Constructing and evaluating energy futures – life cycle environmental impacts, material demand and transparency of energy scenarios

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Vorwort

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(4) Junne, T.; Xiao, M.; Xu, L.; Wang, Z.; Jochem, P.; Pregger, T. How to assess the quality and transparency of energy scenarios: Results of a case study. Energy Strategy Reviews 2019, 26, 100380, DOI: https://doi.org/10.1016/j.esr.2019.100380.

Other Papers

(5) Moreno-Leiva, S.; Haas, J.; Junne, T.; Valencia, F.; Godin, H.; Kracht, W.; Nowak, W.; Eltrop, L. Renewable energy in copper production: A review on systems design and methodological approaches. Journal of Cleaner Production 2020, 246, 118978, DOI: https://doi.org/10.1016/j.jclepro.2019.118978.

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(7) Vandepaer, L.; Junne, T.; Gibon, T.; Fernandez Astudillo, M.; Bauer, C.; Amor, B. The integration of life cycle assessment into energy system models: best practices, current challenges and aim for the next decade. Submitted. Renewable and Sustainable Energy Reviews.

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Abstract

The transformation of the energy system may contribute to a number of environmental challenges and is associated with high material use. Therefore, when analyzing future energy systems, it is necessary to quantify the effects on the environment and the material requirements to maintain the functionality of the ecosystems and to identify potential material bottlenecks of transformation strategies. However, planning and transforming the energy system while quantifying the impacts on natural and human systems and the material requirements is a difficult task with many dimensions and complex dynamics. Sound statements can therefore only be made using a transdisciplinary approach and several numerical models.

In this thesis, analytical frameworks are developed for the environmental assessment and for quantifying the abiotic resource demand of future energy systems. The first framework quantifies environmental indicators using the method of life cycle assessment (LCA). The second framework quantifies the material demand using material flow analysis (MFA). These methods are then combined with energy system models (ESMs) and energy scenarios to gain insight into the environmental co-benefits and adverse side effects of the energy transition and to assess the pressure on the supply system of abiotic resources.

In order to obtain environmental indicators that correspond with the forward-looking nature of ESMs, this thesis develops a prospective LCA approach based on the integration of global scenarios for the electricity sector into the life cycle inventory (LCI) database used. Thus, future versions of the LCI database will be generated for several time steps in different global scenarios. This database is supplemented with additional LCI data from energy technologies present in the ESMs applied. The term ‘energy technologies’ encompasses all energy-related technologies, such as power generation, conversion and transport technologies. In order to couple LCI data with ESMs, adjustments must first be made to the LCI data of the energy technologies that are included in the ESM. In a case study for Germany, it is shown that the transformation of the energy system leads to improvements for a majority of environmental indicators, but is accompanied by additional land use and increased depletion potential of abiotic resources (Paper 1). This Paper also shows that the inclusion of global scenarios for the electricity sector in the LCI database can have a considerable influence on the environmental profiles of the energy scenarios. However, these so-called ex-post assessments of energy scenarios have the disadvantage that they assess the environmental impacts of mostly purely minimum-cost systems. The environmental impacts are not incorporated into the expansion and operational decisions of the technologies considered in the ESMs.

Therefore, in Paper 2, environmental impacts of energy technologies are endogenously integrated into an optimizing ESM. In addition, the option of

minimizing impacts is added to the objective function of the ESM to enable the environmental optimization of the energy system from a life cycle perspective. A case study in Paper 2 considers not only system costs but also life cycle climate impacts. The results allow an analysis of the environmental and economic interactions of energy systems. The results show that the energy systems considered, which are highly ambitious in terms of avoiding direct carbon dioxide emissions, still generate significant greenhouse gas (GHG) emissions, which are mainly caused by the upstream supply chains of the energy technologies. A reduction of life cycle GHG emissions compared to the cost optimal system leads to a technology shift towards an increased expansion of wind power plants (offshore and onshore) at moderate cost increases. The reduction of life cycle GHG emissions also leads to significant environmental benefits, such as for human health, air pollution, ozone depletion, and acidification. Adverse side effects occur in particular with regard to water consumption and ionizing radiation. The methodological approach followed in Paper 2 demonstrates the added value of combining ESM and LCA, which has been largely neglected so far: the possibility to create and assess energy scenarios that result from a reduction in the environmental impact of energy technologies over their entire life cycle.

The results of coupling ESMs and LCA in Paper 1 and 2 show the importance of considering a wide range of impact categories in the assessment of the energy system transformation. However, there are uncertainties in LCA, especially with regard to the LCI data used.

Papers 1 and 2 illustrate that ambitious energy scenarios in terms of avoiding direct CO_2 emissions have an increased potential for abiotic resource depletion compared to today and/or less ambitious scenarios. This depletion potential is driven not only by bulk materials such as steel and copper, but also by the demand for other metals such as lithium, cobalt or rare earths. The indicator for assessing abiotic resource depletion potential in LCA is based on current conditions and is of limited use for assessing possible future demand dynamics and material bottlenecks. Therefore, in Paper 3, the methodology of dynamic MFA is applied to estimate the demand for lithium, cobalt, dysprosium and neodymium in global energy scenarios and to compare this demand with estimates of reserves, resources and annual production. It is shown that potential shortages may especially affect the use of lithium and cobalt in batteries for electromobility as well as for stationary storage applications.

The combination of energy scenarios and ESMs with LCA and MFA shows a great potential that has so far only been used to a very limited extent. The methods developed in Papers 1, 2 and 3 are the basis for a robust and comprehensive construction of energy scenarios and of the derivative energy policies.

The use of energy scenarios is regarded as a valid concept for a systematic analysis of the design of future energy systems. Thus, energy scenarios have become a central element in the societal debate about the design of future energy supply systems, and the construction process of the scenarios should be accessible and comprehensible for everybody who is interested in this topic. Paper 4 refrains from working with scenarios and ESMs themselves (Papers 1-3) and addresses the question to what extent current scenario studies meet the criteria of quality and transparency defined in the scientific literature. An analysis of three scenarios shows that the underlying model-based methods lack information on data exchange between models, a transparent description of model couplings, and a discussion of the rationality of method selection and of the strengths and weaknesses of the approaches applied. Based on these findings, general advice is provided for energy scenario developers on how to ensure transparency and traceability in future energy scenario studies.

Zusammenfassung

Die Transformation des Energiesystems trägt potenziell zu einer Reihe von ökologischen Herausforderungen bei und ist mit einem hohen Materialeinsatz verbunden. Daher ist es bei der Analyse zukünftiger Energiesysteme notwendig, Auswirkungen auf die Umwelt und den Materialbedarf zu quantifizieren, um die Funktionalität der Ökosysteme zu erhalten und potenzielle Materialengpässe von Transformationsstrategien zu identifizieren. Die Planung und Transformation des Energiesystems bei gleichzeitiger Quantifizierung der Auswirkungen auf die natürlichen und menschlichen Systeme und des Materialbedarfs ist jedoch eine schwierige Aufgabe mit vielen Dimensionen und komplexer Dynamik. Fundierte Aussagen können daher nur mit einem transdisziplinären Ansatz und mehreren numerischen Modellen getroffen werden.

In dieser Arbeit werden analytische Modellierungsansätze für die Umweltbewertung und für die Quantifizierung des abiotischen Ressourcenbedarfs zukünftiger Energiesysteme entwickelt. Der erste Modellierungsansatz quantifiziert Umweltindikatoren mit der Methode der Ökobilanz (LCA). Der zweite Modellierungsansatz quantifiziert den Materialbedarf mit Hilfe der Materialflussanalyse (MFA). Diese Methoden werden dann mit Energiesystemmodellen (ESMs) und Energieszenarien kombiniert, um Einblicke in die ökologischen Zusatznutzen und negativen Nebeneffekte der Energiewende zu gewinnen und den Druck auf das Versorgungssystem abiotischer Ressourcen zu bewerten.

Um Umweltindikatoren zu erhalten, die dem zukunftsorientierten Charakter von ESMs entsprechen, wird in dieser Arbeit ein prospektiver LCA-Ansatz entwickelt, der auf der Integration globaler Energieszenarien für den Elektrizitätssektor in die verwendete Lebenszyklusinventardatenbank (LCI-Datenbank) basiert. So werden zukünftige Versionen der LCI-Datenbank für mehrere Zeitschritte unter verschiedenen globalen Szenarien erzeugt. Diese Datenbank wird mit zusätzlichen LCI-Daten von Energietechnologien, die in den verwendeten ESMs vorhanden sind, ergänzt. Der Begriff "Energietechnologien" umfasst alle energiebezogenen Technologien, wie z. B. Stromerzeugungs-, Umwandlungs- und Transporttechnologien. Zur Kopplung von LCI-Daten mit ESMs ist es zunächst notwendig Anpassungen der LCI-Daten von Energietechnologien vorzunehmen, die im ESM berücksichtigt sind (Paper 1). In einer Fallstudie für Deutschland wird in Paper 1 gezeigt, dass die Transformation des Energiesystems zwar zu Verbesserungen bei einem Großteil der Umweltindikatoren führt, aber mit zusätzlichem Flächenverbrauch und erhöhtem Erschöpfungspotenzial von mineralischen Ressourcen einhergeht. In dieser Arbeit wird auch gezeigt, dass Berücksichtigung globaler Szenarien für den Elektrizitätssektor in der LCI-

Datenbank wesentlichen Einfluss auf die Umweltprofile der bewerteten Energieszenarien haben kann. Diese sogenannten Ex-post-Bewertungen von Energieszenarien haben jedoch den Nachteil, dass sie die Umweltauswirkungen von meist reinen kostenminimalen Systemen bewerten. Die Umweltauswirkungen fließen nicht in die Ausbau- und Einsatzentscheidungen der in den ESMs berücksichtigten Technologien ein.

Daher werden in Paper 2 die Umweltauswirkungen von Energietechnologien endogen in ein optimierendes ESM integriert. Zusätzlich wird die Zielfunktion des ESM um die Option der Minimierung der Umweltauswirkungen erweitert, um die Umweltoptimierung des Energiesystems aus Sicht des Lebenszyklus zu ermöglichen. Eine Fallstudie in Paper 2 betrachtet nicht nur die Systemkosten, sondern auch die lebenszyklusbasierten Treibhausgas-Emissionen (THG-Emissionen). Die Ergebnisse erlauben eine Analyse der ökologischen und ökonomischen Wechselwirkungen von Systemen. Es wird gezeigt, dass in den betrachteten Systemen, die in Bezug auf die Vermeidung direkter Kohlendioxid-Emissionen sehr ambitioniert sind, signifikante THG-Emissionen verbleiben, die hauptsächlich durch die vorgelagerten Lieferketten der Energietechnologien verursacht werden. Eine Reduktion der Lebenszyklus-THG-Emissionen gegenüber dem kostenoptimalen System führt zu einem Technologiewandel hin zu einem verstärkten Ausbau von Windkraftanlagen (offshore und onshore) bei moderaten zusätzlichen Kosten. Die Reduktion der Lebenszyklus-THG-Emissionen führt darüber hinaus zu erheblichen Umweltvorteilen, z. B. für die menschliche Gesundheit, die Luftverschmutzung, den Ozonabbau und die Versauerung. Ungünstige Nebeneffekte treten insbesondere beim Wasserverbrauch und bei ionisierender Strahlung auf. Der in Paper 2 verfolgte methodische Ansatz zeigt den Mehrwert der Kombination von ESM und LCA, der bisher weitgehend vernachlässigt wurde: Die Möglichkeit, Energieszenarien zu erstellen und zu bewerten, die aus einer Verringerung der Umweltauswirkungen von Energietechnologien über ihren gesamten Lebenszyklus resultieren.

Die Ergebnisse der Kopplung von ESM und LCA in Paper 1 und 2 zeigen, wie wichtig es ist, bei der Bewertung der Energiewende neben den direkten Kohlenstoffemissionen eine Vielzahl von ökologischen Wirkungskategorien zu berücksichtigen. Allerdings gibt es in der Ökobilanz Unsicherheiten, insbesondere hinsichtlich der verwendeten LCI Daten.

Paper 1 und 2 verdeutlichen, dass ambitionierte Energieszenarien im Sinne der Vermeidung direkter CO_2 Emissionen im Vergleich mit heute und/oder weniger ambitionierten Szenarien ein erhöhtes Potenzial für die Erschöpfung abiotischer Ressourcen aufweisen. Neben Massenmaterialien wie Stahl und Kupfer wird dies auch durch andere Metalle wie Lithium, Kobalt oder Seltene Erden getrieben. Der Indikator zur Bewertung des abiotischen Ressourcenerschöpfungspotenzials in der Ökobilanz basiert auf aktuellen

Bedingungen und ist für die Bewertung möglicher zukünftiger Nachfragedynamiken und Materialengpässe nur bedingt geeignet. Daher wird in Paper 3 die Methodik der dynamischen MFA angewendet, um den Bedarf an Lithium, Kobalt, Dysprosium und Neodym in globalen Energieszenarien abzuschätzen und mit Schätzungen der Reserven, Ressourcen und der jährlichen Produktion zu vergleichen. Es wird gezeigt, dass insbesondere der Einsatz von Lithium und Kobalt in Batterien für die Elektromobilität sowie für stationäre Energieanwendungen potenziellen Engpässen unterliegen könnte.

Die Kombination von ESM und Energieszenarien mit LCA und MFA zeigt ein großes Potenzial, das bisher nur in sehr geringem Umfang genutzt wird. Die in den Papern 1, 2 und 3 entwickelten Methoden sind die Grundlage für eine robustere und umfassendere Erstellung und Bewertung von Energieszenarien und daraus resultierender Energiepolitik.

Energieszenarien werden als Konzept für eine systematische Analyse der Gestaltung zukünftiger Energiesysteme angesehen. Damit sind Energieszenarien zu einem zentralen Element der gesellschaftlichen Debatte um die Gestaltung der zukünftigen Energieversorgung geworden und der Erstellungsprozess sollte jedem, der sich für dieses Thema interessiert, zugänglich und nachvollziehbar sein. Paper 4 nimmt Abstand von der Arbeit mit Szenarien und ESMs selbst (Paper 1-3) und geht der Frage nach, inwieweit aktuelle Szenariostudien den in der wissenschaftlichen Literatur definierten Qualitäts- und Transparenzkriterien entsprechen. Die Analyse von drei Szenarien zeigt, dass es den zugrundeliegenden modellbasierten Methoden an Informationen zum Datenaustausch zwischen den Modellen, an einer transparenten Beschreibung der Modellkopplungen sowie an einer Diskussion der Rationalität der Methodenwahl und der Stärken und Schwächen der verwendeten Ansätze mangelt. Basierend auf diesen Ergebnissen werden allgemeine Ratschläge für Entwickler von Energieszenarien gegeben, wie Transparenz und Nachvollziehbarkeit in zukünftigen Energieszenariostudien sichergestellt werden können.

