independent models' (p. 730). Brock and Durlauf [49] further suggest Bayesian analysis as a method to quantify model uncertainty, but argue that a robustness analysis is most appropriate for models which are characterized by rather similar purposes. An example for an uncertainty analysis in ESS using a Bayesian model is given by Culka [56].

To attribute the effect of input parameter and the model selection on the results, both sensitivity and robustness analyses are listed as criteria in the ESS transparency checklist.

Conclusions and recommendations of model-based ESS

Although the ESS transparency checklist aims at ensuring model comprehensibility for experts in the first place, making the model exercise transparent is not sufficient to justify conclusions. As a fundamental part of a scientific study, the conclusions represent, in contrast to the model outputs, the outcome of the whole modeling framework. Especially, this part of the checklist assists ESS users to fully grasp the studies' outcomes. The conclusions are supposed not to be drawn only from the model results, but also to take into consideration the underlying assumptions. Concerning communication of the latter, the Progressive Disclosure of Information (PDI) strategy offers a detailed guideline [21].

As in ESS, 'Conclusions and recommendations', in general, are mostly intended to give some kind of advice to decision-makers, and another level of information detail is required to assess the study's outcome in terms of answering the overarching research question. This means that even if the necessary information for an uncertainty assessment by external experts is provided, we recommend that ESS authors give a statement about the effect of uncertainties, because they are the most knowledgeable about the model exercise. For instance, it can be explicitly stressed which alternative future developments are also possible even if they are not covered by the studies' results.

Information on how the uncertainties have been dealt with is required not only for the formulation of the conclusions but also for the formulation of the recommendations. Depending on the degree of uncertainty, three types of statements are possible: probabilistic, possibilistic or deterministic. This has an influence on how recommendations are communicated. As an example for improving current practice, ESS authors could learn from climate research which delivers a prototype for giving policy advice taking into account uncertainty communication [57]. Probabilistic statements for explorative scenarios rarely can be made since the capability to predict future developments is limited [58]. A common misinterpretation by ESS users is mistaking of business-as-usual scenarios as predictions of what *will* happen (instead of what *can* happen).

In addition, the missing transparency of how concrete proposals for decision-making are derived from the theoretical model exercise was a major critique on existing model-based ESS during the process of developing the transparency criteria. The ESS authors face the risk that their recommendations are perceived as untraceable or, in extreme cases, arbitrary if they fail to clarify the relationship between their conclusions and their recommendations. In order to mitigate this risk, the ESS authors should provide a clear argument for their recommendations. This would mean that the description of the causal chain captured by their model is complemented by argumentation analysis to support their recommendations, thereby highlighting the process by which the results-recommendation relationship is created.

Limitations of the ESS transparency checklist

The ESS transparency checklist as a first step to improve transparency in ESS is an expert-to-expert tool. This entails a restricted perspective of the issue of lacking transparency in ESS as well as a limited transferability to non-experts. However, the difference in perspective between experts (here, modelers or ESS authors) and non-experts is important. For example, Walker et al. [50] explicitly distinguish, in the context of uncertainty, between the modeler's view and the decision-makers' or policymakers' view. To some extent, the transparency criteria in their current form are beneficial for non-experts as they provide a first insight into the key assumptions and methodologies of an ESS. Nevertheless, although this may be of value to non-experts, addressing their needs in a more comprehensive manner requires an approach that differs from the ESS transparency checklist. For instance, an adaptation or enlargement of the transparency checklist might ensure applicability to a broader audience.

Furthermore, asking ESS authors to fill out the checklist by themselves may raise the question of quality assurance and as a qualitative empiric tool the checklist includes potential conflicts of interest of energy modelers. However, with regard to this, for quality assurance, we rely on the practice of good scientific conduct in the modeling community.

Finally, the ESS transparency checklist facilitates and also requires a certain level of standardization, which is a key element in order to provide comparability of model-based ESS. Consequently, it determines to some extent in which way ESS are presented (i.e. what information is conveyed and at what level of transparency). However, it is important to stress that standardization is not a panacea, since ESS are very diverse and the current version of the checklist naturally does not exhaust all reporting possibilities. This is one reason why ESS authors might find it challenging to apply the checklist to their study.

Conclusions and outlook

If ESS are to meet their purpose, openness to public scrutiny is needed. We argue that a high degree of transparency in consonance with scientific standards is still pending in model-based ESS. In this paper, an instrument to tackle this issue has been proposed in the form of the ESS transparency checklist. This tool is conceived as an addition to transparency approaches such as open source which represent so called glass box (i.e. high level of transparency) models. It presents the key information of model-based ESS in a compact and standardized manner. In practical cases where, for various reasons, ESS authors are unable to provide their glass box model, the checklist may be used as a tool that meets a minimum requirement for transparency.

The ESS checklist is the outcome of a process which includes literature review, expert interviews and expert validations. Its structure follows the method of data and information processing within a model-based ESS. Therewith, it distinguishes between input parameter modification in advance of the modeling (pre-processing) and post-processing which aims at condensing rare model outputs (post-processing). Stressing, especially, the importance of assumptions communication and model documentation, the checklist considers different levels of detail to provide information for study users with different degrees of knowledge about a modeling exercise. Although the ESS transparency checklist appears to be a useful tool for modeling experts in the first place, it is the first step for a standardized communication protocol between performers and assessors of complex studies in the field of energy scenarios.

We do not expect to leave this issue completely resolved. Instead, an attempt is made to highlight one weakness in ESS, and we put forward our initial suggestion for improvement. For instance, we suggest the development of transparency criteria for a broader spectrum of addressees, such as the public or policy-makers. The reduced version of the ESS transparency checklist (see Additional file 1) can be a valuable starting point for this purpose, but further questions (e.g. 'What does a solver routine do?') need to be considered as well. In order to identify transparency criteria, e.g. for politicians or public stakeholders, we suggest further surveys, specially adapted to these addressees taking into account customized communication strategies as proposed by Kloprogge et al. [21]. A useful manner of addressing the needs of non-experts may be by means of producing a modeling guide for non-experts. Such a guide could contain fundamental issues and answers to questions a non-expert user should ask about the model exercise.

We think that the ESS transparency checklist is a simple but very helpful tool for authors and readers of ESS and expect that its adoption will help improve the quality of such studies in the future. We would like to invite potential users to benefit by applying it to their studies and reports. Comments and critiques from the research community and experienced users of model-based ESS are welcomed.

Endnotes

[1] In this paper, we refer to the following definition of the word 'scenario' given by the Intergovernmental Panel on Climate Change (IPCC): 'A plausible and often simplified description of how the future may develop, based on a coherent and internally consistent set of assumptions about driving forces and key relationships' (p. 86) [59].

[2] 'Availability bias' describes the tendency of ESS authors to include their knowledge of historic events (e.g. the past development of electricity prices) and own experience into the rationale behind their model parametrization or model methodology. In consequence, unexpected or disruptive elements might be neglected in the modeling approach. For the availability heuristic and availability biases in the context of risk, see [61, 62].

[3] In this paper, a 'model' is defined as a mathematically consistent framework including an inter-dependent set of equations which aims to analyse how phenomena occur in a complex system. It is usually in the form of a computer algorithm.

[4] In general the terms 'reader' or 'user' are reserved to designate those people who—expert or not—use the outcome of ESS, e.g. for decision making or subsequent modeling exercises. Note that this paper addresses expert users in particular.

[5] By assumptions, we mean reasonable, best guess definitions for unknown values or relationships between variables which are supposed to be plausible but cannot be directly validated by measured data. In ESS, this applies either for future developments, generalization in order to reduce complexity (of data or models) or incomplete data sets for which measurements are not fully available. Thus, assumptions may differ depending on the professional background, intention, or even ideology of persons who make them.

[6] The term 'ESS author' refers to those people who develop ESS. Thus, in this paper, ESS authors can be understood as modeling experts having the intention to document an ESS. Often ESS authors are also readers of ESS.

[7] A complete summary of the questions from the workshop is attached to the 'Appendix' section below.

[8] These normative assumptions are a part of the storyline. For instance, they do influence the distinction of what is (not) included in the data processing and therefore define the system boundaries of the model(s).

Appendix

Questionnaire for the initial collection of transparency criteria

Assumptions

What assumptions about price paths and technology costs in the future were made and how do they affect the scenario results and derived recommendations? Is there sufficient transparency to assess this? Are the assumptions well-founded or could other developments be assumed just as well?

Scenario methods

How can the basic methodology of the scenario construction be described and how can we distinguish it from other approaches? In particular, which methodology has been used to develop future technology splits for the electricity, heat and transport sectors and how far have economic and infrastructural aspects been taken into account (keyword: system costs)? Is the study sufficiently transparent to assess this?

Consistency

Are assumptions and scenario results consistent (consumption and demand drivers in the energy sectors, supply/generation, costs, and conclusions)? Is there sufficient transparency to judge this? Are interactions between the electricity, heat and transport sectors considered?

Uncertainty

How does the study communicate uncertainties of its main findings? Are scenarios considered to be plausible worlds, or possible future pathways, or likely evolutions of the energy system? Do the main findings of the studies represent possibility statements? Are uncertainties expressed in a probabilistic way, either qualitatively or quantitatively? Does the study pretend to arrive at robust results? And is the specific way the study presents uncertainties adequate?

Policy advice

Does the study derive policy recommendations from the scenarios? If so, how? And is this reasoning valid? Which additional normative assumptions enter the derivation of policy recommendations and are they made sufficiently transparent?

Reception

How has the study been received (in the public, by stakeholders, in the media, etc.)? Has this reception been politically biased? Were the findings over-simplified and did this seriously distort the original content of the study?

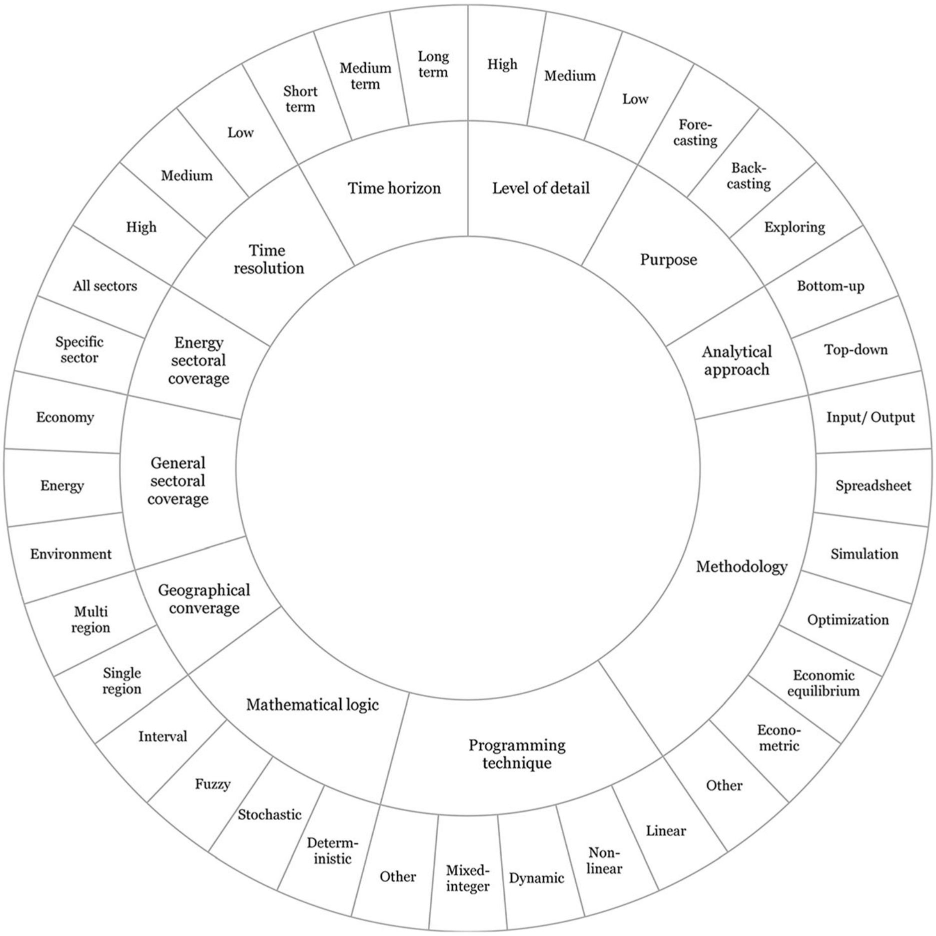


Fig. 2 Classification of energy system models based on [81]

Table 2 Full version of the ESS transparency checklist

Criterion	Transparency question	Examples and further description	Applied study and page number
General Information			
1. Author, Institution	–Who are the ESS authors and for which institution(s) do they work?	–John Doe (Scenarios Inc.).	–[40], pp. 2–3 displays information on the study partners, the name of the project manager and lead author, the names and institutes of the research team (co-authors) and the editors.
	–In case of a collaborative ESS, what are the authors' contributions in detail?	–'John Doe developed the model, while Jane Doe was responsible for the interpretation of the results.'	
2. Aim and funding	–Who are the costumers requesting the study? –Is there external funding? If yes, what is the source and to which proposal does it refer? –What is the purpose (hypothesis) and research question of the study? –What is different in comparison to the current state of research?	–Study commissioned and fully funded by Energy Inc. –'Giving policy advice to show whether Nuclear Phase-out in Germany by the end of 2022 is affordable.' –'A novel methodology is used, beside new cost parameters which were included.'	–[24], pp. ii expresses that the study is funded by an Agency of United States government. –[60], pp. I present the core objective of the study which is to show a pathway of moving toward a nuclear-free European Union.
3. Key term definitions	–How are key terms used in the study's context?	–Different terms to address the same matter: 'Grid balancing' and 'power system flexibility' both mean the availability of an energy system to shift power to match supply and demand. –The same term used for different matters: 'Demand' can be interpreted as useful demand or final energy consumption.	–In the context of car propulsion, [61], pp.76–78 clarifies the different automotive technologies. The study also includes a list of acronyms (p.145), but not a glossary.
	–Where are key terms defined?	–'Key terms are defined in the main text'/'The study includes a glossary section.'	
Empirical data			
4. Sources	–What are the sources of empirical data?	–'Power-plant capacity and spatial distribution base on Enipedia [62].' –'Economic statistics, such as electricity or gas prices, are provided by Eurostat [63].'	–[64] Allows online visualization of the data used in the study and the possibility to download the data in an Excel file. For transport, such a file contains information on the units but not the source of data for historical values.
5. Pre-Processing	–Are empirical data used directly as model input or are data pre-processed? –How is the characteristic of the empirical data adapted to the input requirements of the model(s)?	–'The spatial resolution of the empirical data is national energy demand of a country (e.g. Germany). The model needs a spatial resolution for administrative regions (e.g. Berlin). Therefore, the national energy demand is multiplied by distribution factors for each administrative region.'	–[65], p.32 use output from different models and studies and modify with regard to their application. In this specific example, they aim to calculate the total earnings from construction and operation in a 100 % renewable energy based scenario. They therefore use raw, unscaled earning values from JEDI models (Economic Development Impact) and scale them in accordance with their prices to account for changes in wages and labor hours.
Assumptions			
6. Identification of uncertain factors	–What are the (main) uncertain factors and corresponding assumptions (quantitative and qualitative)?	–'All considered uncertainties concerning future developments can be found in the supplementary section.'	–[66], p.6 describes how the selection of uncertain factors was done, who was included, and which method was use. Pp. 7, 8, 10 list those factors which are explicitly considered in the study.

Table 2 Full version of the ESS transparency checklist *(Continued)*

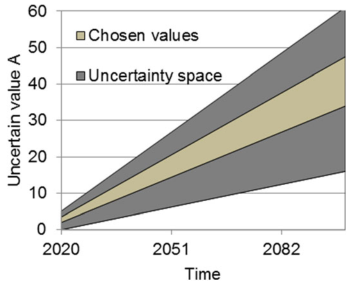
	–Which uncertain factors are explicitly considered in the study?	–'For all types of power plants a general standard efficiency is assumed according to the following table…' –'We take into account lifestyle changes (qualitative factor), as well as the growth rate of the oil price (quantitative factor).'	
7. Uncertainty consideration	–How do you deal with the uncertain factor you have identified?	–'Lifestyle changes are considered indirectly by their impacts on other factors (e.g. demand and efficiency).' –'Oil price is considered directly as an assumption of the model application by an expert's opinion.'	–[67], pp. 387–389 explain the key driving forces of the scenario study and their assumed alternative developments in the future. They also mention how the assessment was done.
	–Which (alternative) development paths are assumed for the uncertain factors?	–Qualitative assessment: 'Lifestyles could be oriented towards sustainability, materialism or economics by 2050.' –Quantitative assessment: 'Oil price growth can be at least 0 %, but not more than 80 % by 2050.' –'GDP growth is fixed to 1.6 % per year.'	
	–What are the sources of the chosen development paths?	–Heuristic. –Empirical (expert knowledge e.g. 10 economists, 10 consumers, literature review).	
	–Why and how are individual values chosen from a bandwidth of possible values?	 –'The chosen values are based on own assumptions/desk research/expert workshop/ literature review.'	
8. Storyline construction	–What narrative description of scenarios is used which highlights the main scenario characteristics and dynamics? –What is the relationship between the key driving forces?	–Qualitative narratives can vary in length from brief titles to very long and detailed descriptions.	–[68], pp. 763–764 mention which groups of actors were included in the construction process of the narratives (stakeholder visions) and furthermore describe the methodology, how the visions were created. On p. 766 a description of the applied visions can be found.
	–Which method is used to construct the storyline(s)?	–Interdisciplinary expert workshop (social scientist, psychologist, engineer, economist). –Intuitive scenario construction (no specific method).	
	–Which normative assumptions are included in the storylines?	–Political targets for green house reductions	

Table 2 Full version of the ESS transparency checklist *(Continued)*

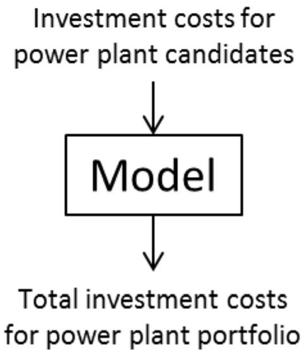
9. Which assumptions are related to the modification of model input?	–For the mentioned example in the section 'Empirical data': The pre-processing is done by splitting up the national energy demand by population density. The assumption related to this is that the energy demand is proportionally distributed to the population density.	–In [69] pp.30–31 a description is given how the nationally installed capacities of renewable power generation are distributed on a regional level.	
Model exercise			
10. Model fact sheet	–Which kind of modeling approach is used?	–Bottom-Up, Top-Down, Hybrid. –Optimization, Simulation.	–[41], p.85 lists the geographical scope (European Union) as well as the models' time horizon (1990–2050).
	–What is the geographical coverage of the model? –What temporal resolution and time horizon uses the model?	–Global, 2005–2050, hourly time steps. –For a comprehensive overview on model classification see also Fig. 2.	
	–Which sector is addressed by the model?	–Energy (power, heat,…), economy, environment.	
	–How does the model deal with uncertainties?	–'The model is deterministic and does not include random elements.' –'The model is mainly deterministic but incorporates stochastic components (e.g. includes Monte Carlo simulations based on probability distribution assumptions for key parameters).' –'The model is mainly stochastic as it is based on probability theory (e.g. econometric model).'	
11. Model specific properties	–What are the main specific characteristics (strengths and weaknesses) of this model regarding the purpose of the recommendation? –What are the new equations or essential equations?	–'High level of technology detail.' –'It is assumed that demand can be derived from GDP with a linear formulation which could also be formulated nonlinearly.' –'For modeling shareholder strategies new equations are implemented and the objective function is extended.'	–[70], pp.8–25 lists several models with their specific strengths regarding the spatial or sectoral focus.
12. Model interaction	–What is the input and output data of the model exercise? –Does the model exercise include several models? If so, which data do these models exchange?	–Flow chart:  	–[71], p.57 shows the interaction of several models.

Table 2 Full version of the ESS transparency checklist *(Continued)*

–Interaction matrix:

	Model A	Model B
Population	In	
Power Demand	Out	In
Power generation cost		Out

13. Model documentation	–Is there a complete documentation of the model available? –Where are the units and symbols used in the equations documented? –Is the model's source code accessible?	–'All used equations can be found in appendix A.' –'The open source model can be downloaded at…' –See also [29, 33, 35–37]	–The Mobility Model in [72], pp.369–378 is fully documented in the Appendix but it is not available for download.
14. Output data access	–Where can one find the numerical values (output) of the model?	–'All output values can be found in appendix B.'	–[73] shows the key model output at the beginning of the study (p. 2) and some key values in the 'Conclusions' section (p. 74). The numerical values can be obtained from their model (freely available on their website).
15. Model validation	–What kind of validation method is used?	–[74] and [18] distinguish between structural and behavioral validation. –[75] illustrates 12 types of tests.	–[76], pp.130–134 devotes a chapter section to the model validation, including structural, parameter and behavior validation (cf. his Table 21).
Results			
16. Post-processing	–Are the presented results directly taken from the models' output or are they modified? –Are additional assumptions applied for this modification?	–'The model outputs are on a regional level, while the research questions aim at recommendations regarding a national level. Therefore, the output data is simply summated.'	–[77] project highway fuel demand based on their estimation of vehicle stock. Table 3 (pp. 160–161) shows that post-processing is undertaken for total vehicles for 2030.
17. Sensitivity analyses	–How sensitive are the model results to parameter values variations?	–Univariate and multivariate sensitivity analyses: numerical, behavioral and policy sensitivity. –Extreme conditions tests.	–[78], pp. 61–62 perform detailed sensitivity analyses for the total system cost of European Energy System.
18. Robustness analyses	–Are the model results within the expected deviation compared to commensurable models?	–See also [55] –'All considered uncertainties concerning future developments can be found in the supplementary section.'	–[79] perform a robustness analysis of their model POWER against three other power system models.

Table 2 Full version of the ESS transparency checklist *(Continued)*

<table>
<tr><td colspan="4">Conclusions and Recommendations</td></tr>
<tr><td>19. Results – recommend-dation - relationship</td><td>–How do specific recommendations correspond to the results (e.g. output value or interpretation)?
–How do results of the model exercise support normative recommendations with respect to the assumptions?
–How far can the recommendations be differentiated?</td><td><table>
<tr><th></th><th>Categorical</th><th>Conditional</th></tr>
<tr><td>Probabilistic</td><td>With a probability of 0.2 climate goals will be reached.</td><td>If CO_2-certificates are more expensive, climate goals will be reached with a probability of 0.2</td></tr>
<tr><td>Possibilistic</td><td>It is possible to reach the climate goals.</td><td>If CO_2-certificates are more expensive, it is possible to reach the climate goals.</td></tr>
<tr><td>Deterministic</td><td>Climate goals will be reached.</td><td>If CO_2-certificates are more expensive, climate goals will be reached</td></tr>
</table></td><td>–[80], p. 3 recommends a global average fuel economy target based on emissions reductions and oil savings results.</td></tr>
<tr><td>20. Uncertainty communication</td><td>–Which normative assumptions are considered for deriving recommendations?</td><td>–‘Based on the assumption that the expansion targets for renewable energies will still be the same for the next 20 years, we recommend to further stimulate investments into new renewable technologies by applying the following…’</td><td></td></tr>
<tr><td></td><td>–How reliable are the results due to the uncertainty of the assumptions and the modeling (e.g. system boundaries, model simplifications)?</td><td>–‘The specific oil-price development being used is highly uncertain. The only thing we know is that such a development is possible. And we also checked that all other assumptions being used to calculate the output are consistent with each other. Hence, what we calculated is possible.’
–‘If we use these simplifications it can be checked in a smaller model, that this simplification leads to an underestimation of….’</td><td>–With the summary for policy makers the IPCC [57] states comprehensively the uncertainties, for instance by differentiating the likelihood of the results and outcomes on p. 4.</td></tr>
</table>

Additional file

Additional file 1: The ESS transparency checklist is freely available from [10.1186/s13705-016-0090-z]. The xls-file named "Cao et al. (2016) Additional file 1_Checklist" contains the reduced version. Both the reduced and the full versions of the ESS transparency checklist are shown in 'Appendix' section. (XLSX 39.5 kb)

Abbreviations

ABM: Agent-based modeling; DOE: US Department of Energy; ESS: Energy scenario studies; FAQ: Frequently asked questions; IPCC: Intergovernmental Panel on Climate Change; ODD: Overview, Design concepts and Details; PDI: Progressive Disclosure of Information; SD: System dynamics; TRACE: Transparent and comprehensive ecological modeling evaluation; UML: Unified Modeling Language

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Authors' contributions

All mentioned authors were involved in the conception and refinement of the ESS transparency checklist as well as the writing and revision of the manuscript, but with different main responsibilities. The transparency checklist was discussed and elaborated within workshops conducted by KKC, FC, BM and SP, and the expert interviews within that process were carried out mainly by FC and BM. The article structure was mainly elaborated by JGV as well as the first draft of the abstract, introduction and the conclusions. JGV and BM were mainly responsible for the literature review, SP for the section about the construction of the transparency checklist and KKC for the results section. Apart from those main responsibilities, all sections also include designed or drafted parts by other authors. KKC and FC integrated all feedback, comments and revisions in the paper and revised the paper according to the journals standards. Finally, all authors (KKC, FC, JGV, BM and SP) helped integrate the reviewers' comments. All authors read and approved the final manuscript.

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Competing interests

The authors declare that they have no competing interests.

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References

1. European Environmental Agency (2011) Catalogue of scenario studies. Knowledge base for forward-looking information and services. EEA Technical report No. 1. Available via: http://scenarios.pbe.eea.europa.eu/. Accessed September 2015
2. Gregory WL, Duran A (2001) Scenarios and acceptance of forecasts. In: Principles of Forecasting 30. Springer US, New York, pp 519–540. doi:10.1007/978-0-306-47630-3_23
3. Lempert RJ, Popper SW, Bankes SW (2003) Shaping the next one hundred years: new methods for quantitative, longer-term policy analysis. Santa Monica, Pittsburgh
4. Wright G, Goodwin P (2009) Decision making and planning under low levels of predictability: enhancing the scenario method. Int J Forecast 4:813–825
5. Dieckhoff C, Appelrath HJ, Fischedick M, Grunwald A, Höffler F, Mayer C, Weimer-Jehle W (2014) Schriftenreihe Energiesysteme der Zukunft: Zur Interpretation von Energieszenarien. Analysis ISBN: 978-3-9817048-1-5, Deutsche Akademie der Technikwissenschaften e. V., München
6. Dieckhoff C, Fichtner W, Grunwald A, Meyer S, Nast M, Nierling L, Renn O, Voß A, Wietschel M (2011) Energieszenarien: Konstruktion; Bewertung und Wirkung - "Anbieter" und "Nachfrager" im Dialog. KIT Scientific Publishing, Karlsruhe, 89. doi:10.5445/KSP/1000021684
7. Börjeson L, Höjer M, Dreborg KH, Ekvall T, Finnveden G (2006) Scenario types and techniques: towards a user's guide. Futures (7), 723–739 doi:10.1016/j.futures.2005.12.002
8. Möst D, Fichtner W, Grunwald A (2008) Energiesystemanalyse: Tagungsband des Workshops "Energiesystemanalyse" vom 27. November 2008 am KIT Zentrum Energie. Proceedings, Universität Karlsruhe, Karlsruhe
9. Hoffman KC, Wood DO (1976) Energy system modeling and forecasting. Annual Review of Environment and Resources (1), 423–453
10. Keles D, Möst D, Fichtner W (2011) The development of the German energy market until 2030—a critical survey of selected scenarios. Energy Policy 2(39):812–825. doi:10.1016/j.enpol.2010.10.055
11. Jebaraj S, Iniyan S (2004) A review of energy models. Renew Sust Energ Rev 10(4):281–311. doi:10.1016/j.rser.2004.09.004
12. Connolly D, Lund H, Mathiesen BV, Leahy M (2010) A review of computer tools for analysing the integration of renewable energy. Applied Energy, 1059–1082
13. Bhattacharyya SC, Timilsina GR (2010) A review of energy system models. International Journal of Energy Sector Management 4(4):494–518. doi:10.1108/17506221011092742
14. Droste-Franke B, Paal B, Rehtanz C, Sauer DU, Schneider JP, Schreurs M, Ziesemer T (2012) Balancing renewable electricity: energy storage, demand side management, and network extension from an interdisciplinary perspective, 1st edn. Springer, Heidelberg. doi:10.1007/978-3-642-25157-3
15. Droste-Franke B, Carrier M, Kaiser M, Schreurs M, Weber C, Ziesemer T (2014) Improving energy decisions towards better scientific policy advice for a safe and secure future energy system, 1st edn. Springer, Switzerland. doi:10.1007/978-3-319-11346-3
16. Després J, Hadjsaid N, Criqui P, Noirot I (2015) Modelling the impacts of variable renewable sources on the power sector: reconsidering the

typology of energy modelling tools. Energy 80(1 February 2015), 486–495 doi: 10.1016/j.energy.2014.12.005

17. Schüll E, Gerhold L (2015) Nachvollziehbarkeit. In : Standards und Gütekriterien der Zukunftsforschung. VS Verlag für Sozialwissenschaften, Wiesbaden 197
18. Bossel H (2007) Systems and models: complexity, dynamics, evolution, sustainability. Books on Demand GmbH, Norderstedt
19. Weßner A, Schüll E (2015) Code of Conduct - Wissenschaftliche Integrität. In: Standards und Gütekriterien der Zukunftsforschung. VS Verlag für Sozialwissenschaften, Wiesbaden 197
20. Grunwald A (2011) Energy futures: diversity and the need for assessment. Futures (8), 820-830 doi:10.1016/j.futures.2011.05.024
21. Kloprogge P, van der Sluijs J, Wardekker A (2007) Uncertainty communication—issues and good practice. Report ISBN: 978-90-8672-026-2, Copernicus Institute for Sustainable Development and Innovation, Utrecht
22. International Risk Governance Council (2015) Assessment of future energy demand—a methodological review providing guidance to developers and users of energy models and scenarios. Concept Note, International Risk Governance Council http://www.irgc.org/wp-content/uploads/2015/05/IRGC-2015-Assessment-of-Future-Energy-Demand-WEB-12May.pdf
23. Menzen G (2014) Bekanntmachung Forschungsförderung im 6. Energieforschungsprogramm "Forschung für eine umweltschonende, zuverlässige und bezahlbare Energieversorgung". Bundesanzeiger, 18
24. Sullivan P, Cole W, Blair N, Lantz E, Krishnan V, Mai T, Mulcahy D, Porro G (2015) Standard scenarios annual report: U.S. Electric Sector Scenario Exploration., Golden
25. Lawrence Berkeley National Laboratory (2015) Resource planning portal. Available via: http://resourceplanning.lbl.gov. Accessed 15 July 2015
26. Openmod initiative (2015) Open energy modeling initiative. Available via: http://openmod-initiative.org/manifesto.html. Accessed 09 November 2015
27. NFQ Solutions (2015) PriceProfor Engine. Available via: http://ekergy.github.io/. Accessed 29 Aug 2016.
28. U.S. Department of Energy (2014) Available via: http://www.energy.gov/sites/prod/files/2014/08/f18/DOE_Public_Access%20Plan_FINAL.pdf. Accessed 23 October 2015
29. Benz J, Hoch R, Legovic T (2001) ECOBAS—modelling and documentation. Ecological Modelling (1–3), 3–15 doi: 10.1016/S0304-3800(00)00389-6
30. Schmolke A, Thorbek P, DeAngelis DL, Grimm V (2010) Ecological models supporting environmental decision making: a strategy for the future. Trends Ecol Evol 25(8):479–486
31. Grimm V, Augusiakd J, Focksd A, Franke BM, Gabsif F, Johnstong ASA, Liug C, Martina BT, Melij M, Radchukc V et al (2014) Towards better modelling and decision support: documenting model development, testing, and analysis using TRACE. Ecological modelling., pp 129–139. doi:10.1016/j.ecolmodel.2014.01.018
32. Rahmandad H, Sterman JD (2012) Reporting guidelines for simulation-based research in social sciences. System Dynamics Review (4), 396–411 doi:10.1002/sdr.1481
33. Grimm V, Berger U, Bastiansen F, Eliassen S, Ginot V, Giske J, Goss-Custard J, Grand T, Heinz SK, Huse G et al (2006) A standard protocol for describing individual-based and agent-based models. Ecological Modelling., pp 115–126
34. Grimm V, Berger U, DeAngelis DL, Polhill JG, Giske J, Railsback SF (2010) The ODD protocol: a review and first update. Ecological Modelling., pp 2760–2768
35. Martinez-Moyano IJ (2012) Documentation for model transparency. System Dynamics Review (2), 199–208 doi: 10.1002/sdr.1471
36. Gass SI, Hoffman KL, Jackson RHF, Joel LS, Saunders PB (1981) Documentation for a model: a hierarchical approach. Commun ACM 24(11):728–733
37. Dodds EP, Keppo I, Strachan N (2015) Characterising the evolution of energy system models using model archaeology. Environmental Modeling & Assessment 20(2):83–102
38. Wassermann S (2015) Das qualitative Experteninterview. In : Methoden der Experten-und Stakeholdereinbindung in der sozialwissenschaftlichen Forschung. Springer, Wiesbaden doi: 10.1007/978-3-658-01687-6
39. Betz G, Pregger T (2014) Helmholtz Research School on Energy Scenarios: advanced module—case studies. 17-20 February 2014, Stuttgart, Karlsruhe http://www.energyscenarios.kit.edu/
40. Greenpeace (2012) energy [r]evolution - a sustainable world energy outlook 4th edn. Greenpeace International http://www.greenpeace.org/international/Global/international/publications/climate/2012/Energy%20Revolution%202012/ER2012.pdf
41. European Commission (2011) EU Energy Roadmap 2050—impact assessment and scenario analysis Part 2/2. Available via: https://ec.europa.eu/energy/sites/ener/files/documents/sec_2011_1565_part2.pdf. Accessed 30 Mar 2015
42. Bogner A, Littig B, Menz W (2009) Expert interviews—an introduction to a new methodological debate. In: Interviewing Experts. Palgrave Macmillan, United Kingdom. doi:10.1057/9780230244276_1
43. Cuhls K (2009) Delphi-Befragungen in der Zukunftsforschung. In : Zukunftsforschung und Zukunftsgestaltung. Springer, Berlin Heidelberg doi: 10.1007/978-3-540-78564-4_15
44. Landeta J (2006) Current validity of the Delphi method in social sciences. Technol Forecast Soc Chang 5(73):467–482. doi:10.1016/j.techfore.2005.09.002
45. Ohlhorst D, Kröger M (2015) Konstellationsanalyse: Einbindung von Experten und Stakeholdern in interdisziplinäre Forschungsprojekte. In : Methoden der Experten- und Stakeholdereinbindung in der sozialwissenschaftlichen Forschung. Springer, Wiesbaden doi: 10.1007/978-3-658-01687-6_6
46. Acatech (2015) Mit Energieszenarien gut beraten. Anforderungen an wissenschaftliche Politikberatung. Deutsche Akademie der Technikwissenschaften, Deutsche Akademie der Naturforscher Leopoldina und Union der deutschen Akademien der Wissenschaften, Berlin
47. International Energy Agency; International Renewable Energy Agency Policies and Measures Databases (PAMS). Available via: http://www.iea.org/policiesandmeasures/renewableenergy/. Accessed April 2016
48. European Regulators' Group for Electricity and Gas (2010) Comitology Guidelines on Fundamental Electricity Data Transparency. Initial Impact Assessment, European Regulators' Group for Electricity and Gas, Brussels http://www.poyry.co.uk/sites/www.poyry.co.uk/files/17.pdf
49. Brock WA, Durlauf SN (2005) Local robustness analysis. Theory and application. J Econ Dyn Control 29(11):2067–2092. doi:10.1016/j.jedc.2005.06.001
50. Walker WE, Harremoës P, Rotmans J, van der Sluijs JP, van Asselt MBA, Janssen P, Krayer von Krauss MP (2003) Defining uncertainty. A conceptual basis for uncertainty management in model-based decision support. Integr Assess 4(1):5–17. doi:10.1076/iaij.4.1.5.16466
51. Trutnevyte E, Guivarch C, Lempert R, Strachan N (2016) Reinvigorating the scenario technique to expand uncertainty consideration, 34th edn. Springer, Netherlands, p 135. doi:10.1007/s10584-015-1585-x
52. Trutnevyte E, Barton J, O'Grady Á, Ogunkunle D, Pudjianto D, Robertson E (2014) Linking a storyline with multiple models: a cross-scale study of the UK power system transition. Technological Forecasting and Social Change., pp 26–42
53. Object Management Group (2011) Object Management Group. Available via: http://www.omg.org/spec/UML/2.4.1/Superstructure/PDF/. Accessed 09 September 2015
54. Hamby DM (1994) A review of techniques for parameter sensitivity analysis of environmental models. Environ Monit Assess 32(2):135–154
55. Weisberg M (2006) Robustness analysis. Philos Sci 73(5):730–742
56. Culka M (2016) Uncertainty analysis using Bayesian model averaging: a case study of input variables to energy models and inference to associated uncertainties of energy scenarios. Energy, Sustainability and Society 6(1)
57. Mastrandrea MD, Mach KJ, Plattner GK, Edenhofer O, Stocker TF, Field CB, Matschoss PR (2011) The IPCC AR5 guidance note on consistent treatment of uncertainties: a common approach across the working groups. Clim Chang 8(4):675–691. doi:10.1007/s10584-011-0178-6
58. Betz G (2010) What's the worst case? The methodology of possibilistic prediction. Analyse & Kritik (1), 87–106
59. Intergovernmental Panel on Climate Change (2008) Synthesis report. Contribution of working groups I, II and III to the fourth assessment report of the intergovernmental panel on climate change. In: Climate Change 2007. IPCC, Geneva, p 86
60. Resch G, Liebmann L, Lamprecht M, Hass R, Pause F, Kahles M (2014) Phase out of nuclear power in Europe—from vision to reality. Report, GLOBAL 2000, Vienna http://www.bund.net/fileadmin/bundnet/publikationen/atomkraft/130304_bund_atomkraft_phase_out_nuclear_power_europe_dt_kurzfassung.pdf
61. WETO (2011) World and European energy and environment transition outlook. Available via: http://espas.eu/orbis/document/world-and-european-energy-and-environment-transition-outlook. Accessed 03 30 2015
62. Davis CB, Chmieliauskas A, Dijkema GPJ, Nikolic I Enipedia. In: Energy & Industry group, Faculty of Technology, Policy and Management, TU Delft. Available via: http://enipedia.tudelft.nl/wiki/Main_Page. Accessed April 2016
63. European Commission Eurostat. Available via: http://ec.europa.eu/eurostat/. Accessed April 2016
64. International Energy Agency (2014) The future and our energy sources—ETP 2014 report. Available via: http://www.iea.org/etp/etp2014. Accessed 30 March 2015

65. Jacobson MZ, Delucchi MA, Bazouin G, Bauer ZAF, Heavey CC, Fisher E, Morris SB, Diniana JYP, Vencill TA, Yeskoo TW (2015) 100% clean and renewable wind, water, and sunlight (WWS) all-sector energy roadmaps for the 50 United States. Energy & Environmental Science., pp 2093–2117
66. Vögele S, Hansen P, Poganietz WR, Prehofer S, Weimer-Jehle W (2015) Building Scenarios on energy consumption of private households in germany using a multi-level cross-impact balance approach. Preprint, Institute of Energy and Climate Research, Julich
67. O'Mahony T, Zhou P, Sweeney J (2013) Integrated scenarios of energy-related CO2 emissions in Ireland: a multi-sectoral analysis to 2020. Ecological Economics., pp 385–397
68. Trutnevyte E, Stauffacher M, Scholz RW (2012) Linking stakeholder visions with resource allocation scenarios and multi-criteria assessment. European Journal of Operational research., pp 762–772
69. Feix O, Obermann R, Strecker M, König R (2014) 1. Entwurf Netzentwicklungsplan Strom. Report, German Transmission System Operators, Berlin, Dortmund, Bayreuth, Stuttgart http://www.netzentwicklungsplan.de/file/2674/download?token=BbPkl0OO.
70. Suwala W, Wyrwa A, Pluta M, Jedrysik E, Karl U, Fehrenbach D, Wietschel M, Boßmann T, Elsland R, Fichtner W et al (2013) Shaping our energy system—combining European modelling expertise: case studies of the European energy system in 2050. Energy System Analysis Agency, Karlsruhe
71. Weber C (2005) Uncertainty in the Electric Power Industry. Springer, New York. doi:10.1007/b100484
72. International Energy Agency (2009) Transport, energy and CO2: moving toward sustainability. Report ISBN: 978-92-64-07316-6, International Energy Agency, Organisation for Economic Co-operation and Development, Paris
73. Façanha C, Blumberg K, Miller J (2012) Global transportation energy and climate roadmap—the impact of transportation policies and their potential to reduce oil consumption and greenhouse gas emissions. Report, International Council on Clean Transportation, Washington http://www.theicct.org/sites/default/files/publications/ICCT%20Roadmap%20Energy%20Report.pdf
74. Barlas Y (1996) Formal aspects of model validity and validation in system dynamics. Syst Dyn Rev 3(12):183–210. doi:10.1002/(SICI)1099-1727(199623)12:33.0.CO;2-4
75. Sterman J (2000) Business dynamics: systems thinking and modeling for a complex world. Mcgraw-Hill Education Ltd, Boston
76. Wansart J (2012) Analyse von Strategien der Automobilindustrie zur Reduktion von CO2-Flottenemissionen und zur Markteinführung Alternativer Antriebe. Springer Gabler, Wiesbaden doi: 10.1007/978-3-8349-4499-3
77. Dargay J, Gately D, Sommer M (2007) Vehicle ownership and income growth, worldwide: 1960-2030. Energy J 4:143–170
78. Brouwer AS, van den Broek M, Zappa W, Turkenburg WC, Faaij A (2015) Least-cost options for integrating intermittent renewables in low-carbon power systems. Applied Energy., pp 48–74
79. Frew BA, Becker S, Dvorak MJ, Andresen GB, Jacobson MZ (2016) Flexibility mechanisms and pathways to a highly renewable US electricity future. Energy 101:65–78
80. Global Fuel Economy Initiative (undated) 50by50. Available via: http://www.fiafoundation.org/connect/publications/50by50-global-fuel-economy-initiative. Accessed 30 March 2015
81. Tomaschek J (2013) Long-term optimization of the transport sector to address greenhouse gas reduction targets under rapid growth: application of an energy system model for Gauteng province, South Africa. Dissertation, Universität Stuttgart, Stuttgart. doi:10.18419/opus-2313

2.2 PUBLICATION 2

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Applied model	REMix Germany
Specific objective	Development and evaluation of a new methodology that allows for network partitioning for Energy System Optimization Models
Thesis-overarching objectives	2.a) Implementation of methods for modeling power flows in large-scale energy systems 2.b) Parameterization of a spatially highly resolved model 2.d) Analysis of the impact of regionalization and model simplification by spatial aggregation
Methodology	Spectral clustering of nodal, marginal power generation costs and aggregation of spatially resolved data
Key outcome	More accurate, spatially aggregated ESOM instances than used before and software tools that allow dynamic changing of spatial resolution.

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Article

Incorporating Power Transmission Bottlenecks into Aggregated Energy System Models

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Abstract: Energy scenario analyses are able to provide insights into the future and possible strategies for coping with challenges such as the integration of renewable energy sources. The models used for analyzing and developing future energy systems must be simplified, e.g., due to computational constraints. Therefore, grid-related effects and regional differences are often ignored. We tackle this issue by presenting a new methodology for aggregating spatially highly resolved transmission grid information for energy system models. In particular, such approaches are required in studies that evaluate the demand for spatially balancing power generation and consumption in future energy systems. Electricity transmission between regions is crucial, especially for scenarios that rely on high shares of renewable energy sources. The presented methodology estimates transmission line congestions by evaluating the nodal price differences and then applies a spectral clustering on these particular link attributes. The objective of the proposed approach is to derive aggregated model instances that preserve information regarding electricity transmission bottlenecks. The resulting models are evaluated against observables such as the annual amount of redispatched power generation. For a selection of defined performance indicators, we find a significantly higher accuracy compared to the commonly used, spatially aggregated models applied in the field of energy scenario analysis.

Keywords: energy scenario; power system modeling; spectral clustering; spatial aggregation; grid and storage expansion

1. Introduction

1.1. Motivation

Optimizing energy system models (ESMs) are frequently applied tools that are used for the analysis and development of energy scenarios [1]. In the context of strategic and political decision making, these scenarios are often used for gaining orientations concerning future developments or to show pathways towards the achievement of targets, such as the reduction of greenhouse gases [2]. One of the advantages of choosing optimization models for analyzing energy scenarios is that these targets can be easily integrated into a mathematical description of a whole system while examining a broad spectrum of technological solutions for meeting such constraints (Bottom-Up modeling) [3]. Hereby, ESMs typically aim for a cost-optimal energy system configuration, where a mix of electricity generators must cover the electrical load at any given time. System sizes range from local to international scales [4]. However, driven by greenhouse gas reduction targets, long-term energy scenarios also have to consider large shares of power generation from renewable energy resources [5,6]. Given the variability of electricity provision from wind turbines or photovoltaics, challenges arise for modeling energy scenarios. A broader set of technologies such as electricity grids, batteries or demand response needs to be included as well as approaches towards cross-sectoral analyses [7].

Recent energy scenario studies address the need for both flexible power generation and consumption by integrating technological flexibility measures into ESMs [8]. The complexity of the underlying multi-area optimization problem is not only affected by the enlargement of considered technologies but especially increases due to the stronger coupling of both time steps and modeled regions. The examination of necessary investments into flexibility options thus becomes a co-optimization problem for the extension of generation, transmission and energy storage capacities [9,10].

Recently, spatial resolutions in ESMs have been increased substantially with better data availability [7]. On the European level, most energy scenarios are characterized by ESMs where each country is represented by either a single or only a few modeled regions [11,12]. Therefore, spatial data are aggregated, or in other words, the total power generation and consumption of a defined region are concentrated at one point while neglecting intra-regional power flows. Such ESMs consist of a network of aggregated regions (often referred to as "copper plates"), observe only inter-regional power flows, and, hence, necessary investments into transport capacities. For energy scenarios that rely on high shares of variable renewable energy sources (vRESs) this translates into neglecting possible transmission grid congestion, caused by the fact that electricity demand centers and resource hotspots are typically remote from one another.

Besides the increasing renewables penetration, further challenges such as market integration or deregulation [13] require appropriate methodologies that can account for limited power exchange capabilities of transmission grids. To tackle these challenges (rather than simply increasing the spatial resolution of an ESM), network clustering and reduction approaches appear to be a suitable way of capturing effects on local levels without a significant increase in the typical computing times of an ESM.

Such approaches, which spatially aggregate data of an ESM, are effective since they reduce the number of linking constraints from the underlying optimization problem. By linking constraint we mean a specific type of constraint that couples variables that belong to individual blocks and prevent a faster solution of the mathematical optimization problem. In particular, spatial aggregation leads to a reduction of power flow constraints which link regions with each other. If all power flow constraints are removed from an ESM, it could be solved by solving smaller optimization problems for each region (in parallel). Mathematical decomposition techniques, such as that applied in [14], make use of this effect, however at the expense of an iterative solution process.

1.2. Objective

This paper aims to develop a methodology that derives spatially aggregated ESM instances from a highly resolved model (referred to as the reference model). In this regard, such instances provide similar results (e.g., power flows and power plant operation) when compared to the solution of the reference model. Spatial details should be reduced to a level that is computationally manageable.

Therefore, two necessary methodological steps are distinguished. First, aggregated regions have to be defined. This directly refers to the selection of transmission links that should be included in the optimization. Second, the process of aggregating spatial data itself needs to be conducted. However, the focus of this paper relies on the former for which the following requirements can be defined:

- The approach must enable the identification of transmission links that show frequent congestions in operation.
- Real-world electricity transmission grids are networks that cover large geographical scales and consist of several thousands of nodes. To manage the appropriate amount of data, an automatized process is preferable.
- A reproducible method is required that is adjustable to changes in generation and consumption patterns. This becomes important to identify intra-regional bottlenecks over a long-term time horizon by myopically adjusting the spatial aggregation.

- It can be assumed that with an increasing number of modeled regions, the accuracy of an ESM can be improved and that there is probably an optimal spatial resolution regarding the trade-off between computing time and model accuracy. However, for our study, the spatial resolution should remain on a level that is comparable to the state of the art [15–17], which allows the comparison to typical ESM resolutions.
- To still be able to derive results for regions of interest, e.g., administrative regions, the definition of static overlay-borders should be possible (even if the spatial aggregation is myopically adjusted).
- Aggregation methods that are able to simplify the whole network representation of the model instead of focusing on specific areas are preferred.

1.3. Literature Review: Spatial Aggregation

For the creation of multi-area ESMs by the spatial aggregation of topological data of a power transmission network (in the following, referred to as original network), the two necessary methodological steps are often referred to as 'network partitioning' and 'creation of network equivalents'.

1.3.1. Network Partitioning

With algorithms such as *k*-means and its variations or hierarchical clustering, methods for automatically deriving clusters of spatially highly resolved data are already available in a broad spectrum [18]. Moreover, attributes that define the desired outcome of such algorithms are necessary. An obvious approach for such definitions is thus the assessment of the actual grid (e.g., through analyzing its topology). Since energy scenarios are typically used for policy advice, model regions in ESMs are required to refer to areas of interest. This leads to the investigation of administrative regions [19] or markets [20].

Also, other criteria can play a role in the selection of aggregated regions. In particular, for studies commissioned [21] or conducted [22] by transmission system operators, the distinction of geographical hotspots of power demand and generation centers is also used. For instance, the clustering approach proposed for the project e-Highway2050 [21] assesses several parameters, such as population, vRES potentials, and already installed hydro and thermal capacities as well as the locations of agricultural areas and natural grasslands. In this way, the need for a spatial power exchange is considered by minimizing the self-consumption of a cluster. Nonetheless, frequently congested transmission lines are not directly detected if no power flow study is conducted.

Therefore, information about the actual state of the grid is still necessary, especially topological characteristics such as geographical or electrical distances [23]. However, when using these simple attributes, relevant information about the placement of generation and demand or the usage of transmission lines is ignored. For this reason, the process of network partitioning is often extended with operational data, gathered from running an ESM. In [24], the use of both operational and topological data is proposed to combine information about the distances and to incorporate critical links in the reduced network. One further example for such partitioning approaches is presented by Singh [25]. While the topological information is limited to the geographical proximity, the operational attribute for building clusters is based on nodal prices which are calculated with an optimal power flow model. In particular, the sensitivity of nodal prices to changes of system loading is evaluated to identify classes of similar nodes in the network.

Operational data are also contained in so-called power transfer distribution factor matrices (PTDFs) that can be created from modeling the power flows within a network. For instance, they are used in [26] for network partitioning where, first, critical transmission lines are identified and subsequently, based on the PTDF, regions are clustered by their influence on the power flow of all links. Similar approaches that evaluate topological and operational data are suggested in the context of network vulnerability analysis [27]. Here, an indicator called transmission betweenness is also determined using regional power injections and the transfer capabilities of transmission lines.

1.3.2. Network Equivalents

Once aggregated regions are defined, the creation of network equivalents can be conducted in several ways. In the simplest case, each cluster is treated as a copper plate where no additional measures are applied for adjusting the outputs of an aggregated ESM to their counterparts obtained from a spatially highly resolved ESM. In other words, due to the aggregation, the resulting power flows and dispatch of power plants may differ significantly.

In the context of power flow analysis, methods for deriving representative electrical distances have been used for a long time [28,29]. A typical example for these methods is Kron's reduction which can be used to remove passive buses (buses without power injection) from the nodal admittance matrix of a network. For instance, applying it to a star circuit results in the star-triangle transformation [30]. While a pure Kron's reduction is already applicable when having the topological description of a network by its admittance matrix, the creation of Ward- and Extended-Ward equivalents additionally takes into account information from a solved power flow problem. This is also used for the determination of the Radial Equivalent Independent (REI), which adds representative loads and generators to the aggregated regions. Therefore a Gaussian elimination is applied to the external buses. The power injections of these buses are preserved by aggregating them to artificial generators which are connected to a representative, radial network which is referred to as REI [23]. Nevertheless, the objective of these network representatives is to divide the original network into an internal and external part, whereas the former remains in full resolution. This, however, is not the first priority if energy scenarios are modeled through equivalent network representations. Therefore, PDTF-based approaches, such as presented in [26,31], appear to be more suitable.