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Table of abbreviations

COP 21	Paris Climate Conference
CSP	Concentrated Solar Power
ESM	Energy System Model
ESOM	Energy System Optimization Model
ESSM	Energy System Simulation Model
EUNA	Europe and North Africa
FRITS	Framework for the Assessment of Environmental Impacts of Transformation Scenarios
GDP	Gross Domestic Product
GHG	Greenhouse Gas
IAM	Integrated Assessment Model
JRC	Joint Research Centre
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MFA	Material Flow Analysis
N.B.	Nota Bene
NEEDS	New Energy Externalities Developments for Sustainability
PtM	Power-to-Methane
PV	Photovoltaic
REMIND	Regional Model of Investment and Development
REMix	Renewable Energy Mix
THEMIS	Technology Hybridized Environmental-Economic Model with Integrated Scenarios
TIMES	The Integrated Markal Efom System

1 Introduction

1.1 Background and motivation

1.1.1 The role of energy scenarios for the energy system transformation

Fundamental changes in the energy system are necessary to achieve the goals of the Paris Climate Conference (COP 21), namely limiting the global temperature increase to well below 2°C in order to limit the harmful effects of global warming [2]. It is expected that these changes will be strongly influenced by government policies and international cooperation on environmental, technological, and economic aspects [3]. To inform these policies and collaborations, energy scenarios are indispensable for the assessment of the energy transition and for the design of a future energy system [4].

Energy system models (ESMs) help design mitigation strategies by incorporating and comparing technologies that provide similar system services but have different technical and economic characteristics. Well-known examples of models that are used to assess future energy systems are integrated assessment models (IAMs) [5], energy system optimization models (ESOMs) [6] and energy system simulation models (ESSMs) [7, 8]. Among these model types, bottom-up ESOMs and ESSMs with a high level of technology detail are commonly used for long-term analysis of large-scale energy systems with varying regional focus (e.g. national [9] or global [10]). The model results usually include the consumption of different primary energy carriers, energy technology capacities and their operation, as well as system costs and direct, on-site carbon emissions.

The driver of these models is the exogenously defined demand for energy services, which is usually estimated based on key factors such as assumptions regarding population development, gross domestic product (GDP), consumer behavior, and efficiency increase through technological progress. On the one hand, these models can be used to explore the effects of political decisions on the development of the energy system with so-called explorative scenarios. On the other hand, so-called normative scenarios can be used to quantify the efforts required to achieve certain goals, such as limiting carbon dioxide (CO_2) emissions [11].

However, the deployment of energy infrastructure as well as the operation of technologies is associated with impacts on human health, on ecosystems, and on abiotic as well as biotic resources that go beyond the ‘traditional’ system boundaries of ESMs. These impacts have not yet received much attention in energy scenario analysis. In addition to broadening the scope of assessment criteria, the increasingly high complexity of scenario analyses calls for addressing the overarching issue of the comprehensibility and transparency of scenario studies in order to ensure that they are understandable to all relevant stakeholders.

1.1.2 The need to consider life cycle environmental impacts in energy scenario modeling

In order to achieve a systemic change that keeps global warming below 2°C, large-scale deployment of low-carbon energy supply technologies is necessary along with other measures. However, as energy supply switches from fossil fuels to renewable sources, environmental impacts tend to shift to processes not captured by 'traditional' ESMs, which typically map only direct, on-site carbon emissions during operation [12].

Life cycle assessment (LCA) has been increasingly used in recent years to comprehensively assess the potential environmental impacts of various goods and services throughout their whole life cycle. Life cycle impact assessment (LCIA) methods aggregate life cycle inventories (LCIs), which include thousands of substance flows, into indicators [13]. The LCIA methods encompass many cause-effect pathways, from particulate matter and its impact on human health to resource consumption and its impact on resource depletion potential [14]. In this context, LCA helps to systematically analyze production systems but also policy directives and to find ways to quantify their impacts on the environment [15]. A key goal of LCA is to avoid burden shifting from one environmental impact to another or from one stage of the life cycle to another [16]. Thus, LCA is a suitable method to fairly compare the environmental impacts of, for example, renewable and fossil fuel-based energy systems. Furthermore, it can be combined with ESMs to compare ambitious energy systems in order to identify potential co-benefits and adverse side effects of certain transformation strategies. Results may help policymakers to initiate appropriate measures and thus avoid undesired environmental effects at an early stage.

This thesis explores the great potential of combining the two methods, energy system analysis on the one hand and LCA on the other. This potential has recently also been recognized by other authors. Hence, a number of case studies first developed and applied methods for LCA-based ex-post assessment of power systems at the time of starting the research for the present thesis or shortly thereafter [17-22]. However, as these studies focused on the power system only, they did not include the assessment of important sectoral interactions such as direct and indirect electrification of transport and heat and their consequences on the environment. These sector interlinkages are also accompanied by methodological challenges in combining LCA and ESMs, which were not addressed in the case studies that exclusively considered electric power generation.

While LCA-based ex-post assessments of energy systems provide meaningful insights into the environmental performance of given scenarios, they do not use the full potential of model coupling to determine environmentally improved system configurations relative to the original model setups. More specifically, these assessments overlook solutions that internalize life cycle environmental impacts. At the start of the present research, integration work was usually characterized by translating life cycle emissions into external costs and including these in the cost optimization [23-25]. Therefore, another area of great, as yet unexplored potential was the integration of LCA indicators into ESMs as additional objective functions.

1.1.3 Application of material flow analysis to estimate potential material shortages arising from the energy transition

The shift towards certain technologies to decarbonize the energy system often also means that varying amounts of different metals have to be utilized. In LCIA, abiotic resource depletion is usually included as an impact category. However, the LCIA methods available evaluate how current natural resource use affects the opportunities of future resource users [26]. For example, the widely used characterization models of abiotic resource depletion are based on the ratio between current annual extraction and the square of natural stock estimates [27]. While they capture the present depletion potential, they are not well suited to assess issues of potential future supply shortages of materials, especially of those materials that are not yet used in large quantities [28].

Currently, energy scenarios mostly neglect the material foundation associated with the transitions outlined. The future demand for specific metals due to the energy technologies deployed in the energy scenarios can be assessed using material flow analysis (MFA). MFA has been defined as “a systematic assessment of the flows and stocks of materials within a system defined in space and time” [29]. Due to the law of conservation of matter, the results of an MFA can be verified by means of a simple material balance comparing all inputs, stocks and outputs of a system [29].

In order to quantify the demand for metals in energy scenarios, studies were conducted at different geographical scales focusing on various metals. The scales vary from single countries [30] or groups of countries [31, 32] to global assessments [33-35], and the studies focus either on specific metals in specific energy technologies or on various metals and their use in various energy technologies. However, few studies included all energy technologies and non-energy sectors that use a particular metal. Furthermore, the technological representation of most energy scenarios is too general (e.g. considering only the technology group ‘Li-ion battery’) to derive quantitative implications for material requirements, hence it is also necessary to investigate possible technological specifications within each technology group (e.g. LiFePO battery) and the resulting uncertainties for future material requirements in more detail.

Primary material demand can be reduced through dematerialization, metal and/or technology substitution, and recycling. Dematerialization is the reduction in the quantities of materials needed to serve economic functions, or the decrease in the mass of materials used in final industrial products over time [36]. Substitution can apply at the level of the metal, the component, or the technology. Metal-for-metal substitution is challenging, as it is only possible with a metal that is produced in greater quantities than the one it is intended to replace [37]. Graedel et al. [38] have investigated the substitution potential for 62 different metals in their main uses and showed that there are no exemplary substitutes for any of the metals that are suitable for all the metals' main uses. Thus, technology-for-technology or component-for-component substitution could have a greater potential for reducing primary material demand than metal-by-metal substitution. Recycling means that at the end of their life cycle, products pass through appropriate recycling chains and can be reused in the manufacture of new products, thus reducing the need for primary materials [39]. To date, however, recycling rates for most metals are still negligibly low [40].

With the use of MFA, it is possible to capture the aforementioned effects on the future demand for materials pivotal to the energy transition. Indications of potential future bottlenecks caused by the deployment of new technologies in the energy and transport system can be derived by comparing annual or cumulative primary material requirements of the energy transition with annual primary production or reserves and resources. This comparison can deliver important information for the management of today's resources and raw materials as well as for economic and environmental policy making. Furthermore, it allows to draw conclusions about which technologies need to be further developed in order to reduce the consumption of potentially critical materials.

Quantifying long-term demand and comparing it to geological deposits also complements current studies on the criticality of metals, which do not provide an assessment of the long-term outlook for potential material shortages. In both the scientific literature and governmental organizations, various criticality indicators have been developed in response to growing concerns about the supply of certain metals due to factors such as the high concentration and the political instability of mining countries, import dependency, and the geographical distribution of reserves. These criticality indicators can be used, for example, by companies or geographical regions, such as the EU [41-46]. However, such indicators mainly refer to the present or the near future, also because many of the factors considered are difficult to project into the longer term (such as the political stability of mining countries) [47].

1.1.4 Evaluating energy scenario studies with regard to their transparency and comprehensibility

The policy relevance of energy scenarios requires the entire scenario development process to be highly transparent. However, in recent years, the transparency had decreased due to the increasing complexity of these studies, even though transparency and comprehensibility are important for society, politics, research and industry. To put it simply, it should no longer be acceptable for research and policy advice to merely present diagrams of the interactions of the models used for scenario building, and the assumptions and reasons for the selection of data and models should be explained and documented in detail. In this context, Cao et al. [48] developed transparency criteria based on expert judgments and provided a transparency checklist for the scientific community. The topic of comprehensibility and transparency of energy scenarios was also addressed and worked on in courses of my PhD fellowship at the 'Helmholtz Research School on Energy Scenarios' [49].

Some scenarios rely on a very strong role of negative emission technologies [50, 51], others on a high share of fluctuating renewables with high shares of electricity storage [52], and others on a substantial role of dispatchable renewables, such as concentrated solar power (CSP) [53, 54]. Scenarios also vary widely in terms of their assumptions about the evolution of energy demand and user behavior. Given these variations in terms of assumptions and strategies for decarbonizing the energy system, it is important to understand the extent to which the quality and transparency of energy scenarios can be evaluated based on published scenario studies.

1.2 Objectives and research questions of the thesis

Grunwald [55] described the life path of energy scenarios, along which many research questions arise that need to be answered by interdisciplinary approaches (Figure 1). The path begins with the 'construction' of energy scenarios on the basis of quantitative models or qualitative assumptions or a combination of both. During this stage, there are fundamental decisions to be made in the context of model building, such as the determination of the system boundaries and the choice of modeling approaches. The scenario construction also includes linking ESMs or their results with other methods (e.g. for environmental impact assessment or to consider implications with regard to the social acceptance of energy technologies). The scenarios can then be evaluated for their content after dissemination. The 'users' evaluation' of energy scenarios is initially aimed at the statements made and the results achieved in the scenario studies. In addition, the objectifiability of the scenario analysis is to be examined. This phase also explores the extent to which it is possible to uncover biases, ideological presuppositions, interests, and premises, all of which have consequences in the ‘usage’ phase of the energy scenarios for decisions, for opinion formation or for the structuring of public debates.

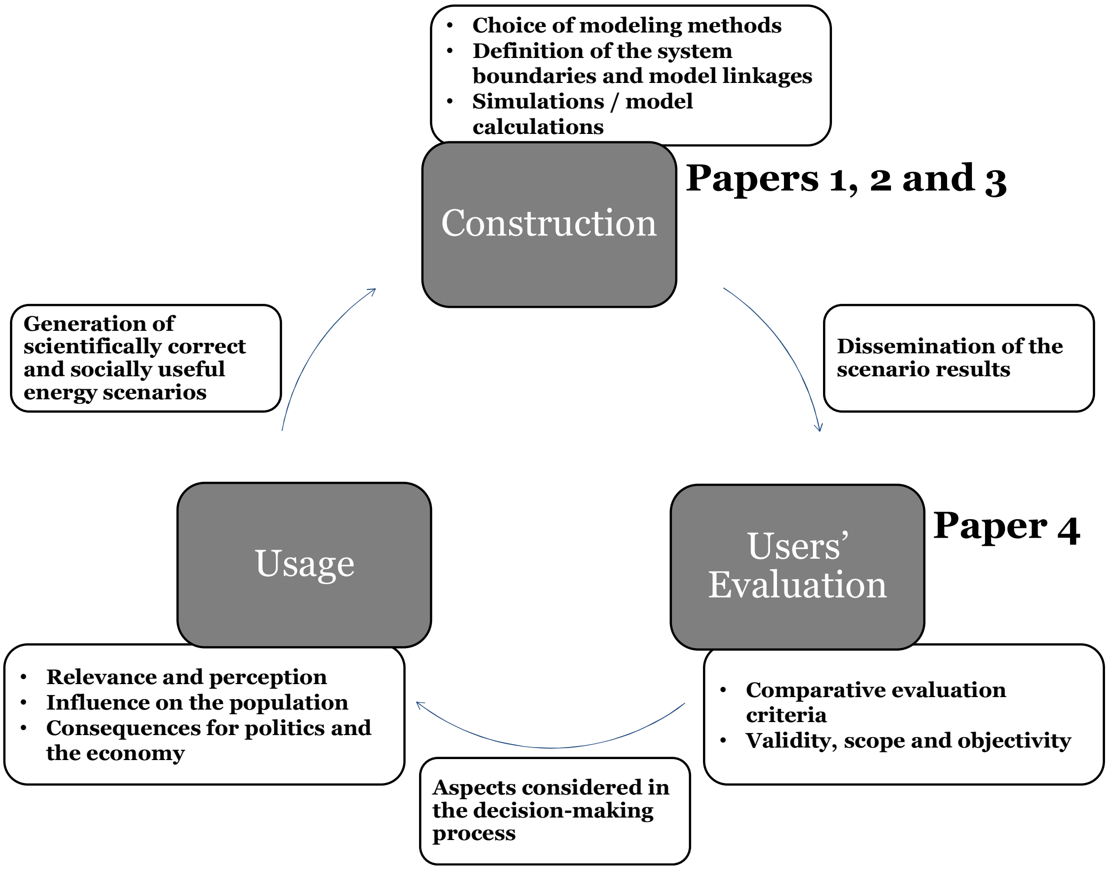

Figure 1. Positioning of the Papers of this dissertation in the life path of energy scenarios as defined by Grunwald [55]. The wording for the individual steps are largely adapted from Schmidt-Scheele [56].

This dissertation addresses two stages in the life path of energy scenarios as defined by Grunwald [55]. First, it contributes to the ‘construction’ phase by developing scenario analysis frameworks that allow for the quantification of the life cycle-based environmental impacts and the material requirements of energy scenarios. Methodologies used for this purpose are LCA and MFA. Furthermore, the scenario calculation itself is modified by adding an additional objective function and an algorithm to perform multi-objective optimization in an ESOM. These contributions to the ‘construction’ phase comprise Papers 1, 2 and 3. Moreover, the ‘users’ evaluation’ phase of energy scenarios is addressed in Paper 4. Here, the objective is to develop a comprehensive approach to evaluate and compare the quality of energy scenario studies. The focus is on aspects of comprehensibility and transparency within and outside the applied modeling approaches in order to gain a deep understanding of the scenario results.

- This dissertation first addresses the methodological challenges of coupling ESMs with LCI data and applies the developed method to energy scenarios with a focus on Germany (Paper 1). Hence, the first aim is to answer the following research questions: *How must LCI data be adapted to evaluate the environmental impact of multi-sectoral energy scenarios? What environmental co-benefits and adverse side-effects can be expected from the transformation of the energy system?*

- While LCAs of existing scenarios provide insights into their environmental performance, they do not use the full potential of method coupling to determine environmentally improved system configurations relative to the original scenario setups. Therefore, an ESOM with a focus on the power system in Europe and North Africa (EUNA) is parameterized with life cycle indicators to calculate a two-dimensional pareto front with the objectives system costs and life cycle GHG emissions (Paper 2). Based on this model enhancement, the following research questions are to be answered: *What are the trade-offs between system costs and life cycle GHG emissions? What is the structure of the power system and what is the electricity grid demand for the calculated solutions on the pareto front?*
- The transformation of the energy system propagated in energy scenarios has consequences for the demand for materials that are essential for the functioning of certain energy technologies. This work also aims to contribute to the quantification of future demand for metals and to assess potential bottlenecks that may occur in the energy transition (Paper 3) by answering the following research questions: *How high is the future global material demand that is related to the technology expansion in different energy scenarios considering different market shares of energy technologies, variations in material demand and recycling rates? Could bottlenecks potentially occur?*
- Improvements of energy scenario studies at the 'users' evaluation' stage are essential in order for them to have a desirable influence on the economy, society and policy (Paper 4). Based on the evaluation of relevant scenarios for Germany, Europe and the world as a whole, the following research questions are answered: *To what extent can scenario analyses be evaluated on the basis of published scenario studies? How can transparency and comprehensibility be improved in future energy scenario studies?*

The research questions and associated objectives of the Papers are summarized in Table 1.

Table 1. Summary of research questions, objectives and classification of the focus.

Research questions	**Objectives**	**Focus on content**	**Focus on methodology**
1) How must LCI data be adapted to evaluate the environmental impact of multi-sectoral energy scenarios? What environmental co-benefits and adverse side-effects can be expected from the transformation of the energy system?	• Identification of necessary adaptions of LCI data for the assessment of multi-sectoral energy scenarios • Development of a framework for the life cycle assessment of energy scenarios • Application of the framework to scenarios for Germany	☐	☒
2) What are the trade-offs between system costs and life cycle GHG emissions? What is the structure of the power system and what is the electricity grid demand for the calculated solutions on the pareto front?	• Enhancement of an ESOM to enable the integration of additional environmental indicators into the objective functions and the ex-post assessment of the results • Implementation of an algorithm for multi-objective optimization • Analysis of the trade-offs between system costs and climate impacts and the associated system configurations	☒	☐
3) How high is the future global material demand that is related to the technology expansion in different energy scenarios considering different market shares of energy technologies, variations in material demand and recycling rates? Could bottlenecks potentially occur?	• Analysis of the influence of market shares and the specific material content of energy technologies on the material demand in global energy scenario • Analysis of possible material bottlenecks • Discussion of the implications of the study from the perspective of energy systems modeling	☒	☐
4) To what extent can scenario analyses be evaluated on the basis of published scenario studies? How can transparency and traceability be improved in future energy scenario studies?	• Review of energy scenarios according to their compliance with predefined transparency criteria • Present general advice for energy scenario developers on how to ensure transparency and comprehensibility in future energy scenario studies	☒	☐

2 Papers

Attached below are the four Papers collected in this dissertation. Essential contextual information as well as methods and main results of each Paper are described in tables. In addition, these tables contain general information, such as the author's contribution to the related scientific process. In each of the attached Papers, the author of this dissertation is the first author (i.e. the lead author).

2.1 Paper 1

Status	**Published in:** Sustainability 12 (9), 8225 (2020), Special Issue Analyzing Development Paths of Emerging Energy Technologies
Title	Environmental Sustainability Assessment of Multi-Sectoral Energy Transformation Pathways: Methodological Approach and Case Study for Germany
Co-Authors	Sonja Simon, Jens Buchgeister, Maximilian Saiger, Manuel Baumann, Martina Haase, Christina Wulf, Tobias Naegler
Publication year	2020
Access	https://doi.org/10.3390/su12198225 ☒ Gold Open Access ☐ Green Open Access ☐ Closed access
Contributions	☒ Conceptualization ☒ Methodology ☒ Software ☒ Validation ☒ Formal analysis ☒ Investigation ☒ Data curation ☒ Writing: original draft preparation ☒ Writing: review and editing ☐ Supervision ☐ Funding acquisition
Specific objective	Development of a novel framework for the assessment of environmental impacts of multi-sectoral energy scenarios.
Thesis-overarching objectives	2.a) Implementation of methods to manipulate the LCI data of foreground technologies for model coupling 2.b) Adjustment of the background LCI database to consider the forward-looking nature of such analysis 2.c) Analysis of the environmental impact of energy scenarios for Germany
Methodology	Manipulation of foreground LCI data, integration of future background scenarios on the power system into the background LCI database, coupling of indicators with output from an ESM.
Key outcome	Framework that allows the assessment of environmental impacts of multi-sectoral energy scenarios (FRITS). More robust statements on environmental co-benefits and adverse side effects in scenario assessments.

sustainability

MDPI

Article

Environmental Sustainability Assessment of Multi-Sectoral Energy Transformation Pathways: Methodological Approach and Case Study for Germany

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Abstract: In order to analyse long-term transformation pathways, energy system models generally focus on economical and technical characteristics. However, these models usually do not consider sustainability aspects such as environmental impacts. In contrast, life cycle assessment enables an extensive estimate of those impacts. Due to these complementary characteristics, the combination of energy system models and life cycle assessment thus allows comprehensive environmental sustainability assessments of technically and economically feasible energy system transformation pathways. We introduce FRITS, a FRamework for the assessment of environmental Impacts of Transformation Scenarios. FRITS links bottom-up energy system models with life cycle impact assessment indicators and quantifies the environmental impacts of transformation strategies of the entire energy system (power, heat, transport) over the transition period. We apply the framework to conduct an environmental assessment of multi-sectoral energy scenarios for Germany. Here, a 'Target' scenario reaching 80% reduction of energy-related direct CO_2 emissions is compared with a 'Reference' scenario describing a less ambitious transformation pathway. The results show that compared to 2015 and the 'Reference' scenario, the 'Target' scenario performs better for most life cycle impact assessment indicators. However, the impacts of resource consumption and land use increase for the 'Target' scenario. These impacts are mainly caused by road passenger transport and biomass conversion.

Keywords: energy system modelling; energy scenario; environmental impact assessment; life cycle assessment

1. Introduction

The threat of irreversible effects of global warming led to the agreement at the Paris Climate Conference (COP 21) that the rise in global temperature should remain well below 2 °C and that net greenhouse gas neutrality must be achieved in the second half of the century [1]. Today, the global energy supply based on fossil fuels is the main source of greenhouse gas emissions. Energy system models (ESMs) are frequently used in order to identify strategies on how to achieve these goals in the most cost-effective and efficient manner. These models depict specific energy conversion sectors such as power supply via the technologies contained therein (e.g., photovoltaic (PV) modules). In the ESMs, the expansion and operation of these technologies are usually driven by techno-economic characteristics combined with CO_2 emission reduction targets for the sectors included. The resulting scenarios at various geographical levels provide important insights into techno-economic and political options for the energy system transformation [2].

However, ESMs generally do not consider other environmental impacts (e.g., effects on ecosystems). In addition, as energy supply shifts from fossil fuels to renewable sources, environmental impacts tend to shift to processes beyond the traditional system boundaries of ESMs, which usually only include emissions during operation [3]. Therefore, processes such as the construction of energy conversion plants and other infrastructure elements must be additionally considered. Life cycle assessment (LCA) provides detailed information on a wide range of sustainability indicators by taking full account of the impact of an energy technology on the environment from cradle-to-grave based on the life cycle inventory (LCI). Due to the complementary nature of technology-focused energy system models and LCA with cradle-to-grave environmental impact assessment, their combination can contribute to a more complete picture and knowledge on the sustainability of energy system transformation pathways.

The combination of technologies modelled in ESMs with LCI data is an emerging field of research, currently mainly focusing on the power sector (see Table 1).

Table 1. Overview of recent studies that carry out environmental ex-post assessments of energy scenarios. The studies are sorted by their publication date (most recent publication on top).

Study	Geographical Scope	Time Horizon	Sectors Assessed			LCI-Database [1]	Prospectivity of LCI Data [2]
			Electricity	**Heat**	**Transport**		
Xu et al. [4]	Europe	2050	✓			Ecoinvent	✓ (F,B)
Luderer et al. [5]	World	2010–2050	✓			EXIOBASE, Ecoinvent	✓ (F,B)
Fernández Astudillo et al. [6]	Quebec (Canada)	2050	✓	✓	✓	Ecoinvent	✓ (F)
Volkart et al. [7]	World	2060	✓	✓	✓	Ecoinvent	✓ (F)
Pehl et al. [8]	World	2010–2050	✓			EXIOBASE, Ecoinvent	✓ (F,B)
Santos et a al. [9]	Brazil	2050	✓			Secondary literature	
García-Gustano et al. [10]	Spain	2015–2050	✓			Ecoinvent, secondary literature	
Volkart et al. [11]	Switzerland	2035	✓	✓	✓	Ecoinvent	✓ (F,B)
García-Gustano et al. [12]	Norway	2010–2050	✓			Ecoinvent	
Shmelev and van den Bergh [13]	UK	2050	✓			Secondary literature	
Sokka et al. [14]	Finland	2020	✓			Secondary literature	
Berrill et al. [15]	Europe	2050	✓			EXIOBASE, Ecoinvent	✓ (F,B)
Menten et al. [16]	France	2007–2030	✓	✓	✓	Ecoinvent	
Igos et al. [17]	Luxembourg	2010–2025	✓	✓		WIOD, Ecoinvent	
Hertwich et al. [18]	World	2015–2050	✓			EXIOBASE, Ecoinvent	✓ (F,B)
Kouloumpis et al. [19]	UK	2010-2070	✓			Ecoinvent	✓ (F)
Portugal Pereira et al. [20]	Japan	2030	✓			GEMIS	
Hammond et al. [21]	UK	1990–2050	✓			Secondary literature	

[1] 'Secondary literature' means that the authors use indicator values from literature without further harmonization of the data. [2] F: Adaptions to future developments (e.g., increasing efficiencies) included for the foreground technologies; B: Adaptions to future developments (e.g., evolving electricity mix) in the background database. LCI: life cycle inventory.

We analysed these studies and classified their approaches in order to identify methodology gaps. Five of the eighteen studies found in the literature assess multi-sectoral energy scenarios that include, next to electricity, also the heating and/or transport sectors [6,7,11,17,22]. Concerning the time horizon, a transformation path over longer time horizons (not just a single year) is assessed by less than half of the studies. Few studies disaggregate the environmental impacts into the life cycle phases corresponding to the investment and operation (and partly decommissioning) of the energy technologies in the scenario [7,8,18]. Therefore, environmental impacts of a transformation path can be allocated to the corresponding points in time. This contrasts with the simplifications of other studies that assess a transformation path but do not distinguish between life cycle phases [10,12,16,17,19].

Since the application of LCA to energy scenarios has a prospective character, some studies include changes to the background LCI database [4,5,8,11,15,18]. However, the approaches and the degree of these adaptions vary greatly depending on the study. For example, in the technology hybridized environmental-economic model with integrated scenarios (THEMIS), applied in [5,8,15,18], the electricity mix of a global energy scenario is integrated into the background LCI database and serves as input to all upstream supply processes that consume electricity (e.g., the construction of electricity generation technologies). Volkart et al. [11] also adapt the background electricity mix for Europe to a scenario for 2030 from literature. In a recent study by Xu et al. [4], the authors integrate the electricity mix of the applied ESM with a focus on Europe to the LCI database. However, as the technologies are manufactured globally, adjusting the electricity mix of a specific region to future developments may have only a minor impact on the environmental profile of the technologies. Many studies do not consider future evolvements of foreground technologies. An exception is the THEMIS model, where LCIs from secondary literature are used to reflect future changes in material composition and efficiency of the electricity generating technologies. In other studies, foreground technologies and their expected future properties are included in the assessment if corresponding LCIs are available [4,7,11,19]. Next to the consideration of future material composition for some technologies, the adaption of conversion efficiencies (e.g., in power generation) to the assumptions of the ESM is the most frequently used method.

Despite the growing number of studies, current attempts to combine ESMs and LCA encounter significant methodological challenges. Firstly, most studies cover only a limited number of technologies or have narrow sectoral boundaries (e.g., electricity supply only). This ignores relevant dynamics and interrelationships such as the direct or indirect electrification of transport, industry and households and their environmental impact on specific sectors and the overall energy system. This will become increasingly relevant with increasing electrification of fuels and heat, as will occur at high shares of renewable energy [2,23,24]. In addition, to the best of our knowledge, no environmental ex-post assessment of multi-sectoral energy system transformation pathways with simultaneous adjustment of the global background electricity mix has been conducted. This would lead to a more precise assessment of environmental impacts, especially in the construction phase, which will also gain relevance with increasing shares of renewable energy in the system (see above).

To overcome these limitations, we develop the FRamework for the assessment of environmental Impacts of Transformation Scenarios (FRITS). FRITS provides a basis for coupling multi-sectoral ESMs that assess energy transformation pathways with a high technological detail with an LCI database. FRITS allows for assessing environmental impacts of the entire energy system (electricity, heat, transport and the generation of biogenic and synthetic fuels and gases). Therefore, it is particularly suited for scenarios with a high degree of sector coupling, i.e., direct and indirect electrification of the transport and heat sectors. It further takes into account a number of prospective elements such as the change of the global electricity mix in the background system, the evolvement of plant efficiencies and operation hours. In contrast to the geographical focus of the aforementioned studies—predominantly European countries and the World—we provide the first assessment of transformation pathways of the German energy system.