2. Materials and Methods

2.1. Overview

The methodology for creating an ESM that incorporates power transmission bottlenecks is composed as follows.

1. Setup of a reference model: This ESM is parameterized and used for conducting an optimal power flow. Its spatial resolution corresponds to the topology of the power transmission grid and thus represents the original network used for the subsequent spatial aggregation.
2. Network partitioning: This step contains the analysis of the operational data, using the differences in nodal marginal costs for the total power supply (in the following, referred to as nodal price differences) as indicators for the connectivity of regions in the original network as proposed in [24]. In other words, the weaker the connectivity of two regions (indicated by the magnitude of nodal price differences) is, the more likely it is that these regions belong to different clusters. The novelty of the presented approach is the application of this particular attribute to a spectral clustering algorithm which can be executed automatically. In contrast to approaches that use spectral clustering for ESMs [32], the topological information of the original network given by its incidence matrix is extended by the operational data. Furthermore, compared to existing studies that use this data in form of nodal prices [25], the purpose of evaluating their differences is rather the determination of relevant congestions in the transmission network than the identification of price zones.
3. Network equivalent: After getting the results from the clustering algorithm, the spatial data of the reference model are aggregated. Therefore, we use the simple approach of creating aggregated areas (in the following, referred to as clusters or zones), which means that power generation capacities and power consumption profiles are summed over all regions within a cluster as well as grid transfer capacities of links that connect regions belonging to different clusters. In a further step, network equivalencing introduced by [26] is applied for assessing the accuracy of the aggregated ESM instances.

The spatial distribution of power generation and consumption could change significantly in the future, for example as a result of an expansion planning approach for which the proposed methodology is suited for. For this reason, the network reduction methodology described above should ideally be applied in a repetitive manner to identify robust investment decisions over a certain time horizon by expansion planning with an ESM (Figure 1).

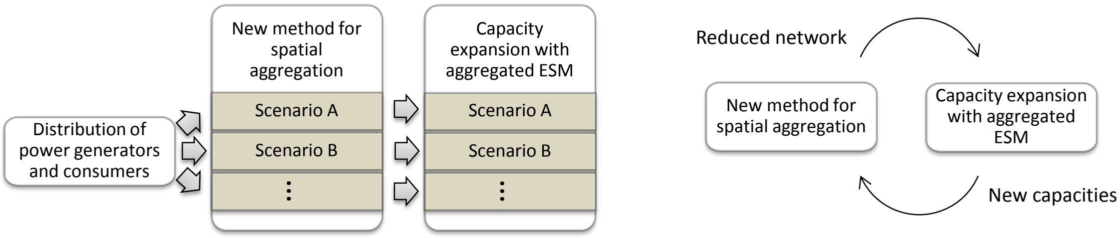

Figure 1. Possible applications of the presented method—examples of data processing using spatially aggregated energy system models (ESMs) for capacity expansion studies, (**left**) stochastic expansion planning, e.g., for a certain scenario year; (**right**) iterative expansion planning, e.g., over a period of scenario years.

On the one hand (Figure 1 left), similar to stochastic optimization, assumptions for the spatial distribution of power generators and consumers (see section Data Pre-Processing) could be changed in the setup of the reference model to proof that the resulting system performs well over a spectrum of different possible futures. On the other hand (Figure 1 right), also expansion planning over a period of scenario years could be iteratively modelled by updating the scenario data. In this way, new capacities required for a certain scenario year could be considered for deriving the aggregated ESM instance for expansion planning of a subsequent year.

However, as this paper emphasizes a new methodology for spatial aggregation of ESMs, in the following, the application of the full approach including the investment optimization is only conducted once (Case study).

2.2. Model Setup

To identify critical transmission links, a spatially highly resolved model (the reference model) is set up based on the grid topology of the German transmission grid. For its creation, a data scrape of the ENTSO-E power map is used [33]. As a case study for developing the algorithm, we initially picked Germany for two reasons: (i) data availability for renewable power generation at high spatial resolution; and (ii) high wind and solar PV penetration, which represents one of the main drivers for transmission grid congestions in the future. For the implementation, the ESM REMix [6] is parameterized using the empirical data for the year 2012. Typical applications of REMix range from theoretical studies concerning future energy supply with different shares of vRES [34] and country specific scenario studies [35,36] to the assessment of system reliability [37] and flexibility requirements [38] of the European energy system in the future. REMix can thus be configured for multiple study purposes. Table 1 shows the model fact sheet of how it is set up for the creation of the reference model where the input data are indicated by references.

To allow an extension of the geographical focus, mainly sources that provide data with a European scope were selected. However, the final input parameters for REMix are partially modified as explained in the subsequent chapter. For example, profiles for power feed-in from vRES are processed for NUTS3 level using potential analyses [39] on meteorological data for the year 2012. As these time series represent potentials, one output of REMix is the amount of usable (or vice versa the amount of curtailed) power generation from vRES.

Table 1 also provides information about the format of input and output data, indicating whether the data differ on the temporal (TM), technological (TC) or spatial (SP) scale. In addition, two different datasets regarding the analyzed year are distinguished. On the one hand, the power plant and transmission grid data reflect the German power system for the year 2012 (validation dataset). However, the objective of the proposed methodology is its application to energy scenarios. Therefore, on the other hand, REMix is parameterized for the year 2030 based on scenario C of the German grid development plan [40] (scenario dataset) that provides technology specific installed power generation capacities as well as a projection for the annual power demand in the year 2030. With regard to grid transfer capacities (GTCs), no grid expansion that goes beyond the values derived from the ENTSO-E power map data scrape is considered.

Despite the fact that REMix is actually used as a power system model, the term 'energy system model' (ESM) is still used in the following since the subsequently presented methodology is also applicable to cross-sectoral optimization models.

Table 1. Model fact sheet of the applied configuration of REMix.

Model Name	**REMix**			
Author (Institution)	German Aerospace Center (DLR), Institute of Engineering Thermodynamics			
Model type	Linear programing Minimization of total costs for system operation Economic dispatch Optimal direct current (DC) power flow (Appendix A)			
Sectoral focus	Electricity			
Geographical focus	Germany			
Spatial resolution	>450 nodes (reference model)			
Analyzed year (scenario)	2012 (2030)			
Temporal resolution	8760 time steps (hourly)			
Input-parameters:		TM	TC	SP
	Conversion efficiencies [41]		√	
	Operational costs [41]		√	
	Fuel prices and emission allowances [42]		√	
	Electricity load profiles [43]	√		√
	Capacities of power generation, storage and grid transfer capacities and annual electricity demand [33,40,44]		√	√
	Renewable energy resources feed-in profiles	√	√	√
	Import and export time series for cross-border power flows [45]	√		√
Evaluated output parameters for clustering	Marginal costs of total power supply			√
	(Nodal balance of total power generation and consumption)			√

2.3. Data Pre-Processing

The raw input data (e.g., from the literature) is often not provided in a format that is directly applicable to the input requirements of a particular ESM (Table 1). Therefore, by data pre-processing we mean the process of preparing empirical data for its use as input data in REMix. As mentioned above, we distinguish two data sets—the validation data set which represents the German power system of the year 2012 and the scenario data set that uses a power plant portfolio of a scenario of the year 2030—for which this preparation process is described in the following.

2.3.1. Disaggregation of Cross-Border Flows

The time series for cross-border power flows (imports and exports to Germany) are given on the country level, where countries are typically connected via several transmission systems. For the reference model, instead of spatially distributing the imported and exported power to each link of the original network, all cross-border links are connected to a single node for each neighbor country. To ensure that the correct total power flows occur, each cross-border node consists of an artificial bus, which generates and consumes power according to the given import and export time series. Data gaps in the accessed physical cross-border flows are filled, either by using the commercial power flows instead or by linear interpolation.

2.3.2. Assignment of Power Generation and Consumption to Network Nodes

Another challenge for setting up an ESM that relies on the nodes and links of the high voltage transmission grid is the assignment of data that are collected for areas (e.g., population of administrative areas) to appropriate nodes. This applies, for example, to decentralized power generators, such as photovoltaic and onshore wind farms, as well as to the annual power demand of a region. For the current purpose, this translates into the mapping of data from areas on the NUTS3 level [46] to nodes indicated as substations in the ENTSO-E power map data scrape. As a previous step, the downscaling of data from coarser resolutions than NUTS3 is also necessary. For the mapping, a common approach is performing a nearest neighbor analysis from the centroid coordinates of the areas to the coordinates of substations if no topological information about the underlying distribution grid is available (see Appendix B for a more detailed description).

2.3.3. Disaggregation of National Scenario Data

Since scenario data are usually available in a spatially aggregated format, e.g., on the country level, a distribution of installed power plant capacities is necessary. To do so, the following steps are performed:

- Central power plants with less total installed capacity compared to the validation dataset: Based on the commissioning year, the sites of the oldest power plants are decommissioned as long as the total installed capacity reaches the same order of magnitude as in the given scenario data.
- Central and biomass power plants with more installed capacity compared to the validation dataset: The installed capacity of existing power plants is equally scaled until the total installed capacity of the scenario data is reached.
- Photovoltaic and onshore wind farms: One-half of the installed capacity of the scenario data is distributed equally to the spatial distribution of the validation dataset. The other half is distributed equally to a technologically specific distribution of capacity factors that are derived from a potential analysis [39].
- Offshore wind farms and pumped storage: Sites of planned power plants [47] are added to the validation dataset.

2.4. Clustering

The process of defining clusters of regions in the network of the reference model is depicted in Figure 2. First, an annual run of the spatially highly resolved reference model is performed. To ensure that the model can be solved, we use a temporally nested heuristic. This approach initially solves the problem in a 6-hr temporal resolution. The obtained results, particularly the values for fuel consumption, shares of allowed annual carbon dioxide emissions, and storage levels, are then used as an input for the following hourly resolved model run.

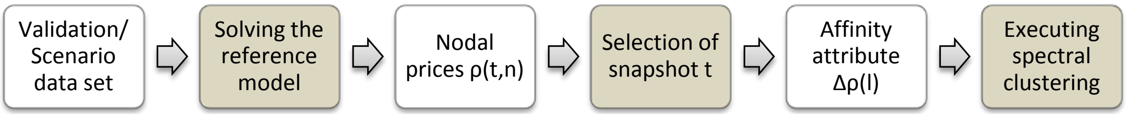

Figure 2. Clustering process, data in white boxes, processes in grey boxes.

From the resulting time series of the nodal price differences of the reference model, certain points in time are selected with the aim of identifying snapshots where a significant share of transmission links within the network are under stress. For this purpose, we define three criteria that can give an indication for such critical situations and apply them to the input or output data of the reference model:

- t_{LoadWind}: hour of the year for which the maximum of the sum of the generated power from wind onshore and the load can be observed; this point in time can be identified by purely analyzing the input time series of the reference model.
- t_{Price}: hour of the year for which the maximum of the nodal price differences can be observed.
- t_{GTC}: hour of the year for which the maximum of the relative grid transfer capacity usage can be observed.

Each of these selection criteria could result in an individual snapshot for each transmission line or region. However, it is very likely that the appropriate hour of the year differs over the several transmission lines and regions. Therefore, we first aggregate the time series of the reference model in space by using a statistical measure and then apply a particular criterion from above. For example, in the case of t_{GTC}, this means that first the 0.95-quantile of the relative power flow over all transmission lines is calculated. Afterwards the maximum value of this spatially aggregated time series is determined to identify the hour of the year that represents the snapshot t_{GTC}. For more details concerning the determination of critical hours see Appendix D.

Although the selection of temporal snapshots is a common approach for analyzing huge electrical networks, it is not ensured that all lines for which a critical state can be observed are captured in this way. However, one major aim of the evaluation is to assess the impact of the proposed clustering approach compared to state-of-the-art modeling, rather than the identification of all critical links. While the latter would be similar to the definition of a worst-case network, we meet this challenge by conducting a stability analysis for a number of different snapshots (see section Clustering of Regions).

The spectral clustering algorithm is set up according to [48]. A detailed description of the conducted data processing is provided in [49]. Based on conducting a number of experiments with the clustering parameters, we use the unnormalized variant by default and thus construct the Laplacian matrix:

$$L_{unnormalized}(n,n') = \sum_{l} K^{T}(l,\ n') \cdot \sum_{l'} \rho_{diag}(l',\ l) \cdot K(\ n,l) n,n' \in N \tag{1}$$

where N is the set of nodes, K is the incidence matrix of the original network, and ρ_{diag} is a diagonal matrix of affinity attribute. The latter can be derived from the vector of nodal price differences (which represents a slice of the appropriate time series determined by applying one of the snapshot selection criteria):

$$\begin{gathered} \Delta\rho(l) = \left| \frac{1}{\sum_n} K(\ n,l) \cdot \rho(n) \right| \\ \text{such that} \\ \sum_n K(\ n,l) \cdot \rho(n) \neq 0,\ \forall l \in L \end{gathered} \tag{2}$$

where L is the set of links in the original network and ρ is the vector of nodal prices. As high values in ρ_{diag} indicate a strong affinity or connectivity, the absolute reciprocal of the nodal price differences is used as an indicator for the similarity of regions in the reference model. Applying a *k*-means algorithm to a matrix, which consists of the eigenvectors that correspond to the *k*-smallest eigenvalues of $L_{unormalized}$, a mapping matrix Π_g can be derived. This matrix represents the final output of the network partitioning process as each region or node of the original network is now assigned to a cluster. These clusters define the regions in the partitioned network of a spatially aggregated ESM instance. In the following, we therefore use the terms "cluster" and "aggregated region" synonymously.

2.5. Derivation of Spatially Aggregated Energy System Models

The process of aggregating the data of the reference model, also referred to as creation of network equivalents, uses Π_g for summing up nodal model parameters, such as installed generation capacities:

$$\begin{gathered} P_{inst,agg}(n_{agg},\tau) = \textstyle\sum_n \Pi_g(n_{agg},\ n) \cdot P_{inst}(n,\tau) \\ \forall n_{agg} \in N_{agg},\ \forall \tau \in \mathrm{T} \end{gathered} \tag{3}$$

where N_{agg} is the set of nodes in the aggregated network and T stands for the set of power generation and consumption technologies. Data that characterize the links of the original network, such as *GTCs*, are aggregated in a similar way:

$$\begin{gathered} GTC_{inst,agg}\left(l_{agg}\right) = \sum_l \Pi_f\left(l,\ l_{agg}\right) \cdot GTC_{inst}(l) \\ \forall l_{agg} \in L_{agg} \end{gathered} \tag{4}$$

where L_{agg} stands for the set of links in the aggregated network, and the mapping matrix Π_f can be derived by evaluating the incidence matrix of the original network and Π_g. Finally, instead of only summing up, the inputs such as load profiles or vRES power generation time series are averaged by the number of aggregated regions per cluster. As a result, the aggregated zones are created from the reference model's regions. These 'copper plates' are connected by inter-zonal links that are derived from combining links of the original network that cross the borders of a zone, while all intra-zonal links are neglected. Concerning the derivation of the nodal admittance matrix of the reduced network, parallel links are aggregated by summing up the appropriate susceptances. In contrast, for the losses estimation, the parallel links are aggregated by averaging to account for the intra-zonal losses.

As this paper emphasizes a new network partitioning approach rather than sophisticated methods for creating network equivalents, further efforts to improve the aggregation procedure are not applied. However, the used network data consist of both passive and active nodes. While the latter are characterized by a certain power generation or consumption, passive nodes are only necessary to branch the network. Since only active nodes contain the relevant information for further analyses, the application of Kron's reduction [30] represents a considerable step towards the simplification of the original network.

3. Results and Discussion

This section is subdivided into several analyses, starting with the validation of the reference model, followed by the comparison of different aggregated ESM instances and a case study where the proposed clustering methodology is applied. For each of this analyses different quality measures or indicators are evaluated. In the following, the results of these different analysis steps are presented in a repetitive manner. Each section consists of the introduction of the evaluation indicator, followed by the description of post-processed output data and a discussion of the appropriate implications.

3.1. Validation of the Reference Model

In the best case, the validation of the reference model provides a test against spatially resolved times series of power flows or the nodal dispatch. Since, up to our knowledge, such a data set for back-testing is not freely available, the validation of the reference model combines tests against different types of historical data. In this context, the entirety of these tests should provide the information to assess the validity of the reference model.

As a first step towards the validation of the model, a simple plausibility check is conducted: To ensure the feasibility of the generated optimization model, slack variables are defined. These slack variables can be interpreted as artificial power generators that generate electricity only if there are no other remaining options to cover the electricity demand in a specific region. This means that the activity of artificial power generators can be interpreted as loss-of-load situations. Since such an event was never recorded in 2012 for Germany, the first plausibility check is conducted by ensuring that no loss-of-load situations occur in the reference model. We therefore use the assumptions for the uniform estimation of GTCs as calibration parameters (see Appendix C). The security margin and the conductor type are iteratively adjusted to avoid the occurrence of the loss-of-load for the validation dataset.

In a second step, the reference model is validated by back-testing against a historic dataset of 2012 which is temporally resolved. To get an idea of the quality of generated temporally resolved data, the observed spot market time series of electricity prices [43] are compared with the marginal costs of the total power supply of the reference model. This is due to the fact that, if a perfect market is assumed, electricity prices should be equal to the marginal costs obtained from an optimization model [50]. We are aware that the consideration of power flows in the spatially highly resolved model implies the inclusion of redispatch measures. The corresponding costs are not contained in the time series of historic electricity prices since the real power market acts like a copper plate model. However, we are of the opinion that a validation against temporally resolved observables is valuable. In this context, time series of market prices are almost the only data which is freely available for this purpose.

The validation is based on hourly data that is used to calculate the Pearson product-moment coefficient (PCC). For a better overview of the analyzed time period of 8760 h, Figure 3 shows the daily rolling average of both the recorded (black curve) and the modeled (red and green dotted curve) data.

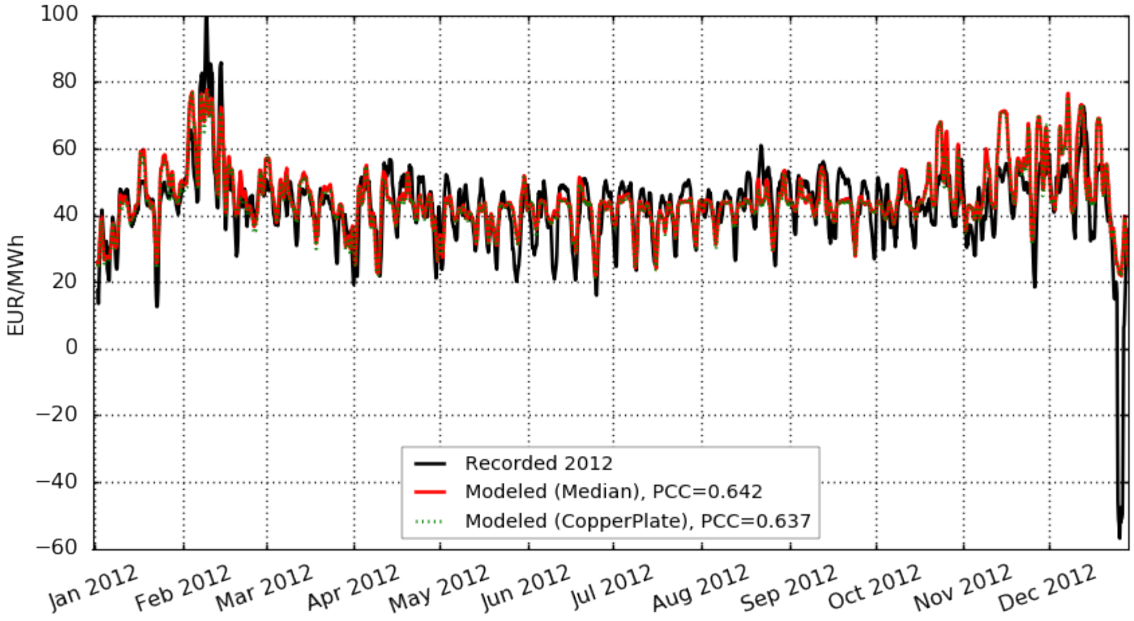

Figure 3. Results of the reference model validation based on a time series of daily electricity prices.

As the reference model actually produces nodal prices (and electricity prices of the spot market are based on one single market zone for Germany), we apply two measures to test against the historical data. First, we determine the median overall nodes of the original network. Second, we spatially aggregate the reference model to a one-node (copper plate) model and use the appropriate marginal costs for validation. Both of these measures have their advantages and disadvantages. The former provides a comparison with the outcome of the spatially resolved reference model, but produces nodal information instead of prices for a single market zone. Although this is not the case for the aggregated copper plate model, this model is not able not provide the data required for spatially resolved analyses, such as the intended identification of congestions in the transmission grid.

Figure 3 shows how the reference model is able to reproduce the times series of the electricity prices of 2012, resulting in a PCC around 0.64. In this context, the almost uniform shape of the modeled curves (red and green dotted) shows that both the median of the spatially resolved model as well as its fully aggregated counterpart perform in a very similar manner. However, peaks and valleys of the observed data are usually underestimated, which is a typical phenomenon of such modeling exercises [51]. This leads to the conclusion that the distribution of modeled prices is flatter than in reality. Possible reasons for this deviation are:

- The strategic behavior of market actors, which is not captured by modeling the fundamental interdependencies of the electricity market.

- Assuming static costs for fuels and emission allowances as well as the classification of power plants by fuel type also results in equalizing specific production costs of large power generation units and, thus, a smaller diversity of marginal costs.
- The chosen economic dispatch model overestimates the flexibility capabilities of certain power plants, e.g., must-run capacities, such as combined heat and power plants.

The last validation step is conducted using observables that provide an insight into the operation of the power system. The advantage of this test is that it is directly related to transmission bottlenecks. However, it can be only evaluated on an annual and spatially aggregated basis.

The amount of redispatched power generation (in the following, referred to as redispatch) is used as an indicator to check whether the reference model shows similar occurrences of congestion events in the grid as reported by the German Federal Network Agency [52]. By performing a run of the reference model with and without constraints introduced for transmission grid modeling (see Appendix A), the redispatch can be derived. Ignoring these constraints is equivalent to a spatial aggregation of the reference model to its single node (copper plate) representation. Hence, we determine the difference of the spatially summed annual power generation of each technology of the reference model output and its spatially fully aggregated counterparts. More details concerning the calculation of the annual redispatch are provided in Appendix E.

According to the results of the comparison of the recorded and modeled redispatch in Table 2, a similar order of magnitude can be reached. A cross-check with slightly different parameters during the calibration of GTCs also showed that the reference model reacts quite sensitively to changes in the security margin (see Appendix C); e.g., reducing it to 0.7 results in a redispatch of 12.62 TWh, while for increasing it to 0.9, a redispatch of 0.11 TWh can be observed. Another trade-off must be made, since an underestimation of GTCs can lead to gaps in the supply of certain nodes. As a consequence, costs for the loss-of-load appear, which significantly affect the nodal prices of the appropriate region. Since such prices are undesirable as input for the subsequent clustering, an exact calibration of the security margin based on the redispatch is therefore not conducted. In this context, it must be noted that the generally applied security margin represents only an approximation of the n-1 criterion which is often considered in power flow models. A possible way to improve the observed behavior of the actual model would therefore be the application of a security-constrained optimal power flow approach [53].

The above-mentioned sensitivity also applies to other annual indicators, such as the total grid losses and the shares of power generation from renewable sources vs. fossil and nuclear power plants. With the exception of the latter, these indicators strongly rely on the assumptions concerning the input parameters, such as the generally applied, specific grid losses factor. In addition, deviations can be explained since the actually used installed generation capacities are derived from a data source that offers large geographical coverage rather than the most accurate information available. Even more insights are provided, when looking at specific transmission lines that are congested (fully utilized) in the reference model. When comparing them to the reported line-specific congestion events, it can be shown that only a part of these events is reproduced by the reference model, but congestions at other sites only appear in the model.

Table 2. Results of reference model validation based on annual observables.

	Observed	**Modeled**
Grid Losses [TWh] [52]	6.2	5.1
Redispatched energy [TWh] [52]	2.6	6.65
Congestion events [52]	7160	17,662
Annual power generation share from vRES [54]	23%	29%

A reason for this behavior is the already-mentioned estimation of grid transfer capacities. The ignorance of the underlying distribution grid may also lead to a deviating assignment of generation capacities to substations and thus to a different spatial pre-balancing of power generation and demand compared to reality.

Furthermore, we observe both more redispatch and a higher share of power generation from vRES in the model (Table 2). This behavior can be explained by the following model characteristics and assumptions: As mentioned above, the applied economic dispatch model generally overestimates the flexibility of large steam power plants. In addition, must-run capacities, such as Combined Heat and Power plants, are not considered separately. This as well as the fact that pumped hydro storage units can operate under perfect foresight conditions, fosters the integration of power feed-in from vRES. Finally, for determining this power feed-in for wind turbines a performance curve of one particular wind energy converter technology is applied to historical weather data. Since the standard use case of the resulting time series is its application to scenario studies, the corresponding performance curve is not representative for all wind turbines operated in Germany in the year 2012.

However, information such as the future distribution of installed capacities or the future performance of certain technologies is not easily derivable for scenario studies. We therefore conclude that the used modeling approach is still suitable for the purpose of the proposed clustering methodology.

3.2. Clustering of Regions

Although the presented clustering approach allows any integer value k for the number of clusters or aggregated regions to be set, we chose a constant value of $k = 20$. This allows for comparison with the commonly used regional model in [22] that consists of 20 regions (see also section *Comparison of Aggregated Models*). However, since the number of clusters correlates with the trade-off between model accuracy and performance, conducting further research on finding an optimal value for k becomes relevant. Some work in the literature already emphasizes this topic on the algorithmic side [55] as well as on the application side [44,56]; however, this goes beyond the focus of the current study.

To get a better idea of the distribution and size of clustered regions, maps of Germany that correspond to the different clustered models are provided in Appendix F.

Another important remark regarding the following results concerns the evaluated dataset. As already mentioned, the objective of the presented clustering methodology is the identification of critical transmission links for energy scenarios. However, it is obvious that for the year 2012, critical links within the German high voltage transmission grid are rare. In the following, we therefore use the scenario dataset (scenario C of the German grid development plan [40]) that is intended to contain a higher number of critical links. This is due to the assumption that the need for electricity transmission and thus the magnitudes of power flows increase with the share of power generation from vRES. As this share is higher for the scenario data set, it can be assumed that more transmission lines reach their limits than in the case of the validation data set.

3.2.1. Preservation of Critical Transmission Links

Based on the three snapshots, three spatially aggregated ESM instances are derived from the reference model. In the following, general characteristics of these clustered models are evaluated.

The preservation of critical transmission links is determined using the relative load (utilization) of transmission lines as indicator from the results of the analyzed ESMs. The idea behind this analysis is the following: The higher the utilization of the entirety of all transmission lines in a model is, the higher is the share of critical links. This means, if we remove, from a given set of links, those ones which show a low utilization (as intended with the proposed methodology), the average load of the remaining transmission lines (the critical ones) should be higher than in the initial network.

Figure 4 shows the appropriate duration curves of the relative utilization of transmission links within the period of 8760 h. The presented curves are derived by dividing the total power flow over each transmission line by its capacity and subsequently calculating the 0.95-quantile over all transmission lines in the network. Compared to the reference model where full utilization does not appear at all for the 0.95-quantile, the duration curves of all aggregated model instances remain for a significantly larger amount of time steps at a level close to 100% GTC usage (Clustered t_{Price}: 1220 h, Clustered $t_{LoadWind}$: 446 h, Clustered t_{GTC}: 687 h).

This means that the intended preservation of critical links is provided by the proposed network partitioning. In other words, since the total number of links is reduced due to aggregation, but lines that show frequently high utilization of GTC remain in the aggregated model instances, the determination of the 0.95-quantile over all links results in a duration curve that is closer to the transversal at 1.0. At first glance, this can be interpreted as an overestimation of critical links for the aggregated network; however, it can be assumed that this effect is compensated to a certain degree as intra-zonal limits on power transmission of the original network are neglected in the aggregated models.

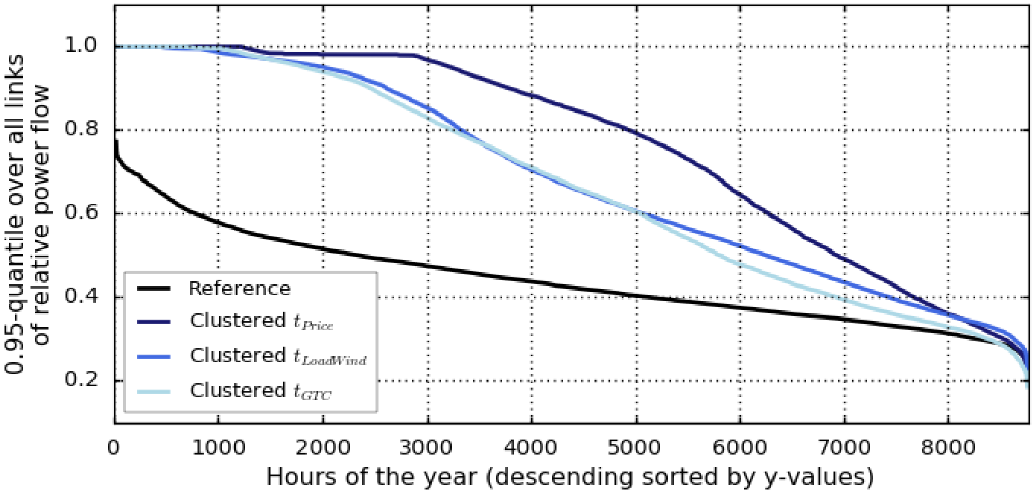

Figure 4. Duration curves of relative grid transfer capacity usage (0.95-quantile over all transmission links).

3.2.2. Stability of Aggregated Regions over Selected Critical States

The network partitioning strongly depends on the operational state, which is used as a snapshot for the selection of nodal price differences. In the best case, a snapshot exists where the majority of critical lines are under stress. However, this is not usually the case. Moreover, even if such a snapshot is detected, due to the predefinition of the number of clusters, not necessarily all stressed links are captured in a single snapshot.

To get an idea of the different clustering results for several critical states, Figure 5 depicts the neighborhood of regions in the reference model. It should be understood as follows: Both the x-axes and the y-axes represent the set of all regions or nodes in the reference model. When depicting the results of the clustering approach, each dot in the plot indicates that the corresponding region on the x-axes belongs to the same cluster as the region on the y-axes (in the following we call those regions neighbors of the regions on the x-axes). For reasons of simplicity (otherwise the plots would be fully inked) Figure 5 shows only all neighbors for 10 randomly selected regions on the x-axes (in the following referred to as analyzed regions). To better distinguish the 10 analyzed regions, the corresponding dots are filled in the same color. For this reason, each subplot in Figure 5 consists of 10 differently colored lines of dots.

Each of the three subplots in Figure 5 refers to the specified snapshot selection criteria introduced above. However, rather than evaluating single snapshots, we order all hours of the year according to the criteria and evaluate the first 20 operational states for each of them. For example, the right subplot is created from taking the 20 h with highest magnitude of the summation of wind power generation and the load, whereas the selected operational states are those for which the highest price differences occur in the output of the reference model. By varying the size of the colored dots in Figure 5 we provide the information about the frequency of how often regions belong to the same cluster while performing the clustering for the first 20 h that fulfill a particular snapshot selection criterion. In the best case this means that, for each of the 20 h, a region on the *x*-axes has the same neighbors. Hence, plotting the best case would result in lines of colored dots of equal size.

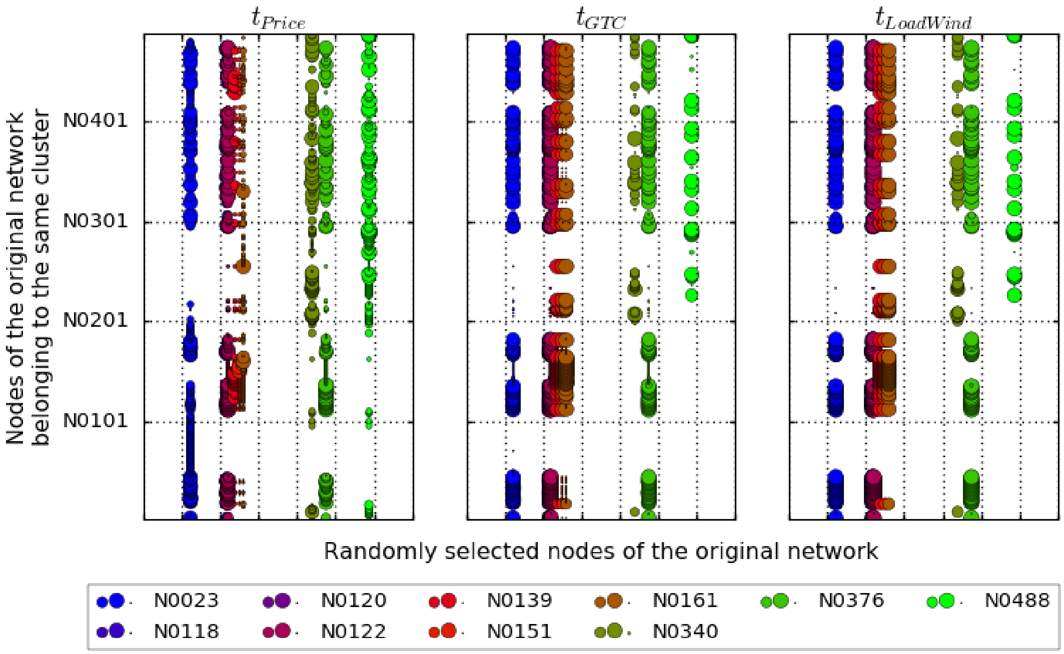

Figure 5. Neighborhood of 10 randomly selected regions after application of clustering based on different criteria: (**left**) t_{Price}; (**middle**) t_{GTC}; (**right**) $t_{LoadWind}$, evaluated for 20 snapshots per criterion.

In this sense, Figure 5 shows the robustness for running the clustering approach for 60 snapshots where a robust clustering is indicated by the following characteristics: For each of the 10 evaluated regions, a relatively small number of equally sized dots appear. In contrast to this, the more colored dots of different sizes, the less robust is the outcome of the clustering. Therefore, it can be stated that the subplot that belongs to $t_{LoadWind}$ shows a more robust clustering than in the case of t_{GTC} and t_{Price}.

To quantify this finding with a more general analysis, Figure 6 depicts the data evaluated for Figure 5 in the form of histograms. They show how often an analyzed region is grouped to a cluster with the same neighbors when performing the clustering 20 times for each snapshot selection criterion. In contrast to Figure 5, which is presented for illustrative purposes, Figure 6 is based on an evaluation of neighborhood for of all regions of the reference model (instead of 10). The best case would therefore result in a single bar at x = 20 and frequency of occurrence at y = 1 (we only need to analyze x = 20 since the other bars, e.g., for x = 19, show the probability of having exactly 19 times the same neighbors when evaluating 20 snapshots).

According to Figure 6, it can be stated that for the criterion $t_{LoadWind}$, the clustering is the most stable. We derive this from the frequency of occurrence at x = 20 which corresponds to number of evaluated snapshots per subplot in the histograms of Figure 6. In the case of $t_{LoadWind}$, it is 63% compared to 40% for t_{GTC} and 14% for t_{Price}. In summary, this means that snapshots based on $t_{LoadWind}$ lead to clusters that are more similar to each other than is the case for the network partitions derived from t_{Price} and t_{GTC}. In other words, using only a single snapshot based on $t_{LoadWind}$ leads to a more reliable clustering of the reference model than in the case of t_{Price} and t_{GTC}.

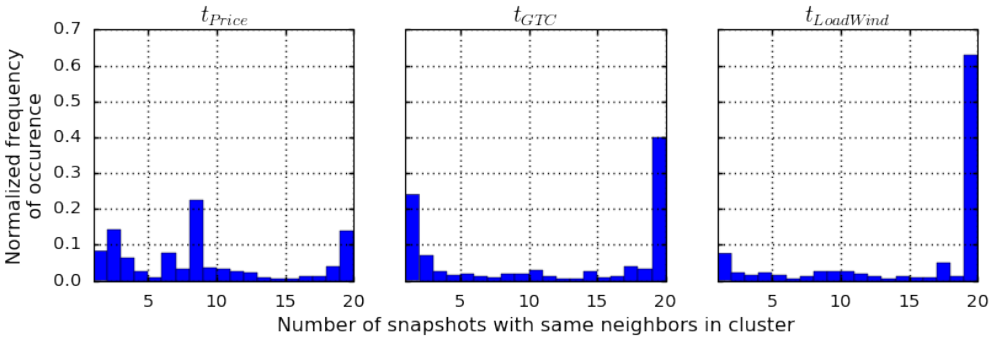

Figure 6. Frequency of occurrence that shows how often two regions are part of the same cluster when applying the clustering 20 times for different criteria, (**left**) t_{Price}; (**middle**) t_{GTC}; (**right**) $t_{LoadWind}$.

Although it can be concluded that for the subsequent steps of spatially aggregating the reference model, ideally multiple snapshots should be considered, we use single snapshot data for our analyses for reasons of simplicity. Thus, for the interpretation of the following findings it must be considered that aggregated ESM instances, especially based on t_{Price} and t_{GTC}, cannot claim to be representative for all states of the ESM where the transmission network is under stress.

3.3. Comparison of Aggregated Models

We evaluated a number of indicators to assess the quality of the three spatially aggregated ESM instances. This is conducted for the results of both the reference model and a set of aggregated benchmark ESMs. It is done to compare the resulting indicators in the context of (i) the best possible performance of the reference model, and (ii) the quality of the results of alternative ESMs (i.e., deviation of the indicators from the reference model).

Concerning the aggregation methodology, the general difference in creating benchmark ESMs lies in the network partitioning process. As already mentioned, the Copper plate ESM represents a single-node model. Since this model shows the lowest spatial resolution, it can be expected that the results of this model show the largest deviations compared to the reference model. The second benchmark ESM "Classical" is the commonly used regional model, which was proposed by the German transmission system operators [22]. As the electricity transmission infrastructure is evolving over time, ESMs that rely on "Classical" need to be frequently updated. However, the network partitioning of this model is based on expert judgment (considering centers of power consumption and power generation form vRES). The applied methodology is therefore not easily reproducible if only publicly available data is used. For this reason, one of the main objectives of the following analyses is to show the implications of statically using this pre-defined spatial aggregation. Lastly, "Simple aggregation" refers to a network partitioning based on the agglomerative clustering approach contained in scikit-learn [18] that obtains topological information in the form of the original network's adjacency matrix as connectivity.

By extending the above-described aggregation process with the determination of PTDF matrices of the aggregated network according to [26], the power flows of the original network can be emulated by the aggregated model instances. However, the appropriate equivalencing process is based on the nodal power injections (balance of nodal power consumption and generation) that occur in the original network. To be consistent with the selection of nodal price differences, the same points in time ($t_{LoadWind}$, t_{Price}, t_{GTC}) are used to select snapshots of nodal power injections. In the following, we refer to these three model instances as extended clustered models.

3.3.1. Redispatch

As for the validation of the reference model, we use the annually redispatched power generation to check whether transmission bottlenecks of the reference model are preserved. From Figure 7, we conclude that the findings from the comparison of capacity values also apply to the assessment of redispatch. The ESM instances derived from clustering nodal price differences show small deviations from the reference model's results. By increasing the number of aggregated regions, it is also likely that this performance can be further improved. More importantly, with values ranging from 0.7% to 4% for Clustered $t_{LoadWind}$, Clustered t_{Price} and Clustered t_{GTC}, the deviation of annually redispatched power generation is closer to the reference than for any of the benchmark ESMs.

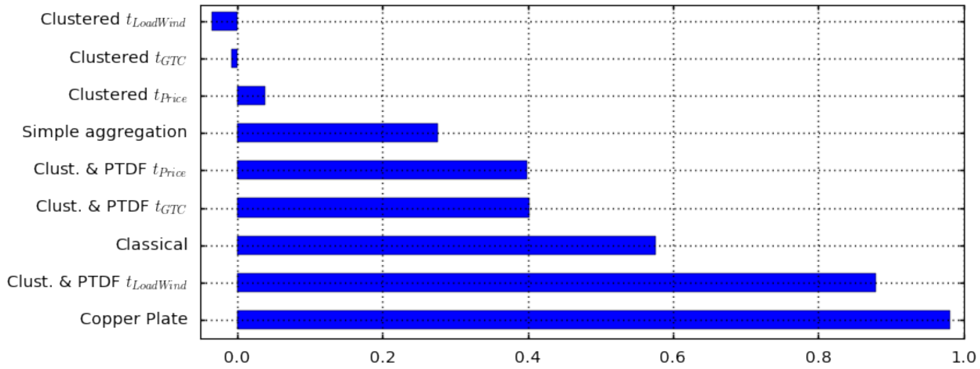

Figure 7. Redispatched power generation, relative deviation from the reference model for different aggregated ESM instances.

Given that Clustered $t_{LoadWind}$ also shows a good performance, and referring to the results from the stability analysis, we deduce that for the application of the presented approach, a fully solved instance of the original problem is not necessarily needed. Since $t_{LoadWind}$ can be identified using only the input time series of the spatially highly resolved model, the reference model needs to be solved only for a pre-defined time slice. In contrast, in the case of t_{Price} and t_{GTC}, each hour of the year must be evaluated with a high spatial resolution.

For the extended clustered model instances, the same spatial aggregations are used, but the distribution of power flows is determined by a reduced PTDF matrix. Therefore, additional information in the form of the nodal power balance from the reference model is considered. With regard to Figure 7, the redispatch of the corresponding model instances deviates significantly (40–88% compared to the reference model). This behavior can be explained by the static distribution of power flows based on power generation and consumption data from the snapshot that is supposed to represent an extreme situation for the grid. The derived PTDF matrices are therefore not representative enough to suitably determine the power flow distribution in the original network for the whole operation period. For more details regarding this redispatch analysis see Appendix G.

3.3.2. Capacity Factors

For a typically assessed indicator, we measure the similarity of power plant operation by comparison of technology-specific capacity factors. Therefore, Figure 8 shows the deviation of capacity factors compared to the reference model for different types of power plants. The compared model instances are grouped by colors, where the benchmark ESMs are depicted in reds and the aggregated models are shown in blues and greens.

In this context, a good performance of an aggregated ESM is indicated by a deviation of the technology-specific capacity factor, which is close to 0%. Furthermore, for each technology, the dark red bar (Copper Plate) gives an indication of the effect of neglecting the power exchange limitations. As expected, wind offshore power plants benefit from neglecting transmission constraints in aggregated ESMs as they are able to distribute generated electricity for nearly zero marginal costs over larger areas. In contrast, coal-fired power plants, open cycle gas turbines and wind onshore turbines are less operated in all of the aggregated model instances. In the case of run-of-river power plants and photovoltaics, almost all ESM instances show the same capacity factors as the reference model. For the investigated case of Germany, this means that for an appropriate simulation of the operational behavior of these power plant types, a high spatial resolution is not essential. This is due to the fact that the corresponding capacity factors can be well approximated with spatially fully aggregated ESM instances, such as the copper plate model.

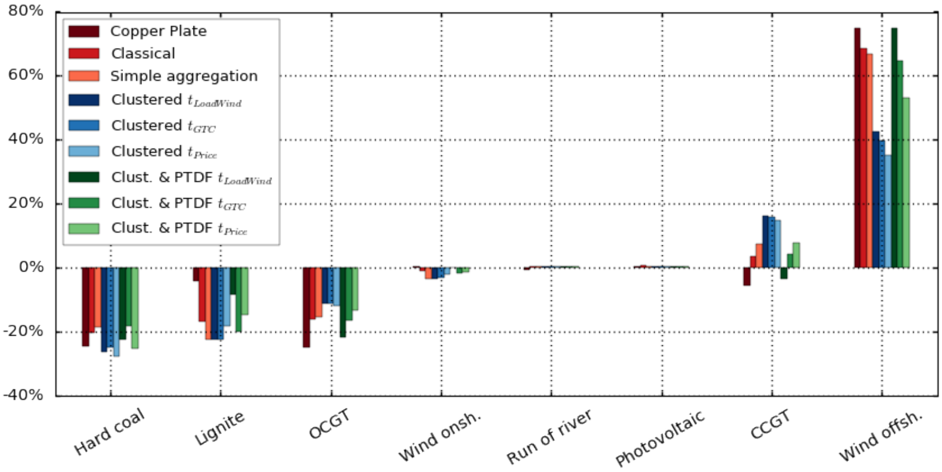

Figure 8. Capacity factors, relative deviations from the reference model for different aggregated ESM instances.

With the exception of combined cycle gas turbines (CCGTs), the blue bars show almost the smallest deviation or they range in a similar order of magnitude, as is the case for the red bars. From an overall perspective, Clustered t_{Price} shows the best performance with a mean deviation of 13.8%, followed by Cluster & PTDF t_{Price} (14.5%), while in the case of the copper plate model, this value is 17%.

Comparing the blue and the green bars confirms the conclusion that it is not advantageous to use the extended clustered models based on power injections of critical situations. This becomes particularly clear when comparing the resulting capacity factor deviations for wind offshore where the extended clustered models show an error between 53% and 75%.

However, with up to 42% deviation, the operational behavior of the simply clustered models (blue bars) is also remarkable. The underlying, significantly higher utilization of offshore wind in the aggregated models stems from bottlenecks that occur in the reference model for links that connect offshore wind farms with the mainland. These connections are not maintained in the clustered models since the observed nodal prices at both ends of the links are usually nearly the same, resulting from strong power generation surpluses at the appropriate substations. At the same time, a downstream bottleneck prevents that this surplus power generation can be transmitted to nodes with higher nodal prices.

As an example, this situation is depicted in Figure 9, which shows an extract of Northern Germany. There are two congested links that connect wind offshore turbines to the mainland. They are vanished when aggregating all nodes of the light blue cluster and thus contribute to the deviation of the capacity factor for offshore wind turbines (Figure 8). However, the downstream bottleneck between the light blue and marine blue cluster is considered in the clustered models. Since this particular bottleneck prevents the efficient transmission of surplus generation from all of the light blue nodes, an increase in its GTC is more pressing than the elimination of the offshore congestions. On the one hand, we understand this effect as an advantage of the chosen clustering approach as it allows prioritizing of critical, but equally utilized, links. On the other hand, although the presented approach generates spatial aggregations where transmission bottlenecks are supposed to be maintained, it is possible that intra-zonal bottlenecks do still appear.

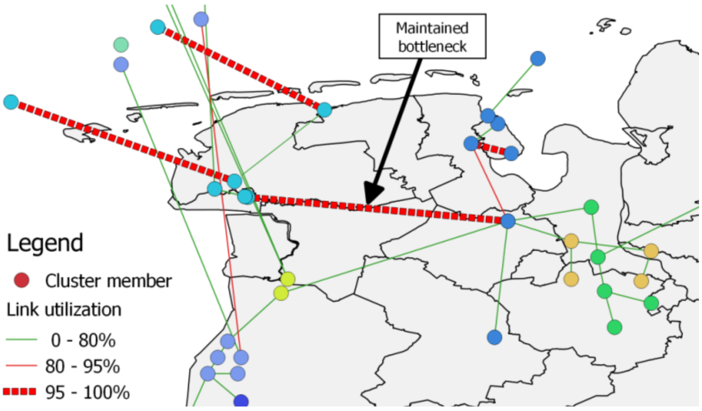

Figure 9. Utilization of transmission lines in the reference model including clustering information (colored dots) for an aggregation based on t_{Price}.

For the practical application of the presented approach, this means that ideally, an alternating process of clustering the spatially highly resolved model (with eventually already increased GTCs) and analysis with the aggregated model instances is conducted. For a better estimation of grid transfer capacities, the approach presented in [57] also appears to be a suitable solution.

3.4. Case Study

To give an example for the application of the proposed ESM clustering and aggregation method, a simplified grid and storage expansion study is conducted. By simplified we mean that we use linear programming and determine investment costs using the equivalent annual costs and assuming an interest rate of 6% (for more details see Appendix H). Accordingly, the presented case study does not claim to provide a robust scenario analysis. Rather, it gives an indication what could happen to the results of a typical ESM use-case if the standard clustering (Classical) is replaced by a spatially aggregated model that relies on spectral clustering of nodal price differences.

While generation capacities are pre-defined by the scenario dataset, the expansion of lithium-ion batteries as well as of GTCs for both alternate current (AC) and direct current (DC) overhead transmission lines is enabled. In case of the latter, this means that the planned High-Voltage Direct Current (HVDC)-connections from north to south Germany [40] are provided as candidates for new links using a capacity-constrained transport model. They are characterized by techno-economic parameters that differ from those of AC transmission lines. The AC grid is modeled by a DC-power flow approximation, while capacity expansion is only possible if a link already exists. Consequently, the available power provision from vRES needs to be balanced, either temporally by new storage units or spatially by the expansion of grid transfer capacities that represent the indicators to assess the performance of different spatially aggregated ESM instances.

In this context, Figure 10 shows the results of the case study by depicting the total sum of model-endogenously added capacities for four different model instances. The results for lithium-ion batteries range between 10.3 and 10.9 GW (110.9 and 113.3 GWh). Having in mind that short-term storage facilities such as batteries are suited to balance variations from power generation by photovoltaics, this similarity in storage expansion corresponds to the equality of capacity factors for the different spatially aggregated ESMs found above (Figure 8). In addition, this result is comparable to the total sum of installed short-term flexibility options (batteries and demand side management: 12 GW) for temporal power balancing in [40].

In contrast, the values for additional GTC in the AC grid differ more significantly among the several aggregated ESMs. In particular, this applies to the Classical model instance that shows 14.7 GW of GTC expansion, which is less than half compared to the aggregated ESMs derived by the presented clustering approach.

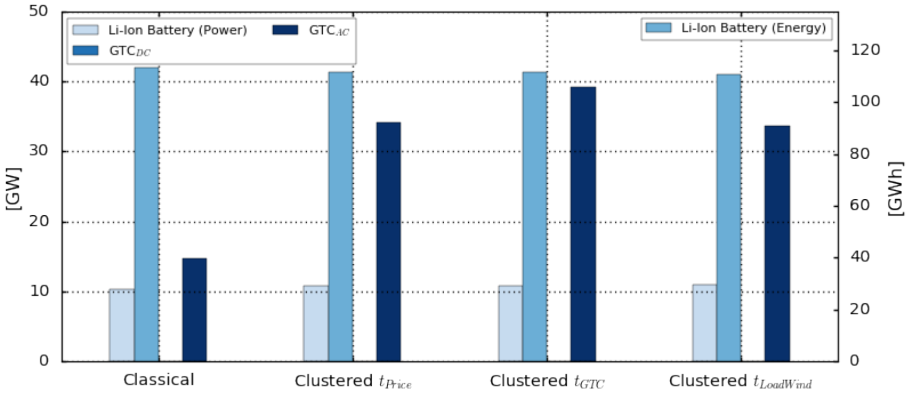

Figure 10. Capacity expansion for lithium-ion batteries and grid transfer capacities in different aggregated models.

When taking into account the lengths of expanded transmission lines, the observed difference for AC grid expansion becomes even larger (Classical 96 GWkm, Clustered t_{GTC}: 554 GWkm, Clustered $t_{PriceDelta}$: 447 GW and Clustered $t_{LoadWind}$ 364 GWkm). Although the amount of added capacity is significantly greater for the clustered models, the resulting total system costs are 1.5–2% lower than in the case of Classical. This is due to the fact that the additional power transmission capacities allow a more intensive utilization of cost-efficient power plants. From this, we conclude that applying the Classical spatial aggregation of Germany from [22] leads to an underestimation of grid expansion needs if a system cost minimizing ESM is used.

Among the clustered instances, the highest value of GTC expansion can be observed for Clustered t_{GTC}. The corresponding snapshot for deriving this aggregated ESM is based on the utilization of transmission lines in the reference model. As this represents a strong indicator for grid congestions, this result is expected. The drawback of using such a clustered model instance is the necessity of solving the reference model for the full time period to identify the required snapshot. However, this is not the case for Clustered $t_{LoadWind}$ where the snapshot identification relies only on the input data. From a practical point of view, a clustering based on $t_{LoadWind}$ is the most favorable since the capacity expansion for the appropriate aggregated model lies in a similar order of magnitude, as for the instances derived from the other snapshot selection criteria.

Remarkably, grid expansion for the HVDC transmission line candidates cannot be observed in any of the evaluated models (indicated by the missing bar for GTC$_{\text{DC}}$ in Figure 10). A reason therefore is that, in the chosen modeling setup, a GTC expansion is only partially necessary to achieve an increase in power flows to be transmitted from the vRES surplus-dominated north to the south of Germany. As this requires mainly investments into additional GTC on congested but short links (<100 km), the enforcing of AC transmission lines is still the more cost-efficient option compared to building new long-distance HVDC connections. However, the advantages of the HVDC technology, such as the capability of having a controlling influence on power flows, are not considered in the applied formulation of a spatially aggregated ESM. For example, the role of loop flows through Eastern Europe cannot be assessed in this way. In addition, the main purpose of the spatially aggregated model instances is to gain better insights into how the balancing of variable power feed-in and demand can be sufficiently realized in future energy systems. They are thus rather less suited to identify the exact need of expansion projects in the electricity transmission grid.

3.5. Comment on Computing Times

This information should be understood as an orientation for other modelers rather than a claim to be a generally valid finding. All spatially highly resolved models were solved on an Intel(R) Xeon(R) CPU E5-1620 v3 @ 1 × 3.50 GHz, 128 GB RAM computer (validation data set) and an Intel(R) Xeon(R) CPU E5-2640 v3 @ 2 × 2.60 GHz, 192 GB RAM (scenario data set) using CPLEX's interior point method with eight threads. Depending on the processor load and the used parameterization (validation or scenario dataset), the total computing times, inclusive of the post-processing routines, ranged between 8 and 34 h. These computing times could be decreased to values between 14 and 24 min for all runs executed on the spatially aggregated ESM instances using an Intel(R) Xeon(R) CPU X5650 @ 2 × 2.67 GHz, 72 GB RAM machine and the same solver settings.

To get an idea of the trade-off of computing time and model accuracy, Table 3 shows the relative values of the total system costs and total computing times for the aggregated model instances in relation to the appropriate values of the reference model. While the deviation of the objective value is not greater than 7.4% for all model instances that consist of 20 regions, the computing time can be reduced to a few percent of the value of the reference model.

Table 3. Trade-off between model accuracy and performance: objective value and total computing time for aggregated ESM instances relative to the appropriate values of the reference model (scenario data set).

Model Instance	Objective Value (Total System Costs)	Total Computing Time
Cluster & PTDF t_{Price}	100.0%	2.8%
Cluster & PTDF t_{GTC}	99.3%	4.8%
Clustered $t_{LoadWind}$	98.4%	3.9%
Clustered t_{GTC}	98.0%	4.4%
Clustered t_{Price}	97.6%	3.2%
Simple Aggregation	94.8%	4.8%
Classical	93.2%	3.8%
Cluster & PTDF $t_{LoadWind}$	92.6%	4.3%
Copper Plate	89.8%	0.7%

As with the reduction of other model scales, for example the reduction of the number of technologies by defining technology classes, the model is downsized. This means, fewer constraints and fewer variables occur in the coefficient matrix of the mathematical optimization problem. Reducing the temporal scale of an ESM—that usually performs analyses over 8760 time steps—by defining representative time slices [58] is therefore effective since reduction ratios >100 can be achieved. Previous analyses showed that the corresponding downsizing factor more or less scales with the achievable speed-up [59].

However, in this paper, the reduction ratio applied to the spatial scale is <10. For example, for the reference model we observe a number of 13,960,164 constraints compared to a number of 2,549,001 for the Classical ESM instance (both after the execution of CPLEX's pre-solve). The main benefit of solving spatially aggregated ESMs instead of their fully resolved versions is caused by another effect—the removal of strongly linking constraints from the original problem. Due to the possibility to transfer power, the power generation and consumption of each individual region could have an effect on all the other analyzed regions of an ESM (the non-zero entries of an appropriate PTDF matrix can give an impression of the interdependencies). In contrast, linking constraints that couple time steps (e.g., applied for modeling storage facilities) usually link pairs of time steps.

Nevertheless, Table 3 cannot claim to provide an exact comparison or derive recommendations regarding an optimal model setting that combines both low computing times and sufficiently accurate model results. This is due to the fact that from a practical point of view the objective value does not represent the best indicator to measure the model accuracy. Rather, specific investigations are needed to identify optimal model settings for different research questions that require the evaluation of certain combinations of model performance indicators. For example, if only the values in Table 3 would be considered, the aggregated ESM Cluster & PTDF t_{Price} appears to be the best choice if the reference model should be aggregated. However, this is not the case when taking into account the evaluation of redispatch from Figure 7.

In summary, the following can be stated. The trade-off between the accuracy and the performance (measured in computing time needed for solving the model) of a spatially aggregated model depends on several aspects. On the one hand, a justifiable error for the indicators that should be analyzed must be defined. On the other hand, there exists a broad spectrum of parameters that can be adjusted (e.g., the optimal number of clusters) to achieve both acceptable computing times and a manageable memory demand with respect to the available computing infrastructure. In this paper, we proposed a new approach that can be used for such model setup optimizations applicable to ESMs that need to incorporate possible bottlenecks in the power transmission grid of the future.

4. Conclusions

With the presented methodology, the aggregated ESM instances could be derived from a spatially highly resolved ESM of Germany that only needed to be solved for defined time-slices (snapshots). We found that evaluating the input time series of potential wind power feed-in and load represents a suitable approach to identify such snapshots. We further proposed a network partitioning based on spectral clustering of nodal differences of the marginal total system costs and compared two approaches for the creation network equivalents. In this way, we developed a methodology to preserve transmission links that tend to represent bottlenecks in future power systems for spatially aggregated ESMs.

With a correlation factor greater than 0.64, a created spatially highly resolved reference model was able to produce times series for electricity prices similar to those recorded in 2012. The evaluation of different performance indicators showed the strengths of aggregated ESM instances that were derived by the presented methodology. Rather than the preservation of critical links, further advantages were observed since annually redispatched energy (error: 0.7–4%) and capacity factors of power plants (mean error: 13.9–15.4%) deviated less from the reference model's outputs than from those of the defined benchmark ESM.

The resulting spatially aggregated ESM instances are intended to be used for capacity expansion studies. We therefore conducted a case study for grid and storage expansion for a scenario of the German power system in the year 2030. Here, we observed a significant lower expansion of grid transfer capacities for a commonly used, spatially aggregated model instance compared to ESM instances derived by the proposed methodology. However, for decentralized technologies, such as photovoltaics and lithium-ion batteries, no differences in the analyzed indicators were found among the several aggregated ESM instances.

An obvious next step of the presented study is the extension of its geographical scope to a European level as well as the claim to cover all energy sectors with the spatially aggregated ESM. However, improvements regarding the availability of spatially highly resolved data are necessary. This applies not only to a more sophisticated determination of the locations of large thermal power plants to be commissioned in the future but also to potential hotspots of vRES power generation. While for an ESM of Germany the used approach of spatially distributing national generation capacities is sufficient, a dataset that consistently provides the locations of decentralized power generation is required for the desired geographical scale. In this context, sophisticated methodologies that evaluate remote sensing data may be applicable. Studies that build on the presented approach would also benefit from the consideration of regionalized load profiles.

From a methodological point of view, the simple creation of copper plates to represent aggregated regions ignores that geographical distances between zones become larger with the geographical expansion of a zone. A correction of distances in the aggregated network thus provides the potential for improving the accuracy of the network equivalent. This also applies to the identification of snapshots used for gaining data from the initial spatially highly resolved ESM. Finally, in the actual study, also short-length transmission lines are considered when running the clustering algorithm. However, since expanding the GTC of such lines is relatively cheap, it seems to be beneficial to perform first a spatial clustering of regions based on geographical distances to avoid that these less relevant links are maintained in the aggregated models.

The spatial aggregation of optimizing energy system models (ESMs) becomes attractive if solving such models reaches computational limits. Given the trend of the increasing complexity of energy systems with high shares of variable renewable power generation, the presented approach can be used for energy scenario analyses that claim to capture both the temporal and spatial balancing needs of electricity demand and generation. It extends the set of available modeling instruments for generating new insights into future energy systems and their possible technological compositions and thus helps to develop strategies to cope with the challenges related to a secure, economically feasible, and sustainable energy supply.

Author Contributions: K.-K.C. conceived and designed the overall methodology; he also performed the modeling exercise, analyzed the data and wrote the paper; J.M. developed and implemented the spectral clustering approach; S.B. contributed to the literature review and did parts of the implementation of the spatial aggregation methodology into the energy system model REMix.

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Abbreviations

CCGT	Combined Cycle Gas Turbines
ENTSO-E	European Network of Transmission System Operators for Electricity
ESMs	Energy system models
HVDC	High-Voltage Direct Current
NUTS	Nomenclature des unités territoriales statistiques
PTDF	Power Transfer Distribution Factors
REI	Radial Equivalent Independent
SP	Spatially differentiated
TC	Technologically differentiated
TM	Temporally differentiated
vRES	variable renewable energy sources
Symbols	
GTC	Grid transfer capacity of a link in the original network
GTC_{agg}	Grid transfer capacity of a link in the aggregated network
K	Incidence matrix
k	Number of clusters
$L_{unnormalized}$	Unnormalized Laplacian matrix of the original network
L	Set of links in the original network (transmission lines in an ESM)
L_{agg}	Set of links in the aggregated network
l	Element of the links set in the original network
l_{agg}	Element of the links set in the aggregated network
N	Set of nodes in the original network (modeled regions of an ESM)
N_{sub}	Subset of N containing only active nodes (nodes with power generation or consumption)
$N_{sub,nearest}$	Subset of N_{sub} containing the three closest substations to the geographical center of a NUTS3 region
N_{agg}	Set of nodes in the aggregated network
N_{NUTS3}	Set of NUTS3 regions considered in the reference model
n	Element of the nodes set in the original network
n_{sub}	Element of the subset N_{sub}
$n_{sub,nearest}$	Element of the subset $N_{sub,nearest}$
n_{NUTS3}	Element of the set of NUTS3 regions considered in the reference model
n_{agg}	Element of the nodes set in the aggregated network
P_{inst}	Installed power generation capacity in the original network

$P_{inst,agg}$	Installed power generation capacity in the aggregated network
T	Set of hourly time steps
t	Element of the set of hourly time steps
t_{GTC}	Selected time step within the set of time steps where a high utilization of transmission lines can be detected in the reference model
$t_{LoadWind}$	Selected time step within the set of time steps where a high magnitude of power demand and power feed-in from wind turbines can be observed in the input data
t_{Price}	Selected time step within the set of time steps where high nodal price differences can be observed in the solution of the reference model
$\Delta\rho$	Nodal price difference
κ	Number of nearest neighbors to be used
Π_f	Mapping matrix between links of the original and the aggregated network
Π_g	Mapping matrix between nodes of the original and the aggregated network
ρ	Nodal marginal system costs for total power supply (nodal prices)
ρ_{diag}	Diagonal matrix of nodal price differences
T	Set of technologies
T_{dec}	Subset of T containing decentral power generation technologies
τ	Element of the set of technologies
τ_{dec}	Element of the subset T_{dec}

Appendix A. Essential Equations of REMix for Performing a DC Optimal Power Flow

For a more complete description of the applied ESM (REMix) the objective function and a selection of essential constraints are listed in the following.

Appendix A.1. Objective Function

The objective function to be minimized is represented by the total annual system costs:

$$\begin{gathered}\sum\nolimits_{\tau,\, y} C_{system}(\tau,\ y) \rightarrow min \\ \text{where}: C_{system}\ \geq\ 0\end{gathered} \tag{A1}$$

τ: Element of the set of all considered technologies.

y: Element of the set of years (either set to y = 2012 for the validation data set or y = 2030 for the scenario data set).

The annual system costs C_{system} contain costs for the system operation and optionally costs for capacity expansion. One the one hand side, the annual operation costs are determined by summation of the variable C_{op} for every time step. On the other hand side, the annual capital/investment costs C_{invest} are not time step dependent and thus are not considered in the summation over the time steps. In addition, link related and node related costs are distinguished. Since it is possible to investigate just a fraction of a year, the annual costs are scaled by the factor f.

$$\begin{gathered}C_{system}(\tau,\ y) = [\sum\nolimits_{l}(C_{invest}(\tau_l,\ y,\ l) + \sum\nolimits_{t} C_{op}(\tau_l,\ y,\ l, t)) + \sum\nolimits_{n}(C_{invest}(\tau_n,\ y,\ n) + \\ \sum\nolimits_{t} C_{op}(\tau_n,\ y,\ n, t))] \cdot f \\ \forall\ \tau, y\end{gathered} \tag{A2}$$

τ_l: Element of the subset of link dependent technologies

τ_n: Element of the subset of node dependent technologies

l: Element of the set of links

f: Scaling factor for sub-annual analyses

For applications that only optimize the dispatch of a given energy system—in this study this applies to all sub-sections of Results and Discussion except Case Study)—no investment costs are considered ($C_{invest} = 0$). The operational costs can be decomposed into a fixed (time independent) and a variable fraction. Besides specific costs per electrical energy generated, the latter contains costs for fuels, emission allowances and estimated costs in case of loss of load events.

Appendix A.2. Essential Constraints

One typical constraint of the mathematical model behind REMix is the power balance constraint. To ensure that the power availability (e.g., given by feed-in time series of power generation from vRES) and the power demand are always balanced, slack variables ($\mathrm{P_{slack}}$) are considered in the model. The amount of the appropriate penalty costs is set to a very high level to ensure that this artificial power generation is always the last option to satisfy the power demand:

$$\begin{gathered}\textstyle\sum_\tau P_{gen}(\tau_{gen},\ y,n,t) - P_{loss}(\tau,y,n,t) - P_{charge}(\tau_{stor},y,n,t) + P_{discharge}(\tau,y,n,t) - \\ P_{export}(\tau_{trans},y,n,t) + P_{import}(\tau_{trans},y,n,t) + P_{slack}(y,n,t) = P_{dem}(y,n,t) \\ \text{where} \\ P_{gen} \geq 0,\ P_{loss} \geq 0,\ P_{charge} \geq 0,\ P_{discharge} \geq 0,\ P_{export} \geq 0,\ P_{import} \geq 0 \\ \forall \tau, y, n, t\end{gathered} \tag{A3}$$

τ_{gen}: Element of the subset of power generation technologies

τ_{stor}: Element of the subset of storage technologies

τ_{trans}: Element of the subset of power transmission technologies

For power generators, storage facilities and power transmission infrastructures capacity limits are considered. In case of the latter the following constraint is applied:

$$\begin{gathered}P_{trans}\ (\tau_{trans},\ y,\ l,\ t) \leq\ GTC_{inst}\ (\tau_{trans},\ y,\ l)\ +\ GTC_{add}\ (\tau_{trans},\ y,\ l) \\ \forall\ \tau_{trans}, y, l, t\end{gathered} \tag{A4}$$

P_{trans}: Power flow in a certain time step t and year y over transmission line l of the transmission technology τ_{trans}.

The relation between the node specific power imports and exports and the link specific power flows is defined by the DC power flow equations which are used to model flows in the AC transmission grid:

$$\begin{gathered}P_{import}\ (\tau_{AC},\ y,\ n,\ t)\ -\ P_{export}(\tau_{AC},\ y,\ n,\ t)\ -\ P_{loss}\ (\tau_{AC},\ y,\ n,\ t) =\ \textstyle\sum_{n'}\ B\ (n,\ n') \cdot \theta\ (y,\ n,\ t) \\ \forall\ \tau_{AC}, y, n \neq n',\ t\end{gathered} \tag{A5}$$

τ_{AC}: Element of the subset of transmission technologies realized as AC grids

B: Nodal susceptance matrix of the considered AC transmission network

θ: Voltage angle at node n in time step t and year y

where the power flows are determined by:

$$\begin{gathered}P_{trans}\ (\tau_{AC},\ y,\ l,\ t) =\ \textstyle\sum_{n,l'} B_{diag}(l,l') \cdot K^T(l',n) \cdot \theta\ (y,\ n,\ t) \\ \forall\ \tau_{AC}, y, n \neq n',\ t\end{gathered} \tag{A6}$$

K^T: Transposed incidence matrix of the considered AC transmission network

B_{diag}: Diagonal matrix of the link susceptances of the considered AC transmission network

and the losses are linearly approximated:

$$\begin{gathered}P_{loss}\ (\tau_{AC},\ y,\ n,\ t) =\ \textstyle\sum_{l \to n} P_{trans}(\tau_{AC},\ y,\ l,\ t) \cdot f_{loss} \cdot d(l) \\ \forall\ \tau_{AC}, y, n \neq n',\ t\end{gathered} \tag{A7}$$

$f_{loss} = 0.02\frac{\%}{km}$: Losses factor

d: Length of the link l

The model also distinguishes between the AC transmission grid and point-to-point HVDC transmission lines for which the power flows are modeled by a simple capacity constrained transport (pipeline). For more details regarding further constraints considered in REMix please see [6].

Appendix B. Assignment of Power Generation and Consumption

For performing the nearest neighbor analysis, the GIS software tool QGIS is applied. As the final result of this pre-processing step, a matrix Π is set up that maps power generation or consumption from areas (NUTS3) to point coordinates (substations):

$$\begin{gathered} P_{inst}(\tau_{dec},\ n_{sub}) = \sum\nolimits_{n_{NUTS3}} \Pi(n_{sub},\ n_{NUTS3}) \cdot\ P_{inst}(n_{NUTS3}, \tau_{dec},) \\ \forall \tau_{dec} \in \mathrm{T}_{dec},\ \forall n_{sub} \in N_{sub} \end{gathered} \tag{A8}$$

where N_{sub} is a subset of the original network's set of nodes. In N_{sub}, passive nodes are removed accordingly. In Equation (A8), T_{dec}, a subset of T, only contains decentralized power generation technologies.

We doubt that the assignment of decentralized power generation from a whole region to one single substation meets reality. Therefore, for each NUTS3 region, we also performed a κ = 3 nearest neighbor analysis to identify the three closest substations of a designated area. The appropriate generation capacity or power demand is then distributed by the weighted share of the reciprocal distance between the area's centroid and the substations. The mapping matrix Π therefore consists of zero and non-zero entries, where for the latter, the sum over all rows is equal to one:

$$\begin{gathered} \Pi(n_{sub},\ n_{NUTS3}) = \frac{d(n_{sub},\ n_{NUTS3})^{-1}}{\sum_{j=1}^{j=3} d\left(n_{sub,j},\ n_{NUTS3}\right)^{-1}} \\ \forall n_{sub} \in N_{sub,nearest},\ \forall n_{NUTS3} \in N_{NUTS3} \end{gathered} \tag{A9}$$

In Equation (A9), $N_{sub,nearest}$, a subset of N_{sub}, contains the three nearest substations for each NUTS3 area. The required distances d are calculated by applying the cosine formula to the point coordinates of the area centroids and substations:

$$\begin{gathered} d(n_{sub},\ n_{NUTS3}) = \mathrm{acos}[\sin(lat_{sub}) \cdot \sin(lat_{NUTS3}) + \cos(lat_{sub}) \cdot \cos(lat_{NUTS3}) \cdot \\ \cos(lon_{NUTS3} - lon_{sub})] \\ \forall n_{sub} \in N_{sub},\ \forall n_{NUTS3} \in N_{NUTS3} \end{gathered} \tag{A10}$$

where N_{NUTS3} is the set of NUTS3 regions and lat and lon either indicate the explicit coordinates of a substation or of a geographical centroid of a NUTS3 region.

For the assignment of nodal demand profiles, the national load profile of Germany is normalized and subsequently scaled by the annual demand. The latter, in turn, is scaled by population data from the national to the NUTS3 level and assigned to substations using the approach mentioned above. In contrast to decentralized electricity generation technologies, large central power plants are directly mapped to their κ = 1 nearest neighbor substation.

Table A1 summarizes the applied assignment approach for each of the considered technologies in the reference model configuration.

Table A1. Applied mapping approach for the assignment of power generation and consumption to substations of the used transmission grid dataset.

Input Parameter	Approach
Installed capacity of central power plants: • Fossil fired power plants • Nuclear power plants • Offshore wind farms • Pumped storage	Nearest neighbor

Table A1. *Cont.*

Input Parameter	Approach
Installed capacity of decentral power plants: • Photovoltaics • Onshore wind farms • Hydro run-of-river • Biomass fired power plants	3-nearest neighbor
Annual electricity demand	3-nearest neighbor

Appendix C. Estimation of the Transmission Capacities from Thermal Limits

The applied transmission grid dataset contains information about the voltage U level as well as the number of circuits $n_{circuits}$. For an estimation of grid transfer capacities GTC, the thermal limits I_{max} of overhead transmission lines need to be known. These limits can be derived from the type of conductors installed per bundle [60]. In order to consider somehow the (n-1)-criterion as well as the fact that the calculated transmission limit for complex power in Equation (A4) needs to be higher than the required upper bound for active power flow in the model, a security margin μ is taken into account:

$$GTC = \sqrt{3} \cdot U \cdot I_{max} \cdot n_{bundles} \cdot n_{systems} \cdot n_{circuits} \cdot \mu \tag{A11}$$

$U = \{220\text{ kV},\ 380\text{ kV}\}$: nominated voltage of a transmission system
$I_{max} = 645\ A$: thermal limit for 243-A1/39-St1A conductors
$n_{bundles} = 4$: number of conductors per line
$n_{circuits} = \{1,\ 2\}$: number of circuits per trace
$\mu = 0.8$: (n-1) security margin

For the selection of an appropriate conductor type applied to all HVAC transmission lines of the grid dataset, a calibration is conducted in advance.

Appendix D. Determination of Snapshots

For spatially aggregating the results of the reference model to identify certain hours of the year as snapshots, a statistical measure is applied over the set of links or the set of nodes in the original network. For this purpose, quantiles are used instead of maximum or minimum values to avoid an overestimation of regionally limited extreme situations. The following formulas show how the points in time, that represent the snapshots which are used for executing the above presented clustering approach, are determined.

$t_{LoadWind}$:

$$\begin{gathered} t_{LoadWind} = t,\ if\ P_{LoadWind}(t) = \max P_{LoadWind}(t) \\ \text{where} \\ P_{LoadWind}(t) = Q_{0.95}(P_{gen}(t,\ n,\ \tau_{wind})) + Q_{0.95}(P_{dem}(t,\ n)) \\ \forall t \end{gathered} \tag{A12}$$

$Q_{0.95}$: 0.95-quantile
$P_{LoadWind}(t)$: Spatially aggregated time series of power generation by wind turbines and power consumption
$P_{gen}(t,\ n,\ \tau_{wind})$: Time series of power generation of wind turbines in each region n
$P_{dem}(t,\ n)$: Time series of power consumption in each region n

t_{Price}:

$$\begin{gathered} t_{Price} = t,\ if\ \rho_{agg}(t) = \max \rho_{agg}(t) \\ \text{where} \\ \rho_{agg}(t) = Q_{0.95}(\rho(t,n)) - Q_{0.05}(\rho(t,n)) \\ \forall t \end{gathered} \tag{A13}$$

$\Delta\rho(t)$: Spatially aggregated time series of power generation by wind turbines and power consumption t_{GTC}:

$$\begin{gathered} t_{GTC} = t,\ if\ f_{agg}(t) = \max f_{agg}(t) \\ \text{where} \\ f_{agg}(t) = Q_{0.95}(f(t,l)) \\ \forall t \end{gathered} \tag{A14}$$

$Q_{0.05}$: 0.05-quantile

$f_{agg}(t)$: Spatially aggregated time series of relative power flows

$f(t,l)$: Time series of relative power flows over each transmission line l

Appendix E. Calculation of Annual Redispatch for the Reference Model

For calculating the amount of annually redispatched power generation in a nodal pricing model, the following processing of the model results is conducted. We subtract the technology specific annual power generation of the copper plate model from the spatially summed power generation for each technology of the reference model. The result is a power balance that shows which technologies generate more or less electricity due to the consideration of power flow constraints. The annual redispatch is than observed by subtracting the power transmission losses (which do not occur in the copper plate model) either from the sum of positive values or the sum of negative values in this balance, e.g.,:

$$\begin{gathered} E_{RD} = \sum_{\tau_{gen}} E'_{RD}(\tau_{gen}) - \sum_{l,t} P_{loss}(\tau_{trans}, l, t) \\ E'_{RD} \in \mathbb{R}^{+} \\ \text{where} \\ E'_{RD}(\tau_{gen}) = \sum_t \left(\sum_n P_{gen}(\tau_{gen},\ n, t) -\ P_{gen,CP}(\tau_{gen}, t) \right) \\ \forall \tau_{gen} \end{gathered} \tag{A15}$$

E_{RD}: Annually redispatched energy

Appendix F. Clustering Maps

Figure A1 shows maps of Germany where substations (regions of the reference model) are same colored if they belong to the same cluster. The thick lines between the colored dots represent transmission lines that are maintained after performing the network reduction.

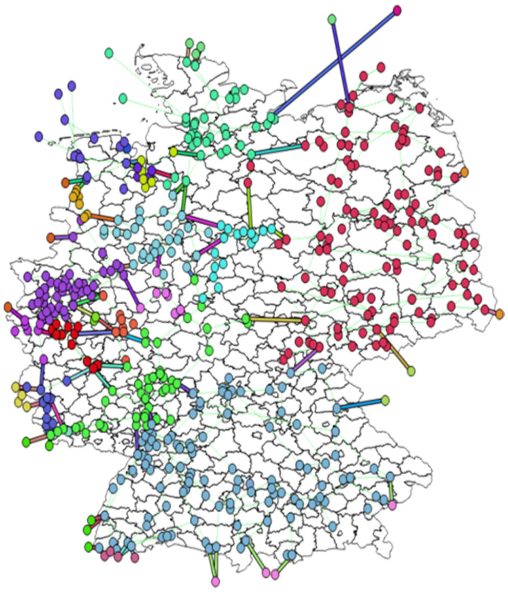

Figure A1. *Cont.*

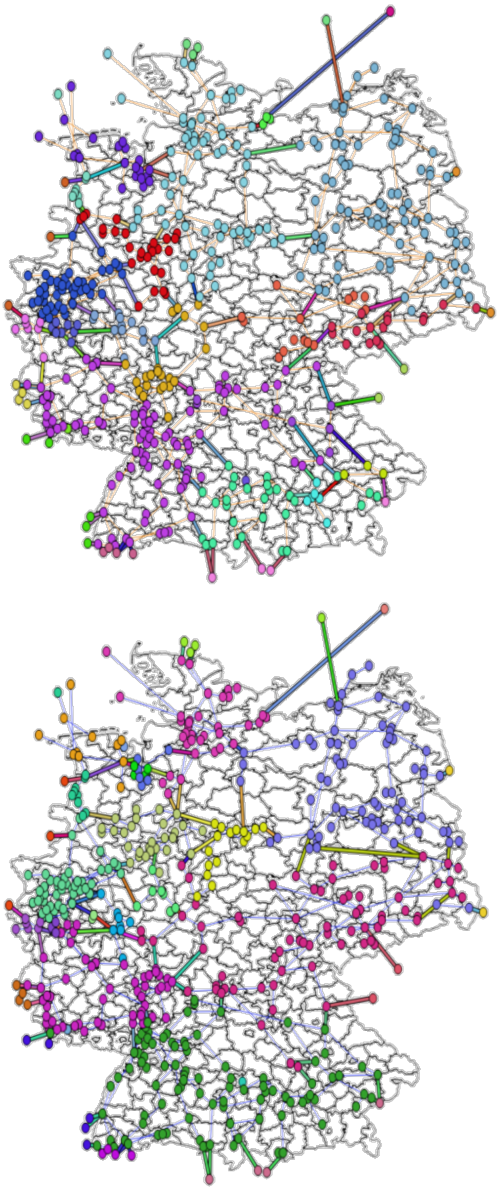

Figure A1. Maps of the German electricity transmission grid model after applying the presented clustering approach based on the validation data set and different snapshot selection criteria (**top**) t_{Price}, (**middle**) $t_{LoadWind}$ (**bottom**) t_{GTC}.

Appendix G. Concurrency of Redispatch Measures

To give an example of when the redispatch for different aggregated model instances (Figure 7) takes place, Figure A2 shows the curtailment of one specific technology for a selected period of time. Given that the curtailment of wind offshore power generation is caused by transmission grid congestions, it can be presumed that the points in time, when the curtailment takes place, correspond to the hours of the year when redispatch measures would occur.

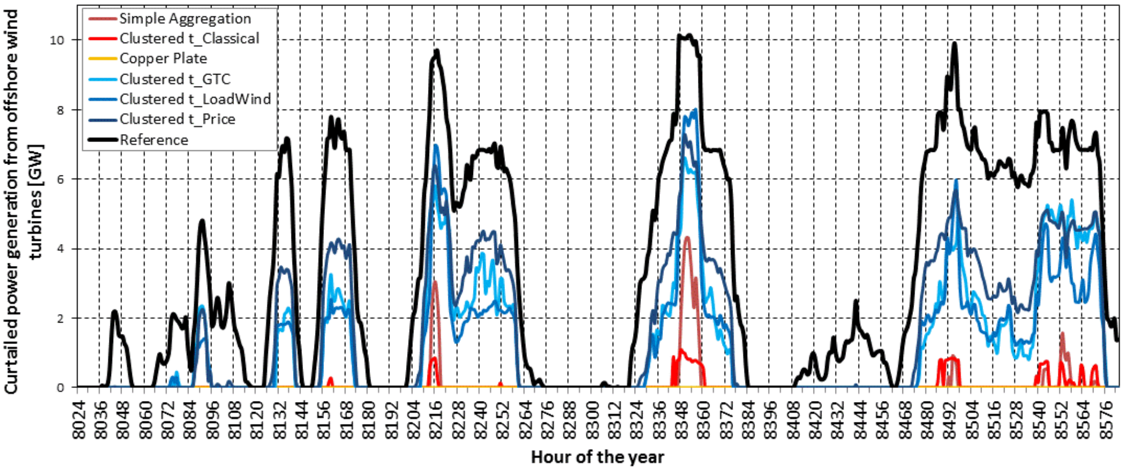

Figure A2. Curtailed power generation of wind offshore turbines for different aggregated ESM instances.

From Figure A2 we deduce the following:

- As it could be expected, in case of the copper plate model no curtailment can be observed since no power transmission limits are considered in this aggregated ESM instance.
- The reference model (black curve) shows the highest magnitudes while the aggregated ESM instances (colored curves) underestimate these effects. However, the ESM instances determined with the spectral clustering of nodal price differences (blue curves) are closer to the reference than it is the case for the aggregated benchmark models (red curves). This corresponds to the findings deduced from Figure 7.
- The frequency of the occurrence of non-zero values in Figure A2 gives an indication for the points in time when redispatch takes place. If the colored curves show this behavior, the black curve indicates non-zero values as well. On other words, the aggregated models are able to detect curtailment or redispatch events like the reference model. This is more often the case for the blue curves than for the red ones (e.g., in hour 8132). We therefore conclude once again, that Clustered $t_{LoadWind}$, Clustered t_{Price}, and Clustered t_{GTC} perform better than the benchmark cases. However, it must be noted that they are not able to capture all relevant curtailment events of the reference model (e.g., between hours 8408 and 8456).

Appendix H. Expansion Planning in the Case Study

For performing the expansion planning study, additional constraints are taken into account which determine the investment costs for a particular technology. For example, in the case of the expansion of GTCs in the AC transmission grid, they are calculated as follows:

$$C_{invest}\left(\tau_{AC}, y, l_{agg}\right) = c(\tau_{AC}, y) \cdot GTC_{add}\left(\tau_{AC}, y,\ l_{agg}\right) \cdot d\left(l_{agg}\right) \cdot f_A(\tau_{AC}, y) \\ \forall \tau_{Ac},\ y, l \tag{A16}$$

c: Specific investment costs for AC grid expansion

$f_A = \frac{(i+1)^{a_l} \cdot i}{(i+1)^{a_l} - 1}$: Annuity factor

In this context, Table A2 shows the used cost parameters for all technologies for which expansion planning is enabled in the case study.

Table A2. Cost parameters for expansion planning of lithium-ion storage and grid transfer capacities.

Technology	Specific Investment Costs c_{AC}	Life Time a_l (Years)
Lithium-ion batteries	225 €/kWh	22
GTC_{AC}	346 €/(km·MW)	40
GTC_{DC}	544 €/(km·MW)	40
Converter station DC	102,000 €/MW	20

References

1. Paltsev, S. Energy scenarios: The value and limits of scenario analysis. *Wiley Interdiscip. Rev. Energy Environ.* **2017**, *6*. [CrossRef]
2. Grunwald, A. Energy futures: Diversity and the need for assessment. *Futures* **2011**, *43*, 820–830. [CrossRef]
3. Herbst, A.; Toro, F.; Reitze, F.; Jochem, E. Introduction to energy systems modelling. *Swiss J. Econ. Stat.* **2012**, *148*, 111–135. [CrossRef]
4. Connolly, D.; Lund, H.; Mathiesen, B.V.; Leahy, M. A review of computer tools for analysing the integration of renewable energy into various energy systems. *Appl. Energy* **2010**, *87*, 1059–1082. [CrossRef]
5. Schlachtberger, D.P.; Brown, T.; Schramm, S.; Greiner, M. The benefits of cooperation in a highly renewable European electricity network. *Energy* **2017**, *134*, 469–481. [CrossRef]
6. Gils, H.C.; Scholz, Y.; Pregger, T.; de Tena, D.L.; Heide, D. Integrated modelling of variable renewable energy-based power supply in Europe. *Energy* **2017**, *123*, 173–188. [CrossRef]
7. Pfenninger, S.; Hawkes, A.; Keirstead, J. Energy systems modeling for twenty-first century energy challenges. *Renew. Sustain. Energy Rev.* **2014**, *33*, 74–86. [CrossRef]
8. Kondziella, H.; Bruckner, T. Flexibility requirements of renewable energy based electricity systems—A review of research results and methodologies. *Renew. Sustain. Energy Rev.* **2016**, *53*, 10–22. [CrossRef]
9. Krishnan, V.; Ho, J.; Hobbs, B.F.; Liu, A.L.; McCalley, J.D.; Shahidehpour, M.; Zheng, Q.P. Co-optimization of electricity transmission and generation resources for planning and policy analysis: Review of concepts and modeling approaches. *Energy Syst.* **2015**. [CrossRef]
10. Haas, J.; Cebulla, F.; Cao, K.; Nowak, W.; Palma-Behnke, R.; Rahmann, C.; Mancarella, P. Challenges and trends of energy storage expansion planning for flexibility provision in low-carbon power systems—A review. *Renew. Sustain. Energy Rev.* **2017**, *80*, 603–619. [CrossRef]
11. Schmid, E.; Knopf, B. Quantifying the long-term economic benefits of European electricity system integration. *Energy Policy* **2015**, *87*, 260–269. [CrossRef]
12. Spiecker, S.; Weber, C. The future of the European electricity system and the impact of fluctuating renewable energy—A scenario analysis. *Energy Policy* **2014**, *65*, 185–197. [CrossRef]
13. Lumbreras, S.; Ramos, A. The new challenges to transmission expansion planning. Survey of recent practice and literature review. *Electr. Power Syst. Res.* **2016**, *134*, 19–29. [CrossRef]
14. Wang, S.J.; Shahidehpour, S.M.; Kirschen, D.S.; Mokhtari, S.; Irisarri, G.D. Short-term generation scheduling with transmission and environmental constraints using an augmented Lagrangian relaxation. *IEEE Trans. Power Syst.* **1995**, *10*, 1294–1301. [CrossRef]
15. Zerrahn, A.; Schill, W.-P. Long-run power storage requirements for high shares of renewables: Review and a new model. *Renew. Sustain. Energy Rev.* **2017**, *79*, 1518–1534. [CrossRef]
16. Göransson, L.; Johnsson, F. Cost-optimized allocation of wind power investments: A Nordic-German perspective. *Wind Energy* **2012**, *16*, 587–604. [CrossRef]
17. Bucksteeg, M.; Trepper, K.; Weber, C. Impacts of renewables generation and demand patterns on net transfer capacity: Implications for effectiveness of market splitting in Germany. *IET Gener. Transm. Distrib.* **2015**, *9*, 1510–1518. [CrossRef]
18. Pedregosa, F.; Varoquaux, G.; Gramfort, A.; Michel, V.; Thirion, B.; Grisel, O.; Blondel, M.; Prettenhofer, P.; Weiss, R.; Dubourg, V.; et al. Scikit-learn: Machine Learning in Python. *J. Mach. Learn. Res.* **2011**, *12*, 2825–2830.
19. Moeller, C.; Meiss, J.; Mueller, B.; Hlusiak, M.; Breyer, C.; Kastner, M.; Twele, J. Transforming the electricity generation of the Berlin–Brandenburg region, Germany. *Renew. Energy* **2014**, *72*, 39–50. [CrossRef]

20. Kurzidem, M.J. *Analysis of Flow-Based Market Coupling in Oligopolistic Power Markets*; ETH Zurich: Zürich, Switzerland, 2010.
21. Anderski, T.; Surmann, Y.; Stemmer, S.; Grisey, N.; Momo, E.; Leger, A.-C.; Betraoui, B.; Roy, P.V. *Modular Development Plan of the Pan-European Transmission System 2050—European Cluster Model of the Pan-European Transmission Grid*; e-Highway2050: Brussels, Belgium, 2014.
22. German Transmission System Operators. *Übersicht über die Voraussichtliche Entwicklung der Installierten Kraftwerksleistung und der Leistungsflüsse in den Netzgebieten der Deutschen Übertragungsnetzbetreiber (Regionenmodell Stromtransport 2013)*; EnBW Transportnetze AG: Karlsruhe, Germany; RWE Transportnetz Strom GmbH: Dortmund, Deutschland; Transpower Stromübertragungs GmbH: Bayreuth, Deutschland; Vattenfall Europe Transmission GmbH: Berlin, Germany, 2013.
23. Shayesteh, E.; Hamon, C.; Amelin, M.; Söder, L. REI method for multi-area modeling of power systems. *Int. J. Electr. Power Energy Syst.* **2014**, *60*, 283–292. [CrossRef]
24. Lumbreras, S.; Banez-Chicharro, F.; Pache, C. *Modular Development Plan of the Pan-European Transmission System 2050—Enhanced Methodology to Define Optimal Grid Architectures for 2050*; e-Highway2050: Brussels, Belgium, 2015.
25. Singh, H.K.; Srivastava, S.C. A reduced network representation suitable for fast nodal price calculations in electricity markets. In Proceedings of the IEEE Power Engineering Society General Meeting, San Francisco, CA, USA, 16 June 2005.
26. Shi, D.; Tylavsky, D.J. A Novel Bus-Aggregation-Based Structure-Preserving Power System Equivalent. *IEEE Trans. Power Syst.* **2015**, *30*, 1977–1986. [CrossRef]
27. Gang, L.; Dongyuan, S.; Jinfu, C.; Xianzhong, D. Automatic identification of transmission sections based on complex network theory. *IET Gener. Transm. Distrib.* **2014**, *8*, 1203–1210. [CrossRef]
28. Papaemmanouil, A.; Andersson, G. On the reduction of large power system models for power market simulations. In Proceedings of the 17th Power Systems Computation Conference (PSCC), Stockholm, Sweden, 22–26 August 2011; pp. 1308–1313.
29. Akhavein, A.; Firuzabad, M.F.; Billinton, R.; Farokhzad, D. Review of reduction techniques in the determination of composite system adequacy equivalents. *Electr. Power Syst. Res.* **2010**, *80*, 1385–1393. [CrossRef]
30. Dorfler, F.; Bullo, F. Kron Reduction of Graphs with Applications to Electrical Networks. *IEEE Trans. Circuits Syst. I Regul. Pap.* **2013**, *60*, 150–163. [CrossRef]
31. Cheng, X.; Overbye, T.J. PTDF-based power system equivalents. *IEEE Trans. Power Syst.* **2005**, *20*, 1868–1876. [CrossRef]
32. Hamon, C.; Shayesteh, E.; Amelin, M.; Söder, L. Two partitioning methods for multi-area studies in large power systems. *Int. Trans. Electr. Energy Syst.* **2015**, *25*, 648–660. [CrossRef]
33. Wiegmans, B. *GridKit Extract of ENTSO-E Interactive Map*; Zenodo: Oldenburg, Germany, 2016. [CrossRef]
34. Scholz, Y.; Gils, H.C.; Pietzcker, R.C. Application of a high-detail energy system model to derive power sector characteristics at high wind and solar shares. *Energy Econ.* **2017**, *64*, 568–582. [CrossRef]
35. Gils, H.C.; Simon, S. Carbon neutral archipelago—100% renewable energy supply for the Canary Islands. *Appl. Energy* **2017**, *188*, 342–355. [CrossRef]
36. Gils, H.; Simon, S.; Soria, R. 100% Renewable Energy Supply for Brazil—The Role of Sector Coupling and Regional Development. *Energies* **2017**, *10*, 1859. [CrossRef]
37. Gils, H.C.; Bothor, S.; Genoese, M.; Cao, K.-K. Future security of power supply in Germany—The role of stochastic power plant outages and intermittent generation. *Int. J. Energy Res.* **2018**. accepted for publication. [CrossRef]
38. Cebulla, F.; Naegler, T.; Pohl, M. Electrical energy storage in highly renewable European energy systems: Capacity requirements, spatial distribution, and storage dispatch. *J. Energy Storage* **2017**, *14*, 211–223. [CrossRef]
39. Scholz, Y. Renewable Energy Based Electricity Supply at Low Costs: Development of the REMix Model and Application for Europe. Ph.D. Thesis, Universität Stuttgart, Stuttgart, Germany, 2012.
40. Rippel, K.M.; Preuß, A.; Meinecke, M.; König, R. *Netzentwicklungsplan 2030 Zahlen Daten Fakten*; German Transmission System Operators: Brussels, Belgium, 2017.
41. Teruel, A.G. *Perspestective of the Energy Transition: Technology Development and Investments under Uncertainty*; Technical University of Munich: Munich, Germany, 2015.

42. Egerer, J.; Gerbaulet, C.; Ihlenburg, R.; Kunz, F.; Reinhard, B.; von Hirschhausen, C.; Weber, A.; Weibezahn, J. *Electricity Sector Data for Policy-Relevant Modeling: Data Documentation and Applications to the German and European Electricity Markets*; Data Documentation; DIW: Berlin, Germany, 2014.
43. Open Power System Data Data Package Time Series. (Primary Data from Various Sources, for a Complete List See URL), Version 2017-07-09. Available online: https://data.open-power-system-data.org/time_series/2017-07-09 (accessed on 21 July 2017).
44. Hörsch, J.; Brown, T. The role of spatial scale in joint optimisations of generation and transmission for European highly renewable scenarios. In Proceedings of the 2017 14th International Conference on the European Energy Market (EEM), Dresden, Germany, 6–9 June 2017; pp. 1–7.
45. ENTSO-E Transparency Platform Cross-Border Commercial Schedule and Cross-Border Physical Flow. Available online: https://transparency.entsoe.eu/content/static_content/Static%20content/legacy%20data/legacy%20data2012.html (accessed on 29 June 2017).
46. Eurostat European Commission Eurostat. *NUTS—Nomenclature of Territorial Units for Statistics*; European Commission: Brussels, Belgium, 2017.
47. *Bundesnetzagentur Kraftwerksliste zu der Genehmigung des Szenariorahmens für die Netzentwicklungspläne Strom 2017–2030*; Bundesnetzagentur: Bonn, Germany, 2017.
48. von Luxburg, U. A tutorial on spectral clustering. *Stat. Comput.* **2007**, *17*, 395–416. [CrossRef]
49. Metzdorf, J. Development and Implementation of a Spatial Clustering Approach Using a Transmission Grid Energy System Model. Ph.D. Thesis, University of Stuttgart, Stuttgart, Germany, 2016.
50. Pape, C.; Hagemann, S.; Weber, C. Are fundamentals enough? Explaining price variations in the German day-ahead and intraday power market. *Energy Econ.* **2016**, *54*, 376–387. [CrossRef]
51. Grote, F.; Maaz, A.; Drees, T.; Moser, A. Modeling of electricity pricing in European market simulations. In Proceedings of the 2015 12th International Conference on the European Energy Market (EEM), Lisbon, Portugal, 20–22 May 2015; pp. 1–5.
52. Bundesnetzagentur. *Monitoringbericht 2013*; Bundesnetzagentur: Bonn, Germany, 2014.
53. Zhu, J. *Optimization of Power System Operation*; John Wiley & Sons: Hoboken, NJ, USA, 2015; Volume 47.
54. ENTSO-E. *Memo 2012, Provisional Values as of 30 April 2013*; ENTSO-E: Brussels, Belgium, 2013.
55. Zelnik-Manor, L.; Perona, P. Self-tuning spectral clustering. In *Advances in Neural Information Processing Systems*; The MIT Press: Cambridge, MA, USA, 2005; pp. 1601–1608.
56. Breuer, C.; Moser, A. Optimized bidding area delimitations and their impact on electricity markets and congestion management. In Proceedings of the 11th International Conference on the European Energy Market (EEM14), Kraków, Poland, 28–30 May 2014; pp. 1–5.
57. Mohapatra, S.; Jang, W.; Overbye, T.J. Equivalent Line Limit Calculation for Power System Equivalent Networks. *IEEE Trans. Power Syst.* **2014**, *29*, 2338–2346. [CrossRef]
58. Pfenninger, S. Dealing with multiple decades of hourly wind and PV time series in energy models: A comparison of methods to reduce time resolution and the planning implications of inter-annual variability. *Appl. Energy* **2017**, *197*, 1–13. [CrossRef]
59. Cao, K.-K.; Gleixner, A.; Miltenberger, M. Methoden zur Reduktion der Rechenzeit linearer Optimierungsmodelle in der Energiewirtschaft? Eine Performance-Analyse. In Proceedings of the 14th Symposium Energieinnovation, Graz, Austria, 10–12 February 2016.
60. Oeding, D.; Oswald, B.R. *Elektrische Kraftwerke und Netze*; Springer: Berlin, Germany, 2011; ISBN 9783642192456.

2.3 PUBLICATION 3

Status	**Published** in: ETG-Fb. 158: International ETG Congress 2019, Power Engineering Society in the VDE (ETG) (Hrsg.), Das Gesamtsystem im Fokus der Energiewende
Title	Grid Expansion, Power-To-Gas and Solar Power Imports - Multi-Scenario Analysis of Large Infrastructure Options for the Decarbonization of the European Energy System
Co-Author	Thomas Pregger
Publication year	2019
Access	https://ieeexplore.ieee.org/document/8835978 https://elib.dlr.de/127573/ ☐ Gold Open Access ☒ Green Open Access ☐ Closed access
Contributions	☒ Conceptualization ☒ Data maintenance ☒ Formal analysis ☐ Funding acquisition ☒ Investigation ☒ Methodology ☒ Project administration ☒ Resources ☒ Software ☒ Supervision ☒ Validation ☒ Visualization ☒ Writing: original draft preparation ☐ Writing: review and editing
Applied model	REMix Europe
Specific objective	Assessing the role of different technologies to ensure system adequacy in European energy scenarios. Special focus on technologies that require large infrastructures such as grid expansion, power-to-gas and solar power imports considering cross-sector coupling of electricity, heat and individual transport.
Thesis-overarching objectives	2.e) Analysis of the impact on model results of different approaches for modeling power flows in ESOMs 3.a) Definition of scenarios and parameterization of an ESOM that allows for power transmission and grid expansion among alternative technological options for load-balancing 3.b) Analysis of the role of power transmission as load-balancing measure in order to ensure system adequacy
Methodology	Definition and development of consistent European energy scenarios by generation expansion planning. Investigation of these scenarios with capacity expansion studies for load-balancing technologies such as power transmission and energy storage. Comparison and discussion of multiple indicators that characterize the different energy scenarios and parameter variations.
Key findings	The availability of load-balancing technologies and sector-coupling generally reduces the need for backup power plants while power-to-gas solutions are more expensive for reaching the examined CO_2 mitigation targets (55% and 85% reduction compared to 1990). For a broad spectrum of scenarios and parameter variations (>50), power transmission results as cost-efficient solution for ensuring system adequacy.

Grid Expansion, Power-To-Gas and Solar Power Imports – Multi-Scenario Analysis of Large Infrastructure Options for the Decarbonization of the European Energy System

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Abstract

Grid expansion measures, Power-To-Gas and imports from concentrating solar power plants are technological options for integrating renewable energies into the energy system, which pose enormous challenges for the development of energy supply infrastructures. Analyses of the potential benefits of these technologies must therefore show a broad spectrum of possible futures. This paper provides a comparative assessment of more than 50 European energy scenarios and sensitivity cases, which vary network expansion costs, weather years and load time series as well as the methodology for modelling interregional power flows.

1 Introduction

1.1 Motivation

Ensuring system adequacy in future power systems with increasing sector coupling and high shares of renewable energies (RE) requires a sufficient amount of generation capacities. Moreover, far-reaching adjustments and extensions of existing supply infrastructures are under discussion. In addition to the expansion of electricity transmission grids already required today, these include the exploitation of large electricity storage potentials, i.e. with power-to-gas, or the import of solar power from remote power plants in areas with high levels of solar radiation.

Temporally and spatially resolved simulations of future power supply scenarios have shown the importance of expanding power grids and energy storage facilities within Europe in the long-term [1], [2]. Due to the high sensitivity model results to a large number of assumptions, however, comprehensive scenario analyses which

1) model the overall energy system on a large scale including the above mentioned infrastructure options as well as sector coupling and
2) evaluate a broad spectrum of possible future developments by a consistent variation of input data and assumptions

are still necessary.

1.2 Objective

The objective of this paper is the evaluation of the different infrastructure options, i.e. grid expansion, power-to-gas and solar power imports taking into account potentials for central and decentral energy storage as well as demand side management and sector coupling in a European context with focus on Germany. For this investigation, energy scenarios are set up and analyzed on the basis of indicators which, go beyond a pure evaluation of cost-efficiency and required backup generation capacities by assessing the importance of certain technologies for the operation and composition of the entire energy supply system.

2 Methodology

2.1 Scopes

The desired indicators are derived by scenario analyses that rely on a macroeconomic cost minimization approach. Therefore a multi-regional modeling framework is set up using the optimizing energy system model REMix [4]. The regional scope covers all European and North African countries which are represented by their national transmission system operators as members of the ENTSO-E. Exceptions are Turkey, Island and Cyprus, which are not considered. With regard to the temporal horizon, scenarios of future power systems of the years 2030 and 2050 are defined considering CO_2 emission reductions in the European power sector by approximately 55% and 85% compared to 1990, respectively.

2.2 General modeling approach

The conducted general modeling approach is divided into two basic steps of applying REMix (see Figure 1). First, base scenarios are determined by generation expansion planning taking into account normative restrictions, such as emission limits or national self-sufficiency quotas. However, the availability of technological options for spatially and temporally balancing of power demand and generation (in the following referred to as flexibility options) is simplified. In particular, expansion of only one representative of the respective flexibility option is allowed. Besides the desired emission reduction, the resulting European power plant parks differ primarily in the consideration of the large-scale use of hydrogen for both synthetic fuel supply and energy storage and the possibility of direct solar power imports.

For these basic power plant parks, scenario variants are derived which take into account different storylines with regard to the expansion of the transmission grid. In addition, in this modeling step, the entire spectrum of flexibility options, such as demand side management, controlled charging of electric vehicles, heat storage or the expansion planning of short, medium and long-term storage facilities, is considered.

2.3 The optimizing energy system model REMix

The model "Renewable Electricity Mix for a sustainable energy supply" (REMix) is a linear, bottom-up energy system model written in GAMS that is developed for temporally and spatially resolved analysis of long-term energy scenarios with high shares of variable renewable energies (VRES). The target function is a cost function which represents the system costs, i.e. operating costs and annuities of the technologies under consideration. These are minimized with respect to technical-physical restrictions. Similar models that use this modelling approach with a focus on the electricity system are often used as fundamental electricity market models. However, previous applications range from country specific cross-sectoral energy system analyses [3] to multi-regional [4] and spatially highly resolved power system analyses [5]. In this paper, we use REMix for dispatch optimization on a sub-annual, hourly basis as well as for expansion planning.

2.4 Scenario definition

When defining scenarios and associated "narratives" it is important to address possible tipping points. These can be determined by political and social framework conditions, but also by technological leaps or other disruptive developments. For this study, we identified two major tipping points, i.e. the emergence of a hydrogen-based economy and the availability of large solar-fed power generation capacities in Northern Africa, respectively. But we assume that these technologies will only become system-relevant after 2030.