Germany's energy system transformation is guided by ambitious political targets until 2050, such as increasing the share of renewable energies in gross final energy consumption to 60% and reducing greenhouse gas emissions by 80–95% (compared to 1990) [25]. Thus, it can serve as a role model for the transformation of a highly industrialized country. We compare a number of environmental co-benefits and adverse side-effects of an ambitious scenario that meets these political targets ('Target') with the current energy system and a baseline ('Reference') scenario to deliver insights for policy planning. Specifically, the following research questions are addressed:

- How can LCI data be used to evaluate energy system transformation scenarios? Which adjustments need to be made to available LCI data in order to become consistent with the energy scenario, especially in the case of very ambitious scenarios with a central role of power-to-x (admixtures) and biofuels? (Section 2)
- What co-benefits and adverse side effects arise in the transformation of the energy system compared to today? (Section 3.1.1)
- Which indicators decrease or increase at, collectively, the scenario level, the sectoral level (e.g., power generation) and the end-use level when comparing life cycle based environmental impacts for two scenarios for Germany? (Sections 3.1.2 and 3.1.3)
- How do life cycle assessments improve the perspective on environmental impacts compared to considering only the direct emissions caused by operation and use? (Section 3.2)
- What influence does the global background electricity mix have on the scenarios assessed? (Section 3.3)

The scenarios are described in Section 2.5. Associated uncertainties, as well as further steps to improve the assessment are discussed in Section 4. Finally, conclusions are provided in Section 5. With this study, we contribute to the integration of knowledge from the ESM and LCA communities with the aim to increase the robustness of energy scenario assessments. The outputs of FRITS may also serve as inputs for multi-criteria decision making (MCDM).

2. Materials and Methods

Figure 1 describes the methodological steps of the framework and provides a reference to the relevant sections of this chapter, where they are explained in detail.

2.1. Energy System Model for Scenario Development

The ESM used in this study is MESAP/PlaNet (MESAP in the following) [26], which has been used in several studies with various geographical foci: global [2,27], national [28–30] and regional [31]. The MESAP accounting framework allows the integration of a wide variety of assumptions into the energy system scenario from other models and studies as well as exogenously defined premises. Table 2 lists sectors and sub-sectors considered in MESAP (the respective technologies are listed in the Supplementary Materials). The MESAP output relevant for FRITS comprises the following quantities (each on an annual basis):

- The annual generation of electricity, heat, synthetic fuels and gases and biogenic energy carriers,
- gross new installed capacities (including replacement capacities) for the generation of power, heat, synthetic fuels, synthetic gases, biofuels, biogas and solid biomass, as well as electricity storage,
- development of vehicle fleet and energy demand in transport by energy carrier,
- annual average blending quota (such as share of biodiesel and/or synfuels in total diesel fuel demand, the share of hydrogen and/or synthetic methane in the natural gas grid, etc.).

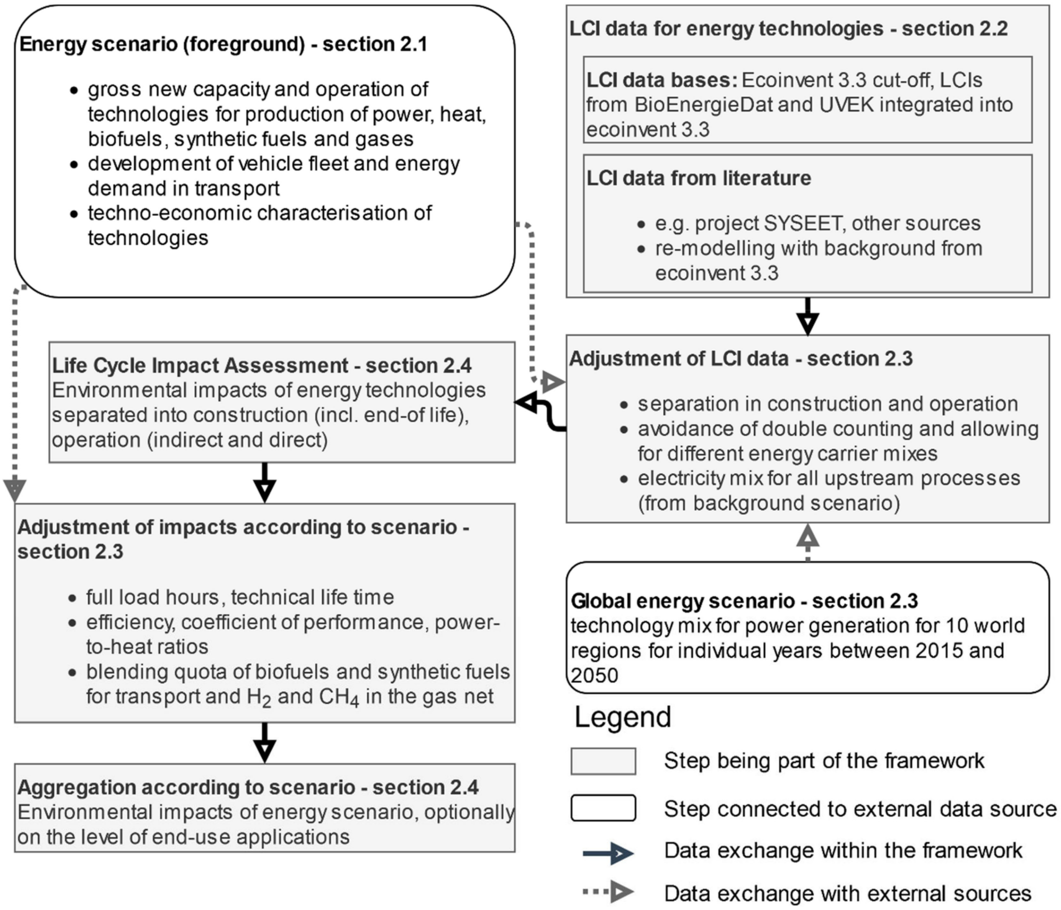

Figure 1. Methodological steps in the FRamework for the assessment of environmental Impacts of Transformation Scenarios (FRITS). The details of each step are described in more detail in the indicated sections.

This output is then combined (soft-coupled) with the LCA impacts of the individual technologies. Detailed explanations on the processing of the LCI data can be found in the following subsections. Note that FRITS is not limited to scenarios generated with MESAP, but can be applied to any model output if the aforementioned data is provided.

2.2. *Life Cycle Inventory Database and Software*

The LCI data for energy and transport technologies from the attributional ecoinvent v3.3 cut-off database [32] are supplemented by LCI data for biomass conversion from BioEnergieDat [33], UVEK LCI data for PV systems [34], for synthetic fuels from the project on the system comparison of storable renewable energy sources (SYSEET) [35] and for single technologies from various other sources (see Table S1 in the Supplementary Materials), which either provide more recent data or geographically specific data for Germany. All non-ecoinvent datasets have been integrated into the database in order to ensure consistent modelling of background data, system boundaries and time frames. The LCI data adaptions described below are performed with the LCA software openLCA version 1.8. A Python plugin based on GreenDelta [36] is used and adapted to update the parametrized electricity markets within ecoinvent (see Section 2.3.2) and to perform the life cycle impact assessment (LCIA) calculations.

Table 2. Overview of main sectors, sub-sectors and end-use applications that are explicitly considered in the foreground system of MESAP.

Main Sector	Sub-Sectors	End-Use Applications
Residential	Space Heat (SH) Hot Water (HW) Combined Heat and Power Auto-Production (CHP)	Space Heat (SH) Hot Water (HW) Electric Appliances [1]
Commerce, Trade and Services	Space Heat & Hot Water (SH/HW) Process Heat (PH) Combined Heat and Power Auto-Production (CHP)	Space Heat & Hot Water (SH/HW) Process Heat (PH) Electric Appliances [1]
Industry	Space Heat & Hot Water (SH/HW) Process Heat (PH) Combined Heat and Power Auto-Production (CHP)	Space Heat & Hot Water (SH/HW) Process Heat (PH) Electric Appliances [1]
Transport	Road Passenger Transport Road Freight Transport Rail Transport Navigation Aviation	Road Passenger Transport Road Freight Transport Rail Transport Navigation [2] Aviation [2]
Conversion	Power Plants CHP (public) Heating Plants Synthetic Fuels and Gases [3] Bioenergy Conversion [4]	
Storage	Electricity Storage	
Import	RES Power Imports	

[1] All electric appliances except those generating useful heat (e.g., electric heat pumps); [2] domestic only; [3] generation of synthetic gases (H2, CH4) and synthetic fuels (Power-to-Liquid), [4] generation of fuels and gases of biogenic origin (biomass-to-liquid, biogas, biofuels and solid biomass).

2.3. Matching and Adapting the Life Cycle Inventory Data to the Energy System Model

When coupling LCI data to an ESM, a distinction must be made between processes and flows that are assigned to the foreground and those in the background system. The foreground system is defined as all conversion technologies that are used in the ESM. The background system comprises all flows and activities that are outside the system boundary of the ESM.

2.3.1. System Boundaries and Technology Mapping

In MESAP, the foreground system comprises all sectors and technologies generating electricity, heat, non-fossil fuels (biofuels, power-to-liquid (P_2L)), non-fossil gases (biogas, H_2 and synthetic CH_4) and road transportation (passenger and freight). Note that since many current scenarios for Germany assume a net import of electricity and/or synthetic fuels and gases, the electricity generation and conversion technologies used abroad for this purpose are also treated as foreground technologies in FRITS.

Table 2 gives an overview of the sub-sectors and end-use applications (EUAs). The output generated by these sub-sectors (electricity, heat, transport, fuels) is used by the EUAs.

Technologies in the ESM are matched with a corresponding LCI data set. Ideally, the LCI data represents the respective energy system technology precisely with regard to the technology type used and the model region. If this is not the case, we select proxy data sets that most closely correspond to the process of the energy system model. We also account for technology deployment scenarios on subtechnology level in FRITS (see Excel supplement). In MESAP, the supply of fossil fuels and gases, as well as uranium, and the construction of energy technologies and auxiliary infrastructure are considered outside the energy system. The LCI data of those (background) processes rely exclusively on the ecoinvent database.

2.3.2. Integration of Future Global Electricity Supply Scenarios into the Background Database

The ecoinvent database distinguishes processes in transformation activities and markets (consumption mixes). The aggregation of activities in markets simplifies the identification and modification of relevant parameters such as the shares of technologies that provide the same output in a given geographical region. In this study, the electricity markets are manipulated, most of which are at country level or higher such as provinces. To account for an evolving electricity mix in FRITS, we integrate the global power mix of the 2.0 °C scenarios from Teske et al. [2] for the scenario years 2015, 2020, 2030, 2040 and 2050 in ecoinvent. Next to the 2.0 °C scenario, we also integrate the 5 °C scenario from Teske et al. [2] to test the influence of the adapted electricity mix on both foreground scenarios (see Section 3.3). The 5.0 °C scenario describes a global energy system pathway strongly following the World Energy Outlook (WEO) 2017's 'Current Policies' scenario of the International Energy Agency [37], whereas the 2.0 °C scenario describes a global energy system pathway consistent with temperature increase of below 2.0 °C compared to pre-industrial levels. For further details on the manipulation of the electricity markets, see Appendix A. The reference power plants are listed in Table S4 of the Supplementary Materials.

2.3.3. Separation of Life Cycle Phases

When the traditional per-output LCI data (e.g., kWh electricity from coal power plants) are used for the assessment of energy transformation pathways, assumptions in the LCI data on both the technical lifetime and full load hours of the technologies would be implicitly included in the analysis. Furthermore, such a single impact coefficient per energy output is not adequate to represent energy transformations pathways as the impacts (especially of renewable technologies) mainly occur during a short construction period. To correctly allocate the environmental impacts in time in line with the outputs of MESAP, the LCI data sets are divided into two life cycle phases: construction and operation. The bases for the separation are the unit processes (e.g., for electricity generation) from which the construction processes are excluded and merged in separate data sets (see Table S1 in the Excel supplement).

2.3.4. Harmonisation of Technical Characteristics of the Technologies

Technical characteristics of the energy technologies assumed in the LCI data sets have to be adapted to those of the ESM. The ESM provides detailed data on the technical characteristics in Germany, such as the efficiency, the output ratios (e.g., in the case of CHP plants the power-to-heat ratio) and the coefficient of performance (COP) of heat pumps. In order to harmonise efficiencies and estimates of the COP, it is assumed that all impacts associated with the operation of a technology scale linearly with those parameters in the ESM. If the respective efficiencies of the model (η_{MOD}) and those assumed in the LCI data (η_{LCI}) diverge, the output from these process are adjusted by their ratios (Out_{LCI}: output from the original LCI dataset, Out_{ADJ}: output adjusted to model efficiency):

$$\mathrm{Out_{ADJ}} = \mathrm{Out_{LCI}} \cdot \frac{\eta_{\mathrm{LCI}}}{\eta_{\mathrm{MOD}}} \tag{1}$$

The same is true for adjustments in the COP of heat pumps. For CHP technologies in ecoinvent (cut-off), LCIs are already pre-allocated to heat and power generation. For those technologies, first the total efficiencies (sum of heat and power output divided by fuel input) are calculated from the documented (separate) efficiencies with respect to heat generation, to power generation and the power-to-heat-ratios of the respective LCI data sets. The environmental impacts are then adjusted to total efficiency assumptions in the energy system model according to the equation above. Total impacts from CHP are subsequently allocated to heat and power generation according to the heat and power output (energy allocation).

2.3.5. Avoiding Double Counting in the Foreground System

The foreground system assessed in this study comprises both EUAs (e.g., electric heat pump or residential gas heater providing space heat) and conversion technologies (such as power plants or technologies for the production of synthetic gases). Thus, in order to avoid double counting of environmental impacts, any inputs of energy sources generated by other foreground technologies have to be excluded from the LCI datasets (see exemplary illustration in Figure 2).

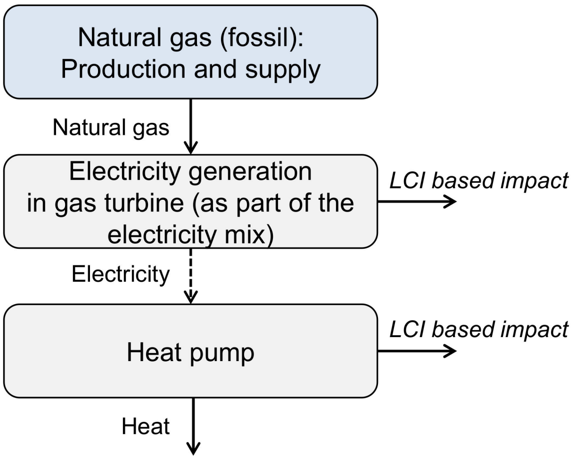

Figure 2. Adaption of life cycle inventory (LCI) data to avoid double counting of impacts in FRITS. Light blue boxes indicate technologies or flows of energy carriers that are not part of the energy system model (ESM). Light grey boxes show technologies or flows of energy carriers that are part of the (foreground) model. Dashed arrows represent flows that are excluded from the original LCI data sets on which the arrow points in order to avoid double counting of impacts.

With this approach, the environmental impact of the production of these secondary or final energy carriers is assigned to the conversion technologies (e.g., electricity generation in a gas turbine).

2.3.6. Impacts of Energy Carrier Mixes

Some technologies (e.g., a gas burner for heat generation) of the foreground system can be operated by a mix of energy sources generated both in the background (e.g., natural gas) and in the foreground (e.g., H_2) (see Figure 3).