In order to conduct a model-based scenario analysis, defined development paths must be quantifiable. Accordingly, in the following, the further definition of energy scenarios consists of a projection of sector specific annual energy demands and the composition of the future power plant portfolio in Europe and Northern Africa.

2.4.1 Energy demand

One of the key drivers of the used modeling approach is the projection of the future energy demand which is highly affected by demographic and economic developments. We use the basic assumptions made in [6] to derive the corresponding input data for REMix. Associated assumptions are, among others, that the German economy will grow by 1 % p.a. in the medium and long term. This growth will be slowed by the declining population (73 million by 2050). Industry will retain its central importance for the German economy. Accordingly, the gross value added rises continuously by an average of 1.2 % annually.

On the European level a continuous population increase (560 million by 2050) and a moderate economic growth (1.8 % p.a.) are assumed. These values refer to the scenarios defined in the e-Highway2050 study [7] and are considered to be in-line with the above assumed developments for Germany. Therefore, we also use the annual power demand values from the corresponding scenarios as a basis for the electricity consumption of “conventional” consumers. However, in addition to technologies that use electricity already today, the future power demand is composed of the demand from new electricity consumers. These consumers mainly appear in the heat and transport sector. Assumptions on the energy demand of transport can vary within a wide range. This is due to the fact that compared to assuming a full sector-penetration with electric vehicles, the greater the use of fuels from electricity, such as synthetic methane, the greater the demand for electricity generation. Accordingly, we distinguish two development paths regarding the effective electricity demand in the transport sector based on scenarios defined in [8]. Concerning the electricity demand for heat generation with heat pumps or electric boilers for peak load coverage of other heat generators, we also built up on these scenarios as well as on the analyses conducted in [9], [16].

2.4.2 Power plants

A hydrogen economy enables both the use of long-term renewable energy storage facilities and the provision of synthetic fuels to be used in the transport sector. Nevertheless, downsides of this option are mainly worse power-to-power conversion efficiencies as well as a limited availability of geologically suitable cavern sites which results in additional transport infrastructure requirements. The latter applies also to solar imports which are associated with high capital expenditures into power transmission infrastructure. However, they provide additional access to huge renewable resources that can be used for demand-oriented power generation with thermal power plants.

It can be thus assumed that the composition of the European and North African power plant parks varies significantly if one or both of the above mentioned developments is considered. Taking this aspect into account, we define the following scenarios:

- **Base** where neither hydrogen nor solar imports are considered**,**
- a reference case **(REF)** that is equally parameterized to Base but with a strongly restricted access to flexibility options (only expansion planning of gas turbines) and
- the already mentioned scenarios where solar imports **(CSP)** or hydrogen (**H_2**) play an important role as well as a combination of these two development paths (**CSP&H_2**).

Furthermore, an additional scenario is derived from the "Small and Local" scenario presented in the project e-Highway 2050 [10]. To harmonize this scenario according to our assumptions concerning the development of the cross-sectoral energy demand, the corresponding scenario **eHighway** is characterized by additional generation capacities. These stem from performing modeling step 1 using the power plant park from "Small and Local" as a starting point for generation expansion planning.

2.5 Model setup and input data

2.5.1 Generation expansion planning

In this modeling step mainly power generation capacities are optimized. It is performed seven times varying the historical weather years from 2006 to 2012. As for the scenario **eHighway,** also starting points for the installed capacities are applied for determining the power plant parks of the rest of scenarios. For thermal power plants such as coal and nuclear-fired units we use the installed capacities given in [11] and apply assumptions for technology specific life-times to receive decommissioning dates that allow us to define which capacities are still installed in the considered time horizons. In the case of renewable energies we define the installed power generation capacities provided in [12] as starting point.

The results of the expansion planning are restricted by normative constraints that we apply to receive, from a today's point of view, more plausible power plant parks. In particular, we determine emission caps using energy balances of the year 2010 [13] and emission factors from [14] to receive specific CO_2 emissions per kWh. Defining a reduction of 90 % of CO_2 emissions compared to 1990 for Germany in 2050 and assuming constant emissions per capita within Europe, the resulting annual CO_2 budgets per country lead to total mitigation quotas of more than 50% and 80% for 2030 and 2050, respectively. Another restriction for this modeling step is achieved by the application of a country specific self-sufficiency rate of 80% of the annual power demand. Similarly, also firm capacities of 80% of the annual peak load of each country are enforced. Both quotas are deduced from preliminary conducted sensitivity analyses that varied both the share of self-sufficiency and firm capacity as well as the input time series for power generation of VRES based on historical data of the years 2006 to 2012.

Further assumptions for this modeling step are a phase-out of coal use all over Europe and a the realization of all projects of the "Ten-Year Network Development Plan" (TYNDP) 2016 [15]. Consequently, all power generation technologies but coal-fired power plants are optimized by expansion planning. Finally, for reasons of simplicity, investments into flexibility options except of power generations are only possible for lithium-ion batteries and transmission capacities; sector-coupling is only considered by inflexible electricity demands time series of the transport and heat sector, while combined heat and power plants (CHP) are only considered by must-run factors that also stem from preliminary analyses.

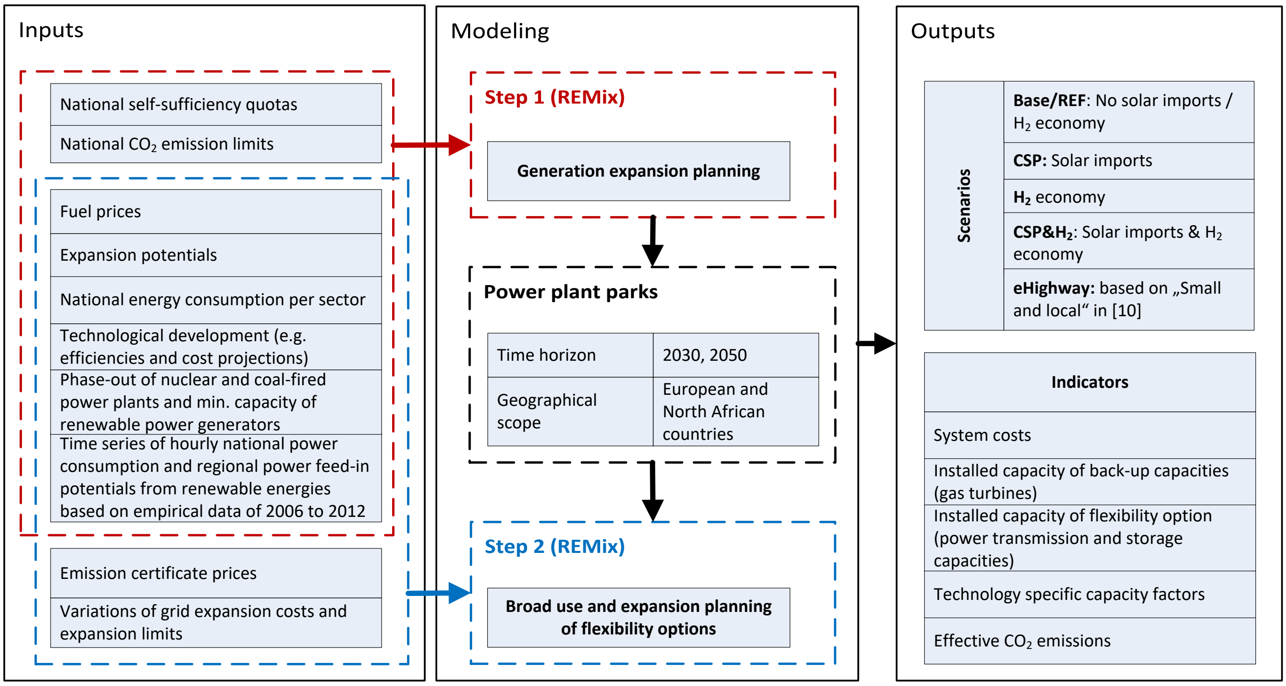

Figure 1: Schematic representation of the conducted data processing and modeling approach

2.5.2 Deployment of flexibility options

The second step of the application of REMix focuses on the deployment of a broad spectrum of flexibility options to balance the generation and demand of electricity. This means generation capacities are almost fixed based on the power plant parks of the five defined scenarios. To avoid presetting of over-dimensioned generation capacities, from the variation of weather years, we select the power plant parks with the smallest total generation capacity for Europe. Expansion planning is basically only applied for gas turbines (backup capacities) to be interpreted as an indicator of security of supply.

With regard to energy storage we consider pumped hydro storage and adiabatic compressed air storage units as well as lithium-ion and vanadium-redox-flow batteries to be optimized. Moreover, demand side management of industrial consumers and controlled charging of electric vehicles can be used to temporally balance load and generation in the short-term.

Also sector-coupling is modeled in a much more detailed way than in modeling step 1. Using the modeling concept from [16], heat demand is fully considered and can be covered by conventional heating technologies such as gas burners or CHP-fed district heating networks. Additionally, the capacity of electric heat generators, e.g. heat pumps is optimized. Capacities of this technology as well as of electric peak load boilers and heat storage units are determined model-endogenously.

For scenarios where hydrogen is considered, expansion planning for hydrogen generation and storage facilities is enabled. The appropriate modeling concept and input data are adapted from [17]: Hydrogen produced by large electrolyzers is stored in salt caverns and can either be used as fuel in the transport sector if fuel stations lie within a radius of 100 km around cavern sites. For gas stations further away, we assume an on-site production with small electrolyzers and storage of hydrogen in pressure storage units. In addition, power reconversion is possible by cofiring of renewable methane in all open and combined cycle gas turbines that belong to the same “hydrogen pool” as a cavern. Therefore, we define 9 “hydrogen pools” which can be interpreted as equivalents to the so called “copper plates” on the electricity transmission side.

2.5.3 Grid-related scenario variants

The transmission grid infrastructure has a significant influence on the transformation of the energy system towards high shares of power supply with VRES. With regard to future network expansion, four different narratives are defined, which differ primarily in the implementation of different transmission technologies, the design of the infrastructure and the implementation speed of the TYNDP:

Trend: The trend scenario represents the standard case. It is assumed that, despite some delays, all major TYNDP projects will be successfully implemented by 2030. The basic structure of the transmission and distribution grids will be retained. With regard to the model setup, transmission capacities of existing transmission lines can be increased up to a limit of 20 GW.

Super Grid: This scenario is characterized by remote power generation. Initially driven by the massive expansion of offshore wind energy, there is the possibility to build up an overlay network based on multi-terminal HVDC transmission to supplement the existing AC high voltage grid. Accordingly, it is assumed that transmission expansion planning is considered for both new HVDC lines and the AC overhead lines.

Smart Grid: Assuming an increasing coupling of the electricity, heat and transport sectors, decentral power generation in combination with extensive use of combined heat and power contribute to the self-sufficiency of large areas. This makes power transmission over long instances less important. The TYNDP is therefore only partially implemented by assuming projects "Under Consideration" to be not realized. Investments in the transmission network infrastructure are associated with higher costs. In addition, decentral generation capacities, i.e. wind turbines or photovoltaics can be further expanded to mainly cover demand on-site.

Protest: Due to continuing resistance against large-scale infrastructure projects, these can only be realized to a limited extent and at considerable financial expense. However, there is still a need to expand the transmission grid infrastructure, as large-scale alternatives, such as cavern storage facilities cannot be realized either. The implementation of the expansion measures in the TYNDP is therefore only partially successful in 2030, but accomplished by 2050. Additional transmission capacities are strictly limited to 2 GW and can only be realized by installing cable routes.

Finally, with regard to the approach for modeling power flows with REMix, we distinguish three applied methodologies. These are

- an implementation of a simple capacity constrained **transport model**,
- the **dc-power-flow** approach that determines the power flow distribution according to distances between the considered regions and
- the application of six temporally clustered **PTDF** matrices that are deduced from AC power flow simulations for the European high voltage transmission grid.

For reasons of consistency with the AC power flow simulation for the latter, the assumed starting point for transmission capacities in these scenario variants is less conservative than in the rest of scenarios.

3 Results

3.1 System costs and backup demand

Figure 2 shows the two major indicators for all defined scenarios and their variants. Those are represented by the colored markers and aim to achieve either a 55% or 85% reduction of CO_2 emission on the European level compared 1990. The indicator on the x-axis is the required backup generation capacity. On the other hand, the resulting overall system costs (operational and capital expenditures) are plotted on the y-axis. Both indicators are presented as the difference to a one of the reference cases (85%-REF), where except of capacity expansion of gas turbines no additional balancing measures are available to the energy system.

The markers of all scenarios are located left of the vertical blue line, which represents the backup capacity in the reference case **85%-REF**. It can be thus concluded that in all scenarios a higher degree of system adequacy can provided. The availability of flexibility options can be assessed by comparing the **REF** scenarios (red markers) with the **Base** scenarios (light blue markers). In all cases significant reductions in backup requirements can be observed, e.g. 75 GW in the case of the **55%**-scenarios up to 165 GW in **eHighway**. The generally lower backup requirement compared to the other scenarios are due to their greater installed capacities of thermal power plants. This also affects the level of the total system costs, which in both cases is higher than in the most of the scenarios that aim for an 85% CO_2 mitigation target.

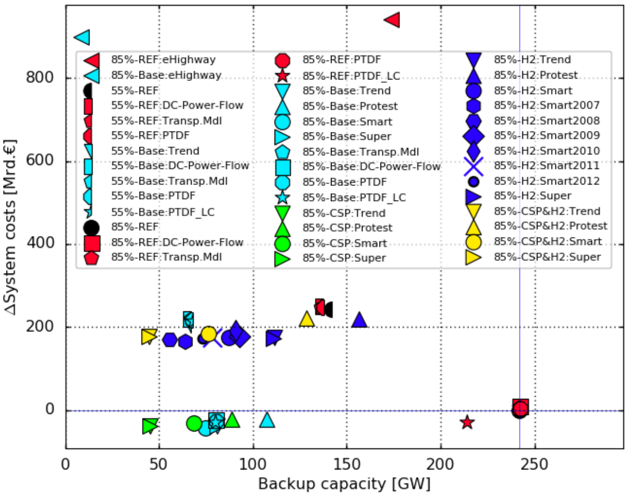

Figure 2: Difference (compared to REF) in system costs and required backup generation capacity across all scenario variants

The blue, green and yellow markers represent the scenarios, which differ in the use of solar power imports and/or the availability of hydrogen. However, the results in Figure 2 show that the latter is only possible with higher overall system costs compared to the reference case. E.g., for the **Trend** variant, the total system costs of **CSP&H2** lie €169 billion above the ones of **REF** (reference value: €2.23 trillion). In contrast, with cost reductions of € 46 billion **Base:Trend** and **CSP:Trend** show lower values regarding the system costs. In addition, for the latter, the demand for gas turbines is 35 GW smaller than in **Base:Trend.** However, this must be seen against the background that in scenarios with solar power imports a further power generation technology is considered for generation expansion planning. Accordingly, gas turbine power plants can possibly be replaced by CSP plants. With regard to the grid-related scenario variants, it can be stated that these have a less significant impact on system costs rather than on the requirements for backup generators. In this context, enabling expansion of an overlay grid using HVDC technology (**Super**) did not lead to significant changes of the analyzed indicators compared to scenario variants without this option (**Trend**). The locations of the upright triangles in Figure 2, show that with up to 157 GW in **H2,** the **Protest** variants require the most backup capacities. On the contrary, when there are no solar power imports considered, **Smart** shows the best performance in terms of both indicators (e.g. **Base:Smart:** (75 GW; €-42 billion.), even though investments into additional transmission capacities are much more expensive than for **Trend** or **Super**.

3.2 Multi-indicator comparison

For better understanding of the interplay of technologies across the **85%-**scenarios, Figure 3 shows a series of key indicators, each characterized by its unit (e.g. [CF%]: capacity factor, [GW]: total installed capacity) in a radar plot. In this context, it must be noted, that in the case of storage technologies only the added storage capacity (long-term storage) or converter capacity (short-term storage) is indicated rather than the total capacity.

With regard to CO_2 emissions, it can be stated that, compared to **Base**, the use of hydrogen leads to higher emissions, whereas imports of solar power result in a reduction of the same. Characteristic of the latter is are the higher values for grid expansion, which even increase significantly for **CSP&H2:Trend** - when combined with a hydrogen infrastructure. Especially, in **Base:eHighway** an increased utilization of the gas-fired power plants can be observed. However, this and the greater power plant park in terms of thermal generation capacities result in less needs of both spatial and temporal load balancing by electricity grids and energy storage, respectively.

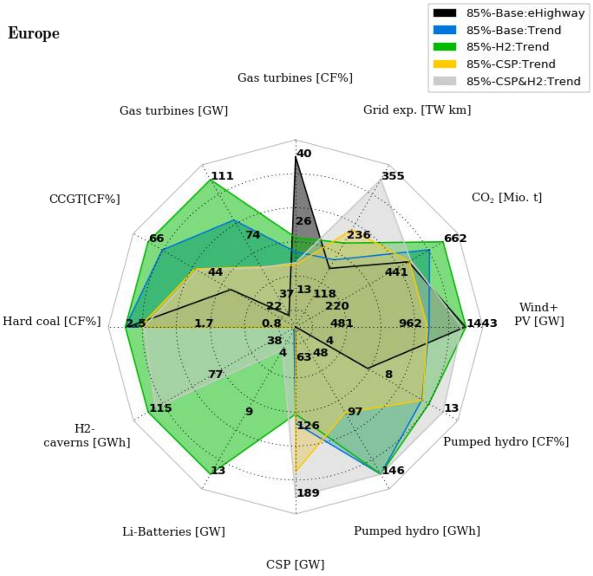

Figure 3: Key indicators in the scenarios with 85% CO_2 reduction target in Europe

It is also conspicuous that only in scenarios with hydrogen expansion of lithium-ion batteries (approx. 14 GW) takes place. Rather, the option of building other storage technologies, such as vanadium-redox-flow batteries or adiabatic compressed air storage is never taken.

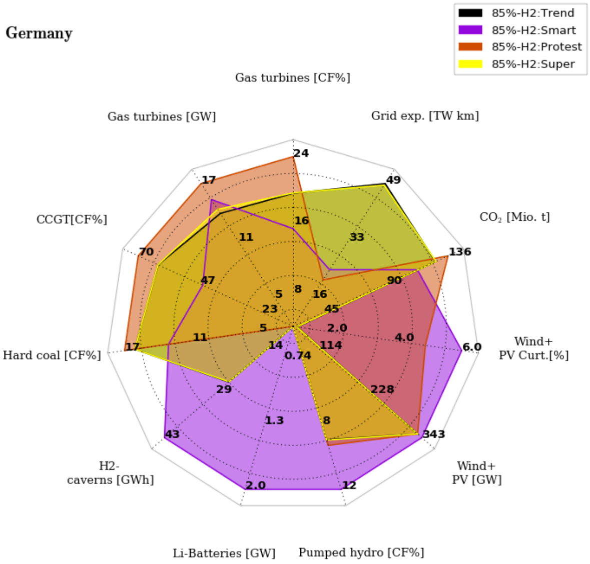

Figure 4: Key indicators in the scenario variants with hydrogen use in Germany

It is even more remarkable as lithium-ion batteries only play a role in scenarios where salt caverns are available for the long-term storage of and reconversion of hydrogen. For this reason, Figure 4 gives a more detailed view of the **H2** scenario using the example of Germany. Since significant capacities of lithium-ion batteries can only be obtained in **Smart** it can be concluded that the observed expansion of 14 GW takes place apart from Germany. In fact, this expansion is limited to locations with significantly high capacities of photovoltaics installed (e.g. Spain) where the deployment of lithium-ion batteries obviously represents a more cost-sufficient option than balancing hydrogen demand and production from renewables with pressure storage tanks. Figure 4 also shows the shift from using power transmission (**Trend/Super**) to the utilization of thermal power plants in **Protest** to the greater utilization energy of storage in **Smart**.

4 Conclusions

In this paper, we presented a multi-scenario analysis focusing the role of technological options to balance power generation and demand for decarbonizing the energy system by high shares of renewable power generation. Rather than an exclusive examination of the requirements for flexibility options such as energy storage, we emphasized the impact of large infrastructure measures for providing an optimal system adequacy. We therefore investigated scenarios with varying power transmission needs by high voltage grids as well as a broad implementation of power-to-gas or electricity imports from North Africa.

As expected, the availability of flexibility options and sector-coupling generally reduced the need for backup power plants (gas turbines) and thus the system costs. In contrast, the consideration of power-to-gas particularly lead to significantly higher overall system costs. Positive effects, however, could be identified if imports of solar generated electricity were possible. They especially reduced the need for backup generation capacities.

We found that strong CO_2 mitigation targets cannot be achieved by exclusively implementing energy-storage based solution; even though local power transmission capabilities were already overestimated by the applied modeling approach that mainly relies on a spatial resolution on country level. In the majority of the analyzed scenarios, we observed that grid expansion robustly appeared beyond the level of TYNDP measures rather than expansion of all kinds of considered energy storage. More restricted power transmission, however, required more generation capacities in combination with energy storage inclusively backup power plants. Nevertheless, those measures were not able to adequately replace power transmission by high voltage grids in terms of cost-efficiency and CO_2 mitigation. With regard to the investigated variants of grid modeling, for a delayed or limited network expansion (**Protest**) the highest system costs and worst system adequacy was observed across all scenarios. The opposite was found for scenarios which are characterized by additional decentral generation capacities (**Smart**). In particular, despite more cost-intensive grid expansion, we observed a further reduction in backup requirements and system costs.

5 References

[1] D. P. Schlachtberger et al., “The benefits of cooperation in a highly renewable European electricity network,” *Energy*, vol. 134, pp. 469–481, 2017.
[2] F. Steinke et al., “Grid vs. storage in a 100% renewable Europe,” *Renewable Energy,* vol. 50, pp. 826–832, 2013.
[3] H. Gils et al., “100% Renewable Energy Supply for Brazil—The Role of Sector Coupling and Regional Development,” *Energies,* vol. 10, no. 11, p. 1859, Nov. 2017.
[4] H. Gils et al., “Integrated modelling of variable renewable energy-based power supply in Europe,” *Energy*, vol. 123, pp. 173–188, 2017.
[5] K.-K. Cao et al., “Incorporating Power Transmission Bottlenecks into Aggregated Energy System Models,” *Sustainability*, vol. 10, no. 6, p. e1916, 2018.
[6] M. Schlesinger et al., “Entwicklung der Energiemärkte - Energiereferenzprognose”, 2014.
[7] K. Bruninx et al., “E-highway2050: D2. 1 Data sets of scenarios for 2050.” 2014.
[8] J. Nitsch et al., “Langfristszenarien und Strategien für den Ausbau der erneuerbaren Energien in Deutschland bei Berücksichtigung der Entwicklung in Europa und global”, 2012.
[9] Y. Scholz et al., “Möglichkeiten und Grenzen des Lastausgleichs durch Energiespeicher, verschiebbare Lasten und stromgeführte KWK bei hohem Anteil fluktuierender erneuerbarer Stromerzeugung”, 2014.
[10] A. Vafeas et al., “e-HIGHWAY 2050: Modular Development Plan of the Pan-European Transmission System 2050 - Technology assessment from 2030 to 2050”, 2014.
[11] PLATTS, “World Electric Power Plants Database.”, 2015.
[12] ENTSO-E, “TYNDP 2016 Market Modelling Data.” Nov-2015.
[13] IEA, “Energy Balances of OECD Countries, 2014 edition,” International Energy Agency (IEA), 2014.
[14] J. Repenning et al., “Klimaschutzszenarien 2050 - 1. Modellierungsrunde”, 2014.
[15] ENTSO-E, “Project list TYNDP2016 assessments: Reference capacities.” Nov-2015.
[16] H. Gils, “Balancing of Intermittent Renewable Power Generation by Demand Response and Thermal Energy Storage,” Universität Stuttgart, http://dx.doi.org/10.18419/opus-6888, 2015.
[17] C. Noack et al., “Studie über die Planung einer Demonstrationsanlage zur Wasserstoff-Kraftstoffgewinnung durch Elektrolyse mit Zwischenspeicherung in Salzkavernen unter Druck”, 2014.

2.4 PUBLICATION 4

Status	**Published** in: Energies, 2019, 12(24), 4656; Special Issue Energy Complex System Simulation, Design, and Optimisation
Title	Classification and evaluation of concepts for improving the performance of applied energy system models
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Applied model	REMix Germany
Specific objective	Comprehensive overview about approaches to reduce the computing times of large, non-generic Energy System Optimization Models on conventionally applied shared-memory computers and determination of achievable speed-up.
Thesis-overarching objectives	2.c) Implementation of approaches to ensure solvability of the spatially highly resolved model
Methodology	Implementation and systematic benchmark analyses of several approaches that are supposed to significantly reduce computing times of Energy System Optimization Models.
Key outcome	Total computing times can be reduced down to 10% compared to conventional computing approaches while maintaining accuracy losses within acceptable ranges.

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Classification and Evaluation of Concepts for Improving the Performance of Applied Energy System Optimization Models

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Abstract: Energy system optimization models used for capacity expansion and dispatch planning are established tools for decision-making support in both energy industry and energy politics. The ever-increasing complexity of the systems under consideration leads to an increase in mathematical problem size of the models. This implies limitations of today's common solution approaches especially with regard to required computing times. To tackle this challenge many model-based speed-up approaches exist which, however, are typically only demonstrated on small generic test cases. In addition, in applied energy systems analysis the effects of such approaches are often not well understood. The novelty of this study is the systematic evaluation of several model reduction and heuristic decomposition techniques for a large applied energy system model using real data and particularly focusing on reachable speed-up. The applied model is typically used for examining German energy scenarios and allows expansion of storage and electricity transmission capacities. We find that initial computing times of more than two days can be reduced up to a factor of ten while having acceptable loss of accuracy. Moreover, we explain what we mean by "effectiveness of model reduction" which limits the possible speed-up with shared memory computers used in this study.

Keywords: energy systems analysis; energy system optimization models; linear programming; mathematical decomposition; model reduction; REMix

1. Introduction

1.1. Motivation

Deregulation and growing decentralization have led to an increasing complexity of energy systems. Given the envisaged creation of a common European energy market and the transformation of energy supply towards sectoral coupling and electricity generation from variable renewable energy sources (vRES), this trend can be expected to continue.

In this context, new energy policies are often investigated with the help of linear optimization models [1]. However, the increasing complexity of the system to be modelled results in energy system models that quickly reach their limits in terms of memory demand and reasonable computing time. Existing and especially future research questions in the field of energy system analysis can thus only be addressed to a limited extent. In applied studies, this challenge is tackled with different strategies. Out-of-the-box solutions that enable the use of massively parallelized high performance computers are not available, since therefore additional knowledge, e.g., about the matrix structure of the mathematical optimization problem is necessary. Therefore, the majority of currently applied speed-up strategies still rely on the application of commercial optimization software executed on shared memory hardware. However, the implementation costs and not the effectiveness often dominate the decision for an appropriate performance enhancement approach. In addition, the heterogeneity of applied strategies results in the fact that the comparability of model-based scenario studies is more difficult and the trade-off between implementation costs and achievable performance is often unknown. Since the used models show similarities in essential characteristics (e.g., with regard to fundamental equations or applied solver software packages), it can be assumed that effective speed-up strategies for energy system models are transferable.

Therefore, this article presents a systematic evaluation of such strategies. The characterization of the discussed linear optimization models, which are referred to as "Energy System Optimization Models" (ESOMs), is followed by a categorization and a qualitative description of known approaches for shortening computing times. Subsequently, the implementation for a selection of performance enhancement approaches is introduced and the framework for the conducted benchmark analysis is presented. Finally, an outlook on further possibilities on the reduction of computing time in ESOMs is given.

1.2. Energy System Optimization Models: Characteristics and Dimensions

In the context of energy systems analysis a broad spectrum of research questions is addressed by ESOMs to support decision making in both energy politics and energy industry. In particular, this concerns the development of future strategies such as energy scenarios for mitigation of climate change [2] or fundamental analyses of electricity markets [3] and investment planning by system operators [4,5]. Therefore, the objective of the associated optimization problems (OPs) is either the optimal operation or the optimal configuration of the analyzed system which consist of a diverse set of technologies. With regard to electricity generation, the former is originally known as Unit Commitment (UC) or Economic Dispatch (ED) problem [6], while the latter is referred to as Generation Expansion Planning (GEP) [7]. If these problems are resolved on the spatial scale, the consideration of transport infrastructures, such as high voltage transmission grids, and thus modeling of multi-area OPs becomes relevant. Typical examples are Optimal Power Flow (OPF) problems [8] on the operational side and Transmission Expansion Planning (TEP) [9] on the configurational side.

Furthermore, due to the increasing relevance of renewable energy sources in todays and future energy systems, also the evaluation of strategies which make use of electricity storage facilities to integrate fluctuating power generation becomes more and more important [10].

The problems addressed by energy systems analysis are typically combinations of the above mentioned aspects which result in integrated bottom-up models that differentiate three major scales: technologies, time and space. Table 1 shows these scales together with their characteristics for exemplary applications. Two kinds of characteristics are distinguished here. While the descriptive characteristic is related to the description of the underlying real world problem, the model characteristic refers to the way how this problem is translated into a mathematical model formulation.

Table 1. Characteristics of Optimizing Energy System Models.

Dimension	Model Characteristic	Descriptive Characteristic	Example	
Time	Set of time steps		Short-term (sub-annual operation)	Long-term (configuration/ investment)
		Temporal resolution Planning horizon	hourly one year	each 5 years from 2020 until 2050
Space	Set of regions	Spatial resolution Geographical scope	Administrative regions (e.g., NUTS3 [11]) European Union	
Technology	Variables and constraints per technology	Technological detail	Consideration of start-up behavior, minimum downtimes	
	Set of technologies	Technological diversity	Power and heat generation, transmission grids and storage facilities	

Depending on the application, the three dimensions are differently pronounced or resolved in energy system analysis. For example, on the one hand, ESOMs are strongly spatially resolved with the aim of cost-optimized network expansion planning by TEP. On the other hand, also the temporal resolution becomes important as soon as a study tries to capture the variability of power generation from renewable energy sources. However, formulating a mathematical model with these characteristics usually results in coupling of time, space and technology among each other. Even more importantly, the need of addressing flexibility demands in future energy systems [12] also leads to couplings within these dimensions. In particular, these couplings are caused by temporally shifting of generation and consumption with storage facilities or demand side management measures which links discrete points in time, by power exchange over transmission grids that results in an interdependency of regions as well as by cross-sectoral technologies such as combined heat and power (CHP) plants.

1.3. Challenges: Linking Variables and Constraints

One substantial common characteristic of optimization models, we refer to as ESOMs, is the use of a cost-based objective function conjunction with a power balance equation. For example, Equations (1) and (2) are typical for ED problems (to better distinguish model parameters and variables, in the following, variables are denoted in bold):

Objective function:

$$Minimize: \sum_{t\in T}\sum_{n\in N}\sum_{u\in U} c(t,n,u)\cdot \boldsymbol{p}(t,n,u) \tag{1}$$

Subject to:

$$\begin{gathered}\sum_{u\in U}\boldsymbol{p}(t,n,u) = \boldsymbol{d}(t,n)\\ \forall t\in T,\ \forall n\in N,\ \boldsymbol{p}(t,n,u)\geq 0\end{gathered} \tag{2}$$

where: $\boldsymbol{p}$: (activity-) **variable** of total power supply, c: specific costs, $\boldsymbol{d}$: power demand, T: set of time steps, N: set of modeled regions and U: set of technologies.

Although different ESOMs consist of a large variety of further constraints, such as capacity-activity, flow or security constraints, they share another similarity concerning the structure of the coefficient matrix **A** of the appropriate linear program (Figure 1).

The abovementioned interdependencies of time, space and technologies translate either into linking variables or linking constraints. Both are characterized by the fact that they prevent the OP from being solved by solving independent sub-problems (indicated by the colored blocks in Figure 1). In this context, we refer to the corresponding OPs to be monolithic.

From an applied point of view, linking means, for example, that for a selected time frame the dispatch of reservoir power plants cannot be determined without the information about the storage level. However, the storage level of the actual time frame also relies on the dispatch of previous points in time.

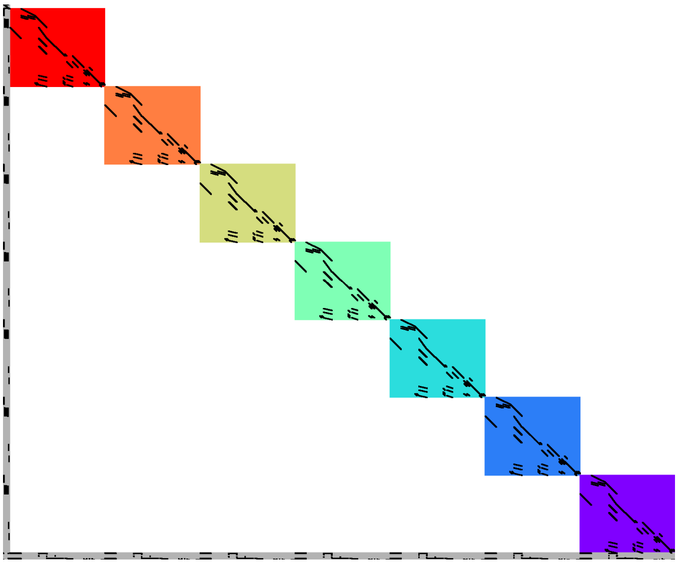

Figure 1. Non-zero entries (black dots) in an exemplary coefficient matrix A of an integrated Energy System Optimization Model (ESOM) with linking variables (grey area at the left), linking constraints (grey area at the bottom) and independent blocks (colored blocks).

In this context, variables that occur simultaneously in several equations are generally referred to as linking variables (or sometimes complicating variables). Provided that an appropriate permutation is given, as shown in Figure 1, linking variables appear as vertical lines of non-zero entries in the coefficient matrix. With regard to the temporal scale, representatives of linking variables in ESOMs appear in expansion planning problems as the appropriate investment decision variables (e.g., opposed to activity variables) are not defined for each time step of the operational time horizon. This is illustrated by inequality (3) which is defined for each time step t, but the variable $\boldsymbol{I}$ stays the same for each t.

Capacity-activity constraint:

$$\begin{gathered} \boldsymbol{p}(t,n,u) \leq P(n,u) + \boldsymbol{I}(n,u) \\ \forall t \in T; \forall n \in N; \forall u \in U \end{gathered} \tag{3}$$

where: $\boldsymbol{I}$: variable of capacity expansion and P: existing capacity

In contrast to linking variables, horizontal lines of non-zero entries in the coefficient matrix indicate linking constraints (Figure 1), sometime referred to as complicating constraints. For example, fuel availability constraints, such as used for modeling biomass fired power plants, typically define a temporally non-resolved value as an annual limit. To ensure that the total fuel consumption within the operation period stays within this limit, a linking constraint couples the involved variables:

Fuel-availability constraint:

$$\begin{gathered} \sum_{t \in T} \sum_{u \in U_{Bio}} \boldsymbol{p}(t,n,u) \cdot \frac{1}{\mu(u)} \leq F(u) \\ n \forall N;\ U_{Bio} \subset U \end{gathered} \tag{4}$$

where: F: available fuel, μ: conversion efficiency and U_{Bio}: set of biomass power plants.

2. State of Research

2.1. Classification of Performance Enhancement Approaches

We distinguish two methodological layers for approaches to enhance the performance of an ESOM (Figure 2). On the one hand, in the technical layer measures are emphasized that can be taken on the solver side in order to generally solve an OP. Thus, it concerns all methods that are applied in a solver package, such as CPLEX, Gurobi, Xpress or MOSEK, whether it is a specific implementation of solution algorithms or the tuning of the same by an appropriate parameterization. On the other hand, the conceptual layer refers to the translation of a real world problem into an OP. This means, for example, that several possibilities exist on how to address a research question with different model formulations. Model-based measures to improve the performance of an ESOM, thus rely on specific domain knowledge provided by developers of ESOMs. This refers to both the treatment of data in order to reduce the amount of data used in the model as well as the application of heuristics and model-based decomposition methods. In the following, we discuss the state-of-research with regard to model reduction, heuristics and mathematically exact decomposition methods applied to the time, space and technology dimension in ESOMs. Although solution algorithms such as Interior point are applied, we do not focus on improvements on the algorithm side (technical layer). This means that also meta-heuristics like particle swarm optimization or genetic algorithms are not considered.

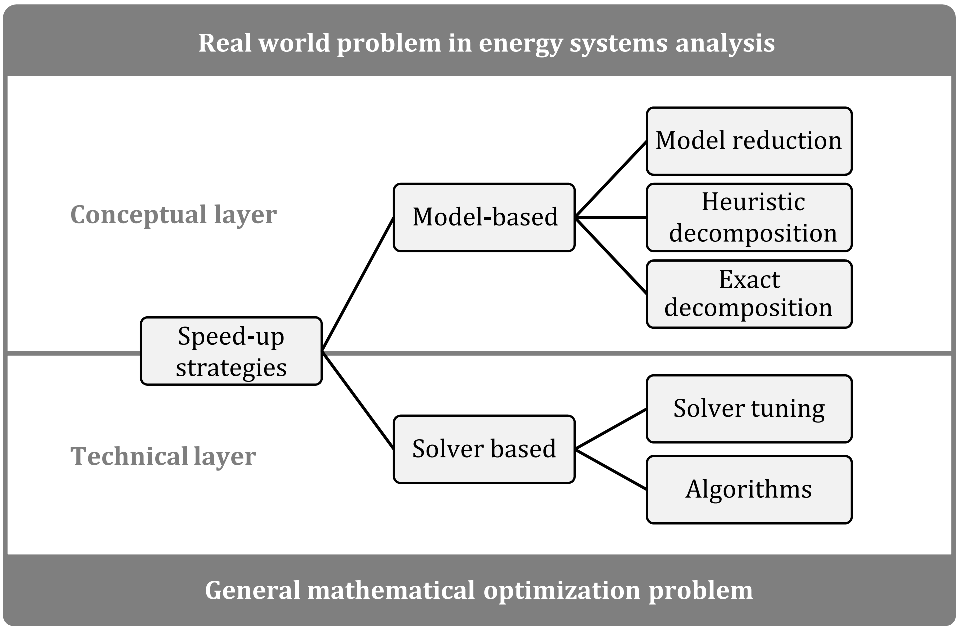

Figure 2. Classification of performance enhancement approaches.

2.2. Model Reduction

Model reduction approaches are very common since they are effective due to the reduction of the total size of the OP (less variables and constraints). Furthermore, they are also implicitly applied to ESOMs, for instance, due to limited input data access. Thus, these approaches usually manipulate input data in a pre-processing step, instead of changing the way how an ESOM is solved. Based on the treatment of available data we distinguish two forms of model reduction techniques: (i) slicing and (ii) aggregation.

2.2.1. Slicing

Slicing approaches translate into focusing to a specific sub-problem by ignoring existing interdependencies or considering only a part of the input data that could be used. This means, for example, excluding technologies such as CHP plants from a model [13] or ignoring power exchange beyond neighboring regions on the spatial side [14]. Regarding the temporal dimension, analyses are conducted only for a specific target year [15] or time-slices are selected [16]. These sub-sets represent either critical situations, such as the peak load hour, or typical time periods which are supposed to be characteristic for the entire set of operational time steps. By this means, slicing approaches can lead to significant deviations of results compared to the global optimum of the full OP as they do not ensure that all relevant information within the available data is captured. However, if for the selection of specific slices a pre-analysis is conducted, we do not refer to this process as simple slicing since it aims to take into account all input data. This is rather typical for aggregation approaches. Therefore, they reduce the input data set in a way that relevant information is maintained as far as possible. In the context of ESOMs, aggregation can also be described as coarsening of resolutions for each of the characteristic model dimensions.

2.2.2. Spatial Aggregation

The treatment of large, spatially explicit data sets is a common challenge in the context of power network analysis. However, corresponding to the area of responsibility of system operators, methods for power networks were developed to study certain slices of the entire interconnected network. The objective of these traditional network reduction techniques is therefore to simplify the neighborhood of the area of interest by the derivation of network equivalents based on given power flows. These equivalents, such as derived by Ward or Radial Equivalent Independent (REI) methods, represent the external area which is required to show the same electrical behavior as the original network [17]. In the case of Ward equivalents, the networks' nodal admittance matrix is reduced by Kron's reduction [18]. In contrast, however, the REI procedure applies a Gaussian elimination to external buses. Power injections are preserved by aggregating them to artificial generators which are connected to a representative, radial network which is referred to as REI.

The principle of creating network equivalents is also applicable to ESOMs, although their scope is rather the interaction of different technologies than the exclusive assessment of stability or reliability of electrical networks. Recently, Shayesteh et al. [19] adapted the REI approach to use-cases with high vRES penetration. However, this step of creating aggregated regions for a multi-area ESOM needs to be preceded by a partitioning procedure which allows for defining of regional clusters. In general, the clustering algorithms, such as k-means, group regions or buses with similar attributes together. In [19] the admittance between two buses is used to account for strongly connected regions. Opposed to this, Shi and Tylavsky [20] as well as Oh [21] derive network equivalents based on reduced power transfer distribution factor (PTDF) matrices which rely on the linearization of certain system operating points.

Despite the availability of a broad spectrum of sophisticated aggregation techniques, in the context of energy system analysis, the applied literature is governed by simple spatial aggregation approaches. In particular, they are usually characterized by a summation of demand and generation capacities, whereas intra-regional flows are neglected and regions are grouped based on administrative areas, such as market or country borders [15,22,23]. Reasons therefore are, on the one hand side, the availability of required, large data sets of spatially explicit data for the broad diversity of technologies, such as potentials and existing infrastructure. On the other hand, the majority of network equivalents are based on pre-computed system states of the spatially highly resolved model, for example, a solved power flow study. This in turn requires the application of nested approaches (Section 2.3), where first simplifications to other scales of an ESOM are required in order to obtain the power flows of the entire network. By this means, reasonable simplifications are the use of time-slices in form of operational snapshots and the summation of power supply from all generation technologies.

Nevertheless, concerning scenarios of the European energy system Anderski et al. [24], as well as Hörsch and Brown [25] take a step towards improved methodologies regarding aggregation of spatially highly resolved data sets. Both use power demand as well as installed generation capacities as attributes for state-of-the art clustering algorithms. However, while in [24] PTDF-based equivalents are built, the authors in [25] apply a more or less straight forward process for creating spatially aggregated regions.

2.2.3. Temporal Aggregation

Temporal aggregation refers to representative time periods or the process of down-sampling data derived from a highly resolved initial data set. Down-sampling is a method where time series based input data is coarsen to a lower temporal resolution (e.g., by averaging from 1-hourly to 6-hourly). In ESOMs, down-sampling typically affects demand profiles (e.g., electric or heat load) and the power feed-in from vRES. Although the approach is an effective way to reduce computing times—Pfenninger [26], for example, shows a reduction of computing time by up to 80% (scenario 90% 2014)—the method is rarely applied. This is due to the claim to capture the dynamics of variable power provision from renewable energy technologies. By this means, ESOMs typically rely on their highest resolved data and often use hourly input [27]. Exceptions can be found in studies that analyze the impact of different temporal resolutions in unit commitment approaches, e.g., in Deane et al. [28] (5, 15, 30 and 60 min) or in O'Dwyer and Flynn [29] as well as in Pandzzic et al. [30] who both compare a 15 min resolution with hourly modeling.

More common is the combination of down sampling and the selection of representative time periods, such as applied in [31] or [32]. Representative time periods are intended to illustrate typical or extreme periods of time. These time intervals are then weighted to derive the overall time horizon, e.g., one year. Moreover, also challenges exist to account for the chronological relationship between hours which in particular becomes important if time-linking constraints are incorporated in an ESOM. One approach to tackle this issue is presented by Wogrin et al. [33] who define transitions between system states derived by applying a k-means-like clustering algorithm to wind and demand profiles. As stated in [26], the selection of time-slices is either based on a clustering algorithm, such as *k*-means [34], hierarchical clustering [35], or simple heuristics [36].

While temporal aggregation is an effective method to reduce computing times, it is not always clear which error is introduced by it. This issue has been tackled by a number of recent papers, such as Pfenninger [26], Haydt et al. [37], Ludig et al. [31], and Kotzur et al [38]. The studies unanimously highlight the rising importance of high temporal resolution with increasing vRES share. The authors also state that there exists no best practice temporal aggregation and emphasize that it strongly depends on the modeling setup. For instance, Merick [39] recommends ten representative hours for robust scenarios when only variable demand is considered. This number, however, increases significantly when vRES and especially several profiles per technology are taken into account. With regard to representative days, he finds that the number of 300 is appropriate. This represents a clear difference compared to the sufficient number of six representative days resulting in [35]. Nahmmacher et al. [35] use the same clustering technique, but assess model outputs, such as total system costs, rather than the variance of clustered hours of the input time series.

2.2.4. Technological Aggregation

We define technology resolution as the abstraction level in a modeling approach to characterize the technologies relevant for the analysis. In this context, it can be stated that the higher the abstraction level, the better the performance of an ESOM. This applies to both the aggregation of input data and the mathematical model of a particular technology. The former, for example, refers to the representation of generation units (electricity, heat, fuels) or flexibility options (e.g., grid, storage). More precisely, classifications of power plant types can be based on several attributes such as rated power, conversion efficiency, and fuel or resources type. Technological resolutions therefore range from very detailed modeling of individual generation units [40] to general distinctions based on fuel consumption and resource [41]. However, the methods for deriving appropriate classifications or aggregations are rather based on simple grouping of attributes than on specific clustering algorithms.

Moreover, the classification of technologies is strongly connected to the mathematical description since physically more accurate models typically require more detailed data. In this regard, a broad body of literature investigates the necessary technological detail for power plant modeling. Often, these analyses compare simplified linear programming approaches (ED) with more detailed mixed integer linear programming (UC) models for least cost power plant dispatch. As a result, such studies assess differences in power plant dispatch (e.g., in [42–45]) and, additionally, highlight effects on resulting metrics (e.g., storage requirements in [46] or marginal prices of electricity generation in [47,48]).

The same applies to transmission technologies where Munoz et al. [49], for instance, study modeling approaches (discrete vs. continuous grid capacity expansion) and their effects on the total system costs. Also technological classifications can be made for different voltage levels or objectives of grid operation (e.g., transmission or distribution). Regarding mathematical models, resolutions range from detailed, nonlinear AC-power flow over decoupled and linear DC-power flow to simple transshipment or transport models [50].

2.3. Heuristic Decomposition and Nested Approaches

Although mathematical exact decomposition techniques (see Section 2.4) could be interpreted as nested approaches, in this section, we explicitly refer to methods that usually find near-optimal solutions rather than a theoretically guaranteed exact optimum. In this context, nested approaches are used as a synonym for heuristics. In contrast to meta-heuristics, this concerns methods that imply modifications of the ESOM regarding the conceptual layer and thus base on the same mathematical solver algorithm. In general, nested approaches are built on model reduction techniques (see Section 2.2). Therefore, combinations of several reduced instances of the same initial ESOM (original problem) are usually solved sequentially. This means, that after the solution of the first reduced model is obtained, certain outputs are used as boundary conditions (e.g., in the form of additional constraints) for the following model(s) to be solved.

As mentioned above, ESOMs have linking constraints or variables that globally link points of one dimension. These characteristics are crucial for the decomposition of an OP into smaller instances of the same problem, regardless of whether it should be solved by an exact decomposition (see Section 2.4) or heuristic approach. Often this is intuitively done by the application of nested performance enhancement methods where linking variables, such as power flows or endogenously added capacities are used to interface between the different reduced models.

In the literature, a wide range of examples for the applications of nested performance enhancement approaches exists. For instance, Romero and Monticelli [51] propose an approach for TEP where they gradually increase the technological detail starting with a simple transport model, and finally taking into account Kirchhoff Voltage Law constraints as in a DC-power flow model.

With regard to the spatial scale, one methodology can be described as "spatial zooming", which is similar to the classical methodology applied for power network analysis (see Section 2.2.2). Possible implementations can look like as follows: First a large geographical coverage is considered in a coarse spatial resolution to study macroscopic interdependencies. In a second step, these interdependencies, such as transnational power flows, can be fixed in order to conduct a detailed analysis of the region of interest [52]. In [53] the spatial dimension is simplified by the derivation of network clusters, while for the solution of the original problem a selection of binary variables related to pipelines and suppliers is restricted.

Comparing the different reduced models used in a nested approach, typically, a decrease of resolution on one scale is accompanied by an increase on another. In this regard, one common approach is decoupling investment decisions by "temporal zooming". First, a power plant portfolio is developed over the analyzed planning horizon using a simplified dispatch model and pre-defined time-slices to simulate the planned operation. In order to check whether the derived power plant portfolio performs well for a selected target year, UC constraints are added and capacities are fixed in the subsequent model run(s) [13,43,54]. Babrowski et al. call a similar method "myopic approach" [55]. In this case, for each year of the planning horizon a model run is performed, whereas the resulting generation expansion is taken as an offset of installed power generation for the subsequently analyzed target year.

In applied energy system analysis, ESOMs often need to consider large sets that represent the temporal scale (i.e., time series of 8760 h) in order to capture the variability of vRES [26], rather than high resolutions on the technological or spatial scale. In the following, we therefore introduce two heuristic methods for this particular dimension in detail.

2.3.1. Rolling Horizon

Although the definition of nested approaches does not perfectly fit to rolling time horizon methods, we introduce these heuristics as a preliminary stage to temporal zooming (see Section 2.3.2). The general idea behind rolling horizon methods is to split up the temporal scale (temporal slicing) into smaller intervals to obtain multiple reduced ESOMs to be solved sequentially. In particular, these methods are used for two reasons. One is to account for uncertainties by frequently updating limited knowledge concerning the future. This applies, for instance, to forecasts of load or electricity production from renewable energy sources. Although the main principles of a rolling horizon approach apply to both operational and investment planning, in the following we mainly refer to the former, the rolling horizon dispatch. Therefore, a typical application is short-term scheduling of power systems with a high penetration of renewables [56–58].

The other purpose of implementing a rolling horizon approach to an ESOM is the premise that the total computing time for solving individual partial problems stays below the one for obtaining a solution for the original problem. Marquant et.al [59] report of a wide variety of achieved speed up factors ranging from 15 up to 100.

An optimal number of time windows usually exists depending on the model size, since the computational overhead for creating reduced models increases with the number of intervals. Furthermore, the planning horizon of an individual time window usually includes more time steps than necessary for the partial solution. In the context of energy system analysis, this overlap is important to emulate the continuing global planning horizon. Especially the dispatch of seasonal storage units is strongly affected by this as, without any countermeasures, it is more cost-efficient to fully discharge the storage until the end of an operational period. Also time-linking variables and constraints, such as annual limits on emissions, can barely be considered in this way since global information regarding the temporal scale can only be roughly estimated for each time window. For this reason, inter alia indicated by a trend to overestimate the total system costs [59], the aggregation of interval solutions does not necessarily end up at the global optimum of the original problem.

2.3.2. Temporal Zooming

Concerning their capability to improve the performance of an ESOM, rolling horizon approaches have one particular disadvantage. Since each partial solution is updated by a subsequent one, the reduced ESOM instances are sequentially coupled. This prevents parallel solving.

The heuristic, we refer to as temporal zooming, overcomes this issue and allows for solutions closer to the exact optimum of the original problem. Therefore, the rolling horizon approach is adapted in the following way. In a first step, time-linking information is gathered from the solution of an additional ESOM instance which is reduced on the temporal scale. But, in contrast to the reduced ESOMs which consider specific intervals within the full operational horizon, the temporal resolution is down sampled. This in turn allows optimizing the dispatch of the original problem for the full planning period. Values of variables from this first model run can subsequently be used to tune the consideration of global time-linking variables and constraints within the intervals. Despite the need for an additional model run, total computing times for obtaining a final solution can be expected to be at least competitive compared to rolling horizon approaches. This is due to the fact that overlaps are not required and the temporally sliced ESOMs can be solved in parallel.

2.4. Mathematically Exact Decomposition Techniques

Decomposition approaches are a well-known instrument for reducing the computing time in OPs. In this case, an OP is broken down into interlinked partial problems. With regard to the structure of the OP's coefficient matrix, the decomposition can be exploited for the creation of individual blocks. Ideally, block structures with globally linking variables or constraints can be isolated from the sub-problems, making them solvable independently of each other, for example in parallel.

Despite this similarity to nested approaches, such as temporal zooming, the crucial difference concerning exact decomposition techniques is the theoretically proven guarantee to find the optimal solution of the original problem [60]. However, this typically requires an iterative solution of partial problems. Therefore, it can be stated, that compared to nested approaches, decomposition techniques provide the best accuracy possible, but at the expense of additional computing time.

2.4.1. Dantzig-Wolfe Decomposition

In particular, approaches that can treat linking constraints are Dantzig-Wolfe decomposition and Lagrangian relaxation. The general idea behind both is to remove the linking constraints from the original problem to observe a relaxed problem that decomposes into sub-problems. In the case of Dantzig-Wolfe decomposition the objective function of the appropriate master problem consists of a linear combination of solutions of the relaxed problem. Starting from an initial feasible solution, the subsequent iterations extend this function if the new solution of the relaxed problem verifiably reduces the objective value (i.e., costs). Accordingly, this process is called column generation since the iterations literally creates also new columns in the master problems' coefficient matrix. Flores-Quiroz et al. [61] use this approach in order to decouple discrete investment decisions from dispatch optimization for a GEP with UC-constraints. Although performance enhancements are examined for realistic applications of different sizes these improvements are only quantified for small model instances due to memory issues of not-decomposed benchmark models (ca. 3 times faster, 95% less memory usage).

2.4.2. Lagrangian Relaxation

The Lagrangian relaxation is derived from the common mathematical technique of using Lagrange multipliers to solve constrained OPs where linking constraints are considered in the form of penalty terms in the objective function of the master problem. In the applied literature, Lagrangian relaxation is used by Virmani et al. [62] to treat the linking constraints, that couple individual generation units in the UC problem. More recently, Wang et al. [63] applied Lagrangian relaxation on a security-constrained OPF problem in order to decouple a security constraint that links variables of two scales, contingencies and circuits. However, as the treated problem consists of both linking constraints and linking variables, Benders decomposition is applied additionally.

2.4.3. Benders Decomposition

Opposed to the previously described decomposition approaches, Benders decomposition can be applied to OPs with linking variables. The general concept of splitting an OP by this approach is based on fixing the linking variables in the sub-problem(s) using their values from the master problem's solution. To improve the solution of the master, the sub-problems are approximated by additional constraints. These so called Benders cuts in turn rely on the dual variables of the obtained solutions in the sub-problems.

As ESOMs are often formulated as linear programs, due to duality of these problems, a translation of linking constraints into linking variables is possible and thus Benders decomposition can be applied to almost all kinds of ESOMs. Accordingly, it is a frequently exploited decomposition technique in the applied literature. Table 2 lists a number of publications that apply decomposition techniques to ESOMs that are at least partially formulated as linear programs (LPs) or mixed-integer linear programs

(MIP). However, due to the non-linearity of AC-power flow constraints, also non-linear programs (NLPs) are a typical use case considered here.

Table 2. Overview decomposition techniques applied to ESOMs.

Authors	**Math. Problem Type**	**Descriptive Problem Type**	**Decomposed Model Scale**	**Decomposition Technique**	**Decomposition Purpose**
Alguacil and Conejo [64]	MIP/NLP	Plant and grid operation	Time, single sub-problem	Benders decomposition	Decoupling of UC and multi-period DC-OPF *
Amjady and Ansari [65]	MIP/NLP	Plant operation		Benders decomposition	Decoupling of UC and AC-OPF **
Binato et al. [66]	MIP/LP	TEP		Benders decomposition	Decoupling of discrete investment decisions and DC-OPF
Esmaili et al. [67]	NLP/LP	Grid operation		Benders decomposition	Decoupling of AC-OPF and congestion constraints
Flores-Quiroz et al. [61]	MIP/LP	GEP	Time, 1-31 sub-problems, sequentially solved	Dantzig-Wolfe decomposition	Decoupling of discrete investment and UC
Habibollahzadeh et al. [68]	MIP/LP	Plant operation		Benders decomposition	Decoupling of UC and ED
Khodaei et al. [69]	MIP/LP	GEP-TEP	Time, two sub-problem types, sequentially solved	Benders decomposition	Decoupling of discrete investments into generation and transmission capacity, security constraints and DC-OPF
Martinez-Crespo et al. [70]	MIP/NLP	Plant and grid operation	Time, 24 sub-problems, sequentially solved	Benders decomposition	Decoupling of UC and security constraint AC-OPF
Roh and Shahidehpour [71]	MIP/LP	GEP-TEP	Time, up to 10 × 4 sub-problems, sequentially solved	Benders decomposition and Lagrangian Relaxation	Decoupling of discrete investments into generation and transmission capacity, security constraints and DC-OPF
Virmani et al. [62]	LP/MIP	Plant operation	Technology (generation units), up to 20 sub-problems, sequentially solved	Lagrangian Relaxation	Decoupling of unit specific(UC) and cross-park (ED) constraints
Wang et al. [72]	LP/MIP	Plant and grid operation	Space, 26 sub-problems, sequentially solved	Lagrangian Relaxation	Decoupling of DC-OPF and UC
Wang et al. [73]	MIP/NLP	Plant and grid operation	Scenarios and time, 10 × 4 sub-problems, sequentially solved	Benders decomposition	Decoupling of UC, scenario specific system adequacy constraints and network security constraints
Wang et al. [63]	LP	Plant and grid operation	Technology (circuits) and time (contingencies), two sub-problem types, sequentially solved	Lagrangian Relaxation and Benders decomposition	Decoupling of DC-OPF, system risk constraints and network security constraints

* Direct Current Optimal Power Flow, ** Alternating Current Optimal Power Flow

2.4.4. Further Aspects

Besides the already presented decomposition techniques, also further mathematically exact approaches exist that are based on individual information exchange between partial problems. Zhao et al. [74], for instance, use this marginal based approach for independent scheduling in a multi-area OPF problem. Compared to the heuristics presented above, this can be interpreted as the spatially decomposed counterpart to the (temporally decomposed) rolling horizon approach.

Although decomposition approaches provide the capability to improve the performance of solving independent sub-problems of an ESOM in parallel, these techniques are mostly applied for another purpose which results in the iterative solution of a master and one sub-problem. A complicated mathematical problem, such as a large NLP, is simplified by splitting it up into two problems, a smaller NLP on the one hand and a less complicated problem, such as a MIP, on the other. This applies especially to the examples in Table 2 for which nothing is listed in the column "Decomposed model scale". And even though the most frequently identified, decomposed model scale is found to be the temporal dimension, this usually refers to the separation of sub-annual operation scheduling and long-term investment planning in GEP or TEP. According to Table 2, the other typical application of exact decomposition techniques is decoupling of power-flow or security constraints from an UC model which generally refers to a spatial decomposition.

The computational benefits of parallel computing are especially exploited in the context of stochastic OPs. Here the temporal scale is extended by almost independent branches which are referred to as scenarios. These scenarios represent different possible futures which can be determined in parallel (sub-problems) while the assessment of these several alternatives is done by the master problem. Besides the classical decoupling of investment and operation decisions, this approach is also suitable in the context of short-term scheduling. For example, Papavasiliou et al. [75] apply Lagrangian relaxation to decompose by scenarios for a stochastic unit commitment model with DC power flow constraints. Opposed to most ESOMs, they solve their model on a high performance computer with distributed memory architecture. As is it can be expected, Papavasiliou et al. [75] find a significant speed-up due to parallelization. This performance increase, however, poorly scales with the number of cores (e.g., speed-up factor 7 for a hundred times the number of cores). Nevertheless, the main goal of the presented approach is to stay below a threshold of computing time that is suitable for day-ahead operation planning.

2.5. Aim and Scope

Despite the existence of a large number of speed-up approaches for ESOMs, it is not clear which methods are the most promising ones to improve the performance of ESOMs that are used in the field of applied energy system analysis. In addition to the arrow-head structure of the coefficient matrix (presence of linking constraints and linking variables, see Section 1), a majority of these models share three characteristics [27]:

(1) To be able to increase the descriptive complexity of the models, the mathematical complexity is often simplified. This frequently means the formulation of large monolithic linear programs (LPs) which are solved on shared memory machines.
(2) Due to the assessment of high shares of power generation from vRES the time set that represents the sub-annual time horizon shows the largest size (typically 8760 time steps)
(3) A great number of applied ESOMs are based on mathematical programming languages such as GAMS (General Algebraic Modeling System) or AMPL (A Mathematical Programming Language") rather than on classical programming languages. Those languages enable model formulations which are close to the mathematical problem description and take the task of translation into a format that is readable for solver software. For this reason, the execution time of the appropriate ESOMs can by roughly divided into two parts, the compilation and generation of the model structure requested by the solver and the solver time.

For the following analyses, we also use GAMS which is, according to a review conducted by Zerrahn and Schill [27], a very popular modelling language in the field of energy systems analysis. We focus on initially large GAMS models for which total computing time is mainly dominated by solver time.

The general aim of this paper is to systematically assess the effectiveness of different performance enhancement approaches for ESOMs that share the above mentioned characteristics. Rather than the comparison of models that deliver exact the same results, we explore possible improvements in terms of required computing time that can be achieved by implementing different conceptual speed-up techniques into an ESOM while staying within a sufficient accuracy range.

By this means, our aim is not to compare all above presented speed-up approaches, but those which are able to achieve the comprehensibly best performance enhancement. In this context, our hypothesis for the selection of model-based speed-up approaches to be systematically evaluated relies on three basic premises:

(1) We focus on very large LPs that have a sufficiently large size for the computing time to be dominated by the solver time and still maintaining the possibility to be solved on a single shared memory computer. If we implement an approach that allows for reduction or parallelization of the initial ESOM by treating a particular dimension, the highest potential therefore can explored by applying such an approach to the largest dimension. Accordingly:
(2) We emphasize speed-up strategies that treat the temporal scale of an ESOM. A high potential for performance enhancement still lies in parallelization, even though, for this study, it is limited to parallel threads on shared memory architectures. Exact decomposition techniques have the advantage to enable parallel solving of sub-problems. However, we claim that each exact decomposition technique can be replaced by a heuristic where the iterative solution algorithm is terminated early. In this way, the highest possible performance should be explored, because further iterations only improve the model accuracy; however they require more resources in terms of computing time. In addition, according to the literature in Table 2, it can be concluded, that mathematically exact decomposition techniques are applied less often with the objective of parallel model execution, but the separation of a more complicated optimization problem from an easy-to-solve one. For very large LPs this is not necessary. For these reasons:
(3) We only analyze model reduction by aggregation and heuristic decomposition approaches.

3. Materials and Methods

3.1. Overview

Our evaluation approach should provide an assessment of model-based performance enhancement approaches for a very large ESOM that is intended to produce results for real use-cases. However, this implies a couple of challenges. A proper adaption of a large applied ESOM for the comparison of a broad set of speed-up strategies is very time-consuming. Accordingly, we limit the evaluation to the following performance enhancement approaches:

- model reduction by spatial and temporal aggregation
- rolling horizon
- temporal zooming

Moreover, to meet the requirement for an evaluation of very large ESOM instances, we want to prevent the implementation of speed-up strategies into a model that is easily solvable by a commercial solver. Nevertheless, for having references for benchmarking this must still be possible. Hence, we select an existing ESOM for which we know from experience that obtaining a solution is hard but not impossible.

Besides, for fair benchmarking, it must be ensured that the reference model already performs well, e.g., with regard to solver parameterization. To meet this requirement our first methodological step is to conduct a source code review for the applied ESOM and follow recommendations by GAMS developers and McCarl [76]. Although most of the corresponding hints of the latter aim at the reduction of the GAMS execution time, the main objective of this review step is the identification of source code snippets that cause the creation of redundant constraints. In practical terms, this means an explicit exclusion of unnecessary cases by broadly applying conditional statements ($-conditions). Otherwise, needlessly large models would be passed to the solver.

Finally, it is essential that all model instances that should be compared are executed on identical hardware which should be exclusively available for the ESOM-related computing processes. Ensuring this across the whole evaluation exercise would require a large number of computers with comparatively large memory (>200 GB) to conduct the analysis within practical time spans. Due to a limited access to such equally equipped computers, we guarantee this only for benchmarks across each particular performance enhancement strategy.

The remainder of this section is structured as follows: The modeling setup consisting of a description of the applied ESOM and its characteristics and data as well as the used solver and its basic parameterization are described in Section 3.2. The implementations of speed-up approaches to be evaluated are then presented in Section 3.3. Finally, we set up an evaluation framework that ensures at least a fair comparison of model performance and accuracy across different parametrizations of a particular speed-up approach.

3.2. Modeling Setup

REMix (Renewable Energy Mix for a sustainable energy supply) can also be regarded as a modeling framework since several parameterizations of the REMix model exist which share the same source code but focus on various research questions and thus have different scopes in terms of available technologies, geographical study area and time horizon. The analyses for this study were conducted with two model setups which were partially extended. Although most of our analyses are performed for both of them, the results presented in Section 4 build on the REMix instance presented in [77]. The corresponding LP represents the German power system for an energy scenario of the year 2030. In its basic configuration it is a CO_2-emission-constrained DC-OPF problem that considers renewable and fossil power generators, electricity transport within the high voltage transmission grid as well as storage facilities such as pumped hydro power plants and lithium-ion batteries.

In addition, no generation capacities are optimized but capacities of both transmission lines and energy storage are optionally considered for expansion planning. To be able to observe a significant expansion of these technologies, their initial values for installed capacities represent the state of 2015. Hence, the installed capacity of lithium-ion batteries is zero. It needs to be noted that this configuration can lead to loss of load situations if capacity expansion is omitted. This is due to the fact that the power plant portfolio of the underlying scenario relies on the assumption that suitable load balancing capability of the power system can be provided by lithium-ion batteries and additional power transmission capacities.

A fact sheet of the appropriate REMix model setup is shown in Table 3 which also provides information about the input and output data.

Table 3. Model fact sheet of the applied configuration of REMix based on [77].

Model Name	REMix
Author (Institution)	German Aerospace Center (DLR), Institute of Engineering Thermodynamics
Model type	Linear programing Minimization of total costs for system operation and expansion Economic dispatch/optimal dc power flow with expansion of storage and transmission capacities
Sectoral focus	Electricity
Geographical focus	Germany
Spatial resolution	488 nodes
Analyzed year (scenario)	2030
Temporal resolution	8760 time steps (hourly)

Table 3. *Cont.*

Model Name	REMix			
Input-parameters:		Dependencies		
		Temporal	Technical	Spatial
	Conversion efficiencies [78]		x	
	Operational costs [78]		x	
	Fuel prices and emission allowances [79]		x	
	Electricity load profiles [80]	x		x
	Capacities of power generation, storage and grid transfer capacities and annual electricity demand [81–83]		x	x
	Renewable energy resources feed-in profiles	x	x	x
	Import and export time series for cross-border power flows [84]	x		x
Evaluated output parameters	System costs (objective value)			
	Generated power		x	x
	Added storage/transmission capacities			x
	Storage levels	x	x	x

3.2.1. Characteristic Constraints

The majority of the mathematical formulations of REMix is presented in [85]. As discussed in Sections 1.2 and 1.3, the coefficient matrix structure of the corresponding LPs contains linking variables and constraints. Besides variables that are induced by enabling capacity expansion (Equation (3)), a great number of linking elements results from modeling power transmission using the dc approximation (spatially linking) or storage facilities (temporally linking). Furthermore, constraints reflecting normative targets, such as necessary for modeling greenhouse gas mitigation scenarios, cause interdependencies between large sets of variables (spatially and temporally linking). For a better comprehensibility Equations (5) to (8) describe these constraints in a simplified manner, i.e., without conditional statements, additional index sets or scaling factors (as implemented in REMix):

Storage energy balance:

$$\begin{aligned} \boldsymbol{p}_{s+}(t,n,u_s) - \boldsymbol{p}_{s-}(t,n,u_s) - \boldsymbol{p}_{\boldsymbol{ls}}(t,n,u_s) \;&=\; \tfrac{E_s(t,n,u_s)\;-\;E_s(t-1,n,u_s)}{\Delta t} \\ \forall t \in T; \forall n \in N;\; \forall u \in U_s; U_s &\subset U \end{aligned} \tag{5}$$

where U_s: set of storage facilities.

DC power flow:

$$\begin{aligned} \boldsymbol{p}_{\boldsymbol{im}}(t,n) - \boldsymbol{p}_{\boldsymbol{ex}}(t,n) - \boldsymbol{p}_{\boldsymbol{lt}}(t,n) \;&=\; \sum_{n'} B(n,n') \cdot \boldsymbol{\theta}(n',t) \\ \forall t \in T; \forall n &\in N \end{aligned} \tag{6}$$

$$\begin{aligned} \boldsymbol{p}_{f+}(t,l) - \boldsymbol{p}_{f-}(t,l) \;&=\; \sum_{l}\sum_{n} B_{diag}(l,l') \cdot K^T(l,n) \cdot \boldsymbol{\theta}(n,t) \\ \forall t \in T; \forall l &\in L \end{aligned} \tag{7}$$

where: $\boldsymbol{p}_{\boldsymbol{im}}/\boldsymbol{p}_{\boldsymbol{ex}}$: power import/export, $\boldsymbol{p}_{\boldsymbol{lt}}$: transmission losses, $\boldsymbol{p}_{f+}/\boldsymbol{p}_{f-}$: active power flow along/against line direction, $\boldsymbol{\theta}$: voltage angle, B: susceptance between regions, B_{diag}: diagonal matrix of branch susceptance, K: incidence matrix and L: set of links (e.g., transmission lines).

Emission cap:

$$\sum_t \sum_n \sum_u \boldsymbol{p}(t,n,u) \cdot \eta_e(u) \leq m \tag{8}$$

where: η_e: fuel specific emissions and m: maximal emissions.

3.2.2. Solver Parametrization and Hardware Environment

In preliminary experiments resulting from a broad spectrum of REMix applications, ranging from country specific cross-sectoral energy systems [86,87] to multi-regional [85,88–90] and spatially highly resolved power systems [77], for monolithic LPs, we observed the best performance in terms of computing time and RAM requirements with the following solver parameters when using CPLEX:

(1) LP-method: barrier
(2) Cross-Over: disabled
(3) Multi-threading: enabled (16 if not otherwise stated)
(4) Barrier tolerance (barepcomp)

- $1e^{-5}$ spatial aggregation with capacity expansion
- default ($1e^{-8}$): rest

(5) Automatic passing of the presolved dual LP to the solver (predual): disabled
(6) Aggressive scaling (scaind): enabled

Especially in the case of the first three solver options, LPs that previously could not be solved within time spans of multiple days, turned out to be solvable in less than 24 h. With regard to the solver parameter 5, the amount of required RAM could be significantly decreased. For example, model instances that showed a peak memory demand of 230 GBs when setting predual to −1, otherwise exceeded the available RAM of 300 GBs. For these reasons, all of the following analyses are conducted with GAMS release 25.1.3 using CPLEX 12.8.0 with the above listed solver parameters. In addition, for all implementations of heuristic decomposition approaches either the GAMS option solvelink = 5 (rolling horizon, temporal zooming) or solvelink = 6 (temporal zooming with grid computing) are used to avoid delay times due to frequent read and write operations on the hard disk.

With regard to available hardware, computers with the following (Table 4) specifications are available:

Table 4. Specifications of available computers for solving model instances.

Processor	Available Threads	Available Memory
Dual Intel Xeon Platinum 8168	2x 24 @ 2.7 GHz	192 GB
Intel Xeon Gold 6148	2x 40 @ 2.4 GHz	368 GB

3.2.3. Original REMix Instances and Their Size

As indicated in Table 3 the applied REMix model performs a DC-OPF which is optionally extendable by capacity expansion planning for storage and transmission infrastructures. Depending on this optional setting, two original model instances can be distinguished referred to as "REMix Dispatch" and "REMix Expansion". Due to the different purposes of the decomposition heuristics to be evaluated, the two original models are only investigated for a sub-set of speed-up approaches. The rolling horizon approach is only sufficiently applicable to dispatch problems since investment decisions for especially short time intervals lead to a significant overestimation of required capacity expansion. In contrast, temporal zooming is explicitly suited for problems that account for capacity expansion.

To get an impression of model size, we measure the number of constraints, variables and non-zero elements of the coefficient matrix reported by the solver after performing the pre-solve routines. The appropriate values are indicated in Table 5. They show that enabling expansion planning is costly, especially with regard to the number of constraints. Compared to the number of variables which is increased by approximately 30%, the number of constraints is more than tripled. Nevertheless, this results in a less dense coefficient matrix since the number of non-zeros is only doubled.

Table 5. Characterization of original REMix model instances.

Original Model Instance Name	Applied Speed-Up Approaches	Number of Variables	Number of Constraints	Number of Non-Zeros
REMix Dispatch	• spatial aggregation • temporal aggregation • rolling horizon dispatch	30,579,396	9,214,488	69,752,951
REMix Expansion	• spatial aggregation • temporal aggregation • sub-annual temporal zooming	43,169,135	32,805,201	137,967,269

3.3. Implementations

3.3.1. Aggregation Approaches

The implemented aggregation approaches either treat the temporal or spatial scale. In case of the first, simple down-sampling is applied to load and feed-in profiles from vRES. Those parameters are available in form of hourly time series (temporally resolved). For down-sampling they are averaged to achieve a data aggregation and accordingly a reduction of the model size by factor M. For instance, when transforming a demand time series and, for reasons of simplicity, index sets of the other dimensions are ignored, the appropriate calculation rule is:

$$\begin{gathered} d_{\text{agg}}(t_M) \;=\; \sum_t \Pi_t(t_M, t) \cdot d(t) \\ \forall t_M \in t_M; M \in \mathbb{N} \end{gathered} \tag{9}$$

where: T_M: set of merged (down-sampled) time steps, Π_t: map that assigns time steps to merged time steps and d_{agg}: temporally aggregated power demand time-series.

Setting $M = 4$ thus results in input time series that have a 4-hourly resolution. In other words, instead of $t = 1, \dots, 8760$ only $t_M = 1, \dots, \frac{8760}{4}$ consecutive data points need to be considered in a REMix instance which we refer to be "temporally aggregated".

With regard to the spatial aggregation methodology, we apply the following data processing: First a network partitioning is performed to define which regions of the original model parameterization are to be merged. Therefore, an agglomerative clustering is used by applying the implementation of this algorithm from scikit learn [91] to the adjacency matrix of the original model's network. We chose this clustering methodology as it ensures that merged regions are only built from neighboring regions. In addition, the clustering algorithm itself scales well with regard to various numbers of clusters.

Secondly, we create network equivalents. The applied data aggregation relies on the premise that regions represent so called "copper plates" which means that transmission constraints are ignored within these areas. As a consequence, most nodal properties, such as installed power generation capacity or expansion potentials as well as power demand are spatially aggregated by simple summation. A special case is the aggregation of feed-in time series. Here a case distinction is applied, where the profiles of renewable power generation are aggregated by weighted averaging. The weights are taken from the installed power generation capacities of the respective regions normalized by the sum over the installed capacities within the aggregated region. If there are no capacities installed (e.g., in the case of green-field expansion planning), the maximal capacities resulting from a renewable energy potential analysis are used.

Data that is related to links, such as power transmission lines, is also specially treated: Transmission lines that would lie within an aggregated region are ignored. The transmission capacities of parallel cross-border links are summed up, while link lengths that are used for loss approximation and susceptance of parallel lines are combined as it is common for parallel circuits, for instance:

$$\begin{aligned} B_{\text{agg}}(l_M) \;&=\; \frac{1}{\sum_l \Pi_l(l_M,l) \cdot {}^{1}\!/_{B(l)}} \\ &\forall l_M \in L_M \end{aligned} \tag{10}$$

where: L_M: set of merged links, Π_l: map that assigns links to merged links and B_{agg}: susceptance of merged links.

3.3.2. Rolling Horizon Dispatch

We implement a rolling horizon dispatch into REMix, a decomposition of the original model in time, where the full time horizon of 8760 time steps is divided into a number of overlapping time periods (intervals). For each of these time intervals only the hourly system operation is optimized. Accordingly, capacity expansion is not considered in the appropriate model instances. This is due to the fact that variables that are related to capacity expansion are not resolved on the temporal scale. These temporally linking elements would prevent an easy decomposition in time and thus limit the application of rolling horizon approaches to dispatch optimization problems.

The emission cap (Equation (8)) is also temporally linking and therefore requires changes compared to the native implementation of REMix. A straightforward approach is the distribution of the annual emission budget to the time intervals. In the simplest case the corresponding distribution factors are constant and calculated from the reciprocal of the number of intervals. More sophisticated distributions may take into account input data such as load and feed-in time series to define sub-annual emission caps that correspond to the residual load. However, such a distribution still does not account for regional differences. For reasons of simplicity we use the constant distribution for our implementation of the rolling horizon dispatch.

Storage facilities are only weakly temporally linking as the appropriate energy balance constraint (Equation (5)) only couples neighboring time steps. The error induced by decomposing in time is small as long as the length of time intervals is much greater than the typical energy-to-power ratio of a particular storage technology. Importantly, the overlap prevents that energy storage facilities are always fully discharged at the end of the evaluated part of a time interval to save costs. In the full time-horizon implementation of REMix this undesired effect is addressed by coupling the very last time step to the initial time step. In other words, it is enforced that the storage levels of the first and the last hour of the year are equal. However, this circular coupling is not suitable concerning the boundaries of sub-annual time intervals.

For the rolling horizon approach this means that full discharging still appears by the end of a computed time interval, but it is weakened the longer the overlap. However, there is a trade-off to be made with regard to the length of overlaps since they imply dispatch optimization of redundant model parts and therefore lead to greater total computing times. Another drawback of using overlaps is also that only sequentially solving of multiple model instances is possible.

The discussed characteristics of the rolling horizon approach require a couple of modifications and extensions of the REMix source code especially with regard to the execution phases. In Figure 3 necessary adaptions are visualized.

(1) A new set T_i that represents the time intervals is defined.
(2) The number of overlapping time steps between two intervals as well as a map that assigns the time steps t to the corresponding intervals (with or without overlap) is defined. With a larger overlap more subsequent time steps are redundantly assigned to both the end of the i^{th} and the beginning of the $(i+1)^{th}$ interval.
(3) It must be ensured that all time dependent elements (variables and constraints) are declared over the whole set of time steps, whereas their definitions are limited to a subset of time steps that depends on the current time interval.

(4) A surrounding loop is added that iterates over the time intervals.
(5) With each iteration a solve statement is executed.
(6) The values of all time dependent variables are fixed for all time steps of the current interval but not for those that belong to the overlap.
(7) To easily obtain the objective value of the full-time horizon model, a final solve is executed that considers only cost relevant equations. As all variable levels are already fixed at this stage, this final solve is not costly in terms of performance.

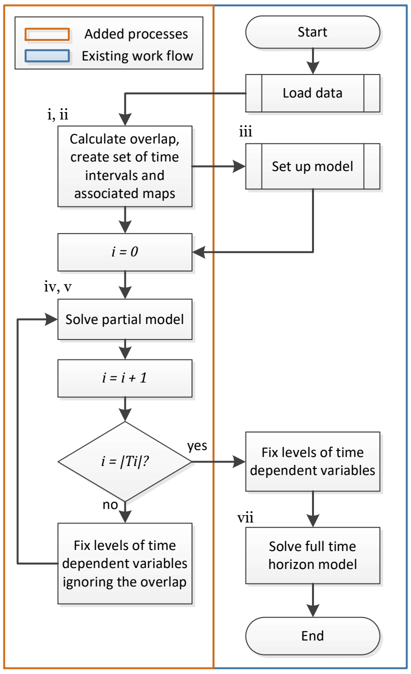

Figure 3. Flow chart of implementation of rolling horizon.

The chosen source code adjustments require a manageable amount of effort and can be seen as a processing friendly implementation since all input data is read in the beginning, whereas data is processed slice by slice. Also partial results are held in memory which facilitates an easy creation of a single output file. Established post-processing routines do not have to be changed. Nevertheless, for memory constrained ESOMs, memory friendly implementations are preferable. Data would accordingly be loaded and written to disc slice by slice. The downside of this solution is the fact that these processes must be executed multiple times which results in additional processing costs. Furthermore, the composition of outputs requires a further post-processing that is characterized by multiple read routines of the partial result files.

3.3.3. Sub-annual Temporal Zooming

Our implementation of the temporal zooming heuristic is an extension of the previously described rolling horizon approach that enables capacity expansion planning. For this reason, also other temporally linking elements can be treated differently. In particular, each time interval represents a sub-problem where, from a global model perspective, missing information is gathered from a temporally down-sampled full time-horizon model run.

In the case of the storage energy balance, at the boundaries of each time interval the storage level variables are fixed to the levels of the corresponding variables of the down-sampled model's result. Furthermore, for each time interval, factors that define the share of annually allowed emissions are determined with respect to the resulting emissions in the down-sampled model run. This allows a much better distribution of these actually time independent parameter values than an equal distribution as in the implementation of the rolling horizon dispatch.

Even though solving a down-sampled model instance causes additional costs in terms of computing time, the advantage of this approach is the independence of partial models where overlaps are no more necessary. However, as the number of parallel threads is limited on shared memory architectures, this parallelization on the conceptual layer is at the expense of less parallelization on the technical layer, i.e., parallel threads when using the barrier algorithm. For this reason, we implement two versions of the temporal zooming approach (where I corresponds to the variable of capacity expansion introduced in Equation (3):

(1) A sequential version that is executed in the same chronological manner as the rolling horizon approach where parallelization only takes place on the solve side (Figure 4).
(2) A parallel version that uses the grid computing facility of GAMS where a defined number of time intervals is solved in parallel. Parallelization takes place on both the model side and the solver side (Figure 5).

Besides the different ways of parallelization the two implementations also differ in the treatment of capacity expansion variables. While in both cases an initial lower bound is defined with regard to the outcome of the down-sampled model run, in the sequential implementation, this lower bound is raised with respect to the results of a particular interval and then shifted to the next interval. On the contrary, the parallel implementation determines the final values of expansion planning variables by selecting the maximum across their interval dependent counterparts.

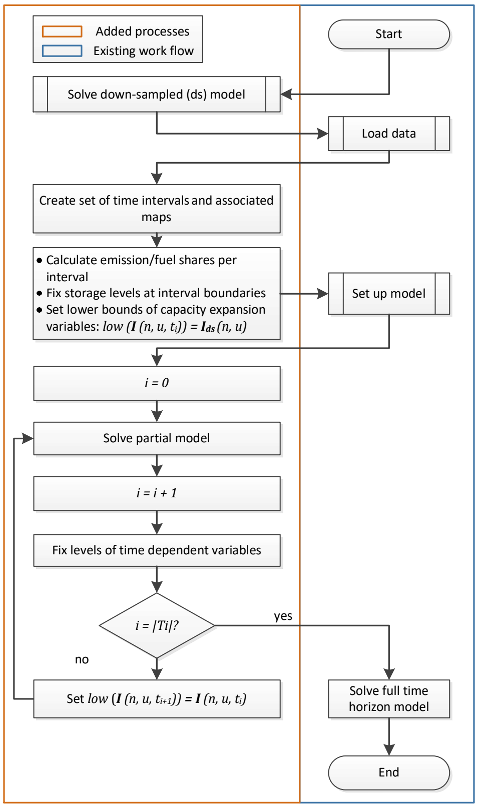

Figure 4. Flow chart of sequential implementation of temporal zooming.

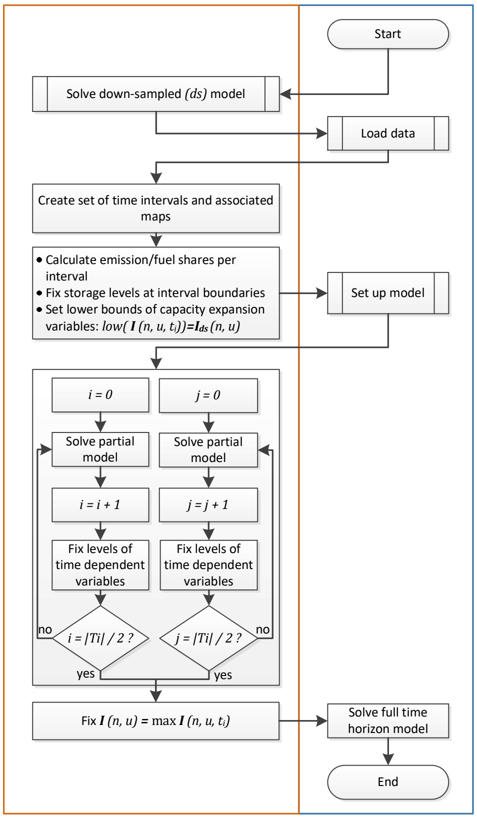

Figure 5. Flow chart of grid computing implementation of temporal zooming, exemplarily shown for two parallel runs.

3.4. Evaluation Framework

3.4.1. Parameterization of Speed-Up Approaches

Each of the implemented model-based speed-up approaches is characterized by parameters that influence the model performance. We refer to these parameters as SAR-parameters (speed-up approach related parameters). In this context, the challenge is to identify SAR-parameter settings that provide both an effective performance enhancement and a sufficient accuracy. We tackle this issue by performing parameter studies. The evaluated parameter value ranges are shown in Table 6.

Table 6. Overview of speed-up approach related parameters and value ranges to be evaluated.

Speed-Up Approach	**Parameter**	
	Name	**Evaluated Range**
Spatial aggregation	number of regions (clusters)	{1, 5, 18, 50, 100, 150, 200, 250, 300, 350, 400, 450, 488}
Down-sampling	temporal resolution	{1, 2, 3, 4, 6, 8, 12, 24, 48, 168, 1095, 4380}
Rolling horizon dispatch	number of intervals overlap size	{4, 16, 52,365} {1%, 2%, 4%, 10%}
Temporal zooming (sequential)	number of intervals temporal resolution of down-sampled run	{4, 16, 52} {4, 8, 24}
Temporal zooming (grid computing)	number of intervals number barrier threads number of parallel runs temporal resolution of down-sampled run	{4, 16, 52} {2, 4, 8, 16} {2, 4, 8, 16} {8, 24}

In the case of aggregation the SAR-parameters are more or less equivalent to the degree of aggregation. It can be expected that there is a continuous relation between these parameters and the achievable performance and accuracy, where increasing the degree of aggregation will reduce the required computing resources at the expense of less accuracy.

However, the implemented rolling horizon as well as the temporal zooming approaches can be tuned by changing a set of SAR-parameters (Table 6). Thus, the relation between speed-up approach parameterization and the evaluated indicators becomes more complex. For instance, one can expect that there is always an optimal number of intervals with regard to total computing time due to the trade of between faster solving of sub-models and the increasing computational burden from GAMS code compilation.

3.4.2. Computational Indicators

When referring to performance we always mean the computing time composed of time spent for model building and solving (solver time). The internal profiling options of GAMS is activated using the command-line option stepsum = 1. All relevant information is then extracted from the logging and listing files of GAMS. The *elapsed seconds* listed in the last step summary represent the total wall-clock time needed for executing all processes. As in our analyses the CPLEX solver is used exclusively, the *solver time* represents the time consumed by CPLEX. This quantity is usually listed above the solver's report summary which also provides the information whether an optimal solution was found. As the CPLEX time reported in seconds can vary depending on the load of the computer system as well as on the used combination of software and hardware, we primarily use the deterministic number of ticks (a computer independent measure) as indicator for required computing time by the solver [92]. The quantity we refer to as GAMS time is accordingly calculated by subtracting solver time from total wall-clock time.

An approximation for peak memory usage is also partially taken from the step summary denoted as Max heap size which represents the memory used by GAMS. An indicator for the memory use on the solver side—in the case of CPLEX's barrier algorithm—is provided by the number of equations and the logging information integer space required [93].

3.4.3. Accuracy Indicators

To measure the accuracy of an ESOM one could argue that all variable levels of a model instance treated by a particular speed-up approach should be compared to their counterparts of the original model. However, especially in the case of aggregation approaches the direct counterparts do not always exist. Besides the fact that the computational effort for such a comparison would be great due to the number of variables, an aggregation of the resulting differences would still be necessary to give an indication of accuracy by only a hand-full of comprehensible values. We therefore use only a selection of partially aggregated variable levels for comparison. Nevertheless, we emphasize indicators which are of practical relevance. As indicated in Table 3 these indicators are:

(1) The "objective value" of the optimization problem.
(2) The technology specific, temporally and spatially summed, annual "power supply" of generators, storage and electricity transmission.
(3) The spatially summed values of "added capacity" for storage and electricity transmission, and
(4) The temporally resolved, but spatially summed "storage levels" of certain technologies.

In the following, these indicators are presented relative to the corresponding result of "REMix Dispatch" or "REMix Expansion" observed for conventional solving according to 0. Hence, for example, the accuracy indicator "wind" is determined as follows:

Accuracy indicator "wind":

$$wind \;=\; \frac{\sum_{t' \in T, n' \in N, u \in U_w} \boldsymbol{p'}(t', n', u)}{\sum_{t \in T, n \in N, u \in U_w} \boldsymbol{p_{REF}}(t, n, u)} \tag{11}$$

where: $\boldsymbol{p'}$: **variable** levels of total power supply in a model instance treated by a speed-up approach, $\boldsymbol{p_{REF}}$: **variable** levels of total power supply in original modeln instance (without speed-up approach), T': set of time steps in a model instance treated by a speed-up approach, N': set of modeled regions in a model instance treated by a speed-up approach and U_w: set of wind enrgy converter technologies.

4. Results

4.1. Pre-analyses and Qualitative Findings

4.1.1. Order of Sets

Concerning an efficient execution of GAMS, in addition to the suggestions mentioned in Section 3.1., we observed that it is always advisable to use a consistent order of sets. An illustrative example considering this issue is provided by Ramos in [94]. We also investigated the hypothesis that ordering the index sets from the largest cardinality to the smallest would reduce the time for the model generation. In summary, reductions of up to 40% of the GAMS generation time are observed in some cases. However, the results strongly vary between different model instances. Furthermore, the time spent for model generation can also increase depending on the used version of GAMS. From this experience we conclude that tuning the source code by using particular index orders cannot be considered as a generally effective improvement of model performance.

4.1.2. Sparse vs. Dense

Especially with regard to the way of implementing the equations for storage energy balance and DC power flow, constraint formulations are conceivable that differ from the ones implemented in REMix (Equations (5) to (7)). These formulations make use of fewer variables and constraints and therefore lead to a smaller but denser coefficient matrix. Equations (12) and (13) give an impression of how such dense formulations can look like.

On the one hand, in the case of the storage energy balance equation, the alternative formulation allows that the storage level variables are no more required. On the other hand, instead of an interdependency of consecutive time steps, the power generation or consumption of each time step is linked with all of its previous pendants. This leads to strong linkages across the temporal scale especially for the balance equations that address the elements at the end of the time set. Concerning the DC power flow, Equation (13) can be derived from substitution of the voltage angle and merging of Equations (6) and (7). However, the resulting PTDF matrix requires a matrix inversion that leads to a dense matrix structure:

Storage energy balance:

$$\sum_{t' = t_0}^{t' = t} \boldsymbol{p_{s+}}(t', n, u_s) - \boldsymbol{p_{s-}}(t', n, u_s) - \boldsymbol{p_{ls}}(t', n, u_s) \;=\; \boldsymbol{p_{s+}}(t', n, u_s) - \boldsymbol{p_{s-}}(t', n, u_s) \\ \forall t \in T; n \in N;\; \forall u \in U_s;\; U_s \subset U \tag{12}$$

DC power flow (dense):

$$\boldsymbol{p_{f+}}(t, l) - \boldsymbol{p_{f-}}(t, l) \;=\; \sum_{n} PTDF(l, n) \cdot \big(\boldsymbol{p_{im}}(t, n) - \boldsymbol{p_{ex}}(t, n) - \boldsymbol{p_{lt}}(t, n)\big) \\ \forall t \in T;\; \forall l \in L \tag{13}$$

where: *PTDF*: power transfer distribution factors

The results of our experiments with these alternative model formulations showed that, for REMix, sparse implementations are usually better in terms of model performance. While already small model instances with the dense storage balance equation are nearly unsolvable, the application of PTDF matrices for the DC power flow turns out to be useable but still less performant compared to the implementation that uses the voltage angle.

In this context, on its left y-axis, Figure 6 shows the computing times for two exemplary scenarios (A and B), where, transmission capacity expansion is either enabled or disabled.

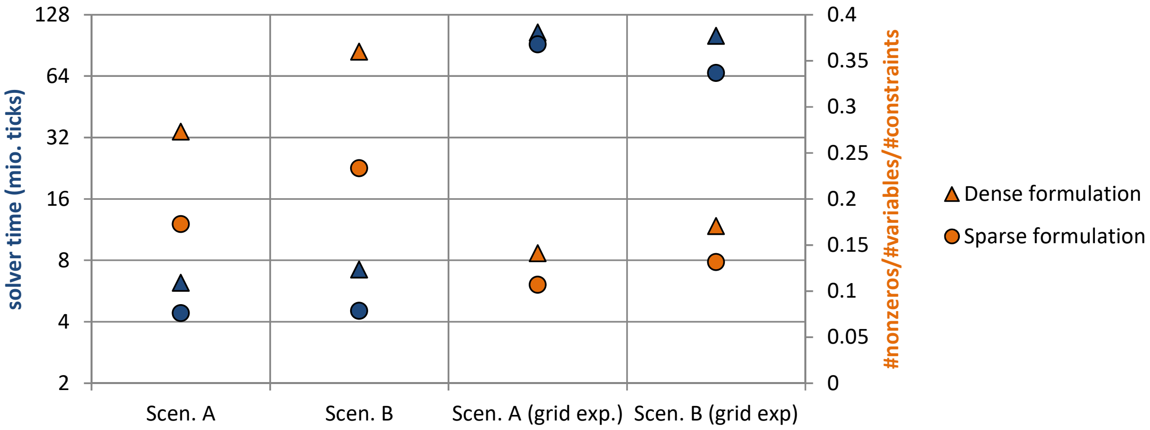

Figure 6. Solver time (blue) and non-zero density of the coefficient matrix (orange) for different DC power flow implementations, circles: sparse (with voltage angle), triangles: dense (with Power Transfer Distribution Factors (PTDF)).

The size of underlying model instances ranges between 20 to 38 million variables and 9 to 24 million constraints. To give an indication of the population density of the corresponding coefficient matrices, the number of non-zeros relative to the product of the number of constraints and the number of variables is plotted on the right y-axis. Each of the resulting four model instances is solved using either the dense (triangles) or sparse (circles) DC power flow formulation. As it can be deduced from comparing the blue markers, the computing times for the PTDF-based instances are 15 to 60% greater than in the case of their sparse counterparts. Due to the results of these preliminary experiments the following analyses are exclusively based on model implementations which aim for sparse constraint formulations.

4.1.3. Slack Variables and Punishment Costs

A common approach to ensure the feasibility of REMix even for scenarios where the power balance Equation (2) would be violated (e.g., by providing too small power generation potentials) is the use of slack generators. These generators do not have a technological equivalent in the reality and represent the last option to be used in the model for covering a given demand. The associated costs for power supply can be seen as the value of loss of load and thus are high compared to costs caused by real technologies. However, even if very high cost values could be particularly justified by macroeconomic damage, from a model performance perspective it is advisable to set these costs in the same order of magnitude as their real counterparts. Figure 7 shows exemplary computing times of identical model instances of a relatively small size (3 Mio. variables, 2 Mio. constraints). We deliberately analyze small models to prevent the model to run into numerical issues. The differences in the resulting solver time are exclusively caused by changing the model parameter that concerns the costs associated with slack power generation. The increasing computing time with increasing values of this parameter are due to worse model scaling.

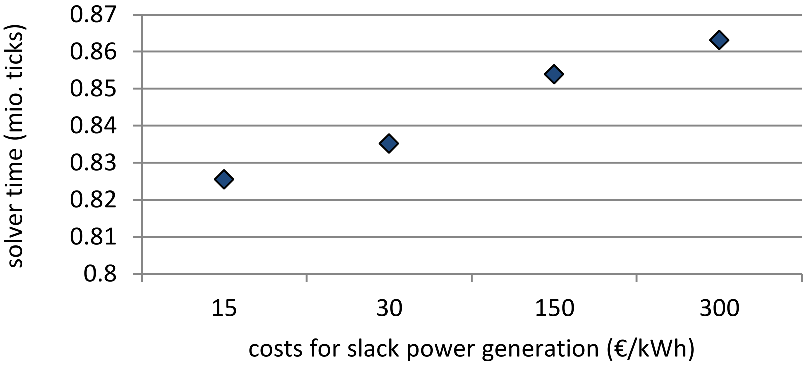

Figure 7. Computing time for different values for power generation costs of slack generators.

Despite the fact that scaling is also automatically applied by the solver, it is advisable that in the coefficient matrix of the resulting LP, coefficients stay within a certain range of order of magnitudes. As described by McCarl [95] the factor between the smallest and largest values should ideally be less than 1e5. Since ESOMs such as REMix consider both operational costs of almost zero (e.g., for photovoltaics) and annuities for investments into new infrastructures of several millions (e.g., large thermal units), the corresponding cost ratios are already out of the ideal range. For this reason, the cost factors for slack power generation should not expand this range. Otherwise, especially for large models, the bad scaling leads to numerical issues of the solver and at least extended computing times.

4.1.4. Coefficient Scaling and Variable Bounds

Also processing of input data during the generation of equations can pose problems concerning the aforementioned maximum range of coefficients. For example, this is relevant when calculating the fuel consumption based on the power generation divided by the fuel efficiency. Moreover, it is advisable to bound variables to restrict the space of possible solutions which may also lead to a better solver performance. However, finding appropriate bounds for future states of the energy system and claiming to analyze a broad range of conceivable developments implies possible contradictions.

To get a more systematic picture, in Figure 8, we compare a selection of model instances in three spatial resolutions with two different solver precisions. The solver precisions are labelled as “$1e^{-5}$” and “Default” ($1e^{-8}$) while further measures such as explicit rounding of parameters and conscious bounding of variables are varied. The idea behind rounding of input time series and efficiencies is to avoid implicit coefficients with more than five decimals. As a further step in the instance denominated as “bounded variables” we add upper bounds on most variables according to model heuristics. For instance, the power production from slack generators is limited to 10% of the exogenously given electricity demand profile. Additionally, we set upper bounds on decision variables for investments into storage and transmission capacities based on the maximum peak load and annual energy demand of the corresponding regions.

In Figure 8 the conducted comparison is shown for three differently sized instances of both the “REMix Expansion” and the “REMix Dispatch” model. The solver time is depicted relative against the number of ticks required to solve the appropriate model with default settings as presented in 3.2. In this context, the black circles represent the reference values at y = 1.0. While for the small instances with 30 and 120 regions the gains from coefficient rounding (blue markers) seem to indicate better performance, in large scale instances the effect is inverse. For the 488-region instance there is an increase in ticks for the barrier algorithm with the presumably improved numerical properties. In contrast, the additional bounds on variables (orange markers) have a rather little impact on the small-sized instances with only a few regions, while the performance gains for the large scale instances are significant by effectively bringing down the solver time to less than 50% compared to instances with default settings.

From the comparison of triangle and circle markers in Figure 8, it can be furthermore concluded, that the observed effects are independent of the solver precision. However, the possible speed-up highly depends on the general model formulation and may not apply for other solution algorithms than interior point.

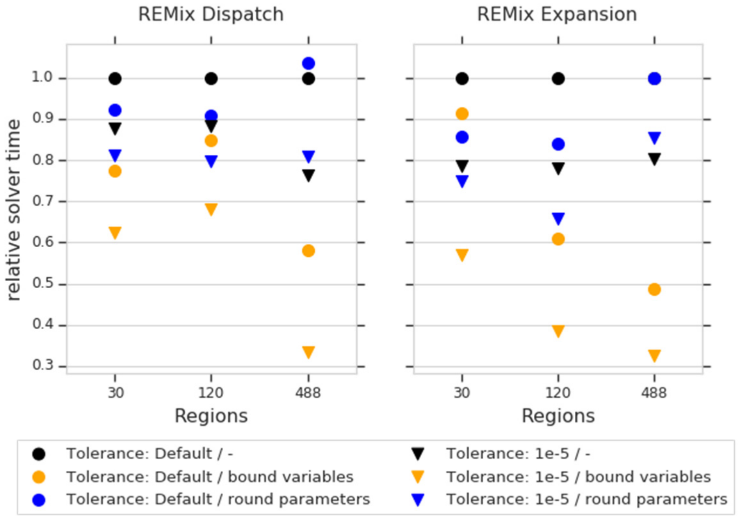

Figure 8. Comparison of solver times as a function of numerical properties and solver accuracy.

4.2. *Aggregation of Individual Dimensions*

This section presents the behavior of performance and accuracy indicators for scaling experiments. This means that the original REMix instances ("REMix Dispatch" and "REMix Expansion") are either reduced by spatial or temporal aggregation whereas the degree of aggregation is varied. The number of aggregated regions or time steps of a respective model instance are depicted on the x-axes of the following evaluation figures. In this context, the degree of aggregation is simply defined by:

Degree of aggregation:

$$a(x,v) = \left(1 - \frac{x(v)}{x_{\text{REF}}(v)}\right) \cdot 100\% \qquad \forall v \in \{\text{spatial}, \text{temporal}\} \tag{14}$$

where: x_{REF}: x-value (number of regions/time steps) of the original model instance.

In the following figures, the curves show computing and accuracy indicators relative to their counterparts of the original model instances. For each indicator, the reference is indicated at the greatest x-value ($x_{\text{REF}}(\text{spatial}) = 488$ regions or $x_{\text{REF}}(\text{temporal}) = 8760$ time steps). Accordingly, the figures are usually read from right to left. The associated absolute y-values are provided in the caption of the respective figure.

4.2.1. Spatial

The results for the spatial aggregation of the "REMix Dispatch" model are shown in Figures 9 and 10. In the former, the computational indicators are depicted by colored curves that represent total wall-clock time, solver time, the number of constraints, the number of non-zeros, and the memory consumed by GAMS as well as an approximation of the memory demand of the solver. On the right hand side, Figure 10 shows the accuracy indicators. Besides the objective value, the annual power generation of selected power generator groups, gas-fired and coal-fired power plants, and wind turbines, is drawn. Even though the REMix model instances consider a broader spectrum of technologies such as photovoltaics, biomass or run-of-river power plants, these technologies are omitted for the sake of clarity.

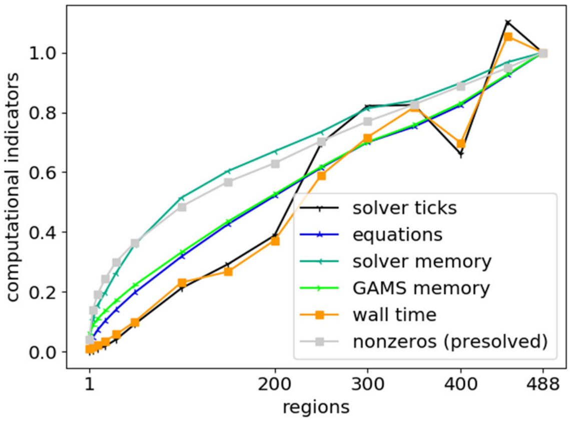

Figure 9. Computational indicators for spatial aggregation of the "REMix Dispatch" model. Reference model: CPLEX ticks 16.3 Mio.; Total memory 79 GB; GAMS time 0.6 h; Total wall-clock time 3.6 h.

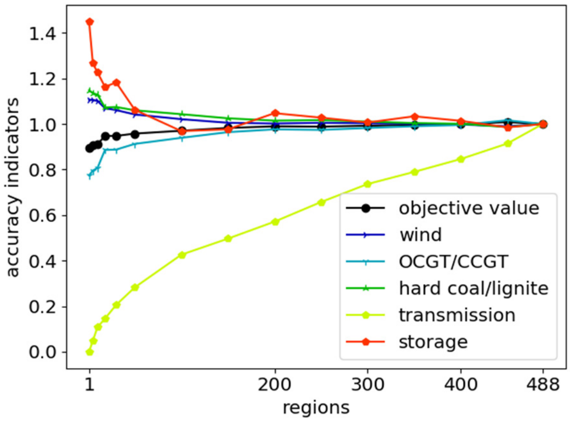

Figure 10. Accuracy indicators for spatial aggregation of the "REMix Dispatch" model. Reference model: Objective value 29.7 Bio €; Objective value (cleaned) 21.9 Bio €; Wind 162 TWh; Gas 174 TWh; Coal 105 TWh; Storage 4.1 TWh; Transmission 434 TWh.