Therefore, several product systems are modelled to allow for a fuel mix. These product systems rely on the original LCI datasets (e.g., transport by a diesel fueled passenger car) from which the original inputs of the fuel supply (e.g., diesel) and the construction (e.g., of the vehicle) are deleted. For technologies where hydrogen is burned (gas burners, gas turbines, etc.), we remove all emissions except NO_x from the original unit process to approximate direct emissions. NO_x emission factors are taken from the original unit process. However, as ecoinvent does not contain any process emissions for the combustion of non-fossil fuels (such as biodiesel or synthetic gas), it is assumed that the emissions are the same as those of the corresponding conventional fuels. For the correct consideration of CO_2 emissions in the impact assessment method, they are characterized as non-fossil (synthetic fuels and gases) or biogenic (biofuels and gases). These adaptions include product systems that have the following primary energy sources as inputs: gas: admixture of biomethane, H_2 or synthetic CH_4; diesel: admixture of biodiesel and synthetic fuels; gasoline: admixture of bioethanol; kerosene and marine diesel: admixture of biomass to liquid (BtL) and synthetic fuels (see Table S1 in the Excel supplement).

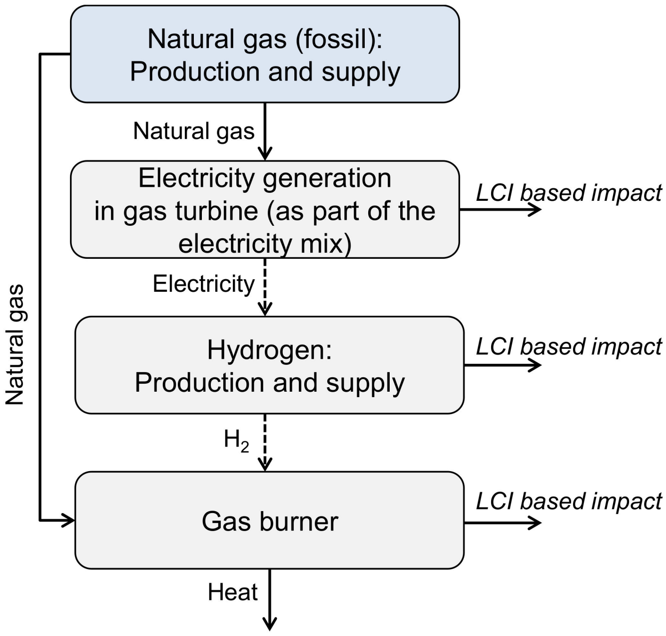

Figure 3. Adaption of LCI data sets in FRITS to model admixtures of fuels that can be produced in the foreground and background system. The specifications of Figure 2 apply.

2.3.7. Avoiding Double Counting in the Background System

When assessing large scale systems, double counting also occurs in other processes (e.g., the construction of power plants), since part of the energy and service inputs (e.g., electricity, heat or transport processes) take place within the geographical system boundary of the scenario assessed. As the ecoinvent database models the electricity supply (in the form of markets) according to a sufficient regional granularity (e.g., for Germany), the supply flows (e.g., electricity production from a wind turbine in Germany) are removed from the German electricity market and thereby from all processes in the database. In other words, the German electricity mix has no impacts in the background. Thus, we avoid double counting on the level of the LCA indicators.

However, double counting is not avoided for heat and transport supply processes due to the insufficiently detailed regional resolution of the database. Since the present analysis covers Germany only, we expect the impact of double counting from the heat and transport activities in in the LCI database to be of limited relevance.

2.4. Linking Scenario Results with LCA Impacts for Scenario Assessment

The impact assessment is based on two of model outputs: (a) annual gross new installations (including replacements after the end of the technical lifetime) of power, heat, gas and fuel generating technologies, electricity storages as well as passenger cars, and (b) annual power, heat, gas and fuel generation and/or the corresponding final energy consumption of those technologies. Gross new installations of power, heat and fuel generating technologies are given in units of MW/a (where the capacity is related to the output). New cars are reported in number of new vehicles. The functional unit for any kind of power, heat, fuel or gas generation is kWh (lower heating value). Passenger and freight transport is given in passenger kilometres and tonne kilometres, respectively. The impact assessment data (per functional unit) are harmonised with the model assumptions (see Section 2.3.4) and then multiplied with the corresponding scenario output to obtain the impacts at the technological, sub-sectoral and scenario levels.

The environmental impacts can also be allocated from the foreground technologies to the 17 EUAs (Table 2) to provide information on the original polluter. This allocation is based on the scenario results (e.g., share of the EUAs in total (net) power demand) and done iteratively on an annual basis.

2.5. Energy Scenarios Used in the Case Study

Two different energy (foreground) scenarios for Germany are used in order to compare life cycle impacts for different transformation paths. The scenario 'Target' is taken from Pregger et al. [30]. It is a normative scenario that describes a technically feasible way of achieving the German targets for reducing greenhouse gas emissions by 80% by 2050. The 'Reference' scenario is inspired by the 'Referenzszenario' (reference scenario) from the BMWi [38]. The main characteristics of the scenarios are shown in Figures 4 and 5.

In the original study from BMWi [38], the 'Reference' scenario describes a business-as-usual (BAU) case with a reduction of energy related CO_2 emissions by ~59% until 2050. However, assumptions on drivers (e.g., population and GDP) and on efficiency improvements differ between Pregger et al. [30] and BMWi [38]. In this study, the aim is to compare the effect of different transformation depths (e.g., shares of renewables) and different technological options, of drivers and assumptions. Thus, the BMWi 'Reference' scenario is adapted to Pregger et al. [30] regarding GDP, population, useful energy demand and transport. In each EUA or conversion sector, technology shares for the 'Reference' scenario are adopted. This leads to a CO_2 reduction of ~65% in 2050 compared to 1990 in the 'Reference' scenario (see Figure 5).

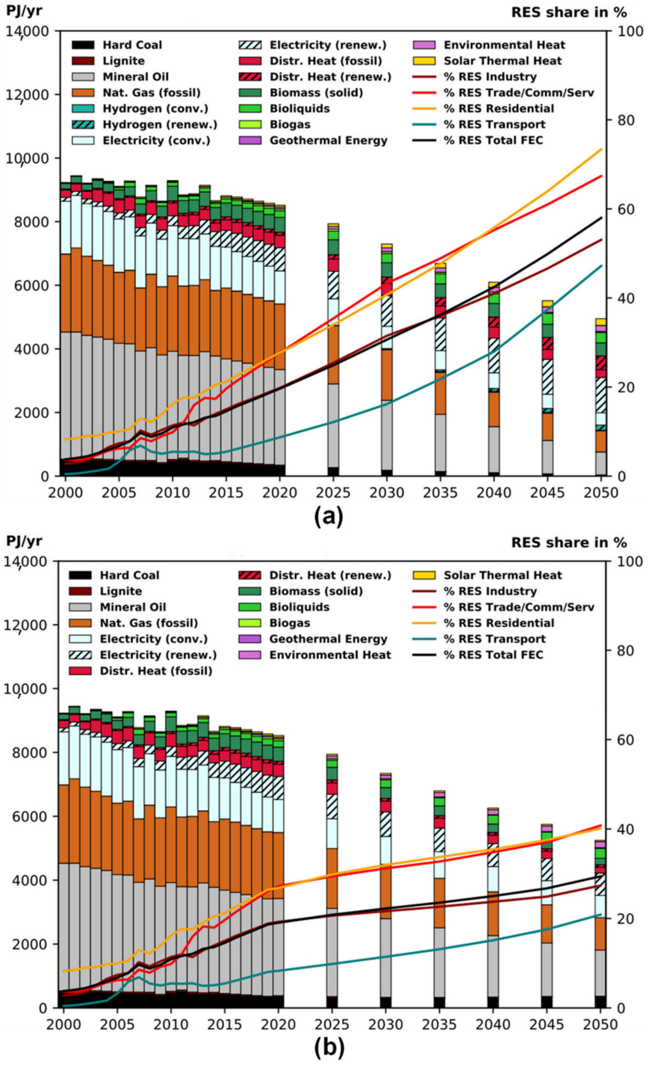

Figure 4. Final energy demand by energy carrier and share of renewable energy sources (RES) in the end-use sectors in the 'Target' (**a**) scenario [30] and the 'Reference' (**b**) scenario [38].

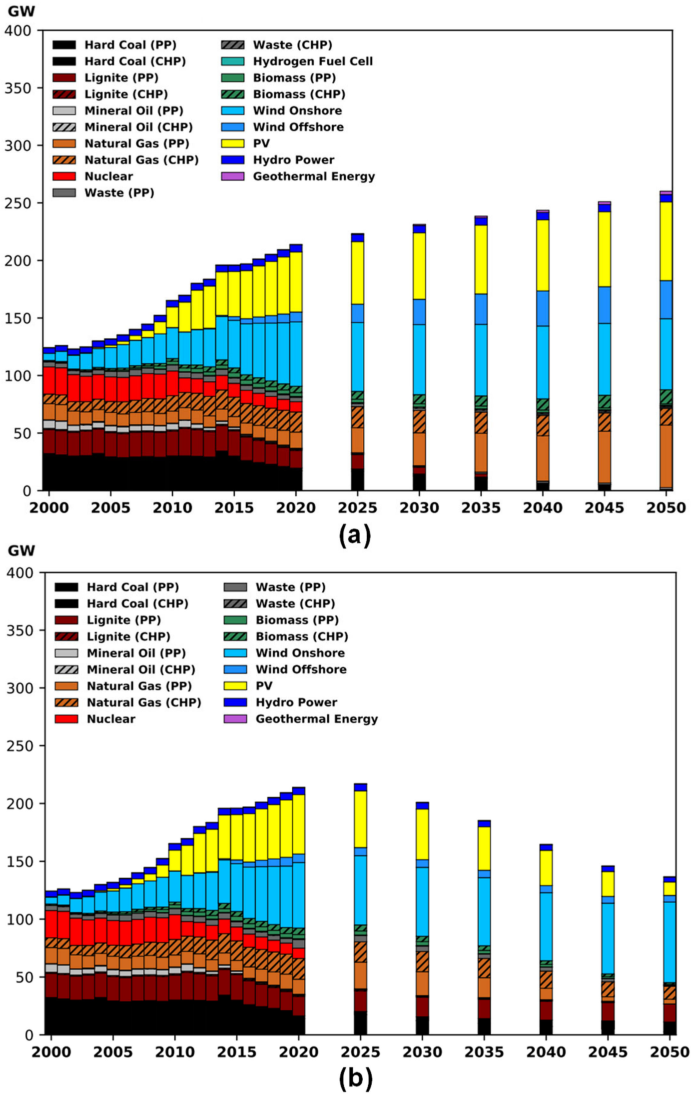

Figure 5. Installed capacities in the electricity sector including in the in the ‘Target’ (**a**) scenario [30] and the ‘Reference’ (**b**) scenario [38].

As these energy scenarios provide only limited information on some transport sectors, we do not account for the impact of new installations of the technologies listed in Table 3 in the following case study. However, operation-dependent life cycle impacts according to the information on the required final demand are considered in the foreground.

Table 3. Overview of the sub-sectors and specifications of the technologies they contain, where the construction is not included in the foreground system.

Sub-Sectors	Specifications of the Technologies
Navigation	Navigation (inland shipping)
Aviation	Airplanes (passenger, freight)
Rail Transport	Rail transport (passenger, freight)
Road Freight Transport	Light and heavy duty vehicles (LDVs, HDVs)

3. Results

In the following case study, we use a selection of midpoint indicators from the ILCD 2.0 2018 method [39]. The impact categories used in this study are listed in Table 4.

Table 4. Overview of the indicators from the ILCD 2.0 2018 method used in this study.

Indicators	Units
Climate change total	kg CO_2 eq
Freshwater and terrestrial acidification	mol H+ eq
Freshwater ecotoxicity	CTUe
Freshwater eutrophication	kg P eq
Marine eutrophication	kg N eq
Terrestrial eutrophication	mol N eq
Non-carcinogenic and carcinogenic effects	CTUh
Ionising radiation	kg U235 eq
Ozone layer depletion	kg CFC-11 eq
Photochemical ozone creation	kg NMVOC eq
Respiratory effects, inorganics	disease incidence
Fossils	MJ
Land use occupation and transformation	points
Minerals and metals	kg Sb eq

3.1. *Co-Benefits and Adverse Side Effects at a Sectoral and Overall Scenario Level*

In the first two sections (Sections 3.1.1 and 3.1.2), the main sub-sector (see Table 2) and the corresponding technology most relevant for each indicator is highlighted. A more detailed sectoral analysis is provided in Section 3.1.3, where we analyse climate change, local emissions and the resulting effects on human health as well as the demand for minerals and metals. The latter two dimensions are selected because they have been recognized in various studies as crucial aspects to monitor when assessing the transformation of the energy system [40,41].

3.1.1. Environmental Co-Benefits and Adverse Side Effects of the Energy System Transformation

Figure 6 shows the impacts of the 'Target' scenario for 2030, 2040 and 2050 relative to the impacts in 2015. It illustrates that both co-benefits (impact ratio < 1) and adverse side effects (impact ratio > 1) of an ambitious transformation path show a clear increasing or decreasing trend for some impacts, while other impacts first increase and then decrease again. The following analysis focuses on those indicators where the difference between 2015 and the 'Target' scenario is at least ±15% in one of the years.

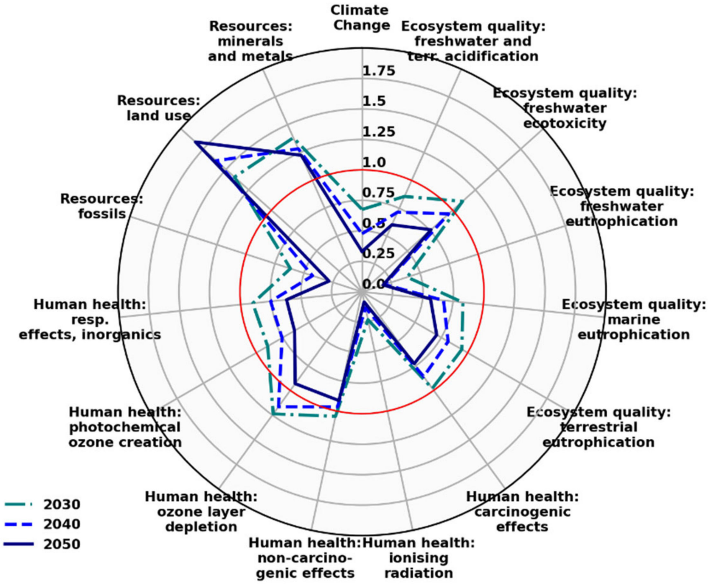

Figure 6. Ratio of impacts of the 'Target' scenario relative to the impacts in 2015. The red line separates adverse side effects (increasing impacts, impact ratio > 1) from co-benefits (decreasing impacts, impact ratio < 1).