With regard to accuracy indicators, up to a degree of aggregation of about 80% (100 regions) most of the curves in Figure 10 show minor deviations within a range of ±5% compared to the reference at $y = 1.0$. While the annual power generation from coal is slightly increasing with stronger aggregation, the opposite can be observed in the case of the objective value and power generation from gas turbines. Wind power and storage utilization are almost constant up to this point. However, for model instances that spatially aggregate to a degree below 100 regions, the use of storage facilities strongly increases. Compared to the reference model, deviations of more than 40% for storage are observable for highly aggregated model instances.

Considering that the number of transmission lines taken into account becomes smaller for more aggregated model instances, it can be expected that most of the effects that come with spatial aggregation stem from unconstrained power transmission. Thus, the strongest influence of this model reduction technique can be observed for the power transmission indicator where deviations greater than 25% already occur for degrees of aggregation >40% (300 regions).

That said, the results can be interpreted as follows: The absence of power flow constraints affects the model accuracy especially when the number of aggregated regions is low and their geographical extent is comparatively large. This facilitates large central power generation units such as pumped hydro storage and coal fired power plants to extensively distribute their electricity in wide areas to the cost of less power generation from probably better sited but more expensive gas turbines.

If the accuracy error for 100 regions is considered to be acceptable for answering a particular research question, the reachable speed-up factor can be determined from Figure 9. For both the solver time (CPLEX ticks) and the total wall-clock time relative to the maximal model time of about 0.2 is observable which corresponds to a speed-up factor of nearly 5. A smaller reduction can be observed for the model size which is characterized by the number of equations as well as the RAM required by the solver ($y \approx 0.4$) and the GAMS ($y \approx 0.3$). In terms of reachable speed-up, a linear reduction of the model size by spatial aggregation usually leads to a more than linear reduction of computing time (e.g., solver time), particularly for weak aggregations. However, especially for these model instances a superposed oscillation of the solver time can be observed which makes the estimation of reachable speed-up more uncertain.

For understanding this oscillation better, we analyzed further indicators provided in the logging and listing files as well as more content-related accuracy indicators such as the number of transmission line congestion events or slack power generation. We found that the number of non-zeros appearing within the Choleksy factorization of the barrier algorithm (reported as "total non-zeros in factor") shows a similar behavior. Nevertheless, no correlation between any of the content-related indicators and the solver time was observed. In addition, we cross-checked our results shown in Figures 9 and 10 by performing the scaling experiment with different solver parameters (barrier tolerance 10^{-5}) as well as based on slightly different clustering algorithm parameters. Both led again to an oscillation of the solver time curve. Thus, we conclude that even if the accuracy indicators scale in a stable manner, especially the solver time depends on how specific nodes are assigned to clusters. Solving of the DC-OPF problem can turn out to be harder for the solver even if the number of regions is smaller than in a less spatially aggregated model instance.

As mentioned in Section 3.2., the initial power plant portfolio of the German power system scenario for the year 2030 is slightly under-dimensioned since storage and power transmission capacities represent the state of the year 2015 ignoring planned expansion of these technologies. In addition, historical weather data of the year 2012 is used which is below the long-time average in terms of renewable power generation. As a consequence the slack power generators are active especially in the "REMix Dispatch" model instances (between 565 and 773 GWh). Total power supply derived from the objective value can thus become more expensive than in the case of "REMix Expansion" depending on the selected specific punishment costs. For this reason, we report two objective values in the caption of the figures of accuracy indictors. Firstly, the objective value of the mathematical optimization problem including costs of punishment terms. Secondly, the cleaned objective value represents costs for total power supply derived from assuming the same costs for slack power generation as for operating fictitious gas turbines.

Figures 11 and 12 show the performance and accuracy indicators for spatial scaling of the "REMix Expansion" model instances. Here, storage (i.e., stationary lithium-ion batteries) and transmission capacities (AC and DC lines) can be added to the system to balance power demand and generation with the installed generation capacities. In accordance to this, the accuracy indicators are extended by storage and transmission expansion. Exceptionally, only the results in this experiment are computed with extensive logging in GAMS's listing files is enabled which automatically leads to an increase of GAMS time.

As reported in the captions of Figures 9 and 11, enabling capacity expansion leads to a significant increase in total computing time from about 3 to almost 50 h. Nevertheless, compared to the "REMix Dispatch" model instances, similarities concerning the over- or underestimation as well as the scaling behavior of the technology specific errors can be observed. For instance, capacity factors of energy storage are increasing for higher degrees of aggregation. This directly affects storage expansion which decreases with the smaller spatial resolution.

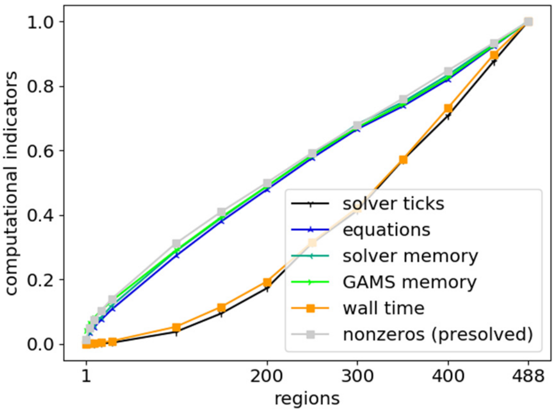

Figure 11. Computational indicators for spatial aggregation of the "REMix Expansion" model. Reference model (only in this experiment): CPLEX ticks 381.3 Mio.; Total memory <256 GB; GAMS time 6.6 h; Total computing time 50.9 h.

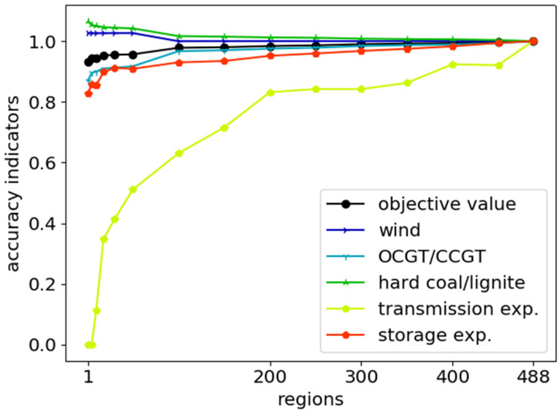

Figure 12. Accuracy indicators for spatial aggregation of the "REMix Expansion" model. Reference model (only in this experiment): Objective value 23.7 Bio €; Objective value (cleaned) 23.2 Bio €; Wind 175 TWh; Gas153 TWh; Coal 115 TWh; Storage expansion 123 GWh; Transmission expansion 28.8 GW.

One exception are power transmission-related indicators where more significant deviations from the reference values occur, especially for degrees of aggregation >60% (<200 regions). On the one hand, model instances with such an aggregation even reach reductions in computing time of more than 80%. On the other hand, transmission capacity expansion already experiences significant deviations (>10% compared to the values of the original model) for degrees of aggregation that go below 400 regions. Remarkably, this has only a minor impact on both the objective value and the generation-related accuracy indicators which is observable from the almost horizontal course of the wind, gas, coal, and storage expansion indicators in Figure 12.

A further similarity to the "REMix Dispatch" model is the linear scaling behavior of computational indicators corresponding to the model size as well as the super-linear scaling of the solver time. However, in Figure 11, the solver ticks resemble a rather exponential curve and no superposed oscillation occurs. This means that enabling the expansion of transmission (and storage) capacities leads to a rather expectable scaling behavior of the computing time: The fewer regions in a spatially aggregated model instance, the smaller the time required for solving the optimization problem. If the slope of the solver time curve is regarded as a measure of effectiveness in terms of model acceleration, it can be concluded that spatial aggregation is mainly effective for degrees up to 40%.

4.2.2. Temporal

The results for temporal aggregation of the "REMix Dispatch" model are shown in Figures 13 and 14.

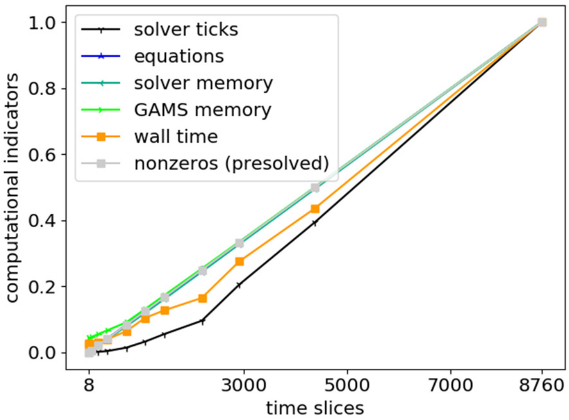

Figure 13. Computational indicators for temporal aggregation of the "REMix Dispatch" model.

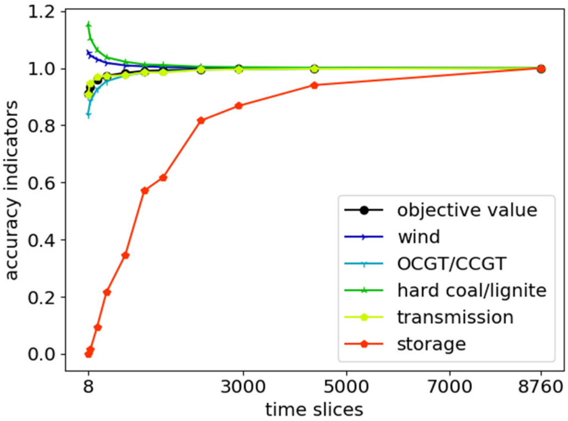

Figure 14. Accuracy indicators for temporal aggregation of the "REMix Dispatch" model.

As in the case of spatial aggregation computational indicators are depicted in the figures on the left while accuracy indicators are illustrated on the right. The reference model is the same as in the spatial scenario. In contrast to spatial aggregation, in Figure 14, the slope of the cost curve (objective value) appears much flatter. However, it should be noted that temporal aggregation representing two-hourly time steps already results in an aggregation factor of 50%. For this reason, all of the observed data points in Figures 13 and 14 are located in the half closer to the y-axis. Concerning the solver time this already leads to speed-ups greater than factor 2. Nevertheless, it is not guaranteed that the total computing time (GAMS time + solver time) can be reduced in the same manner. This is due to the additional computing effort for aggregating hourly input data. Compared to such model instances, the greater GAMS time, e.g., in the case of 4380-time steps, results from this additional input data processing. This effect becomes significant for small model instances where the total computing time is not necessarily dominated by solver time. However, for those model instances total computing time is only a few minutes and thus represents no bottleneck. Opposed to this, for the non-aggregated "REMix Dispatch" model the ratio between solver time and GAMS time is still about a factor of 10.

While the objective value as well as most of the technological specific power generation indicators show an absolute error below 5% even for daily averaged time steps (365 time slices; corresponding speed-up factor: 40), significant deviations can be observed for the storage use. For this technology (i.e., pumped storage power plants) the underestimation of power generation compared to the original model is already 5% in the case of diurnal time steps. Also open cycle gas turbines (OCGT) are affected at degrees of aggregation greater than 70% (e.g., three-hourly time steps). But due to their small electricity production compared to combined cycle gas turbines (CCGT) they have only a minor impact on the slope of the corresponding curve in Figure 14.

Remarkably, power generation from photovoltaics (PV) is almost independent from the degree of temporal aggregation. Because its deviation is less than 0.1‰ across all analyzed model instances, the corresponding curve is not depicted in all figures concerning accuracy indicators. In other words, ignoring day-night periods has no effect on the dispatch of photovoltaics but rather on the need for storage. However, given that in the analyzed model parameterizations the amount of electricity from photovoltaics is only 10% of the annual power generation it becomes clear that PV-integration is possible at almost each point in time. Significant deviations due to temporal aggregation would therefore rather be expected in scenarios with high shares of renewables.

The results for temporal scaling behavior if expansion of storage and transmission capacities is possible can be seen in Figures 15 and 16. For both figures the reference values of the original instance of "REMix Expansion" are denoted a second time. They stay the same for all following analysis with this model.

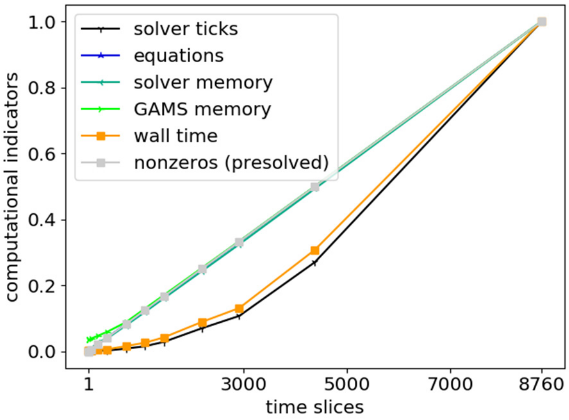

Figure 15. Computational indicators for temporal aggregation of the "REMix Expansion" model. Reference model: CPLEX ticks 534.3 Mio.; Total memory >256 GB; GAMS time 0.6 h; Total computing time 62.3 h.

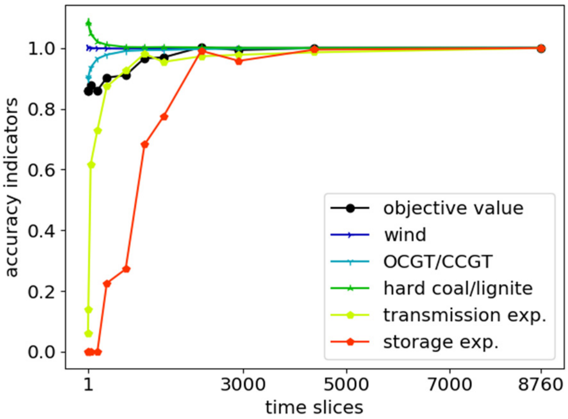

Figure 16. Accuracy indicators for temporal aggregation of the "REMix Expansion" model. Reference model: Objective value 22.8 Bio €; Objective value (cleaned) 22.3 Bio €; Wind 180 TWh; Gas 146 TWh; Coal 117 TWh; Storage expansion 122 GWh; Transmission expansion 29.2 GW.

A difference compared to temporal aggregation of the "REMix Dispatch" model instances is the lager area between the green curve that represents the solver time and the blue and violet curves representing the size of a particular model instance. According to this, the reachable speed-up in terms of solver time is greater for instances with two-hourly (factor 3) or three-hourly (factor 7) time steps. On the other hand, in Figure 15, the slope of the solver ticks is much flatter in its lower part. By this means, going beyond degrees of aggregation of 90% (twelve-hourly time steps) appears to be less effective regarding the reachable speed-up.

Concerning the scaling behavior of model accuracy, significant errors occur for storage-related indicators. Similar to "REMix Dispatch" the annual power generation from storage facilities already decreases by 10% for two-hourly time steps. However, the storage expansion indicator stays below an error of 5% up to an aggregation factor of 75% (four-hourly time steps) while the transmission expansion indicator falls below this value at 730 time slices (twelve-hourly time steps). Therefore, it can be concluded that for observing widely accurate results for capacity expansion of transmission lines and lithium-ion batteries, four-hourly time steps appear to be sufficient, especially assessed against the background of an approximate reduction of computing time by a factor of 13.

4.3. Heuristic Decomposition

4.3.1. Rolling Horizon Dispatch?

This section presents the behavior of computational and accuracy indicators for model-based speed-up approaches that make use of heuristic decomposition techniques applied to the temporal scale of both the "REMix Dispatch" and the "REMix Expansion" model. Since the corresponding benchmark experiments vary over different parameters the appropriate figures are built up on hierarchical indices on the x-axes. However, the relative deviations are depicted for each of the analyzed indicators compared to the monolithically solved instances of "REMix Dispatch" and "REMix Expansion". Rolling horizon dispatch

The "REMix Dispatch" model is executed with the rolling horizon approach presented in Section 3.3.2 while the interval size and the number of intervals are varied. The resulting computational and accuracy indicators are shown in Figures 17 and 18. Both the settings for the overlap size and the number of intervals occur on the x-axis.

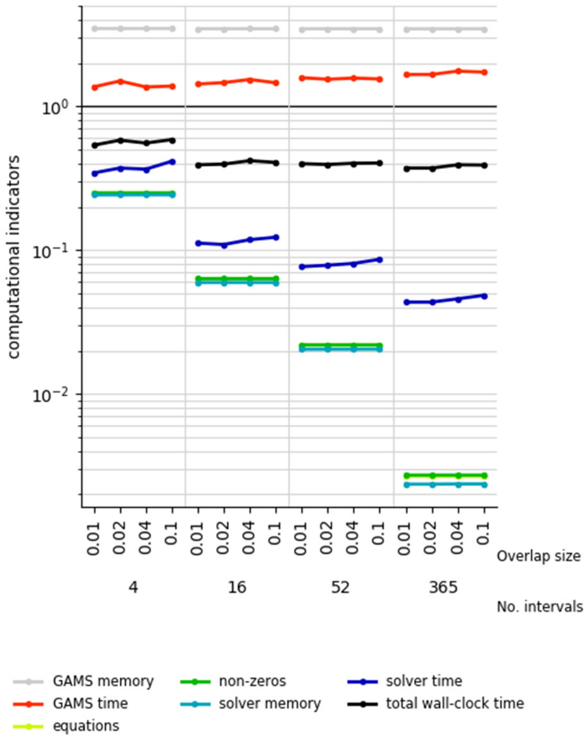

Figure 17. Computational indicators for rolling horizon dispatch applied to the "REMix Dispatch" model.

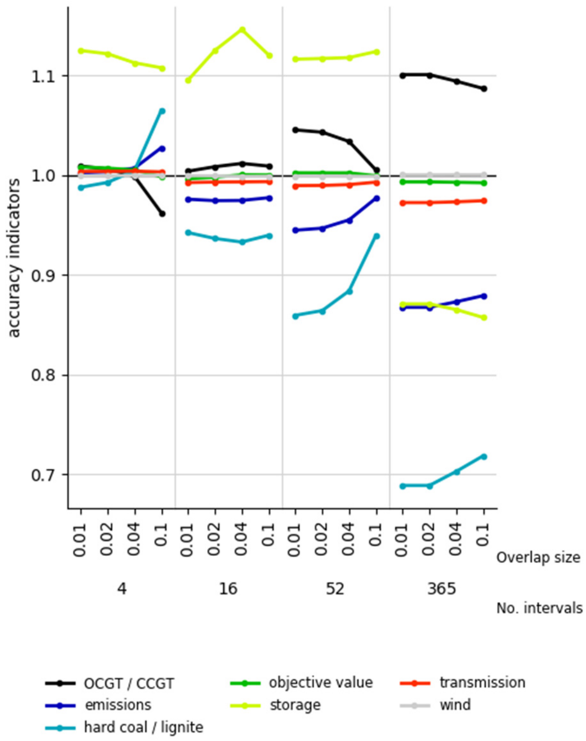

Figure 18. Accuracy indicators for rolling horizon dispatch applied to the "REMix Dispatch" model.

With regard to the first, it is striking that the intended behavior of total computing time is achieved—compared to the original model instance speed-up factors between two and three can be observed especially for model instances that decompose the temporal scale into more than four intervals.

In particular, with increasing numbers of time intervals the total time consumed by the solver decreases (down to less than 5% of the monolithic model) as well as the maximal memory required by the solver. On the contrary, memory required and time elapsed for executing GAMS increase by factors around 1.6 and 3.5, respectively.

This is due to the additional need for generating smaller but multiple sub-model instances to be solved one after another. Even though the ratio between GAMS time and solver time is around factor four in the original model instance, when the rolling horizon approach is used, the GAMS time already dominates all model instances but those with four intervals. The total wall-clock time accordingly barely scales with the number of intervals, especially for those with more than 16 intervals.

The overlap size is determined relative to the absolute length of a particular time interval. Compared to the number of intervals, it has only a minor impact on the computational indicators: As it can be expected, the greater the overlap, the more computing resources are required. This is due to the fact that all model parts that lie within the overlap are redundantly considered and thus, the total amount of equations to be solved as well as the number of non-zeros (and variables) increases for greater overlap sizes. However, even if these model size measures increase by 10% (overlap size: 0.1), the resulting total wall-clock time only experiences changes within a range of 2% (4 intervals) to 5% (365 intervals).

Different observations can be made for the accuracy indicators where comparatively large overlaps mostly improve the accuracy of the corresponding model instances. The objective values as well as the indicators for power transport and electricity production by wind turbines have errors smaller than 3% across all investigated model instances. In this context it needs to be considered that we do not observe lower total costs than for the original model instance. Objective values smaller than 1.0 occur since slack generator costs are not considered.

The dispatch of fossil fired power plants and pumped hydro storage units shows stronger deviations. Remarkably for the latter, first overestimations of around 10% are observable for intervals numbers of four, 16 and 52. However, for intervals on a daily level, the storage accuracy indicator shows an underestimation of more than 10%.

These deviations occur, on the one hand, due to the missing circular restriction for the storage level balance that is omitted when the rolling horizon approach is applied. The appropriate constraint enforces the equality of storage levels at the beginning and at the end of the analyzed time period and thus prevents a total discharge for monolithic model instances with perfect foresight. Opposed to that, without this constraint and due to the limited foresight, (even for large overlap sizes in model instances with rolling time horizons) storage levels still tend to zero at the end of an interval (“discharge effect”) and thus, average storage levels are smaller than when comparatively long time spans are considered. For example, the mean storage level of 4.6 GWh in the model instance with 365 intervals and 10% overlap is significantly smaller than in the case of four intervals with the same overlap size (20.7 GWh).

In particular, when time interval lengths are in the range of typical storage cycling periods (in the presented case daily periods for pumped hydro storage), storage charging over several energy surplus periods is not cost-efficient for an individual time interval and, in addition, the overlap size cannot be large enough to compensate the “discharge effect”. Such a tipping point can be seen in Figure 18 for the 16-interval model instances where storage utilization first increases but decreases as soon as the overlap size changes from 4% overlap (21 h) to 10% (55 h).

On the other hand, the overutilization of energy storage in model instances with less than 365 time intervals stems from another effect. As shown in the upper part of Figure 19, significant deviations between the storage levels of the original (solid black line) and the model instance with seasonal rolling horizon time intervals (solid green line) occur mainly in the middle of the observed scenario year. Furthermore, in the case of weekly intervals (solid grey line), differences from the shape of the black curve appear over the whole time period.

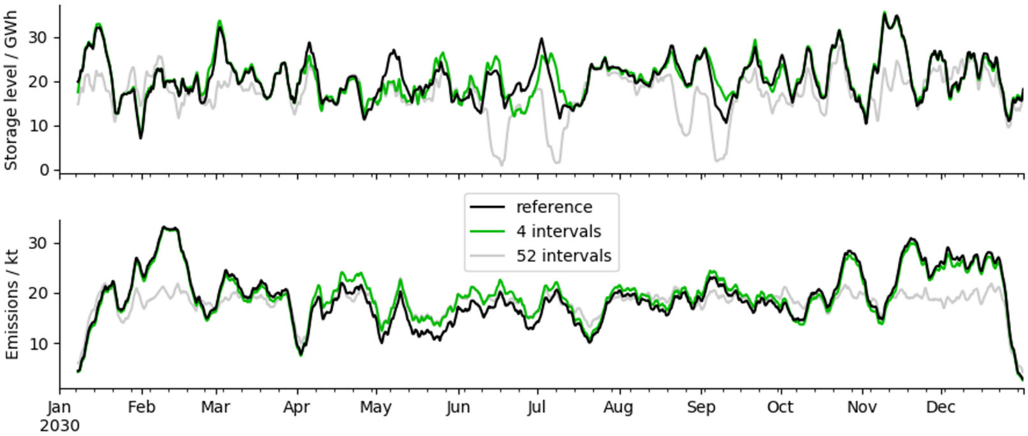

Figure 19. Weekly rolling average of spatially cumulated storage levels (top) and greenhouse gas emission (bottom) for two model instances with four and 52 time intervals, computed with the rolling horizon approach, compared to the corresponding results of the original “REMix Dispatch” model instance (reference).

The deviations in storage dispatch occur independently of the intersection areas of time intervals. The reason for this is related to the treatment of the annual greenhouse gas emission budget. In the current rolling horizon implementation the annual emission budget is simply equally distributed to the individual time intervals:

Proportional emission budgets:

$$\begin{gathered} m_i(i) \;=\; \frac{m}{|T_i| + \left|T_0(i)\right|} \\ \forall i \in \{T_i\} \end{gathered} \tag{15}$$

where: t_0: set of time steps that belong to overlaps

According to Equation (15), the resulting cumulated proportional emission budget can be greater than its annual counterpart. However, this especially applies when the absolute size of overlaps becomes large. The reason therefore is the following: Although emission produced within the overlaps are not considered for the final result, model setups exist where the proportional emission budget (that considers also emissions for the time steps within the overlap) is almost fully utilized within the time steps before the overlap begins and thus the total emission may be higher than intended. In Figure 18 this can be observed for the model instance with 4 intervals and 10% overlap. With regard to emissions we call this "negative overlap effect" in the following.

Apart from that, the equal distribution of allowed greenhouse gas emissions rather leads to less total emissions than in the original model instance as they are caused by fossil-fired power plants which are usually in operation in time periods with less electricity feed-in from renewable energies. Such time periods with high residual load are naturally not equally distributed. Consequently, according to the blue lines in Figure 18 and the grey line in the lower part of Figure 19, the more time intervals are considered the more restrictive the proportional emission budget. This also leads to the decrease in dispatch of coal-fired power plants observable for an increasing number of intervals in Figure 18.

Moreover, also the over-utilization of energy storage can be traced back to this effect: In the case of seasonal time intervals, in time spans with low residual load, the slightly higher emission potential allows a technology shift from flexible gas-fired turbines to less cost-intensive coal-fired power plants where the missing flexibility of that latter is provided by energy storage facilities ("negative interval effect"). This finally results in the deviating storage levels and higher emissions for the seasonally sliced model instance in Figure 19 observable in the middle of the analyzed scenario year. The opposite of this technology shift takes place when the emission limit is binding for time periods with high residual load ("positive interval effect"). In this case emission-intensive power generation of coal-fired power plants needs to be replaced by electricity production based on gas. Energy storage then comes into play to increase the capacity factor of CCGT and OCGT plants. However, as it can be seen especially for weekly time intervals in Figure 18, this "positive interval effect" is compensated by the "negative overlap effect".

4.3.2. Temporal Zooming

This subsection presents the results for the sequential implementation of the temporal zooming approach applied to "REMix Expansion" model. In this regard, sequential means that multi-threading is only used on the solver level. For a better understanding, we refer to the execution of the temporally down-sampled model instance as "first execution phase" while post-sequent solving of multiple temporally decomposed models is denoted as "second execution phase". In Figures 20 and 21 the resulting performance and accuracy are shown where the parameterization of these two execution phases (temporal resolution of the down-sampled model instance and the number of intervals) is varied. As for the visualization of computational indicators in case of the rolling horizon approach, the x-axes in Figure 20 are hierarchically labeled for the variation of two SAR-parameters (see Section 3.4.1). In this figure, computing times represent cumulative quantities while for the GAMS memory the maximum value is shown. Opposed to that, the indicators that concern the number of non-zeros, the number of equations and the memory demand by the solver show average values reported when solving each sub-model.

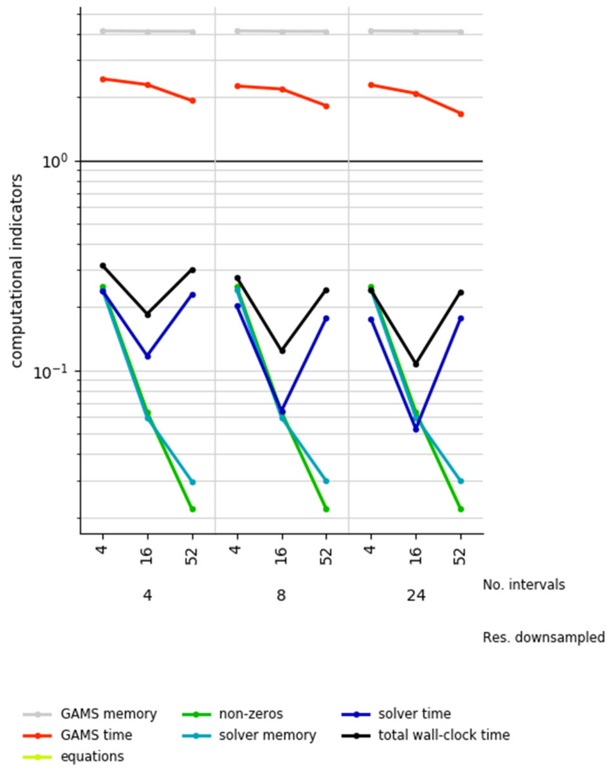

Figure 20. Computational indicators for sequential temporal zooming applied to the "REMix Expansion" model.

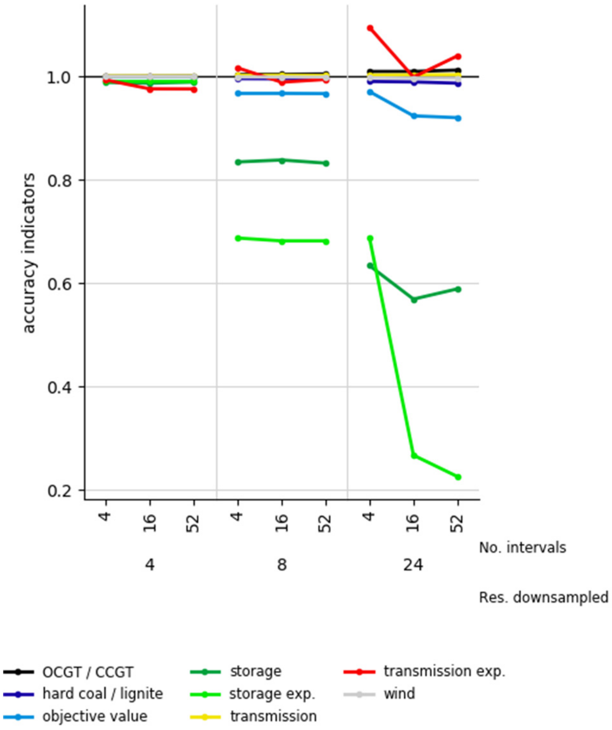

Figure 21. Accuracy indicators for sequential temporal zooming applied to the "REMix Expansion" model.

Given that all computational indicators scale with temporal aggregation (see Section 4.2.2), it can be expected that the stronger the temporal aggregation of the down-sampled model instance, the less memory and computing time is required. This expectation matches the results shown in Figure 20.

Furthermore, obvious similarities compared to the computational behavior of the rolling horizon dispatch (see Section 4.3.1) can be observed for the GAMS related indicators. Both the GAMS time and the required memory significantly increase compared to the monolithic reference model. Nevertheless, opposed to the observations made for rolling horizon, GAMS execution times are slightly reduced for an increasing number of time intervals. The total wall-clock time, however, is significantly dominated by the solver performance as the ratio between solver time and GAMS time is greater than factor 100 for the original model and never below 1 for the model instances computed with temporal zooming. Therefore, in Figure 20, the shape of the black curve mirrors the shape of the dark-blue curve that depicts the solver time.

Concerning the solver time, it is striking that there is a significant minimum observable for 16 intervals. This means, even though the solver time can be reduced due to creation of smaller partial models for shorter time intervals, a tipping point exists, when this reduction cannot anymore compensate the additional computing effort for solving multiple sub-models. It becomes clearer when the super-linear scaling behavior for model instances with different numbers of time steps is taken into account. As discussed for Figure 15 in Section 4.2.2, the slope of the curve that represents the scaling of solver time vs. model size, is much flatter for small models (between one and 168 aggregated time steps) than for large models (between 1095 and 8760 time steps). In a temporally decomposed model with four time intervals, the length of an individual interval lies at 2190 time steps and therefore, a more than linear reduction of solver time can be expected. Opposed to that, for 52 time intervals, the time span that is covered by a single sub-model is 168 time steps. In this area of the scaling curve in Figure 15, a reduction of model size by factor two only causes a reduction of total computing time of less than 0.1%.

This decreasing effectiveness of model reduction is also the reason for the less significant increase of speed-up when comparing the total wall-clock time for different temporal resolutions in the “first execution phase”. Although the model size between the instances with an eight-hourly and a 24-hourly down-sampled basis is reduced by factor three, the reduction in total computing time is around 1–3%. In contrast, when the instances with 4-hourly and 8-hourly down-sampled bases are compared, the model size is only halved, while the total wall-clock time shows a reduction of 2–6%.

In summary, it can be concluded that speed-ups around factor eight to nine can be achieved. However it needs to be considered that, due to the super-linear scaling behavior, saturation takes place in terms of further performance enhancements.

The error of accuracy indicators of the model instances that are treated by the temporal zooming approach is especially small if a temporally down-sampled model instance with four-hourly resolution is used. It stays below 3% for all accuracy indicators whereas, compared to the outcome of the original model, the largest deviation is observable for transmission expansion when more than seasonal time intervals are considered. For stronger temporal aggregations in the “first execution phase”, significant underestimations of storage expansion as well as of storage utilization occur in Figure 21. However, while in case of an eight-hourly resolution the impact of different interval sizes is rather negligible, down-sampling on daily level results in large errors across interval sizes especially for storage expansion.

Given that the storage capacity expansion concerns lithium-ion-batteries that are usually used to smooth the daily feed-in pattern of PV plants, it becomes clear that those energy storage facilities are no longer necessary in the 24-hourly down-sampled model instance. The sudden decrease of the storage expansion for greater numbers of intervals can be accordingly explained as follows:

As for the “second execution phase” lower bounds for investments into new capacities are taken from the results of the “first execution phase”, this lower bound is obviously binding for models based on the eight-hourly down-sampled model instance, regardless of the number of intervals in the “second execution phase”. For this reason, the storage expansion indicator is at approximately $y = 0.7$ (light-green line). Opposed to that, in the 24-hourly case (right section of Figure 21), the lower bound gathered from the “first execution phase” is considerably smaller as it is depicted in the case of weekly time intervals ($y = 0.22$). However, additional storage expansion appears particularly for seasonal time intervals ($y = 0.69$). It can therefore be concluded that the shorter the observed time periods of a sub-model, the less attractive are investments into storage capacities.

The objective value accordingly decreases the less storage capacities are built. In this context, it is necessary to have in mind that the effective objective value still includes additional costs for slack power generation and, opposed to the cleaned costs in Figure 21, total costs for power supply are not automatically lower than in the original model.

4.3.3. Temporal Zooming with Grid Computing

When we apply the GAMS grid computing facility to the temporal zooming approach, an additional SAR-parameter is to be considered. Although the total number of parallel threads is limited by the available processors on a shared memory machine (in the current study we use 16 threads), their utilization is variable in the grid computing case. While in the previous analyses all 16 threads are used for parallelization of the barrier algorithm, in this section, also the capability to run several GAMS models in parallel is examined. Therefore, the variation parameter "Threads", indicated on the x-axes of Figures 22 and 23, distinguishes the number of runs times the number of parallel barrier threads accessible for the solver.

Opposed to the sequential implementation of temporal zooming, we do not show results for a variation of the temporal resolution used in the “first execution phase” but only for model runs based on an eight-hourly down-sampled instance. This is due to the fact that for the relation between this SAR-parameter and accuracy, it can be expected that the findings from Section 4.3.2 also hold true for benchmark experiments with temporal zooming and grid computing. Using a down-sampled model instance with eight-hourly resolution represents a compromise between desired high speed-up and acceptable loss in accuracy.

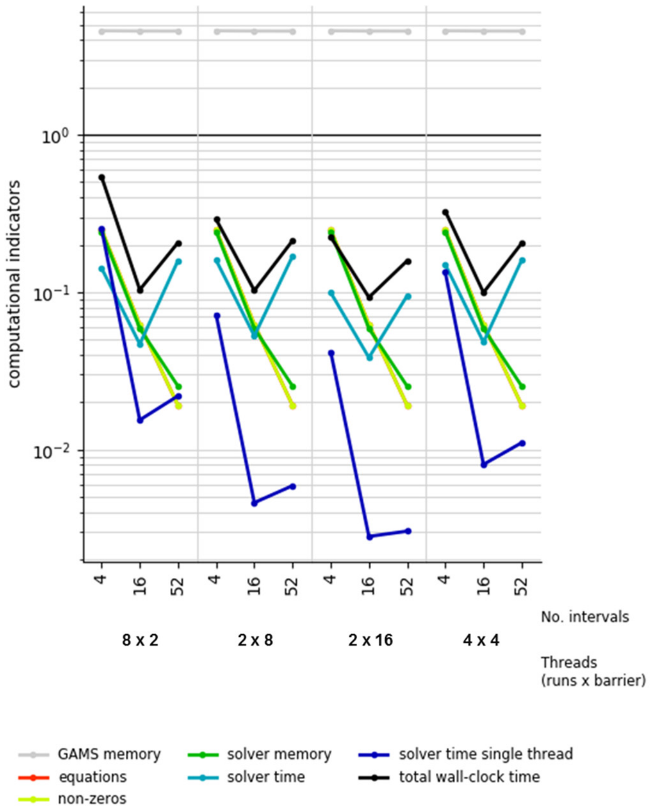

Figure 22. Computational indicators for temporal zooming with grid computing and eight-hourly down-sampled basis applied to the “REMix Expansion” model.

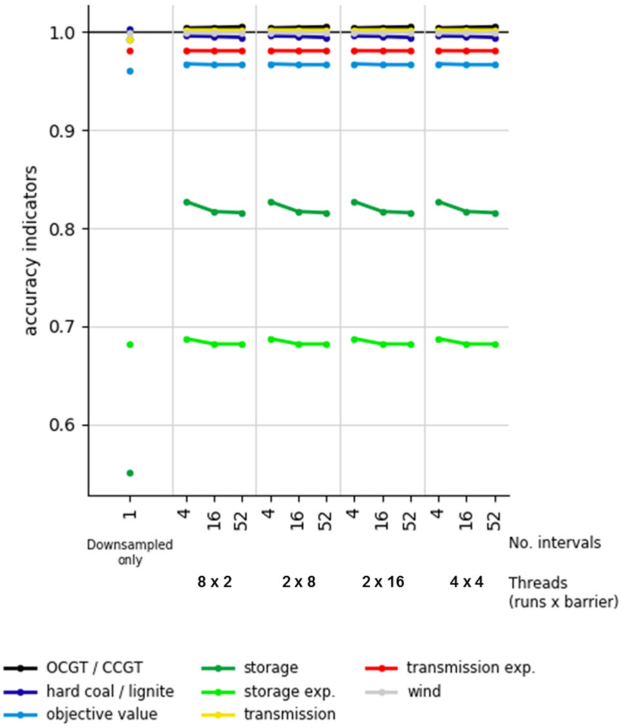

Figure 23. Accuracy indicators for temporal zooming with grid computing and eight-hourly down-sampled basis applied to the "REMix Expansion" model.

Furthermore, for efficient in-memory communication between GAMS and the solver the current analysis is conducted with the GAMS option solvelink = 6. This implies that the sub-models that represent the different time intervals are solved in parallel in an asynchronous manner while partial results are hold in memory.

Depending on the combined settings of the number of intervals and the number of parallel threads, the majority of model instances cannot completely be solved in parallel. For example, in the case of 16 intervals and eight threads (and presuming almost equal solver times) it is likely that two sets of sub-models are treated after each other. First, time interval one to eight is solved within eight parallel threads and afterwards time interval nine to 16. In the following we refer to this as "serial part". However, due to the asynchronous solution process and non-equal solver times, for the described example, it is not guaranteed that each thread processes exactly two sub-models.

Given that the machine independent, total solver time (reported in ticks) is not provided by the GAMS logging files, but for each time interval, we post-process the solver time indicator for the performance evaluation. For this reason, solver time is depicted in two forms in Figure 22: The dark blue line, denoted as "solver time single thread", represents the median calculated over the solver times of all time interval-specific sub-models. To account for the "serial part" we multiply this indicator by a factor α to determine an approximation for the effective "solver time" (light-blue line):

Serial solve factor:

$$\alpha = \frac{|T_i|}{n_g} \tag{16}$$

where: n_g: number of threads for parallel runs when using grid computing.

In this context, a clear distinction between solver time and GAMS time is also difficult since generation (part of the GAMS time) and solving of particular sub-models are executed in parallel. Deriving an approximation for the GAMS time and normalizing it with respect to its counterpart of the original model appears accordingly less useful. The appropriate computational indicator is therefore not depicted in Figure 22.

Looking at the results for the total wall-clock time, a similar relation between computing time and the number of intervals can be observed as for sequential temporal zooming. Independent of the settings regarding the distribution of threads, the best performance occurs for 16 intervals. On the one hand, this is due to the decreasing effectiveness of model reduction as explained in Section 4.3.2. On the other hand, considering the number of parallel runs $n_g = \{2, 4, 8\}$, it becomes clear, that especially instances that are decomposed into a number of intervals that represents an integer multiple of n_g are candidates for high speed-ups. In these cases the available resources (threads) can be equally utilized. This applies to all model instances with 16 time intervals but only occasionally for seasonally and weekly decomposed model instances.

The most important outcome shown in Figure 22 is the achievable speed-up compared to the sequential temporal-zooming approach. For 16 time intervals and 4 x 4 threads the resulting total wall-clock times go down to values of 10% of computing time of the original model. This additional speed-up appears due to the following effects: In contrast to a pure parallelization on the solver level, grid computing also allows to execute the model generation at least partially in parallel. Furthermore, it can be shown that computing times for implementations of the barrier algorithm in commercial solvers often scale only up to 16 parallel threads [96]. A further reduction of computing time by stronger parallelization (>16 threads) is accordingly only beneficial if it is applied elsewhere within the computing process. Logically, the application of grid computing is especially useful, if more than 16 threads are available in total.

However, the current benchmark analysis shows that parallelization by grid computing is similarly effective as solver parallelization for comparably small numbers of threads. As depicted in Figure 22, different distributions of the number of parallel model runs and the number of barrier have a rather small impact on resulting solver and total wall-clock times. Also for more than 16 threads the additional value of grid competing can only poorly be demonstrated: Taking into account the results for the model instance labelled with 2 × 16 threads, it can be stated that despite the total number of threads is doubled, only slight improvements concerning the computing speed are achieved (speed-up factor <10.8).

Apart from that, Figure 23 shows the accuracy for temporal zooming with grid computing relative to the original model instance but also against the outcome of the eight hourly down-sampled model instance used computed in the “first execution phase”. For storage utilization significant improvements are observable: While in the down-sampled model instance the accuracy is only 55%, it reaches levels around 82%. This increase in accuracy, however, comes with the costs of less performance (for pure down-sampling on an eight-hourly basis the speed-up is around factor 37). Nevertheless, as discussed in Section 4.2.2, the strongest errors occur with regard to storage utilization and storage capacity expansion. Other accuracy indicators (e.g., transmission expansion) deviate less than 6% from the solution of the original model instance. If only dispatch-related indicators, such as capacity factors of wind, gas-fired or coal-fired power plants are assessed, the appropriate error is smaller than 1%. This outcome is only slightly affected when the number of intervals differs. As discussed in Section 4.3.2 for Figure 21, this SAR-parameter only plays a role if the “second execution phase” is based on down-sampled model instances that show stronger temporal aggregations than eight hourly time steps.

4.4. Temporal Aggregation Using Feed-in Time Series Based on Multiple Weather Years

This section exemplary shows the response of accuracy indicators against a variation of model input parameters. Rather than a systematic sensitivity analysis of a broad spectrum of parameters and assumptions across all analyzed speed-up approaches, it emphasizes one particular quantity that is associated to high uncertainties for energy scenarios—the availability of power generation from vRES. The appropriate model parameters to be varied are the hourly feed-in time series for electricity generation from wind and solar energy. While in the analyses above this parameter set is always based on weather data of the year 2012, in the following results for additional weather data of the years 2006 to 2010 are shown.

In Figure 24, the accuracy indicators for temporal aggregation (0) applied to "REMix Dispatch" are depicted. Again, each point represents the relative deviation of an aggregated model's result compared to its counterpart of the non-aggregated model. Therefore, for each weather year an individual original model instance is required and computed (and thus all curves in Figure 24 share the point at time slices = 8760 and accuracy = 1.0).

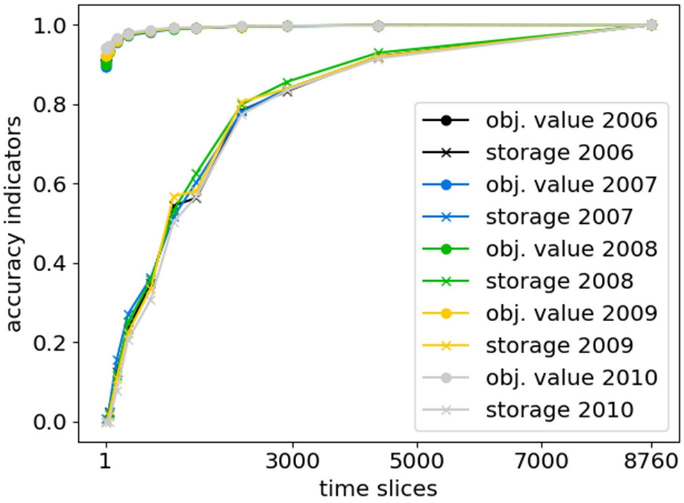

Figure 24. Accuracy indicators for spatial aggregation of the "REMix Dispatch" model for parameter variation concerning power generation from wind and solar energy (weather data from 2006 to 2010).

For the sake of clarity only the curves of the objective value and the annual power consumption of energy storage are shown. Nevertheless, considering the findings from above it can be concluded that also the remaining accuracy indicators would show curves that are very similar if weather years are varied. This even applies to the computational indicators which are not significantly affected by the variation of this parameter sets.

As the results in Figure 24 proof, our findings on the impact of the degree of aggregation on accuracy are robust against a parameter variation of weather years. In the first place, this particularly holds true for the case of temporal aggregation applied to "REMix Dispatch". However, it can be expected that even for spatial aggregation and also in the case of "REMix Expansion" deviations of accuracy indicators across different feed-in time series are comparably small. For more general statements concerning sensitivity of accuracy deviations, however, more extensive parameter variations are required where also different assumptions on cost parameters are considered.

5. Discussion

5.1. Summary

With this paper, we provide systematic evaluations of different approaches to improve the computing performance of applied ESOMs. Besides a number of preliminary measures such as source code reviewing and solver parameterization based on experiences gathered from former model applications, we implemented two kinds of commonly used speed-up approaches to the ESOM REMix. These are, on the one hand, spatial and temporal aggregation methods that showed effective speed-ups up to factor 10 if expansion of storage and transmission capacities is to be considered.

We showed that the majority of analyzed accuracy indicators stay within an error range of about 5% reaching computing time reductions of 60–90% for spatial and temporal aggregation, respectively. Moreover, if particularly affected technologies such as either power transmission or storage are of secondary interest, for dispatch models speed-up factors between 4 and 20 are possible. In this context, it is important to select an appropriate aggregation approach based on the model outputs to be evaluated in particular. For example, if the competition between technologies that provide spatial or temporal flexibility to the energy system is to be examined, the presented aggregation techniques are not suited for this purpose. For model instances that consider capacity expansion, we also observed that significant speed-ups are particularly reached for low to intermediate degrees of aggregation. In contrast, strong aggregations (beyond 90%) showed only relatively small additional improvements in computing performance.

Based on these findings, we conclude that model reduction by aggregation offers the possibility to effectively speeding-up ESOMs by at least factor two without the implication of significant losses in accuracy. In contrast, strong degrees of aggregation are less useful because speed-up gains are comparatively small while accuracy errors reach inacceptable levels ("effectiveness of model reduction").

On the other hand, we applied nested model heuristics that aim at the decomposition of the temporal scale of an ESOM. As these speed-up concepts imply manipulations on the temporal scale of an ESOM, they affect accuracy indicators that are related to modeling energy storage. The benchmark analyses of the rolling horizon approach for pure dispatch-models revealed that large overlap sizes and interval periods that cover full storage cycles are recommendable. Their additional costs with regard to computing effort are low, but may increase accuracy significantly. For the computational performance of the rolling horizon dispatch the ratio between GAMS time and solver time is crucial since only for dominating solver times, significant speed-ups around a factor of 2.5 could be observed for "REMix Dispatch". In this regard, it needs to be considered that "REMix Dispatch" is still a quite easy-to-solve model instance (total wall-clock time <4 h). Based on our knowledge about "effectiveness of model reduction" we assume that this performance enhancement approach will be even faster for larger dispatch models.

Considerably higher speed-ups were observed for the lager "REMix Expansion" model that was treated by the temporal zooming approach. We showed that within the limited capabilities for parallelization on shared memory hardware, speed-ups of more than factor 10 were possible, especially if grid computing was used. However, besides the limitation imposed by hardware resources, the reachable performance enhancement is also restricted due to scaling behavior of very small models. This means, that additionally to the ratio between GAMS time and solver time, it needs to be considered that as soon as sub-models are reduced to a certain size, further size reductions only slightly decrease solver time (downside of "effectiveness of model reduction"). Hence, with regard to speed-up by parallelization, it is remarkable that at first glance, many intervals appear to be more effective. However, according to the results in 0 und 0, medium sized intervals performed best.

5.2. Into Context

Our findings, especially concerning temporal aggregation, are also in-line with those of Pfenninger [26] who reports reductions of computing time of more than 80% at three-hourly time resolution for scenarios of the ESOM Calliope applied to scenarios for the UK. With regard to accuracy, Pfenninger reports the values for capacity expansion of wind energy converters. His results show that the higher the wind penetration of a particular scenario is, the stronger the errors that occur due to temporal aggregation. However, the availability of storage technologies puts the effect of strong deviations compared to an hourly-resolved model instance into perspective.

This indicates that the scaling behavior of computing time rather depends on the model characteristics than on the composition of input parameters. Opposed to this, the scaling behavior of accuracy measures indicates a dependency on the parameter setup. However, our exemplary parameter variation across different feed-in time series for one particular use case also indicated certain robustness of the resulting accuracy errors for different degrees of aggregation.

In contrast to the here applied "REMix Expansion" model, Calliope also considers the expansion of generation capacities. In [26], for a scenario with extensive capacity expansion of renewables, the steep decrease of the curve of computing time for low degrees of aggregation is more pronounced than in our model instances which rather show a smooth transition to the area with a flatter slope ("effectiveness of model reduction").

For the examined heuristic decomposition techniques, our observations concerning accuracy are in-line with expectations derivable from known strengths and weaknesses occurring when differently treating the temporal scale: The down-sampled model instance allows a better approximation of capacity expansion indicators due to the consideration of the full time-horizon to be analyzed. In contrast, solving model instances with the best temporal discretization enables an accurate dispatch of available power generators (and storage units). However, as results for accuracy gains by the latter show, running a temporally decomposed model instance - when the solution for its down-sampled counterpart is known – was only beneficial for observing a more accurate dispatch of storage units or when the temporal resolution in the "first execution phase" was poor. In this case it needs to be considered, that for sufficient accuracy enhancements the selection of an appropriate number of intervals is crucial since errors of accuracy indicators only decrease for comparably large interval sizes.

Given that the "effectiveness of model reduction" becomes more significant when going from the comparatively easy-to-solve "REMix Dispatch" to the more complicated "REMix Expansion" model while it is also observable for different scenarios analyzed by Pfenninger, it can be generally concluded, that already low degrees of aggregation with small accuracy errors become the more valuable the harder it is to solve a particular monolithic ESOM. This makes model speed-up approaches that are based on model reduction techniques even more attractive for application to ESOMs programed with mixed-integer variables.

5.3. Limitations

The claim of conducting analyses for comparably large model instances implies several challenges that only partially could be addressed. As mentioned in Section 3.1., the whole benchmarking should ideally be carried out on the same computer hardware ensuring no influence on the solving process by parallel processes of other applications. However, due to a limited access to equally equipped computers, the instances of the „REMix Dispatch" model with rolling horizon were solved on the JUWELS cluster of the Juelich Supercomputing Center (first row in Table 4). For all of the other benchmark experiments other hardware was used (second row in Table 4).

Also minor bug-fixes were applied to REMix between the different benchmark experiments. One remarkable change is the indicated reduction of solver precision from $1e^{-8}$ to $1e^{-5}$ to reduce total computing times for the experiments related to spatial aggregation with capacity expansion (see Section 3.2.2) while extensive logging in GAMS's listing files was enabled. This obviously changed the ratio between GAMS time and solver time and probably led to smaller speed-ups observed for spatial aggregation with instances of "REMix Expansion".

For these reasons, speed-ups found for the individual performance enhancement approaches are not fully comparable with each other. Despite this circumstance, it can be expected that ideal conditions are also hardly achievable if speed-up approaches are used in applied studies. And still, for large models, the relation between achievable speed-up by a particular performance enhancement approach and impact on the computing time by parallel third-party processes should be negligible.

Moreover, the two selected REMix models that were used for this evaluation of speed-up approaches share many similarities with other applied ESOMs, especially if these are formulated in GAMS. However, we do not claim to provide general findings - such as the specific number of intervals to use for a rolling horizon method - that are representative for all of these models. For instance, because our results are only based on a single model parameterization, the impact of different data sets especially on accuracy indicators could not be assessed which limits the general transferability of our findings. Nevertheless, the outcome of this study provides a clear indication which speed-approaches show the highest potential for significantly reducing computing times. Furthermore, we mainly used straight-forward implementations that can still be tuned towards greater accuracy if required. This is particularly necessary if other indicators than the ones that were used in this study (mainly on an annual basis) are of interest; e.g., shadow prices.

5.4. Methodological Improvements

In this paper, we mainly focused on reachable improvements concerning the computational indicators, i.e., the required total wall-clock time. However, as all of the presented methodological approaches do not provide exact solutions of the original model instances, improvements regarding the accuracy can be considered if necessary. In the case of model reduction, a broad variety of conceivable methods to increase the accuracy of particular model outputs exists (see Section 2.2). As methods such as representative time slices or more sophisticated network equivalences are more or less related to smart treatment or preprocessing of input data, the total time consumption for the overall modeling exercise will not significantly increase.

With regard to the applied rolling horizon dispatch approach, similar improvements are conceivable by using temporally aggregated data for the time steps within the overlap. The idea behind is an extension of the foresight horizon while keeping the number of redundant time steps to be considered low. For instance, for the operation of long-term storage, down-sampling of the residual load for the next annual period would be valuable to avoid the undesired effect of full discharging towards the end of an interval.

Moreover, improved estimations for emission budgets for each interval are conceivable. In the actual implementation the annual emission budget is simply equally distributed which, on the one hand, prevents the dispatch of thermal power plants particularly in points in time with high residual load. On the other hand, time intervals where sufficient renewable energy resources are available may require a smaller emission limit instead. To address this issue, it could be considered to shift unused emissions from one time interval to the next and to select a summer date as starting point for an annual model run and heuristic decomposition approaches such as the presented temporal zooming method offer a starting point for improvements that could go into two directions:

(1) Improved performance can be gained by running the independent model parts (such as the time intervals in case of grid computing presented in 0) on different computers. By this means, the drawback of being limited to memory and CPU resources of shared memory machines could be overcome. In this context, for a better coordination and utilization of available computing resources the application of workload managers such as Slurm [97] would be beneficial.

(2) Improved accuracy can be reached by an extension to an exact decomposition approach that decomposes the temporal scale. However, this requires additional source code adaptions. For instance, in case of Benders decomposition, the distribution of emission budgets to the respective intervals needs to be realized by interval specific variables necessary to create benders cuts. Additionally, it can be expected that due to the need of an iterative execution of master and sub-problems the total computing time would significantly increase. Taking into account the best achievable speed-up of 10 of temporal zooming compared to simply solving the monolithic model, there is only a little room for improvements which may be disproportionate to the implantation effort required.

Finally, the combination of both improved performance and maintaining the accuracy requires iterative methods as well as the utilization of distributed memory computing hardware. However, effective implementations of such performance enhancement approaches require efficient communication between the processes that are executed in different computing nodes. Parallelization should therefore not only be thought at the conceptual level but also on the technical layer (see Figure 2). This goes hand in hand with the parallelization of solvers which is realized with the PIPS-IPM++ solver [98]. This solver provides a HPC-compatible implementation of the interior point method for LPs that are characterized by linking variables and linking constraints.

5.5. Practical Implications

In this study, the presented use case of a German ESOM has a macroeconomic perspective. It is thus suited for decision support in the field of energy policy of national economies. However, very similarly shaped optimization problems are also to be solved in energy industry.

For example, an aggregator which bundles and markets the power generation of decentralized power plants together with a storage facility across energy markets has to make operating decisions while seeking for a margin maximization that also needs to consider a technological, spatial and temporal component. Although time series in such use cases are not as extensive as in our study, manageable computing times are much more crucial as deadlines for bidding define hard time slots which are available for model-based analyses. In particular, rolling horizon approaches are suitable for dealing with weather and electricity price prognoses errors which become smaller with a shorter foresight horizon of a particular time interval. According to our findings both overlaps and interval sizes need to be comparably large for high accuracy (the latter should be, at least, greater than the typical cycling period of the storage facility). In this context, a high accuracy of the objective value (compared to the global optimum under perfect foresight) is to be understood as the potential to reach a higher margin. Our analysis in 0 shows that implications on total computing time by varying overlap and interval sizes are negligible.

However, this still leaves spaces for further and more detailed case studies because recommendations on the discussed SAR-parameters (0) are only valuable if the concrete framework conditions of an applied use case are known. For example, in our study, nearly constant computing times with rolling horizon dispatch were observed for time ratios (interval size divided by size of total foresight horizon) ranging between factor 0.003 and 0.02. If a total foresight horizon of 48 h would be considered in the example of the aggregator, the appropriate interval sizes would range within less than one hour.

6. Conclusions

Energy systems analysis highly depends on modeling tools such as Energy System Optimization models (ESOMs). To fulfill their purpose to provide insights into complex energy systems for decision support they need to be solvable within acceptable time spans.

For the broad spectrum of existing measures to improve the performance of ESOMs, we provided a detailed classification of conceivable approaches. Furthermore, we gave examples on easy-to-use adaptions that already improve computing performance, especially for ESOMs formulated in GAMS. These measures were accompanied by comprehensive benchmark analyses for a set of frequently applied speed-up techniques. The conducted examination included model aggregation approaches on different scales as well as strategies for heuristic decomposition. Both were applied to a spatially (488 regions) and temporally (8760 time steps) highly resolved ESOM of Germany for an energy scenario of the year 2030. While conventional computing with commercial solver software required more than two days for optimal solutions of certain model instances, selected speed-up approaches obtained sufficient solutions after less than six hours.

In particular, the novelty of this paper is the systematic evaluation of a broad set of approaches assessed for an applied ESOM focusing on achievable performance improvements. This allowed statements concerning possible speed-up factors and implied accuracy losses that went far beyond existing, methodologically focused assessments of single approaches with generic model setups.

In this context, Table 7 shows the final overview of the deeply analyzed speed-up approaches of the current study. Here, the "sufficient speed-up" indicates how many times faster a model instance could be solved compared to the total time required to solve the same model in the conventional way. As our analyses emphasized model reduction and heuristic decomposition, "accuracy" was quantified by using a set of pre-defined accuracy indicators. These indicators were determined as the relative deviations of:

- the "objective value" of the optimization problem,
- "power supply" of different electricity generation and load balancing technologies as well as, if appropriate,
- "added capacities" of storage and electricity transmission

against their counterparts calculated with an original, conventionally solved model instance (see also 0). In Table 7, the deviation from 100% accuracy is listed for both, the average over all assessed accuracy indicators and the accuracy indicator that showed the greatest error.

Table 7. Overview of analyzed performance enhancement approaches: observed speed-up and accuracy evaluated across all considered accuracy indicators.

Speed-Up Approach	Sufficient Speed-Up (Model Instance)	Accuracy	
		Average	Worst (Affected Indicator)
Spatial aggregation			
"REMix Dispatch"	>4 (100 regions)	>95%	>70% (power transmission)
"REMix Expansion"	>8 (150 regions)	>95%	>70% (transmission expansion)
Down-sampling			
"REMix Dispatch"	>6 (2190 time steps)	>97%	>81% (storage utilization)
"REMix Expansion"	>10 (2190 time steps)	>97%	>87% (storage utilization)
Rolling horizon dispatch	≈2.5 (16 intervals)	>96%	>87% (storage utilization)
Temporal zooming (sequential)	>8 (1095 time steps/16 intervals)	>93%	>69% (storage expansion)
Temporal zooming (grid computing)	>10 (1095 time steps/16 intervals)	>92%	>68% (storage expansion)

According to Table 7, within our evaluation framework, temporal down-sampling turned out to be the most efficient speed-up approach. The usefulness of this approach is strongly related to the "effectiveness of model reduction". In other words, the larger and more difficult to solve a particular ESOM becomes, the greater the achievable speed-up by already minor model reductions is. Taking into account that solving of linear ESOMs with mixed-integer variables is more complicated than for the model instances considered in this study, we suppose that the presented speed-up approaches are especially effective for such use cases.

As far as only specific model outcomes such as additional transmission capacities are of interest and extensive multi-threading is possible, the presented heuristic decomposition approaches with grid computing (temporal zooming) are also promising as they allow additional speed-ups without increasing loss of accuracy. Moreover, they offer the possibility for executing an ESOM on multiple shared memory computers even though parallelization is only applied to the conceptual layer of the optimization model (see Section 2.1).

Nevertheless, we showed that the appropriate gains in performance are limited depending on the size of a certain model. In this case, the down-side of "effectiveness of model reduction" comes into play: Since the idea behind decomposition is based on solving multiple reduced sub-models, such approaches reach their speed-up limit when the decrease of computing time by model reduction becomes negligible for very small sub-models.

Restrictively, the examined speed-up approaches were implemented and evaluated for a single ESOM framework. In this regard, further systematic evaluations are conceivable where variations of both input data and model specific source code need to be done systematically. This especially applies to the latter because we suppose that differing input data affect the accuracy of an ESOM rather than the computing performance.

In conclusion, the capability to solve very large ESOMs much faster is a pre-condition for best-practice studies in the field of energy systems analysis. Rather than spending time on solving models only for a hand full of scenarios and parameter sets, broad parameter scans become possible for which plenty of model solutions are required. In this manner, the application of effective speed-up approaches highly contributes to the generation of robust and well-founded model-based analyses for the development of decarbonization strategies of the energy system.

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References

1. Baños, R.; Manzano-Agugliaro, F.; Montoya, F.G.; Gil, C.; Alcayde, A.; Gómez, J. Optimization methods applied to renewable and sustainable energy: A review. *Renew. Sustain. Energy Rev.* **2011**, *15*, 1753–1766. [CrossRef]
2. Paltsev, S. Energy scenarios: The value and limits of scenario analysis. *Wiley Interdiscip. Rev. Energy Environ.* **2017**, *6*. [CrossRef]
3. Ventosa, M.; Baíllo, Á.; Ramos, A.; Rivier, M. Electricity market modeling trends. *Energy Policy* **2005**, *33*, 897–913. [CrossRef]
4. Kagiannas, A.G.; Askounis, D.T.; Psarras, J. Power generation planning: A survey from monopoly to competition. *Int. J. Electr. Power Energy Syst.* **2004**, *26*, 413–421. [CrossRef]
5. Wu, F.; Zheng, F.L.; Wen, F.S. Transmission investment and expansion planning in a restructured electricity market. *Energy* **2006**, *31*, 954–966. [CrossRef]
6. Zhu, J.; Hu, K.; Lu, X.; Huang, X.; Liu, K.; Wu, X. A review of geothermal energy resources, development, and applications in China: Current status and prospects. *Energy* **2015**, *93*, 466–483. [CrossRef]
7. Oree, V.; Hassen, S.Z.S.; Fleming, P.J. Generation expansion planning optimisation with renewable energy integration: A review. *Renew. Sustain. Energy Rev.* **2017**, *69*, 790–803. [CrossRef]
8. Frank, S.; Steponavice, I.; Rebennack, S. Optimal power flow: A bibliographic survey I. *Energy Syst.* **2012**, *3*, 221–258. [CrossRef]
9. Quintero, J.; Zhang, H.; Chakhchoukh, Y.; Vittal, V.; Heydt, G.T. Next Generation Transmission Expansion Planning Framework: Models, Tools, and Educational Opportunities. *IEEE Trans. Power Syst.* **2014**, *29*, 1911–1918. [CrossRef]
10. Haas, J.; Cebulla, F.; Cao, K.; Nowak, W.; Palma-Behnke, R.; Rahmann, C.; Mancarella, P. Challenges and trends of energy storage expansion planning for flexibility provision in low-carbon power systems—A review. *Renew. Sustain. Energy Rev.* **2017**, *80*, 603–619. [CrossRef]
11. Eurostat European Commission Eurostat. *NUTS-Nomenclature of Territorial Units for Statistics*; Eurostat European Commission Eurostat: Brussels, Belgium, 2017.
12. Kondziella, H.; Bruckner, T. Flexibility requirements of renewable energy based electricity systems—A review of research results and methodologies. *Renew. Sustain. Energy Rev.* **2016**, *53*, 10–22. [CrossRef]
13. Brouwer, A.S.; Broek, M.; van den Zappa, W.; Turkenburg, W.C.; Faaij, A. Least-cost options for integrating intermittent renewables in low-carbon power systems. *Appl. Energy* **2016**, *161*, 48–74. [CrossRef]
14. Weigt, H.; Jeske, T.; Leuthold, F.; von Hirschhausen, C. Take the long way down: Integration of large-scale North Sea wind using HVDC transmission. *Energy Policy* **2010**, *38*, 3164–3173. [CrossRef]

15. Bussar, C.; Stöcker, P.; Cai, Z.; Moraes, M., Jr.; Magnor, D.; Wiernes, P.; Bracht, N.; van Moser, A.; Sauer, D.U. Large-scale integration of renewable energies and impact on storage demand in a European renewable power system of 2050 Sensitivity study. *J. Energy Storage* **2016**, *6*, 1–10. [CrossRef]
16. Loulou, R.; Labriet, M. ETSAP-TIAM: The TIMES integrated assessment model Part I: Model structure. *Comput. Manag. Sci.* **2007**, *5*, 7–40. [CrossRef]
17. Deckmann, S.; Pizzolante, A.; Monticelli, A.; Stott, B.; Alsac, O. Studies on Power System Load Flow Equivalencing. *IEEE Trans. Power Appar. Syst.* **1980**, *99*, 2301–2310. [CrossRef]
18. Dorfler, F.; Bullo, F. Kron Reduction of Graphs with Applications to Electrical Networks. *IEEE Trans. Circuits Syst. I Regul. Pap.* **2013**, *60*, 150–163. [CrossRef]
19. Shayesteh, E.; Hamon, C.; Amelin, M.; Söder, L. REI method for multi-area modeling of power systems. *Int. J. Electr. Power Energy Syst.* **2014**, *60*, 283–292. [CrossRef]
20. Shi, D.; Tylavsky, D.J. A Novel Bus-Aggregation-Based Structure-Preserving Power System Equivalent. *Power Syst. IEEE Trans. Power Syst.* **2015**, *30*, 1977–1986. [CrossRef]
21. Oh, H. Optimal Planning to Include Storage Devices in Power Systems. *Power Syst. IEEE Trans.* **2011**, *26*, 1118–1128. [CrossRef]
22. Corcoran, B.A.; Jenkins, N.; Jacobson, M.Z. Effects of aggregating electric load in the United States. *Energy Policy* **2012**, *46*, 399–416. [CrossRef]
23. Schaber, K.; Steinke, F.; Hamacher, T. Transmission grid extensions for the integration of variable renewable energies in Europe: Who benefits where? *Energy Policy* **2012**, *43*, 123–135. [CrossRef]
24. Anderski, T.; Surmann, Y.; Stemmer, S.; Grisey, N.; Momo, E.; Leger, A.-C.; Betraoui, B.; Roy, P.V. *Modular Development Plan of the Pan-European Transmission System 2050-European Cluster Model of the Pan-European Transmission Grid*; European Union: Brussels, Belgium, 2014.
25. Hörsch, J.; Brown, T. The role of spatial scale in joint optimisations of generation and transmission for European highly renewable scenarios. In Proceedings of the 2017 14th International Conference on the European Energy Market (EEM), Dresden, Germany, 6–9 June 2017; pp. 1–7.
26. Pfenninger, S. Dealing with multiple decades of hourly wind and PV time series in energy models: A comparison of methods to reduce time resolution and the planning implications of inter-annual variability. *Appl. Energy* **2017**, *197*, 1–13. [CrossRef]
27. Zerrahn, A.; Schill, W.-P. Long-run power storage requirements for high shares of renewables: Review and a new model. *Renew. Sustain. Energy Rev.* **2017**, *79*, 1518–1534. [CrossRef]
28. Deane, J.P.; Drayton, G.; Gallachóir, B.P.Ó. The impact of sub-hourly modelling in power systems with significant levels of renewable generation. *Appl. Energy* **2014**, *113*, 152–158. [CrossRef]
29. O'Dwyer, C.; Flynn, D. Using energy storage to manage high net load variability at sub-hourly time-scales. *IEEE Trans. Power Syst.* **2015**, *30*, 2139–2148. [CrossRef]
30. Pandzzic, H.; Dvorkin, Y.; Wang, Y.; Qiu, T.; Kirschen, D.S. Effect of time resolution on unit commitment decisions in systems with high wind penetration. In Proceedings of the PES General Meeting Conference Exposition, National Harbor, MD, USA, 27–31 July 2014; pp. 1–5.
31. Ludig, S.; Haller, M.; Schmid, E.; Bauer, N. Fluctuating renewables in a long-term climate change mitigation strategy. *Energy* **2011**, *36*, 6674–6685. [CrossRef]
32. Leuthold, F.U.; Weigt, H.; von Hirschhausen, C. A Large-Scale Spatial Optimization Model of the European Electricity Market. *Netw. Spat. Econ.* **2012**, *12*, 75–107. [CrossRef]
33. Wogrin, S.; Duenas, P.; Delgadillo, A.; Reneses, J. A New Approach to Model Load Levels in Electric Power Systems With High Renewable Penetration. *IEEE Trans. Power Syst.* **2014**, *29*, 2210–2218. [CrossRef]
34. Green, R.; Staffell, I.; Vasilakos, N. Divide and Conquerk-Means Clustering of Demand Data Allows Rapid and Accurate Simulations of the British Electricity System. *IEEE Trans. Eng. Manag.* **2014**, *61*, 251–260. [CrossRef]
35. Nahmmacher, P.; Schmid, E.; Hirth, L.; Knopf, B. Carpe diem: A novel approach to select representative days for long-term power system modeling. *Energy* **2016**, *112*, 430–442. [CrossRef]
36. Spiecker, S.; Vogel, P.; Weber, C. Evaluating interconnector investments in the north European electricity system considering fluctuating wind power penetration. *Energy Econ.* **2013**, *37*, 114–127. [CrossRef]
37. Haydt, G.; Leal, V.; Pina, A.; Silva, C.A. The relevance of the energy resource dynamics in the mid/long-term energy planning models. *Renew. Energy* **2011**, *36*, 3068–3074. [CrossRef]

38. Kotzur, L.; Markewitz, P.; Robinius, M.; Stolten, D. Impact of different time series aggregation methods on optimal energy system design. *Renew. Energy* **2018**, *117*, 474–487. [CrossRef]
39. Merrick, J.H. On representation of temporal variability in electricity capacity planning models. *Energy Econ.* **2016**, *59*, 261–274. [CrossRef]
40. Mitra, S.; Sun, L.; Grossmann, I.E. Optimal scheduling of industrial combined heat and power plants under time-sensitive electricity prices. *Energy* **2013**, *54*, 194–211. [CrossRef]
41. Frew, B.A.; Becker, S.; Dvorak, M.J.; Andresen, G.B.; Jacobson, M.Z. Flexibility mechanisms and pathways to a highly renewable US electricity future. *Energy* **2016**, *101*, 65–78. [CrossRef]
42. Palmintier, B.S. *Incorporating Operational Flexibility into Electric Generation Planning: Impacts and Methods for System Design and Policy Analysis*; Massachusetts Institute of Technology: Cambridge, MA, USA, 2013.
43. Poncelet, K.; Delarue, E.; Six, D.; Duerinck, J.; D'haeseleer, W. Impact of the level of temporal and operational detail in energy-system planning models. *Appl. Energy* **2016**, *162*, 631–643. [CrossRef]
44. Raichur, V.; Callaway, D.S.; Skerlos, S.J. Estimating Emissions from Electricity Generation Using Electricity Dispatch Models: The Importance of System Operating Constraints. *J. Ind. Ecol.* **2016**, *20*, 42–53. [CrossRef]
45. Stoll, B.; Brinkman, G.; Townsend, A.; Bloom, A. *Analysis of Modeling Assumptions Used in Production Cost Models for Renewable Integration Studies*; National Renewable Energy Laboratory (NREL): Golden, CO, USA, 2016.
46. Cebulla, F.; Fichter, T. Merit order or unit-commitment: How does thermal power plant modeling affect storage demand in energy system models? *Renew. Energy* **2017**, *105*, 117–132. [CrossRef]
47. Abrell, J.; Kunz, F.; Weigt, H. *Start Me Up: Modeling of Power Plant Start-Up Conditions and Their Impact on Prices*; Working Paper; Universität Dresden: Dresden, Germany, 2008.
48. Langrene, N.; Ackooij, W.; van Breant, F. Dynamic Constraints for Aggregated Units: Formulation and Application. *Power Syst. IEEE Trans.* **2011**, *26*, 1349–1356. [CrossRef]
49. Munoz, F.D.; Sauma, E.E.; Hobbs, B.F. Approximations in power transmission planning: Implications for the cost and performance of renewable portfolio standards. *J. Regul. Econ.* **2013**, *43*, 305–338. [CrossRef]
50. Nolden, C.; Schönfelder, M.; Eßer-Frey, A.; Bertsch, V.; Fichtner, W. Network constraints in techno-economic energy system models: Towards more accurate modeling of power flows in long-term energy system models. *Energy Syst.* **2013**, *4*, 267–287. [CrossRef]
51. Romero, R.; Monticelli, A. A hierarchical decomposition approach for transmission network expansion planning. *IEEE Trans. Power Syst.* **1994**, *9*, 373–380. [CrossRef]
52. Gils, H.C. *Balancing of Intermittent Renewable Power Generation by Demand Response and Thermal Energy Storage*; Universität Stuttgart: Stuttgart, Germany, 2015.
53. Haikarainen, C.; Pettersson, F.; Saxen, H. A decomposition procedure for solving two-dimensional distributed energy system design problems. *Appl. Therm. Eng.* **2016**. [CrossRef]
54. Scholz, A.; Sandau, F.; Pape, C. A European Investment and Dispatch Model for Determining Cost Minimal Power Systems with High Shares of Renewable Energy. *Oper. Res. Proc.* **2016**. [CrossRef]
55. Babrowski, S.; Heffels, T.; Jochem, P.; Fichtner, W. Reducing computing time of energy system models by a myopic approach. *Energy Syst.* **2013**. [CrossRef]
56. Tuohy, A.; Denny, E.; O'Malley, M. Rolling Unit Commitment for Systems with Significant Installed Wind Capacity. *IEEE Lausanne Power Tech.* **2007**. [CrossRef]
57. Barth, R.; Brand, H.; Meibom, P.; Weber, C. A Stochastic Unit-commitment Model for the Evaluation of the Impacts of Integration of Large Amounts of Intermittent Wind Power. In Proceedings of the 2006 International Conference on Probabilistic Methods Applied to Power Systems, Stockholm, Sweden, 11–15 June 2006; pp. 1–8.
58. Silvente, J.; Kopanos, G.M.; Pistikopoulos, E.N.; Espuña, A. A rolling horizon optimization framework for the simultaneous energy supply and demand planning in microgrids. *Appl. Energy* **2015**, *155*, 485–501. [CrossRef]
59. Marquant, J.F.; Evins, R.; Carmeliet, J. Reducing Computation Time with a Rolling Horizon Approach Applied to a {MILP} Formulation of Multiple Urban Energy Hub System. *Procedia Comput. Sci.* **2015**, *51*, 2137–2146. [CrossRef]
60. Conejo, A.J.; Castillo, E.; Mínguez, R.; García-Bertrand, R. *Decomposition Techniques in Mathematical Programming*; Springer: Berlin, Germany, 2006.

61. Flores-Quiroz, A.; Palma-Behnke, R.; Zakeri, G.; Moreno, R. A column generation approach for solving generation expansion planning problems with high renewable energy penetration. *Electr. Power Syst. Res.* **2016**, *136*, 232–241. [CrossRef]
62. Virmani, S.; Adrian, E.C.; Imhof, K.; Mukherjee, S. Implementation of a Lagrangian relaxation based unit commitment problem. *IEEE Trans. Power Syst.* **1989**, *4*, 1373–1380. [CrossRef]
63. Wang, Q.; McCalley, J.D.; Zheng, T.; Litvinov, E. Solving corrective risk-based security-constrained optimal power flow with Lagrangian relaxation and Benders decomposition. *Int. J. Electr. Power Energy Syst.* **2016**, *75*, 255–264. [CrossRef]
64. Alguacil, N.; Conejo, A.J. Multiperiod optimal power flow using Benders decomposition. *IEEE Trans. Power Syst.* **2000**, *15*, 196–201. [CrossRef]
65. Amjady, N.; Ansari, M.R. Hydrothermal unit commitment with {AC} constraints by a new solution method based on benders decomposition. *Energy Convers. Manag.* **2013**, *65*, 57–65. [CrossRef]
66. Binato, S.; Pereira, M.V.F.; Granville, S. A new Benders decomposition approach to solve power transmission network design problems. *IEEE Trans. Power Syst.* **2001**, *16*, 235–240. [CrossRef]
67. Esmaili, M.; Ebadi, F.; Shayanfar, H.A.; Jadid, S. Congestion management in hybrid power markets using modified Benders decomposition. *Appl. Energy* **2013**, *102*, 1004–1012. [CrossRef]
68. Habibollahzadeh, H.; Bubenko, J.A. Application of Decomposition Techniques to Short-Term Operation Planning of Hydrothermal Power System. *IEEE Trans. Power Syst.* **1986**, *1*, 41–47. [CrossRef]
69. Khodaei, A.; Shahidehpour, M.; Kamalinia, S. Transmission Switching in Expansion Planning. *IEEE Trans. Power Syst.* **2010**, *25*, 1722–1733. [CrossRef]
70. Martínez-Crespo, J.; Usaola, J.; Fernández, J.L. Optimal security-constrained power scheduling by Benders decomposition. *Electr. Power Syst. Res.* **2007**, *77*, 739–753. [CrossRef]
71. Roh, J.H.; Shahidehpour, M.; Fu, Y. Market-Based Coordination of Transmission and Generation Capacity Planning. *IEEE Trans. Power Syst.* **2007**, *22*, 1406–1419. [CrossRef]
72. Wang, S.J.; Shahidehpour, S.M.; Kirschen, D.S.; Mokhtari, S.; Irisarri, G.D. Short-term generation scheduling with transmission and environmental constraints using an augmented Lagrangian relaxation. *IEEE Trans. Power Syst.* **1995**, *10*, 1294–1301. [CrossRef]
73. Wang, J.; Shahidehpour, M.; Li, Z. Security-Constrained Unit Commitment With Volatile Wind Power Generation. *IEEE Trans. Power Syst.* **2008**, *23*, 1319–1327. [CrossRef]
74. Xin-gang, Z.; Tian-tian, F.; Lu, C.; Xia, F. The barriers and institutional arrangements of the implementation of renewable portfolio standard: A perspective of China. *Renew. Sustain. Energy Rev.* **2014**, *30*, 371–380. [CrossRef]
75. Papavasiliou, A.; Oren, S.S.; Rountree, B. Applying high performance computing to transmission-constrained stochastic unit commitment for renewable energy integration. *IEEE Trans. Power Syst.* **2015**, *30*, 1109–1120. [CrossRef]
76. McCarl, B.A. *Speeding up GAMS Execution Time*; Materials drawn from Advanced GAMS Class by Bruce A McCarl: College Station, TX, USA, 2000.
77. Cao, K.-K.; Metzdorf, J.; Birbalta, S. Incorporating Power Transmission Bottlenecks into Aggregated Energy System Models. *Sustainability* **2018**, *10*, 1916. [CrossRef]
78. Teruel, A.G. *Perspestective of the Energy Transition: Technology Development and Investments under Uncertainty*; Technical University of Munich: Munich, Germany, 2015.
79. Egerer, J.; Gerbaulet, C.; Ihlenburg, R.; Kunz, F.; Reinhard, B.; von Hirschhausen, C.; Weber, A.; Weibezahn, J. *Electricity Sector Data for Policy-Relevant Modeling: Data Documentation and Applications to the German and European Electricity Markets*; Data Documentation; DIW: Berlin, Germany, 2014.
80. Open Power System Data Data Package Time Series. Available online: https://data.open-power-system-data.org/time_series/2017-07-09 (accessed on 2 August 2017).
81. Rippel, K.M.; Preuß, A.; Meinecke, M.; König, R. *Netzentwicklungsplan 2030 Zahlen Daten Fakten*; German Transmission System Operators: Berlin, Germany, 2017.
82. Wiegmans, B. GridKit Extract of ENTSO-E Interactive Map; 2016. Available online: https://zenodo.org/record/55853 (accessed on 10 July 2017).
83. Hofmann, F.; Hörsch, J.; Gotzens, F. FRESNA/Powerplantmatching: Python3 Adjustments; 2018. Available online: https://github.com/FRESNA/powerplantmatching (accessed on 3 July 2017).

84. ENTSO-E Transparency Platform Cross-Border Commercial Schedule and Cross-Border Physical Flow. Available online: https://transparency.entsoe.eu/content/static_content/Static%20content/legacy%20data/legacy%20data2012.html2012 (accessed on 29 June 2017).
85. Gils, H.C.; Scholz, Y.; Pregger, T.; de Tena, D.L.; Heide, D. Integrated modelling of variable renewable energy-based power supply in Europe. *Energy* **2017**, *123*, 173–188. [CrossRef]
86. Gils, H.C.; Simon, S. Carbon neutral archipelago-100% renewable energy supply for the Canary Islands. *Appl. Energy* **2017**, *188*, 342–355. [CrossRef]
87. Gils, H.C.; Simon, S.; Soria, R. 100% Renewable Energy Supply for Brazil—The Role of Sector Coupling and Regional Development. *Energies* **2017**, *10*, 1859. [CrossRef]
88. Cao, K.-K.; Gleixner, A.; Miltenberger, M. Methoden zur Reduktion der Rechenzeit linearer Optimierungsmodelle in der Energiewirtschaft? Eine Performance-Analyse. In Proceedings of the 14. Symposium Energieinnovation, Graz, Austria, 10–12 February 2016.
89. Scholz, Y.; Gils, H.C.; Pietzcker, R.C. Application of a high-detail energy system model to derive power sector characteristics at high wind and solar shares. *Energy Econ.* **2017**, *64*, 568–582. [CrossRef]
90. Gils, H.C.; Bothor, S.; Genoese, M.; Cao, K.-K. Future security of power supply in Germany–the role of stochastic power plant outages and intermittent generation. *Int. J. Energy Res.* **2018**, *42*, 1894–1913. [CrossRef]
91. Pedregosa, F.; Varoquaux, G.; Gramfort, A.; Michel, V.; Thirion, B.; Grisel, O.; Blondel, M.; Prettenhofer, P.; Weiss, R.; Dubourg, V.; et al. Scikit-learn: Machine Learning in Python. *J. Mach. Learn. Res.* **2011**, *12*, 2825–2830.
92. IBM. *IBM Deterministic Time, Release Notes for IBM CPLEX Optimizer for z/OS V12.5*; IBM: Armonk, NY, USA, 2013.
93. IBM. *IBM ILOG CPLEX Optimization StudioCPLEX User's Manual*; IBM Corporation: Armonk, NY, USA, 2017.
94. Ramos, A. *Good Optimization Modeling Practices with GAMS*; Lecture; Universidad Pontificia Comillas: Madrid, Spain, 2018.
95. McCarl, B. *Bruce McCarl's GAMS Newsletter Number 41*. Available online: https://www.gams.com/fileadmin/community/mccarlarchive/news41.pdf (accessed on 10 June 2019).
96. Breuer, T. Contribution of HPC to the BEAM-ME project. In *Implementation of Acceleration Strategies from Mathematics and Computational Sciences for Optimizing Energy System Models*; Final Workshop; The BEAM-ME Project: Aachen, Germany, 2019.
97. Slurm Workload Manager. Available online: https://slurm.schedmd.com (accessed on 6 July 2019).
98. Breuer, T.; Bussieck, M.; Cao, K.-K.; Cebulla, F.; Fiand, F.; Gils, H.C.; Gleixner, A.; Khabi, D.; Koch, T.; Rehfeldt, D.; et al. Optimizing Large-Scale Linear Energy System Problems with Block Diagonal Structure by Using Parallel Interior-Point Methods. In *Operations Research Proceedings 2017*; Kliewer, N., Ehmke, J.F., Borndörfer, R., Eds.; Springer: Berlin, Germany, 2018.

3 DISCUSSION

In the following, an overview of the results related to the publications summarized in this thesis is provided. In order to discuss them in an overarching scientific context, the section on the "General context", first, explains how the particular publications contribute to answering the research questions raised in section 1.3. The particular new scientific insights and further development potentials are then presented in sub-section 3.2 to 3.5, where the key outcome of each publication is discussed together with its limitations.

3.1 GENERAL CONTEXT

Figure 1 shows the central research questions of this thesis in tabular form. Each of the four publications from section 2 is assigned to one column to show whether the traceability of scenario studies (research question 1), impact of power-flow modeling in ESOMs (research question 2) or the contribution of grid expansion to system adequacy (research question 3) is mainly addressed by the publication. In addition, Figure 1 shows to what extent the associated studies build on each other.

Publication 1 can be seen as starting point as it generally focuses on model-based energy scenario studies, their purpose, state-of-the art methodologies, and challenges especially regarding a transparent execution and presentation of the whole modeling process. This also includes studies, where power flows in ESOMs are modeled. Hence, the findings from the associated broad literature review and the lessons learned concerning transparent documentation are applied to the subsequent Publications 2 - 4. Note that this does not mean that a full transparency can be claimed for these Publications but rather the awareness for providing essential information to modeling experts.

With regard to research question 2, integrating power flows into ESOMs is related to several challenges, which can be distinguished into *model construction*, *model operation* and *new model insights*. In particular, *model construction* refers to the implementation of new functionalities (e.g., by writing source codes), and acquisition and preparation of useable data sets. The latter is strongly connected to *model insights,* if these should go beyond the analysis of generic use cases. For this reason, *model construction* is the focus of Publication 2 for which a new instance of REMix is set up ("REMix Germany"). It allows for conducting studies on transmission grid level for scenarios of the German power system. The strength of the associated case study is the high spatial resolution of the created reference model[12], which enables modeling of real electricity transmission lines and the identification of new battery storage sites for more than 450 regions within Germany.

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[12] Reference model: Fully resolved instance of "REMix Germany" used for deriving and benchmarking of spatially aggregated model instances

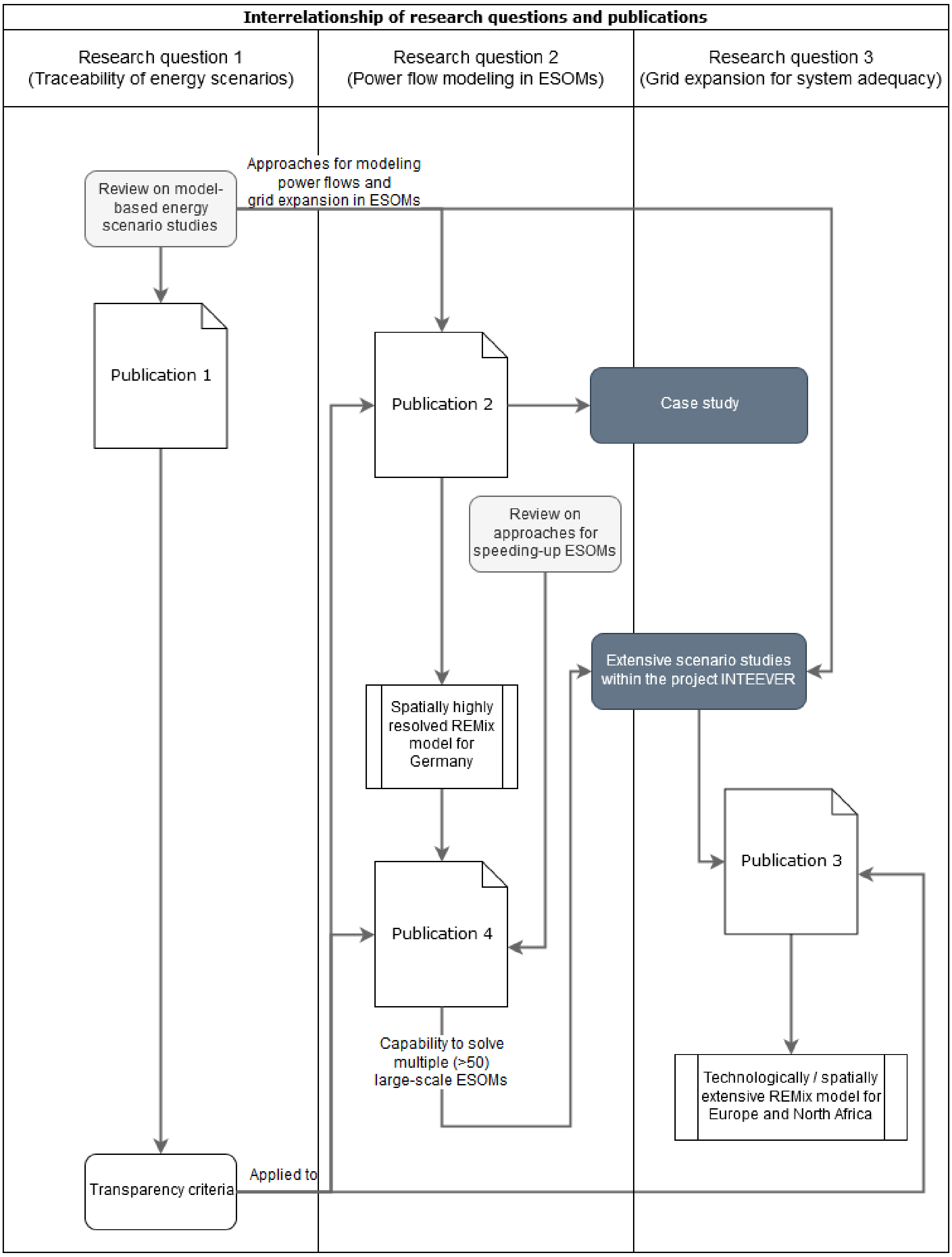

FIGURE 1: INTERRELATIONSHIP OF RESEARCH QUESTIONS AND PUBLICATIONS SUMMARIZED IN THIS THESIS.[13]

However, for Publication 2 simplifications are made with regard to spatial extensity. This limits analyses on one important effect of electricity transmission – spatial load-balancing across wide areas (i.e., country borders). Especially in the case of Germany this should not be ignored due to its central location within Europe, which implies significant cross-border power-flows.

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[13] INTEEVER: Research project (2015-2018) funded by the German Federal Ministry of Economic Affairs and Energy

This issue is addressed in Publication 3, where another new model instance of REMix is set up on European level and which also builds-up on a spatially aggregated representation of the German power system (recall, performing this in a way to maintain transmission bottlenecks is the focus of Publication 2). As this study is about the role of grid expansion for system adequacy as one option among several competing technological alternatives, it is assigned to research question 3. Compared to "REMix Germany", the strength of "REMix Europe" is the consideration of a broad spectrum of technologies for load-balancing (including coupling of energy demand sectors). Since in Publication 3 a high number of scenarios is also analyzed, its content-related findings are more robust than in the case study conducted for Publication 2.

Bringing the strengths of both "REMix Germany" and "REMix Europe" together is one possible way for future research. According to the lessons learned from the studies for Publication 1, a high number of model executions is required to conduct best-practice scenario studies. However, this is only realizable if one central bottleneck can be resolved - impracticably high computing times of large-scale ESOMs.

For this reason, Publication 4 emphasizes the aspect of ensuring the solvability of large ESOMs when power-flow modeling is integrated (*model operation)*. The underlying benchmark analysis studies and suggests approaches for reducing computing times in "REMix Germany" as one representative for such ESOMs.

In summary, Publication 2 provides a technique for constructing spatially aggregated ESOMs (*model construction*). Such an aggregated model is used for the scenario analyses in Publication 3 (*new model insights*), where however, disproportionally high computing times are still a limitation for studying a broad spectrum of conceivable energy futures. The speed-up approaches evaluated in Publication 4 (*model operation*) allow overcoming this issue.

How Publication 1 supports the effective utilization of such scenario studies[14], is discussed in the following chapter.

3.2 TRANSPARENCY CRITERIA FOR DOCUMENTING AND TRACING ENERGY SYSTEM MODELING PROCESSES

When modeling energy scenarios, a proper documentation represents one essential medium to provide traceability. However, although documentation is always taken for granted to ensure best scientific practice [39], in the context of scientific modeling it goes far beyond simply writing down what was done and

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[14] Note that due to a strict page limitation, the Energy Scenario Study checklist is not part of the scenario study in Publication 3. Nevertheless, it is provided with the a more detailed journal article to be published under the title "Analyzing the future role of power transmission in the European energy system" [63].

storing of results. Documentation and thus traceability are rather a multi-faced topic.

Its first or bottom layer is related to model development. Practically, the development of scientific modeling tools is a software engineering process. Therefore, it also shares the challenges with regard to traceability: Like modeling tools in the field of energy systems analysis, modern software in general tends to become more and more complex. The fact that documentation is often less prioritized by developers also is a general issue in software engineering [40]. Accordingly, these challenges were already identified in this domain and concepts that strive on improvements in model development processes exist [41].

The application of a model and all processes and workflows related to using a model represent the top-layer of documentation required for traceability. To a certain extent concepts for best-practice software engineering are also transferable from the model development layer to this layer. For example, this concerns the distinction of target groups into writers, users, and the differentiation of documentation purposes ranging from documentations with introductory character (e.g., tutorials, reference works or narratives) to technical documentations (e.g., descriptions and specifications [42]). Nevertheless, compared to the layer of model development one major difference exists: If all facets of documentation are ignored, there is still the always existing but worst-quality documentation: the source code itself. This means, a minimum of continuous traceability on the model development layer is always achievable by inspecting source code. Due to this fact, open-source modeling is one key element for improving traceability in order to ensure access to this minimal documentation to potential shareholders [43]. However, on the application layer even the existence of this minimal documentation is not guaranteed.

For this reason, Publication 1 directly addresses traceability on the layer of model application in the context of decision support for energy-policy making. Taking the view of both writers and users of energy scenario studies it proposes an easy-to-use documentation concept for increasing transparency – the "ESS transparency checklist"[15]. As scenario modeling represents an important tool for supporting policy making, especially a broad spectrum of potential users is conceivable, which have different levels of knowledge. This makes transparency even more important to get credibility for decisions made on the basis of scenario studies even though the expert knowledge is not given, which is required for fully tracing the model application (see Figure 2).

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[15] ESS: Energy Scenario Studies

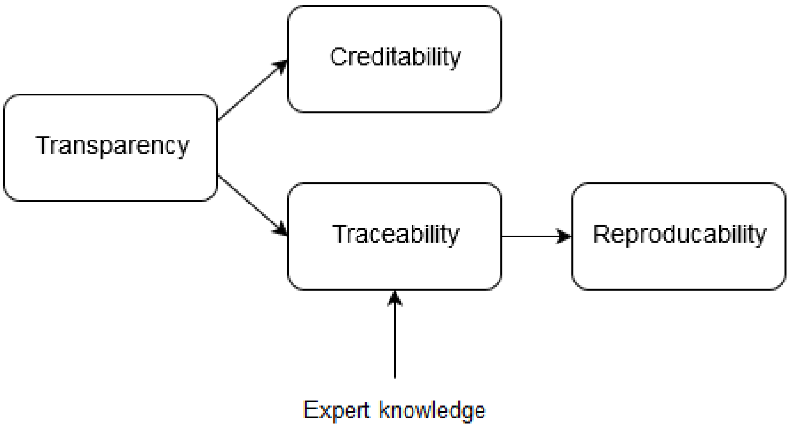

FIGURE 2: RELATION BETWEEN TRANSPARENCY AND TRACEABILITY

In the context of Figure 2, transparency and traceability are defined as follows: While traceability already implies that a process can be comprehensibly followed step by step, transparency represents a precondition for enabling this by providing the relevant information for this procedure.

In the field of ecosystem modeling, documentation schemes such as ODD [44] are already in use. However, before publishing the "ESS transparency checklist" with Publication 1 this was not the case within the energy systems analysis community. Therefore, the added values of Publication 1 are i) discussing the lack of transparency in the field of energy system modeling the first time and ii) proposing a new approach for improvements on transparency in the future.

Recently, the ESS transparency checklist was already applied by Hülk et al. [45]. The authors take an extract of the initial transparency criteria as a basis for a quantitative evaluation of transparency and reproducibility of an applied study conducted by the authors. They also introduce an additional classification of the transparency criteria into background-related general transparency, reproducibility-related and scientific quality-related criteria. In this sense, Hülk et al. extend the initial idea of Publication 1, where transparency is defined as a pre-condition to enable reproducibility and quality assessments. Junne et al. [46] go even further by using the "ESS transparency checklist" as basis to assess three different model-based energy scenario studies on quality and to derive general recommendation to authors of such studies.

The publications by Hülk et al. and Junne et al. show that the purpose of the major outcome of Publication 1 could be met – the "ESS transparency checklist" is used by scientists with both perspectives – the author's and the user's perspective. However, it needs to be stressed that the applicability is still limited to experts. Therefore, the transparency criteria rather contribute to improving the traceability of the scientific workflows, whereas the capability to increase credibility across different user groups is limited. In addition, although traceability facilitates partially reproducibility, to ensure the goal of full reproducibility, further measures are required (e.g., formal documentation processes such as in the case of ODD).

3.3 FROM SPATIALLY AGGREGATED TO HIGHLY RESOLVED MODELS

3.3.1 SPATIALLY AGGREGATED MODELING

As discussed in section 1.3.1, in the past and still today, in applied studies on scenarios of the European energy system, spatial data is conventionally resolved on country level [47] (in the following referred to as "low resolution"). Therefore, accounting for power flows is only possible by means of strong abstraction as usually only cross-border transmission can be considered. Deriving recommendations on infrastructure development (i.e., investments into transmission grids) is possible, albeit in an accordingly abstract manner. Typically, such analyses show that additional cross-border transmission capacities are required to foster the integration of power generation by fluctuating renewable energy sources and thus have positive effects on electricity prices [48,49]. Even the studies conducted for Publication 3 use a similar modeling framework, which leads to the result that, from a pure macroeconomic perspective, grid expansion is the most cost-efficient instrument for ensuring system adequacy in the analyzed European scenarios.

However, similar to previous European studies by Gils [50] or Cebulla [51], a special focus of Publication 3 is on Germany, which is modeled in the same way: It is divided into 20 regions in order to observe intra-national power flows on transmission lines that are candidates for transmission capacity expansion. The used regionalization was initially proposed by the German transmission system operators in a transmission network development study for Germany [52] and considers three main criteria: locations of power generation from renewable energies, locations of significant electricity consumption , and transmission bottlenecks. In the following, such spatial resolutions are referred to as "intermediate resolution".

From a methodological point of view, the 20 regions represent aggregations of spatially explicit data based on the three criteria. Using this established regionalization for modeling Germany also entails disadvantages as the initial process of creating 20 regional clusters is not traceable and thus not reproducible. Hence, if formerly identified transmission bottlenecks are resolved or new centers of power generation and consumption emerge, new regional models may be required.

3.3.2 A TRACEABLE METHOD FOR SPATIAL AGGREGATION

This issue is tackled by the studies conducted in Publication 2, where a traceable methodology for clustering of data from a spatially highly resolved ESOM of Germany is presented. The corresponding ESOM is "REMix Germany", which allows for hourly optimization of the power system operation using an OPF approach. As shown in Table A-1 (see Appendix), additional capacity expansion is possible but, in the case of Publication 2, limited to grid transmission capacities and lithium-ion battery storage.[16]

By applying a state-of-the-art spectral clustering algorithm to the results from "REMix Germany", spatially aggregated ESOM instances can be created with the capability to reproduce or modify the aggregation process. A similar approach of clustering data from the transmission grid level is applied by Hörsch and Brown [53] on a European scale. However, the novelty of the clustering approach proposed in Publication 2 is the application of operational data (nodal differences of marginal costs of total power supply) as clustering criteria, instead of purely relying on almost static topological information. Using these specific attributes has the advantage that relevant information such as locations of high electricity demand or the occurrence of transmission line congestions are already summarized in a single attribute. With this, ESOMs such as "REMix Europe"—with an intermediate spatial resolution striving for the identification of appropriate investments into transmission grid infrastructure—may use the proposed clustering approach to create a customized regionalization depending on the given scenario, especially with respect to different conceivable development stages of the energy system.

3.3.3 INTEGRATED POWER-FLOW MODELING

The philosophy of integrating power flows into ESOMs in "REMix Germany" differs from its counterpart partially used by "REMix Europe" for Publication 3. The underlying approaches are referred to as "Integrated modeling" of power flows in spatially highly resolved ESOMs for the former and "Coupling" of spatially aggregated ESOMs with AC power-flow simulations for the latter (which was partially done in a unidirectional manner for Publication 3).

Despite the fact that, in general, the linear DC power-flow is applied across all REMix instances considered in this thesis, one major difference of "Integrated modeling" and "Coupling" is the calculation of parameters that determine the distribution of power flows. In the case of "Integrated modeling" these factors are calculated model endogenously based on simplified technical parameters of the transmission grid. Opposed to that, when coupled to AC power-flow simulations, these Power Transfer Distribution Factors (PTDF) are derived from spatially aggregating accurately modeled AC power-flows. However, both philosophies of integrating power flows into ESOMs have advantages and disadvantages. In this context, Table 5 provides a general overview.

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[16] Note, that the used techno-economic parameters of the conducted case-study have not been checked to be fully consistent with each other because the focus of Publication 3 is rather to demonstrate the implications of the developed clustering methodology than to perform a sophisticated scenario analysis. Therefore, the author admits that especially the purely literature-based assumption of battery life times being greater than power converts life times is contradicting.

Furthermore, Figure 3 shows how, according to Table 3, mentioned references and the REMix model instances of this thesis can be assigned either to conventional energy system optimization or to power-flow analysis.

With regard to "Integrated modeling", one opportunity for a specific improvement of "REMix Germany" (used for Publication 2) is related to the disaggregation of primary data of power consumption. This data is only publicly available on power market or control-zone level and therefore needs to be distributed in space. While for the annual energy demand statistical data on county-district level is applicable for this scaling procedure (e.g., number of inhabitants), for the temporally resolved profiles of electricity consumption more sophisticated pre-processing approaches for input data become necessary. In the master thesis by Wittekind [54] a tool has been developed to perform this distribution for "REMix Germany" based on additional inputs such as standard load profiles or the gross value added. However, the nodal data used for Publication 2 relies on the same publicly available load curve, which represents the course of hourly power consumption in Germany of the year 2012.