In accordance with previous literature, the energy system transformation causes adverse side effects in the use of minerals and metals as well as in land use [7,11]. The increase in the indicator 'minerals and metals' can be attributed in particular to road passenger transport, with Otto and diesel engines being substituted by plug-in hybrid electric vehicles (PHEVs) and battery electric vehicles (BEVs) from 2020 onwards. Both car types have a higher specific (per car) value for 'minerals and metals', but the increasing sufficiency in road passenger transport assumed in the scenario (lower total passenger km) leads to a slight reduction of this impact category for the years 2040 and 2050 compared to 2030. The widening gap for the indicator 'land use' compared to 2015 is mainly due to the use of agricultural land for the production of wood used directly as pellets or in gasification in the bioenergy conversion sector. The strong impact of energy crop cultivation on land use is also highlighted by Volkart et al. [7].

For the indicators 'ozone layer depletion' and 'freshwater ecotoxicity', the energy transformation first leads to an increase and then to a decrease in 2050 of the indicators compared to 2015. In 2030 and 2040, 'ozone layer depletion' is driven in particular by bioethanol production from winter wheat and grass in the bioenergy conversion sector. The decline in bioethanol production from 2025 to 2050 eventually leads to a better performance of the scenario in 2050 compared to 2015. In 2050, passenger transport, especially BEVs, make the largest contribution to this indicator. The ecosystem quality related 'freshwater ecotoxicity' is dominated by passenger transport in all years. In 2030, this dominance is largely driven by Otto and diesel engines, while between 2040 and 2050, BEVs and PHEVs are increasingly responsible for the reduced impact.

As shown in other studies [6,8,18], the phase-out of fossil power plants, specifically lignite-based power generation, leads to a considerable reduction of the indicators 'climate change', 'fossils', 'carcinogenic effects', 'marine eutrophication', 'freshwater eutrophication' as well as 'freshwater and terrestrial acidification'. The decline in the indicator 'respiratory effects, inorganics' is due to the declining use of Otto and diesel engines in road passenger transport, but also to the decline in the use of coal and the switch to solar thermal production for process heat for industry. Passenger transport also drives most of the reductions in 'photochemical ozone creation' and 'terrestrial eutrophication'. The phase-out of nuclear power plants by 2022 leads to a sharp decline of 'ionizing radiation'.

3.1.2. Comparison of the Impacts of the 'Reference' and 'Target' Scenarios

Figure 7 shows the impacts of the 'Target' scenario relative to the impacts of the 'Reference' scenario for 2030, 2040 and 2050. The differences between the scenarios per indicator mostly follow a clear trend with increasing years. This is also true at the level of the responsible sub-sectors. Therefore, the following analysis focuses on the year 2050. In addition, only indicators where the difference between the 'Target' and 'Reference' scenarios is at least ±15% in 2050 are analysed in more detail.

Significant higher impacts in the 'Target' scenario, i.e., adverse side-effects, can be observed for the indicators 'land use', 'non-carcinogenic effects' and 'terrestrial eutrophication', while 'minerals and metals' is only slightly affected. Higher land use impacts are primarily driven by the bioenergy conversion sector, i.e., agricultural land for energy crops such as short rotation forestry for the production of wood pellets or in gasification as well as rapeseed for biodiesel production. The difference of human-health-related 'non-carcinogenic effects' is driven by the greater share of heat and power co-generation in industry using wood chips and the higher production of biodiesel and biogas in the bioenergy conversion sector. Biogas production from energy crops also accounts for most of the larger impacts in ecosystem quality related 'terrestrial eutrophication'.

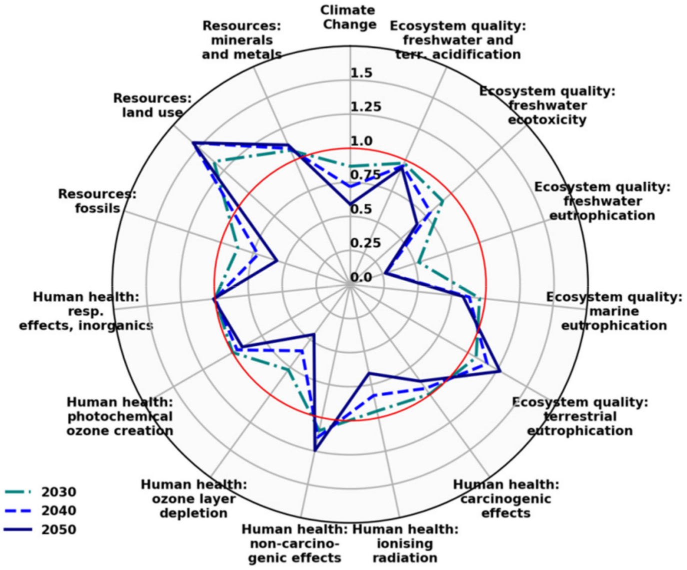

Figure 7. Ratio of impacts of the 'Target' scenario relative to the impacts of the 'Reference' scenario. The red line indicates the line of 'equal impacts'.

Similar impacts of the 'Target' scenario compared to the 'Reference' scenario for all years occur for the indicator 'respiratory effects, inorganics'. The indicators 'photochemical ozone creation', 'carcinogenic effects' and 'freshwater and terrestrial acidification' are slightly lower. Significantly lower impacts can be observed for the indicators 'climate change', 'fossils', 'ozone layer depletion', 'ionising radiation', 'marine eutrophication', 'freshwater eutrophication' as well as 'freshwater ecotoxicity'. Declining impacts of 'climate change' and 'fossils' in the 'Target' scenario are mainly caused by the phase out of lignite-based generation by 2038 and the deployment of electric vehicles which reduces fossil fuel demand and emissions from combustion. The power plant sector is also responsible for most of the differences of 'marine eutrophication' and 'freshwater eutrophication' in 2050. The difference in the human health related indicator 'ozone layer depletion' is mainly caused by the lower production of bioethanol from winter wheat and grass in the bioenergy conversion sector. The latter and road passenger transport, especially the significant reduction of Otto engines, are responsible for the majority of the differences in 'freshwater ecotoxicity' in 2050. The difference in 'ionising radiation' is due to road freight and passenger transport, as less petroleum is produced, the process in which most impacts occur in 2050, e.g., from naturally occurring radioactive material.

3.1.3. Impacts for Selected Indicators at the Level of Technology Groups and End-Use Sectors

In the following section, the assessment is conducted both at sub-sector level and for EUAs (see Table 2) and, if relevant, the technology of the sub-sector responsible for most of the respective impacts is highlighted.

3.1.4. Climate Change

Between 2015 and 2050, total life cycle CO_2 eq decrease by 44% and 67% in the 'Reference' and 'Target' scenario, respectively (see Figure 8). This results in a difference between the two scenarios of 211 Mt CO_2 eq in 2050.

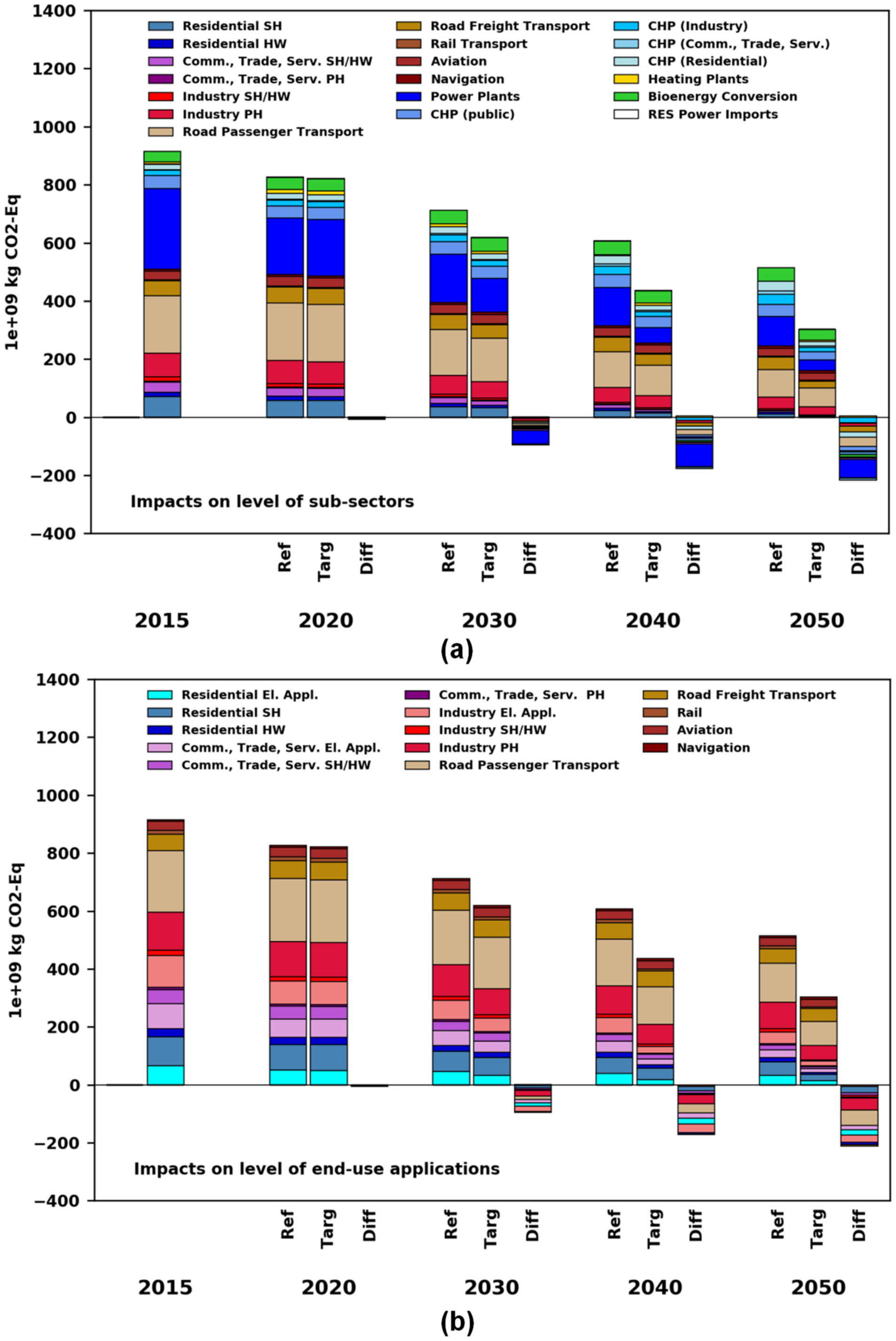

Figure 8. Main drivers for climate change in the 'Target' and 'Reference' scenarios. (**a**) Impact caused by the sub-sectors, (**b**) Impact caused by the end-use applications.

In both scenarios and all years, the main drivers in the sub-sectors (Figure 8a) are road freight and passenger transport as well as power generation. In 2050, the impacts related to freight transport are dominated by light and heavy duty vehicles with diesel engines, although in the 'Target' scenario they are operated to a larger extent with bio-based fuels or hydrogen. In the 'Target' scenario, there is also a greater technological shift in passenger transport with an increased use of PHEVs and BEVs. Thus, the higher direct and indirect electrification of both transport modes in the 'Target' scenario leads to a reduction of total climate change impacts.

As described above, the phase out of coal based generation and the switch to renewable electricity and natural gas in the 'Target' scenario leads to a strong decrease of overall greenhouse gas emissions, in particular during the operation phase of the power plants. In 2050, in addition to the dominant gas-fired power plants, 19% of total emissions in the power sector would be accounted for by rooftop PV. Furthermore, emissions from biomass cultivation and supply in the bioenergy conversion sector are driven by biodiesel production in the 'Target' scenario and bioethanol production in the 'Reference' scenario.

The column 'Diff' shows the difference between both scenarios for each year. If the difference is negative for a given sector, then the impacts from the 'Target' scenario are lower in this sector compared with the 'Reference' scenario. This means that ambitious climate protection has co-benefits in the respective sector and impact category. On the other hand, if the difference is positive, ambitious climate protection comes along with adverse side effects. All the aforementioned sectors emit absolutely less in the 'Target' than in the 'Reference' scenario.

In line with the sub-sectors, all the EUAs perform better in the 'Target' scenario than in the 'Reference' case in all years. In both scenarios, emissions caused by different end-use sectors in 2050 are dominated by passenger and freight cars as well as process heat production for the industrial sector (see Figure 8b). The avoided CO_2 eq in the 'Target' scenario are mainly due to road passenger transport and industrial electric appliances. The large emission differences in power generation between the two scenarios (see Figure 8a) are thus now particularly reflected in passenger road transportation and industrial electric appliances due to the higher degree of direct electrification of these applications in the 'Target' scenario compared to the 'Reference' case.

3.1.5. Disease Incidences

The disease incidences of the two scenarios are reduced by 39% and 38% between 2015 and 2050 respectively for the 'Reference' and 'Target' scenarios (see Figure 9). Over the whole time horizon, both scenarios reveal quite similar impacts on the scenario level, while the shares of the sub-sectors in the overall impact become increasingly different over time between the scenarios.

In 2050 and in both scenarios, the main drivers for disease incidences of the sub-sectors (Figure 9a) are road passenger and freight transport as well as the bioenergy conversion sector. Similar to climate change, the impacts related to freight transport are dominated by light and heavy duty vehicles with diesel engines. Disease incidences from road passenger transport in the 'Reference' scenario mostly stem from vehicles with Otto engines (in the scenario they have almost three times the annual mileage in 2050 compared to diesel engines). In the 'Target' scenario, the impact is dominated by PHEVs with Otto engines but also from BEVs where the impact is shifted towards the construction phase of the vehicle. Most of the impacts in the transport sector are caused by $PM_{2.5}$ emissions. In the bioenergy conversion sector, on the other hand, impacts in the 'Reference' scenario are mainly driven by SO_2, NH_3 and NO_x emissions from cultivating of winter wheat and grass for the production of bioethanol, whereas in the 'Target' scenario NH_3 emissions during the fermentation process for biogas production are the main cause.

The sectors where disease incidences are comparably smaller in the 'Target' scenario compared with the 'Reference' scenario are mainly freight and road passenger transport as well as process heat in industry (Figure 9a). However, these positive effects are counterbalanced by increased impacts for combined electricity and heat production for industry and residents where emissions mainly result from the increasing combustion of solid biomass. Likewise, respiratory diseases in the 'Target' scenario from the electricity sector are higher than those in the 'Reference' case, especially due to the higher installation rate of rooftop PV with high impacts during construction.

In the EUAs perspective, in both scenarios in 2050, passenger and freight cars are clearly the main contributors to respiratory disease impacts due to the large consumption of bio- and synthetic fuels and electricity (see Figure 9b). The impacts of road passenger transport are smaller in the 'Target' scenario compared to the 'Reference' scenario, mainly because of the higher direct and indirect electrification in the ‘Target’ scenario compared to the use of biofuels in the ‘Reference’ scenario. On the other hand, impacts from the residential and industrial electrical appliances are higher in the ‘Target’ than in the ‘Reference’ scenario due to higher impacts from power generation in the former (see Figure 9a). Higher impacts in the EUA residential heat in the ‘Target’ scenario are cause by the greater use of biomass.

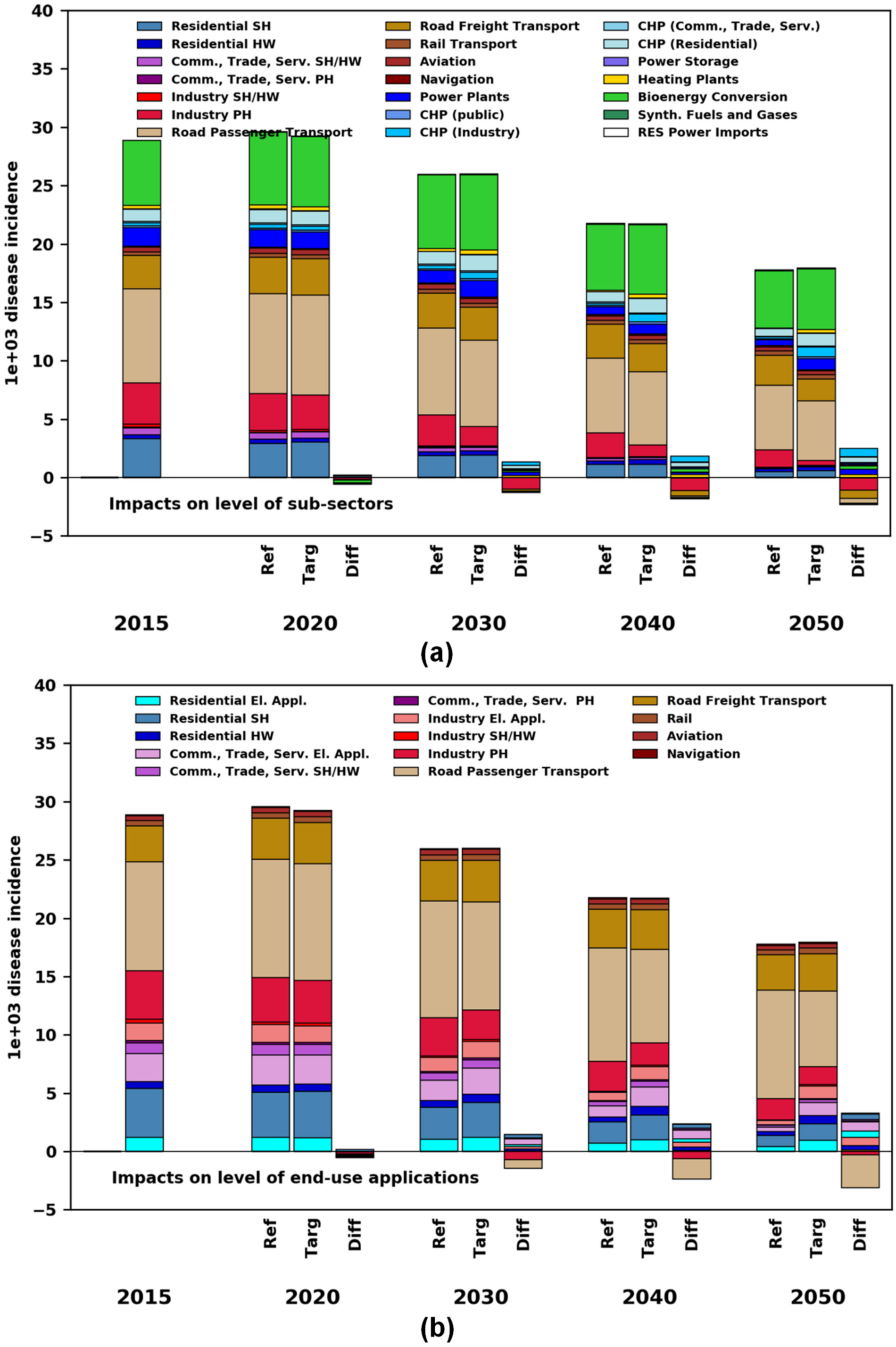

Figure 9. Main drivers for respiratory effects, inorganics in the ‘Target’ and ‘Reference’ scenarios. (**a**) Impact caused by the sub-sectors, (**b**) Impact caused by the end-use applications.

3.2. Resource Depletion of Minerals and Metals

Between 2015 and 2050, the resource depletion of minerals and metals increases by 9% in the ‘Reference’ scenario and by 23% in the ‘Target‘ scenario (see Figure 10).

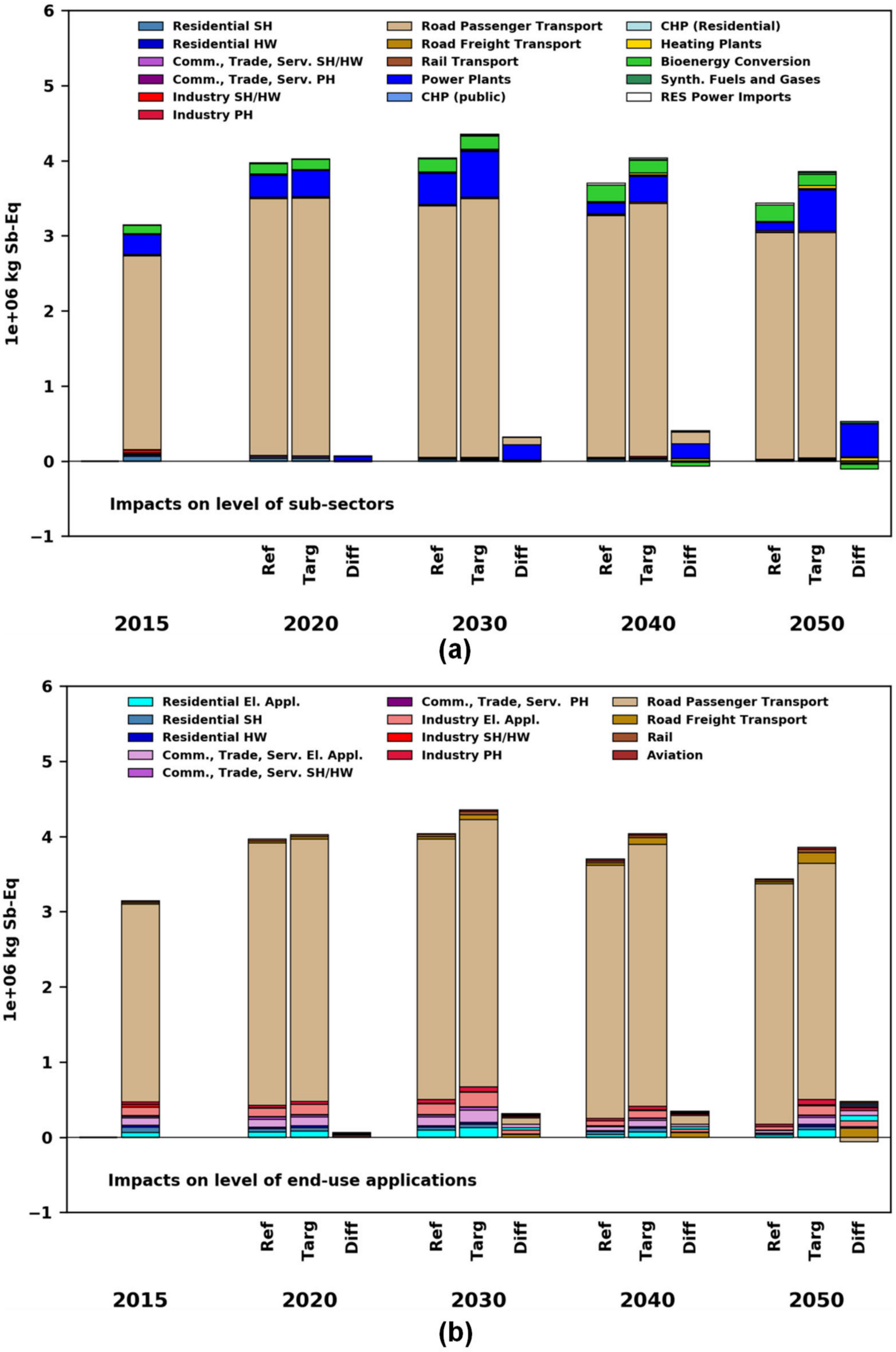

Figure 10. Main drivers for abiotic resource depletion in the 'Target' and 'Reference' scenarios. (**a**) Impact caused by the sub-sectors, (**b**) Impact caused by the end-use applications.

In a sub-sectoral perspective, in both scenarios and for all years, the main driver is road passenger transport (Figure 10a). However, the comparatively stronger expansion of PHEVs with Otto engines and BEVs in the 'Target' scenario only contributes slightly to the adverse side effects. In the electricity sector, which is responsible for most of the higher impacts of the 'Target' scenario, the strong increase in rooftop PV in particular increases the material intensity. While the peak in the 'Reference' scenario in 2030 is also attributed to rooftop PV, the impact in the following years in the 'Reference' scenario is mainly driven by wind-onshore power plants and is noticeably decreasing. Bioethanol production accounts for a large part of the impacts of the bioenergy conversion sector in the 'Reference' scenario.

In the 'Target' scenario, the effects of bioenergy conversion are driven by bioethanol, biodiesel and biogas production, leading to slight co-benefits in this sector. In the 'Target' scenario, the use of flat and tube solar collectors as local heating systems causes most of the impact in this sector.

From an EUAs perspective and in line with the sectoral perspective, passenger cars cause most of the impacts of both scenarios (Figure 10b). Freight transport plays a larger role, as it consumes parts of the liquid biofuels where impacts are associated with the respective infrastructure (e.g., biomass conversion plants). The greater extent of direct electrification results in a comparably higher impact in most other EUAs in the 'Target' scenario compared with the 'Reference' scenario. The only exception is road passenger transport, where slight co-benefits arise due to the larger share of indirect electrification in the 'Target' scenario compared to the 'Reference' scenario via H_2 and the comparatively small contribution of electrolysis to this indicator.

3.3. Influence of Different Life Cycle Phases

To analyse the influence of different life cycle phases in this section, the operation phase is subdivided into direct impacts of the foreground technologies (i.e., direct, on-site operation-dependent emissions) and indirect impacts occurring outside the system boundary of the ESM (e.g., impacts from the production and supply of natural gas). The impacts of the operation that stem from upstream processes are calculated as the difference between the total life cycle impacts of the operation and the direct emissions.

Figure 11 shows the relative contribution of these phases for each impact category considered for 2015 (first bar) and for the 'Reference' (second bar) and the 'Target' (third bar) scenarios in 2050. In general, in can be observed that the relative shares of those life cycle phases vary strongly between the different indicators. They also vary, albeit to a lesser extent, in the time between scenarios.

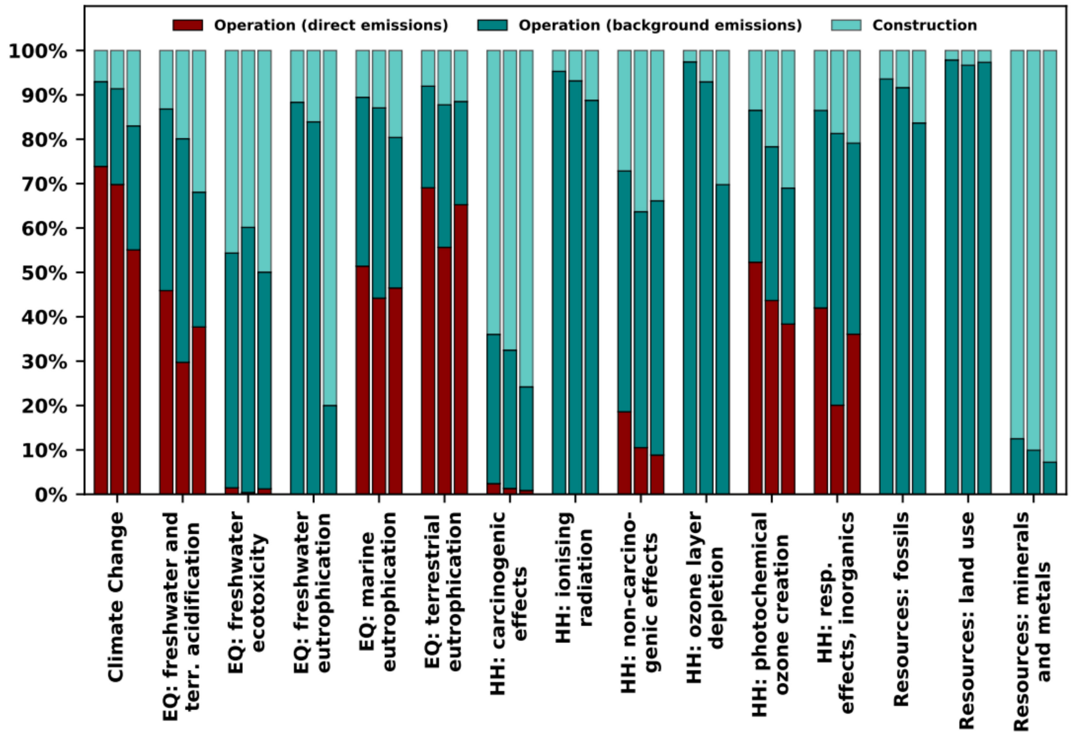

Figure 11. Relative contributions of life cycle phases to total impacts. The first bar chart for each indicator is for the base year 2015, the second and third for the 'Reference' and 'Target' scenarios, respectively, in 2050.

Direct emissions play the dominant role (>50% of absolute impacts) for four out of fifteen indicators in 2015 ('climate change', 'marine eutrophication', 'terrestrial eutrophication', 'photochemical ozone creation'). For most of these indicators, however, there is a shift in the relevance of the life cycle phases towards the construction of energy technologies. In 2050, direct emissions account for an increasingly small proportion of total impacts in most of these impact categories.

For example, the share of direct CO_2 eq emissions in the 'Target' scenario is reduced from 73% in 2015 to 56% in 2050. The limited shift of the LCA phases for 'terrestrial eutrophication' can be explained by the fact that road freight and passenger transport as well as the bioenergy conversion sector, which emit most of NH_3, NO_3 and NO_x, do so at a relatively similar share in 2015 and in 2050 in both scenarios. Especially in the 'Target' scenario, emissions such as NO_x, CH_4 and other volatile organic compounds that contribute to 'photochemical ozone creation' are slightly shifted to the construction phase of the energy technologies, especially in road passenger transport.

For the three indicators 'freshwater and terrestrial acidification', 'non-carcinogenic effects' and 'respiratory effects, inorganics', the share of direct emissions in total impacts is still above 10% in 2015. On the other hand, for all other indicators, direct emissions make only a small to no contribution (<5%) to total impacts. This is the case in all 'resources' type impact categories and for some impact categories that address 'human health' as well as 'ecosystem quality'. Here the effects either occur mostly in the construction phase of the energy technologies or in processes upstream of the operation phase.