TABLE 5: ADVANTAGES AND DISADVANTAGES OF CONSIDERING POWER-FLOW MODELING IN ENERGY SYSTEM OPTIMIZATION MODELS WITH DIFFERENT CHARACTERISTICS

	Integrated modeling of power flows in spatially highly resolved ESOMs	**Coupling** of spatially aggregated ESOMs with AC power-flow simulations
Advantages	+ Explicit modeling of all transmission capacities and bottlenecks with respect to a given development stage of the energy system + Modeling of concrete measures (e.g., realization of specific infrastructure projects)	+ More accurate distribution of power flows + Opportunity of analyses related to conventional power-flow analysis (e.g., security of grid operation)
Disadvantages	- Neglect of changing technical parameters (i.e., susceptance) of transmission lines due to expansion of transmission capacities - Additional input data requirements and parameterization effort for cross-sectoral modeling - Computational heavy, especially if modeled as MIP	- Extensive input data requirements (i.e., detailed technical parameters) for the AC power-flow simulation - Costly model coupling/harmonization procedures (e.g., disaggregation of ESOM results) - Grid expansion planning provides rather abstract results

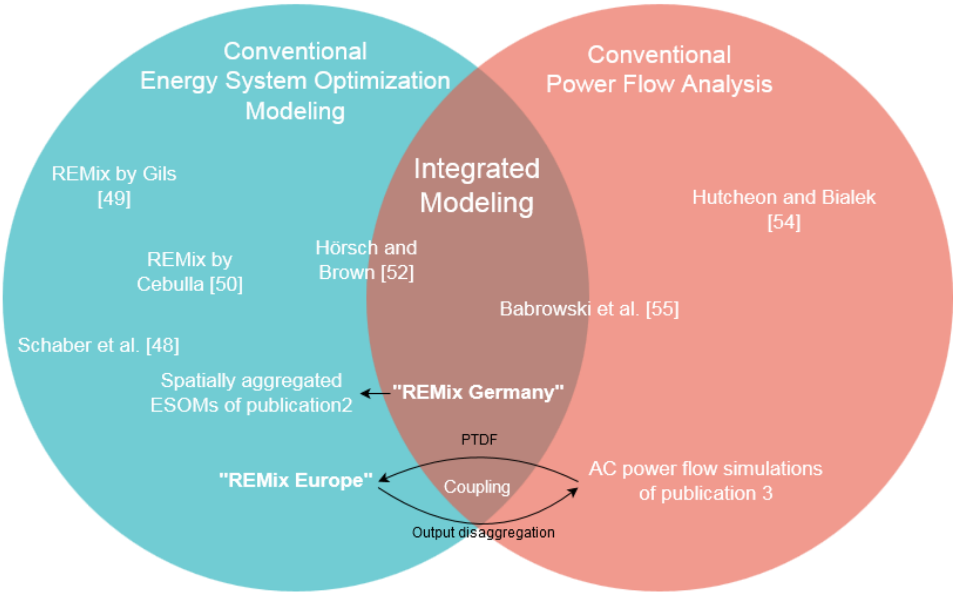

FIGURE 3: LOCATION OF VARIOUS APPLIED MODELS AND STUDIES IN THE CONTEXT OF ENERGY SYSTEM MODELING AND POWER-FLOW ANALYSES FOR EUROPE

If aggregated ESOMs are defined as proposed in Publication 2, the need for operational data from a spatially highly resolved model instance implies the challenge of solving such a model (“REMix Germany”). This is realized by keeping the model size comparably constant by making the following trade-off: As the spatial dimension is increased by higher resolution, the temporal dimension is reduced, which is, according to Table 3, more characteristic for conventional power-flow modeling (e.g., conducted by Hutcheon and Bialek [55]).

Reducing one model dimension in order to gain more detailed insights on another is a typical approach, which, however, requires additional methodologies to perform this reduction. In Babrowski et al. [56], a simple selection of typical time slices by weekday and season is used to keep computing times of a spatially highly resolved ESOM of Germany manageable. For the studies conducted for Publication 2, pre-analyses with different criteria are also made to identify probably critical points within the used time series inputs. In other words, the situations for which grid expansion would become necessary, need to be anticipated by approaches that filter or cluster the extensive input time series of power consumption or power generation from renewable energy sources.

One of the criteria tested in Publication 2 is typical for conventional transmission expansion planning: points in time with high amplitudes of both feed-in from wind-energy converters and power consumption. According to the findings by Agapoff et al. [57] the nodal price differences themselves are also considered as an appropriate selection criterion. Nevertheless, applying a more sophisticated methodology to identify critical time slices for grid expansion is recommendable for further improvements. For this purpose, new methodologies for temporal aggregation for energy system modeling published in recent studies (see section 2.2.3 in Publication 4) could be examined. For example, a more sophisticated approach particularly developed for transmission expansion planning is presented by Torbaghan et al. [58], where the authors apply a k-medoids algorithm to the results of a pre-performed *principal component analysis* in order to reduce the operational states to be considered for grid expansion.

3.4 THE VALUE OF MODEL-BASED SPEED-UP APPROACHES FOR LINEAR ENERGY SYSTEM OPTIMIZATION MODELS

Approaches for spatial aggregation and the determination of representative time slices are only a selection of heuristics for model reduction and thus concepts for enhancing the performance of ESOMs. However, most of the studies that are published on this topic focus on one specific approach and its individual benefits compared to similar methodologies. Opposed to that, Publication 4 takes a more general perspective with the objective to identify those methodologies that pose the largest potential for reducing computing times of ESOMs.

In this regard, the added value of Publication 4 is two-fold as on the one hand, it provides the very first review of popular heuristics applied to linear ESOMs taking into account their cross-model characteristics. These heuristics are discussed in context with alternative approaches such as mathematically exact decomposition or opportunities offered by high performance computing (HPC). On the other hand, an extensive benchmark experiment is conducted, where different speed-up approaches are systematically assessed against the conventional way of solving an ESOM.

Despite its broad focus, the results of Publication 4 are limited to model-based heuristics. This means that, on the one hand, these approaches are always accompanied by a certain loss of accuracy compared to exact approaches (e.g., *benders decomposition)*. For applied ESOMs formulated as LPs and under cost-benefit aspects, however, the added value of exact and thus mostly iterative decomposition approaches is questionable. Regarding the impact on the computing performance, the additional iterations cause losses in speed-up, whereas the gains on the accuracy side are often negligible because the optimum observed for ESOMs is often rather flat [59]. Especially this circumstance implies additional model development effort for iterative approaches, which then have to be adapted case-specifically to achieve convergence in acceptable time spans.

On the other hand, the observed performance enhancement of Publication 4 is still restricted to the changes that can be made by modifying the source code of an ESOM or adjusting the parameters of the applied solver software. Speed-up approaches that allow for massive parallelization by High Performance Computing (HPC) are thus not sufficiently examined. In this regard, a promising approach is the application of the parallel implementation of an interior point solver developed in the research project BEAM-ME [60]. Nevertheless, the findings from Publication 4 are essential for cost-benefit estimations since the application of solvers suited for HPC demand costly model adaptions. Hence, potential users of speed-up approaches are able to decide which acceleration of computing time is available at which implementation effort. In contrast, the use of HPC should be dedicated to problems that otherwise cannot be solved in reasonable time. This applies, for example, to so-called maximum models, which represent the modeled phenomena in the best-possible way. Their solutions can serve as a substitute for the limited validation possibilities in the field of energy system analysis. In this sense, HPC enables the provision of models, which can be used to investigate and derive permissible model simplifications.

The benchmark analyses conducted for Publication 4 use two very similar reference models based on “REMix Germany”, where, compared to the modeling setup presented in Table A-1, the module for heuristic temporal decomposition is applied. Other ESOMs share many of the characteristics of the corresponding reference models but specific implementations and parameters may differ. For this reason, a possible direction for future research are cross-model benchmarks in order to validate the statements made in Publication 4.

Another lesson learned from this publication is the basic knowledge about workflows for accessing and utilizing distributed memory architectures such as used for HPC. The application of job scheduling with professional job management tools (i.e., Slurm [61]) already improved conventional solving routines, which were used for solving the comparably large ESOM instances related to Publication 3 (see Figure 1).

3.5 THE CONTRIBUTION OF GRID EXPANSION TO SYSTEM ADEQUACY

As shown in Figure 1, Publication 3 represents an excerpt of more detailed studies conducted in the research project INTEEVER. Besides the comparison of scenarios that vary the consideration of solar power imports and a hydrogen economy, more detailed analyses concerning the role of grid expansion are conducted and presented in the corresponding technical report [62], and a further journal publication [63].

In this context, the basis of all model-based analyses is “REMix Europe”, which is used for both the determination of scenarios of European power plant portfolios (Table A-2) and for assessing different system configurations with regard to technologies for load-balancing (Table A-3).

One of the key findings from the studies related to Publication 3 is that, for a prescribed European power generation mix, grid expansion makes the most robust contribution to system adequacy (which is measured in the reduction of demand for back-up generation capacities). Without sufficient grid expansion, the integration of renewable power generation and thus the reduction of CO_2 emissions is not possible solely through the use of storage facilities. Otherwise the demand for more generation capacities increases, whereas additional curtailment occurs resulting in a significant higher demand for alternative load-balancing technologies including gas-fired backup power plants. Although these technologies play a major role for the composition of adequate future energy supply systems, especially when grid expansion is low and from a macroeconomic perspective, they can replace grid expansion only at higher cost. However, if ideally sited, gas-fired backup generation capacities can foster a reduction of required grid expansion.

Despite existing model limitations (e.g., neglection of further conceivable technologies, which are not listed in Table A-3, such as *carbon capture and storage*), the strength of the analyses summarized in Publication 3 is that they hold true for a broad variety of scenarios and parameter variations. Especially the role of grid expansion is evaluated for: i) two different starting points of prescribed grid expansion, ii) varying assumptions on investment costs, iii) the effect of bounding capacity expansion, and iv) considering the impact of topographic differences on expansion costs of individual interconnectors (for more details see [63]). Furthermore, the availability profiles of renewable power generation are varied by a parameter variation of weather data. An additional benchmark analysis also shows that, from a macroscopic perspective, the statements above are also robust against the different possibilities of modeling power flows in spatially aggregated ESOMs (i.e., transshipment model, DC power-flow based on simplified technical grid parameters, and DC power-flow based on PTDFs from AC power-flow simulations). The appropriate results indicate that the resulting composition of the energy system technology mix is almost independent of the used approach for modeling power flows in spatially aggregated ESOMs instances such as “REMix Europe”.

A recent study by Brown et al. [64], that is conducted without coupling with AC power-flow simulations, emphasizes the role of grid expansion within a sector-coupled European framework. The authors come to similar conclusions concerning electricity transmission being a robust measure for cost-efficient energy supply across a broad spectrum of considered scenarios. As the applied ESOM accounts for load-balancing by a power-balance constraint, system adequacy is also ensured for each of these scenarios. With regard to greenhouse gas mitigation targets, the scenarios go even further than the ones presented in Publication 3 as they aim at a reduction of 95% of CO_2 emissions compared to

1990. Nevertheless, Brown et al. also find that especially in cases where a broad variety of technologies for load-balancing is available (i.e., due to cross-sector coupling), electricity transmission and grid expansion are much more prominent if unrestrictedly competing with storage technologies. This highlights their role for ensuring system adequacy in highly renewable energy supply systems.

However, regardless of the additional determination of PTDFs by AC power-flow simulations, the weakness of spatially aggregated ESOMs is their implicit assumption of unlimited power transmission within the modeled regions at no costs. In other words, by concentrating all power generators and consumers at country-representing nodes, a non-negligible share of required spatial load-balancing is already done by the abstraction step of spatial aggregation. Hence, additional grid expansion needs are to be identified. This would require that grid expansion measures are also determined on the side of power-flow analyses for the transmission, and moreover, the distribution grid. Especially for the latter, the integration of new electricity producers and consumers, and even so-called prosumers can lead to significant investment needs for adapting the grid infrastructure. The corresponding installation of, for instance, controllable power converters and transformers, or battery storage is often referred to as transition to smart grids. For example, in the case of Germany, the corresponding investments are estimated to be greater than factor 10 compared to the identified grid expansion needs for the transmission grid [65].

Conducting such detailed grid expansion planning in an automated manner would require a power-flow simulation, which also considers investment decisions. With regard to Figure 3, this implies a shift towards optimization. An example for conducting such analyses based on model-coupling with an ESOM is proposed by ENTSO-E [66]. The involved modeling approaches are referred to as market simulation (ESOM) and network simulation (power-flow simulation), which have to be iteratively executed. The underlying idea is back-feeding of costs for intra-regional electricity transmission to the ESOM, which then could consider these costs for a refined model re-execution. However, this is very similar to solving an integrated ESOM by a mathematical decomposition method (see Publication 4) and thus, involves similar challenges concerning computing time and convergence behavior of the coupled models.

Therefore, integrated ESOMs are an equivalent or even more appropriate way for further research on system adequacy, although obstacles such as the costly parameterization and expectable increases in computing time need to be overcome. Nevertheless, expenditures for grid expansion are still hidden for an integrated ESOM as soon as the realization of decentral infrastructures on distribution grid level is to be investigated. At this point, specific but spatially limited power-flow simulations are required since many abstractions that are made on transmission grid level must be considered in higher detail.

4 CONCLUSIONS

Modeling energy scenarios with power-flow constraints is essential for gaining insights on the technological interdependencies and cost-efficient deployment of decarbonized energy systems. In particular, the added value of taking into account power flows is the ability to understand the implications stemming from the fact that locations with suitable potentials for electricity generation from renewable energy resources are often remote from regions with high energy consumption.

Energy System Optimization Models (ESOMs) are frequently applied for modeling energy scenarios. Addressing the complex task of scenario construction with re-executable computer tools offers the capability to ensure reproducibility of energy scenarios as long as the used ESOMs are sustainably accessible. However, sufficiently incorporating power-flow constraints into these equally complex models contributes to increases in model resolutions and extends system boundaries to be modeled and thus complicates the traceability of studies that strive for giving policy advice based on ESOMs.

In order to provide traceability when modeling scenarios of large-scale energy systems, a first step is a sufficient degree of transparency, at least for experts. The studies carried out as part of this thesis contributed to this issue by compiling a comprehensive list of transparency criteria (ESS transparency checklist), which has been applied to both the conception of further studies by the author and by other researchers dealing with energy scenarios.

By implementing and investigating two different approaches for modeling power flows in the transmission grid, this thesis contributed to improved analyses on spatial load-balancing with the ESOM REMix. Among these approaches, especially integrated modeling of power flows in spatially highly resolved ESOMs allows for the detailed investigation of future infrastructure needs. However, further methodological improvements such as the extension to mixed-integer modeling or the capability to conduct path optimizations (instead of the used annuity method) for investment planning are required if seeking for robust implementation measures in the real world.

This also applies to the extent to which possible future developments are considered by energy scenarios. If they are supposed to provide robust decision support, implications of a broad variety of scenarios need to be assessed. By analyzing the macroeconomic usefulness of grid expansion on system adequacy for more than 50 energy scenarios and parameter variations, the studies conducted as part of this thesis have already taken a step forward. In this context, it was found that grid expansion still represents a very cost-efficient measure. However, robust decision making also requires the analysis of extreme or disruptive events and addressing all kinds of uncertainties involved with scenario development. Therefore, the construction of an even larger number of energy scenarios with integrated ESOMs represents a suitable approach for future research on the contribution of grid expansion on system adequacy.

In order to enable researchers to conduct the corresponding extensive model-based scenario analyses, the computing times of ESOMs need to stay manageable. With the systematic evaluation of concepts for reducing computing times of ESOMs, Publication 4 of this thesis provided a comprehensive guideline for modelers who are dealing with this issue. However, the found speed-ups of up to factor 10 still need to be increased if large-scale parameter variations for scenario analyses are to be conducted in the future. In this regard, massive parallelization of ESOMs using High Performance Computing (HPC) represents one conceivable research direction for the future. Today, optimization modeling and in particular energy systems analysis are still at the beginning compared to established applications for HPC.

In summary, the publications associated to this thesis provide the foundations for addressing new partially diverging trends in the application of ESOMs for the macroscopic analysis and construction of future energy systems. In particular, these are the capabilities for traceable documentation, development, and solving of spatially highly resolved ESOMs which are suited for modeling a broad spectrum of scenarios across energy sectors.

5 REFERENCES

[1] IPCC, *Annex I: Glossary [Matthews, J.B.R. (ed.)]. In: Global Warming of 1.5°C. An IPCC Special Report on the impacts of global warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty*, [Masson-Delmotte, V., P. Zhai, H.-O. Pörtner, D. Roberts, J. Skea, P.R. Shukla, A. Pirani, W. Moufouma-Okia, C. Péan, R. Pidcock, S. Connors, J.B.R. Matthews, Y. Chen, X. Zhou, M.I. Gomis, E. Lonnoy, T. Maycock, M. Tignor, and T. Waterfield (eds.)], 2018. Available: Online https://www.ipcc.ch/site/assets/uploads/sites/2/2019/06/SR15_AnnexI_Glossary.pdf.

[2] UNFCCC, "Paris Agreement," Dec. 2015. Available: Online https://treaties.un.org/doc/Treaties/2016/02/20160215%2006-03%20PM/Ch_XXVII-7-d.pdf.

[3] C. Dieckhoff, "Modellierte Zukunft," Universität Stuttgart, 2015.

[4] J. Rogelj, D. Shindell, K. Jiang, S. Fifita, P. Forster, V. Ginzburg, C. Handa, H. Kheshgi, S. Kobayashi, E. Kriegler, L. Mundaca, R. Séférian, and M.V. Vilariño, *Mitigation Pathways Compatible with 1.5°C in the Context of Sustainable Development. In: Global Warming of 1.5°C. An IPCC Special Report on the impacts of global warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty*, [Masson-Delmotte, V., P. Zhai, H.-O. Pörtner, D. Roberts, J. Skea, P.R. Shukla, A. Pirani, W. Moufouma-Okia, C. Péan, R. Pidcock, S. Connors, J.B.R. Matthews, Y. Chen, X. Zhou, M.I. Gomis, E. Lonnoy, T. Maycock, M. Tignor, and T. Waterfield (eds.)], 2018. Available: Online https://www.ipcc.ch/site/assets/uploads/sites/2/2019/05/SR15_Chapter2_Low_Res.pdf.

[5] A.J. Schwab, *Elektroenergiesysteme - Erzeugung, Übertragung und Verteilung elektrischer Energie*, Springer Vieweg, 2017. Available: Online http://link.springer.com/book/10.1007/978-3-642-21958-0.

[6] R. Billinton and R.N. Allan, *Reliability Assessment of Large Electric Power Systems*, Springer Science + Business Media, 1988. Available: DOI 10.1007/978-1-4613-1689-3, Online https://books.google.de/books?id=kYn4BwAAQBAJ&printsec=frontcover&hl=de#v=onepage&q&f=false.

[7] A. Herbst, F. Toro, F. Reitze, and E. Jochem, "Introduction to energy systems modelling," *Swiss journal of economics and statistics*, vol. 148, 2012, pp. 111–135.

[8] V. Krey, "Vergleich kurz- und langfristig ausgerichteter Optimierungsansätze mit einem multi-regionalen Energiesystemmodell unter Berücksichtigung stochastischer Parameter," Ruhr-Universität Bochum, 2006.

[9] A. Zerrahn and W.-P. Schill, "Long-run power storage requirements for high shares of renewables: review and a new model," *Renewable and Sustainable Energy Reviews*, vol. 79, 2017, pp. 1518–1534. Available: DOI https://doi.org/10.1016/j.rser.2016.11.098, Online http://www.sciencedirect.com/science/article/pii/S1364032116308619.

[10] H.-K. Ringkjøb, P.M. Haugan, and I.M. Solbrekke, "A review of modelling tools for energy and electricity systems with large shares of variable renewables," *Renewable and Sustainable Energy Reviews*, vol. 96, Nov. 2018, pp. 440–459. Available: DOI 10.1016/j.rser.2018.08.002.

[11] S. Collins, J.P. Deane, K. Poncelet, E. Panos, R.C. Pietzcker, E. Delarue, and B.P.Ó. Gallachóir, "Integrating short term variations of the power system into integrated energy system models: A methodological review," *Renewable and Sustainable Energy Reviews*, vol. 76, Sep. 2017, pp. 839–856. Available: DOI 10.1016/j.rser.2017.03.090.

[12] D. Connolly, *A Review of Energy Storage Technologies*, University of Limerick, 2010.

[13] I.M. Algunaibet and G. Guillén-Gosálbez, "Life cycle burden-shifting in energy systems designed to minimize greenhouse gas emissions: Novel analytical method and application to the United States," *Journal of Cleaner Production*, vol. 229, 2019, pp. 886–901. Available: DOI https://doi.org/10.1016/j.jclepro.2019.04.276, Online http://www.sciencedirect.com/science/article/pii/S0959652619313678.

[14] U. Remme, “Zukünftige Rolle erneuerbarer Energien in Deutschland : Sensitivitätsanalysen mit einem linearen Optimierungsmodell,” Universität Stuttgart, 2006. Available: Online http://elib.uni-stuttgart.de/opus/volltexte/2006/2817.

[15] R. Schultz and H.J. Wagner, *Innovative Modellierung und Optimierung von Energiesystemen*, LIT Verlag Münster, 2009.

[16] S. Frank, I. Steponavice, and S. Rebennack, “Optimal power flow: a bibliographic survey I,” *Energy Systems*, vol. 3, Sep. 2012, pp. 221–258. Available: DOI 10.1007/s12667-012-0056-y, Online https://doi.org/10.1007/s12667-012-0056-y.

[17] J. Quintero, H. Zhang, Y. Chakhchoukh, V. Vittal, and G.T. Heydt, “Next Generation Transmission Expansion Planning Framework: Models, Tools, and Educational Opportunities,” *IEEE Transactions on Power Systems*, vol. 29, Jul. 2014, pp. 1911–1918. Available: DOI 10.1109/TPWRS.2014.2317590.

[18] F.L. Hitchcock, “The Distribution of a Product from Several Sources to Numerous Localities,” *Journal of Mathematics and Physics*, vol. 20, Apr. 1941, pp. 224–230. Available: DOI 10.1002/sapm1941201224.

[19] T.U. Dresden, “Eltramod - Electricity Transhipment Model,” Aug. 2016. Available: Online https://tu-dresden.de/bu/wirtschaft/ee2/forschung/modelle/eltramod?set_language=en.

[20] S. Nagl, M. Fürsch, M. Paulus, J. Richter, J. Trüby, and D. Lindenberger, “Energy policy scenarios to reach challenging climate protection targets in the German electricity sector until 2050,” *Utilities Policy*, vol. 19, Sep. 2011, pp. 185–192. Available: DOI 10.1016/j.jup.2011.05.001, Online https://www.sciencedirect.com/science/article/pii/S0957178711000324.

[21] ENTSO-E, *2nd ENTSO-E Guideline for Cost Benefit Analysis of Grid Development Projects*, 2018. Available: Online https://tyndp.entsoe.eu/Documents/TYNDP%20documents/Cost%20Benefit%20Analysis/2018-10-11-tyndp-cba-20.pdf.

[22] B. Stott, J. Jardim, and O. Alsac, “DC Power Flow Revisited,” *IEEE Transactions on Power Systems*, vol. 24, Aug. 2009, pp. 1290–1300. Available: DOI 10.1109/tpwrs.2009.2021235, Online http://dx.doi.org/10.1109/TPWRS.2009.2021235.

[23] A.J. Conejo, L.B. Morales, S.J. Kazempour, and A.S. Siddiqui, *Investment in Electricity Generation and Transmission*, Springer International Publishing, 2016. Available: DOI 10.1007/978-3-319-29501-5.

[24] J. Haas, F. Cebulla, K.-K. Cao, W. Nowak, R. Palma-Behnke, C. Rahmann, and P. Mancarella, “Challenges and trends of energy storage expansion planning for flexibility provision in low-carbon power systems – a review,” *Renewable and Sustainable Energy Reviews*, vol. 80, 2017, pp. 603–619. Available: DOI https://doi.org/10.1016/j.rser.2017.05.201, Online http://www.sciencedirect.com/science/article/pii/S1364032117308377.

[25] F. Cebulla and T. Fichter, “Merit order or unit-commitment: How does thermal power plant modeling affect storage demand in energy system models?,” *Renewable Energy*, vol. 105, May. 2017, pp. 117–132. Available: DOI http://dx.doi.org/10.1016/j.renene.2016.12.043, Online http://www.sciencedirect.com/science/article/pii/S0960148116310990.

[26] A. Grunwald, “Energy futures: Diversity and the need for assessment,” *Futures*, vol. 43, 2011, pp. 820–830. Available: DOI https://doi.org/10.1016/j.futures.2011.05.024, Online http://www.sciencedirect.com/science/article/pii/S0016328711001315.

[27] Y. Scholz, “Renewable energy based electricity supply at low costs: development of the REMix model and application for Europe,” Universität Stuttgart, 2012. Available: DOI http://dx.doi.org/10.18419/opus-2015.

[28] H.C. Gils, Y. Scholz, T. Pregger, D.L. de Tena, and D. Heide, “Integrated modelling of variable renewable energy-based power supply in Europe,” *Energy*, vol. 123, 2017, pp. 173–188. Available: DOI http://dx.doi.org/10.1016/j.energy.2017.01.115, Online http://www.sciencedirect.com/science/article/pii/S0360544217301238.

[29] F. Cebulla, T. Naegler, and M. Pohl, “Electrical energy storage in highly renewable European energy systems: Capacity requirements, spatial distribution, and storage dispatch,” *Journal of Energy Storage*, vol. 14, 2017, pp. 211–223. Available: DOI https://doi.org/10.1016/j.est.2017.10.004, Online http://www.sciencedirect.com/science/article/pii/S2352152X17302815.

[30] H.C. Gils and S. Simon, “Carbon neutral archipelago - 100% renewable energy supply for the Canary Islands,” *Applied Energy*, vol. 188, 2017, pp. 342–355. Available: DOI

http://dx.doi.org/10.1016/j.apenergy.2016.12.023, Online http://www.sciencedirect.com/science/article/pii/S0306261916317871.

[31] H.C. Gils, S. Simon, and R. Soria, “100% Renewable Energy Supply for Brazil—The Role of Sector Coupling and Regional Development,” *Energies*, vol. 10, Nov. 2017, p. 1859. Available: DOI 10.3390/en10111859.

[32] H.C. Gils, S. Bothor, M. Genoese, and K.-K. Cao, “Future security of power supply in Germany – the role of stochastic power plant outages and intermittent generation,” *International Journal of Energy Research*, vol. accepted for publication, 2018. Available: Online http://onlinelibrary.wiley.com/doi/10.1002/er.3957/full.

[33] J. Zhu, *Optimization of power system operation*, John Wiley & Sons, 2015. Available: Online http://eu.wiley.com/WileyCDA/WileyTitle/productCd-1118854152.html.

[34] S. Pfenninger, A. Hawkes, and J. Keirstead, “Energy systems modeling for twenty-first century energy challenges,” *Renewable and Sustainable Energy Reviews*, vol. 33, 2014, pp. 74–86. Available: DOI http://dx.doi.org/10.1016/j.rser.2014.02.003, Online http://www.sciencedirect.com/science/article/pii/S1364032114000872.

[35] W. Häfele, *Energy in a Finite World: A Global Systems Analysis (Volume 2)*, Ballinger, 1981.

[36] W. Medjroubi, U.P. Müller, M. Scharf, C. Matke, and D. Kleinhans, “Open Data in Power Grid Modelling: New Approaches Towards Transparent Grid Models,” *Energy Reports*, vol. 3, Nov. 2017, pp. 14–21. Available: DOI 10.1016/j.egyr.2016.12.001.

[37] F. Wiese, I. Schlecht, W.-D. Bunke, C. Gerbaulet, L. Hirth, M. Jahn, F. Kunz, C. Lorenz, J. Mühlenpfordt, J. Reimann, and W.-P. Schill, “Open Power System Data – Frictionless data for electricity system modelling,” *Applied Energy*, vol. 236, Feb. 2019, pp. 401–409. Available: DOI 10.1016/j.apenergy.2018.11.097.

[38] ENTSO-E, *TYNDP 2018 Executive Report - Connecting Europe: Electricity 2025 - 2030 - 2040*, European Network of Transmission System Operators for Electricity, 2018. Available: Online https://tyndp.entsoe.eu/.

[39] *Leitlinien zur Sicherung guter wissenschaftlicher Praxis - Kodex*. Available: Online https://www.dfg.de/download/pdf/foerderung/rechtliche_rahmenbedingungen/gute_wissenschaftliche_praxis/kodex_gwp.pdf.

[40] B. Selic, “Agile Documentation, Anyone?,” *IEEE Software*, vol. 26, Nov. 2009, pp. 11–12. Available: DOI 10.1109/MS.2009.167.

[41] G. Wilson, D.A. Aruliah, C.T. Brown, N.P.C. Hong, M. Davis, R.T. Guy, S.H.D. Haddock, K.D. Huff, I.M. Mitchell, M.D. Plumbley, B. Waugh, E.P. White, and P. Wilson, “Best Practices for Scientific Computing,” *PLoS Biology*, vol. 12, Jan. 2014, p. e1001745. Available: DOI 10.1371/journal.pbio.1001745.

[42] D.L. Parnas, “Precise Documentation: The Key to Better Software,” *The Future of Software Engineering*, Springer Berlin Heidelberg, 2010, pp. 125–148. Available: DOI 10.1007/978-3-642-15187-3_8.

[43] S. Pfenninger, J. DeCarolis, L. Hirth, S. Quoilin, and I. Staffell, “The importance of open data and software: Is energy research lagging behind?,” *Energy Policy*, vol. 101, 2017, pp. 211–215.

[44] V. Grimm, U. Berger, D.L. DeAngelis, J.G. Polhill, J. Giske, and S.F. Railsback, “The ODD protocol: A review and first update,” *Ecological Modelling*, vol. 221, Nov. 2010, pp. 2760–2768. Available: DOI 10.1016/j.ecolmodel.2010.08.019, Online http://dx.doi.org/10.1016/j.ecolmodel.2010.08.019.

[45] L. Hülk, B. Müller, M. Glauer, E. Förster, and B. Schachler, “Transparency, reproducibility, and quality of energy system analyses–A process to improve scientific work,” *Energy Strategy Reviews*, vol. 22, 2018, pp. 264–269.

[46] T. Junne, M. Xiao, L. Xu, Z. Wang, P. Jochem, and T. Pregger, “How to Assess the Quality and Transparency of Energy Scenarios: Results of a Case Study,” *Energy Strategy Reviews (under review)*, 2019.

[47] W. Zappa, M. Junginger, and M. van den Broek, “Is a 100% renewable European power system feasible by 2050?,” *Applied Energy*, vol. 233-234, 2019, pp. 1027–1050. Available: DOI https://doi.org/10.1016/j.apenergy.2018.08.109, Online http://www.sciencedirect.com/science/article/pii/S0306261918312790.

[48] K. Schaber, F. Steinke, and T. Hamacher, “Transmission grid extensions for the integration of variable renewable energies in Europe: Who benefits where?,” *Energy Policy*, vol. 43, 2012, pp. 123–135. Available: DOI http://dx.doi.org/10.1016/j.enpol.2011.12.040, Online http://www.sciencedirect.com/science/article/pii/S0301421511010469.

[49] S. Weitemeyer, D. Kleinhans, L. Wienholt, T. Vogt, and C. Agert, “A European Perspective: Potential of Grid and Storage for Balancing Renewable Power Systems,” *Energy Technology*, 2015, p. n/a–n/a. Available: DOI 10.1002/ente.201500255, Online http://dx.doi.org/10.1002/ente.201500255.

[50] H.C. Gils, “Balancing of Intermittent Renewable Power Generation by Demand Response and Thermal Energy Storage,” Universität Stuttgart, 2015. Available: DOI http://dx.doi.org/10.18419/opus-6888, Online http://dx.doi.org/10.18419/opus-6888.

[51] F. Cebulla, “Storage demand in highly renewable energy scenarios for Europe: the influence of methodology and data assumptions in model-based assessments,” 2017.

[52] Dena, *dena-Netzstudie II. Integration erneuerbarer Energien in die deutsche Stromversorgung im Zeitraum 2015 - 2020 mit Ausblick 2025.*, Deutsche Energieagentur (Dena), 2010.

[53] J. Hörsch and T. Brown, “The role of spatial scale in joint optimisations of generation and transmission for European highly renewable scenarios,” *2017 14th International Conference on the European Energy Market (EEM)*, 2017, pp. 1–7. Available: DOI 10.1109/EEM.2017.7982024, Online http://ieeexplore.ieee.org/document/7982024/.

[54] R. Wittekind, “Development and impact analysis of regionalized load profiles for spatially highly resolved energy system models,” Universtiy of Leipzig, 2019. Available: Online https://elib.dlr.de/126971/.

[55] N. Hutcheon and J.W. Bialek, “Updated and validated power flow model of the main continental European transmission network,” *2013 IEEE Grenoble Conference*, IEEE, 2013. Available: DOI 10.1109/ptc.2013.6652178.

[56] S. Babrowski, P. Jochem, and W. Fichtner, “Electricity storage systems in the future German energy sector: An optimization of the German electricity generation system until 2040 considering grid restrictions,” *Computers & Operations Research*, vol. 66, 2016, pp. 228–240. Available: DOI http://dx.doi.org/10.1016/j.cor.2015.01.014, Online http://www.sciencedirect.com/science/article/pii/S0305054815001227.

[57] S. Agapoff, C. Pache, P. Panciatici, L. Warland, and S. Lumbreras, “Snapshot selection based on statistical clustering for Transmission Expansion Planning,” *2015 IEEE Eindhoven PowerTech*, IEEE, 2015. Available: DOI 10.1109/ptc.2015.7232393.

[58] S.S. Torbaghan, M. Gibescu, B.G. Rawn, and M. van der Meijden, “A Market-Based Transmission Planning for HVDC Grid—Case Study of the North Sea,” *IEEE Transactions on Power Systems*, vol. 30, 2015, pp. 784–794. Available: DOI 10.1109/TPWRS.2014.2332762, Online http://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=6851949.

[59] E. Schmid and B. Knopf, “Quantifying the long-term economic benefits of European electricity system integration,” *Energy Policy*, vol. 87, Dec. 2015, pp. 260–269. Available: DOI 10.1016/j.enpol.2015.09.026, Online http://dx.doi.org/10.1016/j.enpol.2015.09.026.

[60] Y. Scholz, B. Fuchs, F. Borggrefe, K.-K. Cao, M. Wetzel, K. von Krbek, F. Cebulla, H.C. Gils, F. Fiand, M. Bussieck, T. Koch, D. Rehfeldt, A. Gleixner, D. Khabi, T. Breuer, D. Rohe, H. Hobbie, D. Schönheit, H.Ü. Yilmaz, E. Panos, S. Jeddi, and S. Buchholz, *Speeding up Energy System Models - a Best Practice Guide*, 2020. Available: Online https://elib.dlr.de/135507/.

[61] “Slurm Workload Manager, https://slurm.schedmd.com,” 2019. Available: Online https://slurm.schedmd.com/.

[62] K.-K. Cao, T. Pregger, Y. Scholz, H.C. Gils, K. Nienhaus, M. Deissenroth, C. Schimeczek, N. Krämer, B. Schober, H. Lens, T. Kneiske, and B. Idlbi, *Analysis of infrastructural options to integrate renewable energies in Germany and Europe considering security of supply (INTEEVER)*, Federal Ministry for Economic Affairs and Energy, 2019. Available: DOI https://doi.org/10.2314/KXP:1667221795.

[63] K.-K. Cao, T. Pregger, J. Haas, and H. Lens, “Analyzing the future role of power transmission in the European energy system,” *Frontiers in Energy Research*, vol. submitted draft, 2020.

[64] T. Brown, D. Schlachtberger, A. Kies, S. Schramm, and M. Greiner, “Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system,” *Energy*, vol. 160, Oct. 2018, pp. 720–739. Available: DOI 10.1016/j.energy.2018.06.222.

[65] Agora Verkehrswende, Agora Energiewende, and Regulatory Assistance Project (RAP), *Verteilnetzausbau für die Energiewende Elektromobilität im Fokus*, 2019. Available: Online https://www.agora-

energiewende.de/fileadmin2/Projekte/2018/Netzausbau_Elektromobilitaet/Agora-Verkehrswende_Agora-Energiewende_EV-Grid_WEB.pdf.

[66] ENTSO-E, *2nd ENTSO-E Guideline for Cost Benefit Analysis of Grid Development Projects*, European Network of Transmission System Operators for Electricity, 2018. Available: Online https://tyndp.entsoe.eu/Documents/TYNDP%20documents/Cost%20Benefit%20Analysis/2018-10-11-tyndp-cba-20.pdf.

APPENDIX

The following tables provide the project specific configuration of the models “REMix Germany” and “REMix Europe” used in the publications of this thesis. Their purpose is to provide rather technical information to experts in the field of energy system modeling.

The table column denoted as “Technology (class)” corresponds to the general technology modules available from the REMix modeling framework (see subsection 1.2.5). Although a higher number of REMix modules exist, this overview is limited to the modules, which have been at least applied in the context of the publications summarized in this thesis.

In “Used model features” it is indicated how general module settings are configured, which are optional. This column is only filled in if either default settings are changed or the indicated specification is expected to have a strong influence on the model behavior. This applies to the curtailment of renewable power generation, which also could be limited. However, to avoid artefacts by creating situations where surplus power is wasted by exploiting additional losses, it is set to be unlimited. With regard to conventional and combined heat and power plants, there exists the option to specify a substitution of the default fuel. This option is used in “REMix Europe” to model power-to-gas-to-power (indicated as “Synthetic fuel co-firing”). For electric vehicles load shifting can be enabled for different fixed time intervals, which distinguishes modeling of their temporal flexibility from the capabilities of stationary energy storage. Furthermore, there exist several options to restrict the emission of greenhouse gases either by making explicit assumptions on costs of emission allowances or by simply bounding the appropriate variables to a desired value.

In “Specifications” the technologies or other model specific parameters, which are explicitly considered in the appropriate model instance are provided. They are supplemented by information about the consideration of particular technologies and how capacities are determined. As “REMix Germany” and “REMix Europe” are usually executed multiple times, these settings may vary within the analyses of Publication 2 – 4. In order to indicate this in the tick boxes, the check-symbol is occasionally shown in brackets.

TABLE A-1: OVERVIEW OF REMIX MODULES USED AND PARAMETERIZED FOR APPLYING “REMIX GERMANY” IN PUBLICATION 2.

✓ yes
(✓) case-dependent
× no
⦸ irrelevant

	Technology (class)	Used model features	Specification	Considered	Model-exogenous capacities	Capacity expansion
Electricity	Biomass-fired power plants		Biomass power plants	✓	×	×
			Geothermal power plants	×	×	×
	Power generation from fluctuating renewable energy resources	Unlimited curtailment	Wind energy converters (Onshore)	✓	✓	×
			Wind energy converters (Offshore)	✓	✓	×
			Photovoltaic	✓	✓	×
			Run-of-river power plants	✓	✓	×
	Conventional thermal power plants		Lignite-fired power plants	✓	✓	×
			Open cycle gas turbines	✓	✓	×
			Combined cycle gas turbines	✓	✓	×
			Nuclear power plants	✓	✓	×
			Hard coal-fired power plants	✓	✓	×
	Concentrated solar power plants		Concentrated solar power plants	×	×	×
	Conventional power consumers		Conventional power consumers	✓	✓	⦸
	Electric vehicles		Electric vehicles	×	✓	⦸
Renewable Fuels	Electrolysis		Alkali-Elektrolyzers	×	×	×
			PEM-Elektrolyzers	×	×	×
	Hydrogen vehicles		Hydrogen vehicles	×	×	⦸
Heat	Electric boilers		Electric boiler for buildings	×	×	×
			Electric boiler for industry	×	×	×
			Electric boiler for district heating	×	×	×
	Gas boilers		Gas boiler for buildings	×	×	×
			Peak load boilers for biomass-fired cogeneration plants	×	×	×
			Peak load boilers for hard coal-fired cogeneration plants	×	×	×
			Gas boiler for industry	×	×	×
			Gas boiler for district heating	×	×	×
			Peak load boilers for lignite-fired cogeneration plants	×	×	×
	Combined heat and power plants		Hard coal-fired power plants for industry	×	×	×
			Combined cycle gas turbines for district heating	×	×	×
			Open cycle gas turbines for buildings	×	×	×
			Lignite-fired cogeneration plants for district heating	×	×	×
			Biomass-fired congeneration plants for buildings	×	×	×
	Heat pumps		Geothermal heat pumps	×	×	×
			Air heat pumps	×	×	×
	Heat consumers		Industrial heat consumers	×	×	⦸
			Heat consumers (buildings, services)	×	×	⦸
Spatial load balancing	HVAC electricity transmission		Overhead lines / cables	✓	✓	(✓)
	HVDC electricity transmission		Overhead lines / cables / sea cables	✓	×	(✓)
	Synthetic gas transmission			×	×	×
Temporal load balancing	Demand side management		Load shifting	×	×	×
			Load shedding	×	×	×
	Energy storage		Hydro reservoir power plants	×	×	×
			Pumped hydro storage	✓	✓	×
			Vanadium-Redox-Flow batteries	×	×	×
			Adiabatic compressed air storage	×	×	×
			Lithium-Ion batteries	✓	×	(✓)
			Warm water storage	×	×	×
			Pressure vessels for hydrogen	×	×	×
			Cavern storage for hydrogen	×	×	×
Global modeling constraints	Self-consumption quotas		0% / 50% / 80% / 100%	×	⦸	⦸
	Fuels		Unlimited availability	✓	⦸	⦸
	Emissions	Emission cap		✓	⦸	⦸
	Firm capacity		0% / 50% / 80% / 100%	×	⦸	⦸
	Heuristic temporal model decomposition			×	⦸	⦸

TABLE A-2: OVERVIEW OF REMIX MODULES USED AND PARAMETERIZED FOR APPLYING "REMIX EUROPE" FOR THE DEVELOPMENT OF SCENARIOS OF EUROPEAN POWER PLANT PORTFOLIOS IN PUBLICATION 3.

✓	yes
(✓)	case-dependent
×	no
⦸	irrelevant

	Technology (class)	Used model features	Specification	Considered	Model-exogenous capacities	Capacity expansion
Electricity	Biomass-fired power plants		Biomass power plants	✓	×	✓
			Geothermal power plants	✓	×	✓
	Power generation from fluctuating renewable energy resources	Unlimited curtailment	Wind energy converters (Onshore)	✓	✓	✓
			Wind energy converters (Offshore)	✓	✓	✓
			Photovoltaic	✓	✓	✓
			Run-of-river power plants	✓	✓	✓
	Conventional thermal power plants		Lignite-fired power plants	✓	✓	×
			Open cycle gas turbines	✓	✓	✓
			Combined cycle gas turbines	✓	✓	✓
			Nuclear power plants	✓	✓	(✓)
			Hard coal-fired power plants	✓	✓	×
	Concentrated solar power plants		Concentrated solar power plants	✓	×	(✓)
	Conventional power consumers		Conventional power consumers	✓	✓	⦸
	Electric vehicles		Electric vehicles	✓	✓	⦸
Renewable Fuels	Electrolysis		Alkali-Elektrolyzers	(✓)	(✓)	×
			PEM-Elektrolyzers	(✓)	(✓)	×
	Hydrogen vehicles		Hydrogen vehicles	(✓)	(✓)	⦸
Heat	Electric boilers		Electric boiler for buildings	✓	×	✓
			Electric boiler for industry	✓	×	✓
			Electric boiler for district heating	✓	×	✓
	Gas boilers		Gas boiler for buildings	×	×	×
			Peak load boilers for biomass-fired cogeneration plants	×	×	×
			Peak load boilers for hard coal-fired cogeneration plants	×	×	×
			Gas boiler for industry	×	×	×
			Gas boiler for district heating	×	×	×
			Peak load boilers for lignite-fired cogeneration plants	×	×	×
	Combined heat and power plants		Hard coal-fired power plants for industry	×	×	×
			Combined cycle gas turbines for district heating	×	×	×
			Open cycle gas turbines for buildings	×	×	×
			Lignite-fired cogeneration plants for district heating	×	×	×
			Biomass-fired congeneration plants for buildings	×	×	×
	Heat pumps		Geothermal heat pumps	✓	×	✓
			Air heat pumps	✓	×	✓
	Heat consumers		Industrial heat consumers	✓	✓	⦸
			Heat consumers (buildings, services)	✓	✓	⦸
Spatial load balancing	HVAC electricity transmission		Overhead lines / cables	×	×	×
	HVDC electricity transmission		Overhead lines / cables / sea cables	✓	✓	✓
	Synthetic gas transmission			×	⦸	⦸
Temporal load balancing	Demand side management		Load shifting	×	×	×
			Load shedding	×	×	×
	Energy storage		Hydro reservoir power plants	✓	✓	×
			Pumped hydro storage	✓	✓	✓
			Vanadium-Redox-Flow batteries	×	×	×
			Adiabatic compressed air storage	×	×	×
			Lithium-Ion batteries	✓	×	✓
			Warm water storage	×	×	×
			Pressure vessels for hydrogen	(✓)	(✓)	×
			Cavern storage for hydrogen	×	×	×
Global modeling constraints	Self-consumption quotas		0% / 50% / 80% / 100%	✓	⦸	⦸
	Fuels		Unlimited availability	✓	⦸	⦸
	Emissions	Emission cap	Global / national	✓	⦸	⦸
	Firm capacity		0% / 50% / 80% / 100%	✓	⦸	⦸
	Heuristic temporal model decomposition			×	⦸	⦸

TABLE A-3: OVERVIEW OF REMIX MODULES USED AND PARAMETERIZED FOR APPLYING “REMIX EUROPE” FOR ASSESSING THE IMPACT OF DIFFERENT TECHNOLOGIES FOR LOAD-BALANCING ON SYSTEM ADEQUACY IN PUBLICATION 3.

✓ yes
(✓) case-dependent
× no
⦸ irrelevant

	Technology (class)	Used model features	Specification	Considered	Model-exogenous capacities	Capacity expansion
Electricity	Biomass-fired power plants		Biomass power plants	×	×	×
			Geothermal power plants	✓	×	×
	Power generation from fluctuating renewable energy resources		Wind energy converters (Onshore)	✓	✓	(✓)
		Unlimited curtailment	Wind energy converters (Offshore)	✓	✓	×
			Photovoltaic	✓	✓	(✓)
			Run-of-river power plants	✓	✓	×
	Conventional thermal power plants		Lignite-fired power plants	✓	✓	×
		Synthetic fuel co-firing	Open cycle gas turbines	✓	✓	✓
			Combined cycle gas turbines	×	✓	×
			Nuclear power plants	×	✓	×
			Hard coal-fired power plants	×	✓	×
	Concentrated solar power plants		Concentrated solar power plants	✓	✓	(✓)
	Conventional power consumers		Conventional power consumers	✓	✓	⦸
	Electric vehicles	Load shifting for 2h, 4h, 8h	Electric vehicles	✓	✓	⦸
Renewable Fuels	Electrolysis		Alkali-Elektrolyzers	(✓)	×	(✓)
			PEM-Elektrolyzers	(✓)	×	(✓)
	Hydrogen vehicles		Hydrogen vehicles	(✓)	(✓)	⦸
Heat	Electric boilers		Electric boiler for buildings	✓	×	✓
			Electric boiler for industry	✓	×	✓
			Electric boiler for district heating	✓	×	✓
	Gas boilers		Gas boiler for buildings	✓	×	✓
			Peak load boilers for biomass-fired cogeneration plants	✓	×	✓
			Peak load boilers for hard coal-fired cogeneration plants	✓	×	✓
			Gas boiler for industry	✓	×	✓
			Gas boiler for district heating	✓	×	✓
			Peak load boilers for lignite-fired cogeneration plants	✓	×	✓
	Combined heat and power plants		Hard coal-fired power plants for industry	✓	✓	×
		Synthetic fuel co-firing	Combined cycle gas turbines for district heating	✓	✓	×
			Open cycle gas turbines for buildings	✓	✓	×
			Lignite-fired cogeneration plants for district heating	✓	✓	×
			Biomass-fired congeneration plants for buildings	✓	✓	×
	Heat pumps		Geothermal heat pumps	✓	✓	✓
			Air heat pumps	✓	✓	✓
	Heat consumers		Industrial heat consumers	✓	✓	⦸
			Heat consumers (buildings, services)	✓	✓	⦸
Spatial load balancing	HVAC electricity transmission		Overhead lines / cables	✓	✓	✓
	HVDC electricity transmission		Overhead lines / cables / sea cables	✓	✓	✓
	Synthetic gas transmission	Methanation of hydrogen		✓	⦸	⦸
Temporal load balancing	Demand side management		Load shifting	✓	✓	×
			Load shedding	✓	✓	×
	Energy storage		Hydro reservoir power plants	✓	✓	×
			Pumped hydro storage	✓	✓	✓
			Vanadium-Redox-Flow batteries	×	×	✓
			Adiabatic compressed air storage	×	×	✓
			Lithium-Ion batteries	✓	×	✓
			Warm water storage	×	×	✓
			Pressure vessels for hydrogen	(✓)	×	(✓)
			Cavern storage for hydrogen	(✓)	×	(✓)
Global modeling constraints	Self-consumption quotas		0% / 50% / 80% / 100%	×	⦸	⦸
	Fuels		Unlimited availability	×	⦸	⦸
	Emissions	Emission costs		✓	⦸	⦸
	Firm capacity		0% / 50% / 80% / 100%	×	⦸	⦸
	Heuristic temporal model decomposition			×	⦸	⦸

TABLE A-4: OVERVIEW OF REMIX MODULES USED AND PARAMETERIZED FOR APPLYING “REMIX GERMANY” IN PUBLICATION 4.

✓ yes
(✓) case-dependent
× no
⦸ irrelevant

	Technology (class)	Used model features	Specification	Considered	Model-exogenous capacities	Capacity expansion
Electricity	Biomass-fired power plants		Biomass power plants	✓	×	×
			Geothermal power plants	×	×	×
	Power generation from fluctuating renewable energy resources		Wind energy converters (Onshore)	✓	✓	×
		Unlimited curtailment	Wind energy converters (Offshore)	✓	✓	×
			Photovoltaic	✓	✓	×
			Run-of-river power plants	✓	✓	×
	Conventional thermal power plants		Lignite-fired power plants	✓	✓	×
			Open cycle gas turbines	✓	✓	×
			Combined cycle gas turbines	✓	✓	×
			Nuclear power plants	✓	✓	×
			Hard coal-fired power plants	✓	✓	×
	Concentrated solar power plants		Concentrated solar power plants	×	×	×
	Conventional power consumers		Conventional power consumers	✓	✓	⦸
	Electric vehicles		Electric vehicles	×	✓	⦸
Renewable Fuels	Electrolysis		Alkali-Elektrolyzers	×	×	×
			PEM-Elektrolyzers	×	×	×
	Hydrogen vehicles		Hydrogen vehicles	×	×	⦸
Heat	Electric boilers		Electric boiler for buildings	×	×	×
			Electric boiler for industry	×	×	×
			Electric boiler for district heating	×	×	×
	Gas boilers		Gas boiler for buildings	×	×	×
			Peak load boilers for biomass-fired cogeneration plants	×	×	×
			Peak load boilers for hard coal-fired cogeneration plants	×	×	×
			Gas boiler for industry	×	×	×
			Gas boiler for district heating	×	×	×
			Peak load boilers for lignite-fired cogeneration plants	×	×	×
	Combined heat and power plants		Hard coal-fired power plants for industry	×	×	×
			Combined cycle gas turbines for district heating	×	×	×
			Open cycle gas turbines for buildings	×	×	×
			Lignite-fired cogeneration plants for district heating	×	×	×
			Biomass-fired congeneration plants for buildings	×	×	×
	Heat pumps		Geothermal heat pumps	×	×	×
			Air heat pumps	×	×	×
	Heat consumers		Industrial heat consumers	×	×	⦸
			Heat consumers (buildings, services)	×	×	⦸
Spatial load balancing	HVAC electricity transmission		Overhead lines / cables	✓	✓	(✓)
	HVDC electricity transmission		Overhead lines / cables / sea cables	✓	×	(✓)
	Synthetic gas transmission			×	×	×
Temporal load balancing	Demand side management		Load shifting	×	×	×
			Load shedding	×	×	×
	Energy storage		Hydro reservoir power plants	✓	✓	×
			Pumped hydro storage	✓	✓	×
			Vanadium-Redox-Flow batteries	×	×	×
			Adiabatic compressed air storage	×	×	×
			Lithium-Ion batteries	✓	×	(✓)
			Warm water storage	×	×	×
			Pressure vessels for hydrogen	×	×	×
			Cavern storage for hydrogen	×	×	×
Global modeling constraints	Self-consumption quotas		0% / 50% / 80% / 100%	×	⦸	⦸
	Fuels		Unlimited availability	✓	⦸	⦸
	Emissions	Emission cap		✓	⦸	⦸
	Firm capacity		0% / 50% / 80% / 100%	×	⦸	⦸
	Heuristic temporal model decomposition			✓	⦸	⦸

DECLARATION OF AUTHORSHIP

I hereby certify that the dissertation entitled

“Modeling Energy Scenarios with Power-Flow Constraints - Transparency, challenges and system adequacy”

is entirely my own work except where otherwise indicated. Passages and ideas from other sources have been clearly quoted.

Name: Karl-Kiên Cao

Signed: ____________________

Date: ____________________