This analysis shows that solely considering direct impacts during the operation phase significantly underestimates the total environmental impacts of the energy system. However, the amount of underestimation depends strongly on the respective indicator and on the configuration of the energy system itself, but is expected to become increasingly relevant as scenarios become more ambitious in terms of climate protection.

3.4. Influence of the Global Background Electricity Mix on the Scenarios

Figure 12 shows the influence of the global background electricity mix of the 2 °C scenario relative to the 5 °C scenario from Teske et al. [2] on the indicator values of the 'Target' (Figure 12a) and the 'Reference' (Figure 12b) scenarios. The influence of the global background electricity mix on the individual indicators varies in its extent between the 'Target' and the 'Reference' scenario, as the electricity intensity of all upstream processes (in construction and operation) differs for the processes and technologies relevant in the scenarios. As illustrated in Figure 11, the construction phase is more dominant in the 'Target' scenario than in the 'Reference' scenario. Thus, there is a more pronounced influence on the former (Figure 12a). For most indicators, the influence increases with the development of the transformation of the global electricity mix towards deeper defossilisation.

In the 'Target' scenario, the effect of the background scenario is largest (>10%) for the indicators 'climate change', 'fossils', 'freshwater eutrophication' and 'ionizing radiation', whereas in the 'Reference' scenario this effect occurs only for the latter. For the indicator 'freshwater eutrophication', the positive effect in the 2 °C scenario in 2050 weakens somewhat again (especially visible in the 'Target' scenario), since the Si-based open ground and roof-top PV systems increasingly deployed in the 2 °C scenario show relatively high values for this indicator compared to other conventional power plants more dominant in 2040 (e.g., gas-fired power plants). The strongest effect can be seen for the indicator 'ionising radiation', as the 2 °C background scenario, in contrast to the 5 °C background scenario, phases out the use of nuclear and coal-fired power plants, the strongest sources of ionising radiation in power generation. A detailed sectoral and technological analysis of the effect of the background power mix on environmental impacts is subject to future assessments.

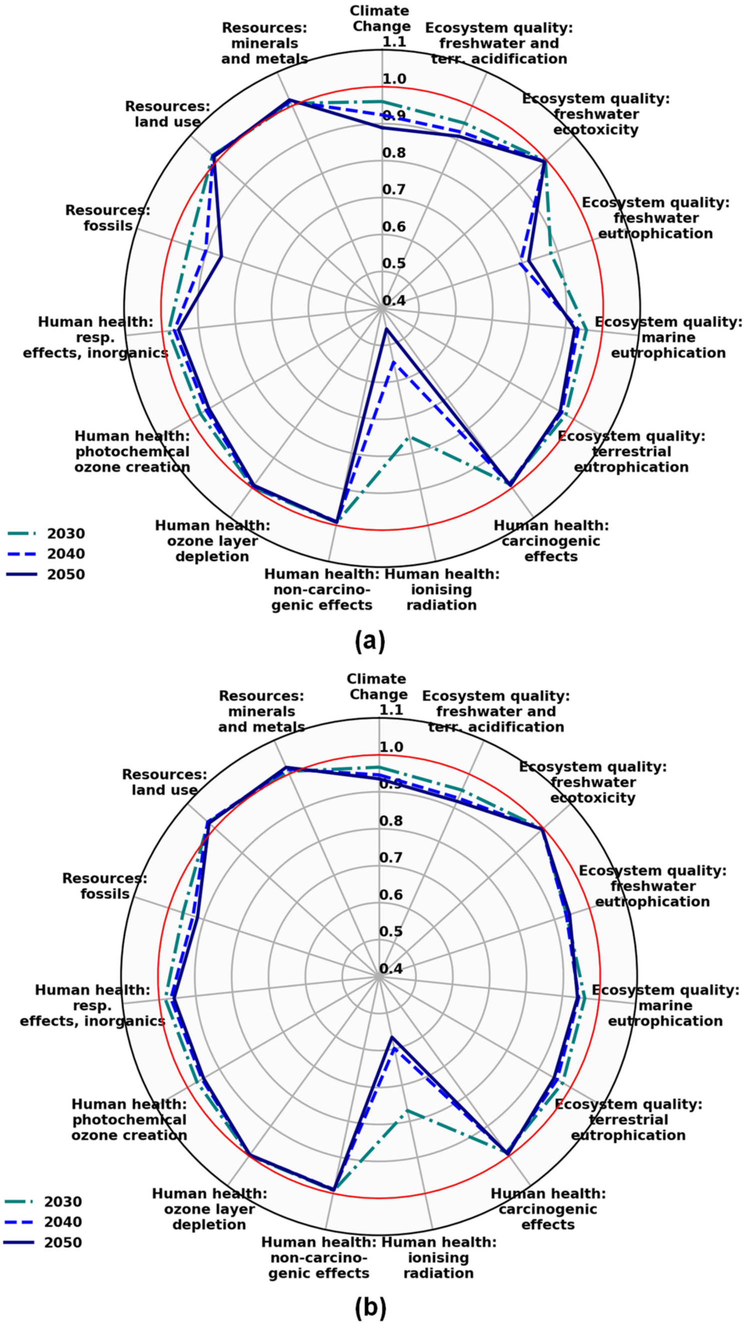

Figure 12. Influence of the global background electricity mix on total environmental impacts in (**a**) the 'Target' and (**b**) the 'Reference' scenario. The figures show the impacts calculated with the 2 °C background scenario relative to impacts calculated with the 5 °C background scenario. The red line indicates the line of 'equal impacts'.

In general, the influence of the background electricity mix on the foreground scenario is particularly relevant for scenarios that are more ambitious in terms of CO_2 emission reduction and thus have a high proportion of impacts embedded in upstream processes, especially in the construction of the necessary infrastructure. This will be even more relevant for scenarios with CO_2 targets on direct emissions beyond a 95% reduction, which are increasingly relevant in the community.

4. Discussion

4.1. Uncertainties Regarding Life Cycle Inventory Data

In line with most previous literature (see Section 1), the ecoinvent database provides most of the LCIs used for this study. The coverage of technologies in ecoinvent 3.3 is good for the electricity sector, although rather limited for non-electricity technologies from the conversion sector (e.g., biofuels, synthetic fuels), transport sector (e.g., BEVs and FCEVs as well as PHEVs) and heat sectors (e.g., industrial heat pumps and solar collectors) and not always fitted to German technologies. In FRITS, some of these shortcomings have been corrected in terms of the level of detail, novelty and completeness of technologies, for example by incorporating LCIs from e.g., BioenergieDat, the SYSEET project, more recent PV data and so far missing technologies such as state of the art electrolysers and heat pumps. In the processes of the bioenergy conversion sector, however, there is still an under-representation of the LCIs on secondary biomass (e.g., biowaste).

Some technologies from the supplemented database had to be assigned to technologies from the model, although their properties do not fully match with respect to the process/technology itself or its scale (e.g., performance class). Future steps will therefore evolve from the best possible completion of technologies in the ESM towards a better harmonization and representation. In some cases, only a single LCI data set is available per technology class, but in reality the system is described by many different subtechnologies for which differentiated LCIs are favorable for future studies.

The LCIs are based on current technologies and future technological developments are considered by adjusting the energy efficiencies (see Section 2.3.4). However, it can be expected that emission factors will change for existing technologies, e.g., due to increased partial load operation or updated emission control systems. Also, for future technologies with different fuel inputs (e.g., biogas in Otto engines) the database has to be extended by respective inventories. Furthermore, material inputs may evolve over time. In future studies, this must be countered either by a further integration of LCIs from the secondary literature that describe a prospective development of the technology under consideration or by the inclusion of generally valid learning curve models (similar to economic learning curve models) to enable the inclusion of material efficiency improvements in existing LCIs and background production processes.

Future global changes in production schemes in the background database were adapted for the electricity mix, which appears to be more relevant as the degree of ambition of the foreground scenario increases and the background becomes increasingly defossilised. Yet, it is to be expected that heat and transport mixes as well as industrial and material extraction processes will also change fundamentally if a defossilisation of the entire energy system is to be achieved.

4.2. Methodological Limitations

Due to the regional structure of the LCI database, it is not possible to distinguish which operation-dependent (indirect) and infrastructure processes and their environmental impacts can be assigned to the geographical system boundary of the ESM (in this case Germany). Further regionalisation of the background database would help to assign processes and impacts to specific regions and would facilitate the inclusion of region-specific scenarios for sectors such as heat and transport. However, this requires not only an adaption in the structure of the database such as the introduction of regionally differentiated markets (e.g., for heat and transport) but also the integration of new LCIs of future relevant processes and scenarios regarding their deployment.

Higher regionalisation of the background database would also have the advantage that double counting and thus the overestimation of environmental impacts at the level of the overall scenario could be better avoided, since the regions considered in the model and the processes depicted in it could be better identified and deleted from the LCI database before the impacts are calculated. The overestimation of impacts due to double counting increases with the inclusion of more sectors (e.g., next to electricity also heat, transport, etc.) and regions (e.g., worldwide) in the ESM. In future studies, input-output tables could be used in order to obtain information on country-specific international trade flows, which in turn could be integrated into LCI databases to increase the regional resolution (e.g., of material, heat and transport supply).

However, such adaptions of the background database are difficult to operationalise with the current software tools. Thus matrix-based approaches, such as those presented in Mendoza Beltran et al. [42], Vandepaer et al. [43] or Fernández Astudillo et al. [6], are becoming increasingly relevant, which also meet the transparency criteria proclaimed by parts of the research community [44,45].

The models used to derive the indicators of the ILCD method are subject to regular quality assessment [39]. While the quality of the indicators 'climate change' and 'respiratory effects, inorganics' analysed in Section 4.1 is considered to be high, the implications of the indicator 'minerals and metals' (next to others) must be treated with great caution. This is because the characterisation factors for each metal are derived from the ratio of annual production to reserves, which fluctuate over time as they are defined by economic considerations not directly related to the depletion problem [46].

Apart from the uncertainty of specific indicators, the linearised approach of the LCIA methods cannot take into account scale variations of impacts, e.g., due to saturation or threshold effects or interactions between different environmental impacts. These issues are partly addressed by the current work of the LCI initiative to improve the LCIA by incorporating further environmental aspects and using harmonised environmental models [47]. Furthermore, impacts are subject to spatial variability, which argues for the use of a spatially differentiated database and regionalized impact assessment methods.

A thorough assessment of all the uncertainties of the assessment stemming from various sources, however, is far beyond the scope of this study. Nevertheless, these aspects point the way for the future development of FRITS.

5. Conclusions and Outlook

The coupling of LCA-based indicators with ESMs enriches the impact assessment of the long-term transformation of energy systems initiated by climate policy. FRITS can provide policy makers and stakeholders with additional information on environmental co-benefits and adverse side effects usually not covered by ESMs. Since it is possible to consider the entire energy system and not only individual energy sectors, the results give a comprehensive picture of the environmental impacts of transformation pathways and can also provide input for subsequent MCDM approaches. FRITS is, in particular, well suited for the assessment of very ambitious climate protection strategies that are characterised by a high share of sector coupling and a prominent role of synthetic gases and fuels for (seasonal) energy storage and the defossilisation of transport and (process) heat. FRITS is transferable to other ESMs that have a different technological and regional scope than the MESAP model used in this paper. It can thus be the basis for future assessments of various mitigation strategies.

The results of the case study show that the ambitious climate protection pathway represented by the 'Target' scenario results in a decrease of environmental impacts relative to 2015 and in comparison to the 'Reference' scenario for most indicators. However, the 'Target' scenario is associated with a significant increase in material and land use and aggravates some human health and ecosystem related impacts. The most controversial picture emerges for the bioenergy conversion sector as it contributes significantly to the adverse side effects but also to the co-benefits of the 'Target' scenario compared to 2015 and to the 'Reference' scenario. The electricity sector accounts for a large consumption of mineral resources but is also one of the main drivers for most of the co-benefits. In absolute terms, road transport (passenger and freight transport) might become the largest source of environmental impacts in the future.

Most of the environmental impacts lie outside the typical system boundaries of ESMs, i.e., they cannot be assessed by the consideration of direct emissions from the energy and transport system alone. Thus, the life cycle perspective is highly important in order to assess all relevant environmental impacts and to disclose the risk of burden shifting to other sectors or regions.

The case study presented here mainly discusses results at indicator and sector level. Future assessments could also be conducted at a deeper technological level for individual life cycle phases and specific indicators and elementary flows. This allows for the detection of environmental hot spots on technology level, to identify needs for action with respect to research and development for individual energy and transport technologies and for regulation measures. However, this type of assessment is still in its beginnings and is subject to high uncertainties. The necessary efforts go beyond the mere integration of new, prospective LCIs. They require the integration of comprehensive scenarios into background databases considering not only future electricity, heat and transport processes, but also future developments in industrial and raw material extraction processes. In general, an open database and platform for coupling ESMs to LCA and vice versa, the integration of results from ESMs into LCAs would greatly facilitate the exploitation of the benefits of combining both methods.

In order to derive increasingly robust, scientifically sound decision support for a sustainable transformation of the energy system, future versions of FRITS will integrate further adaptions of the background database and improvements of the quality of LCIs that represent the foreground technologies.

Supplementary Materials: The Excel supplement available online at http://www.mdpi.com/2071-1050/12/19/8225/s1 contains the following Tables: Table S1: 'Product systems', Table S2: 'Fuel shares', Table S3: 'Assignment to ESM techs', Table S4: 'Background electricity mixes'.

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Appendix A. Adaption of the Background Database and Technology Selection

The ecoinvent database distinguishes processes in transformation activities and markets (consumption mixes). The aggregation of activities in markets simplifies the identification and modification of relevant parameters such as the shares of technologies that provide the same output in a given geographical region. In this study, the electricity markets are manipulated, most of which are at country level or higher such as provinces (see Treyer and Bauer [48] for more information on the electricity markets in ecoinvent v3). The markets for different regions in ecoinvent are first assigned to regions of the scenario (Table A1).

PV technologies in ecoinvent supply electricity at the low-voltage level. For our study, we instead connect PV to the high-voltage level market to properly integrate it in the markets. Furthermore, an equal share of open-ground and rooftop PV in all regions is assumed, since the scenario does not differentiate between the two types. The transmission grid markets and the emissions generated during transmission have not been adjusted and kept at the original level of the inventory data. Power generation technologies that are relevant in the future according to the scenario but are missing in ecoinvent are added to the database's electricity markets. This includes, in particular, concentrated solar power (included from ecoinvent v3.5 and adapted for v3.3) and the use of hydrogen in gas turbines. Data sets for other technologies, e.g., ocean energy, which are missing in ecoinvent and have little relevance in the scenario, are not integrated into the database.

Table A1. Matching of scenario regions to market regions in the ecoinvent database.

Scenario Region	Corresponding Regions of the Electricity Markets in Ecoinvent v3.3
Africa	ZA, TZ
China	CN-GD, CN-GX, CN-GZ, CN-HA, CN-YN, CN-ZJ, CN-AH, CN-BJ, CN-CQ, CN-FJ, CN-GS, CN-HB, CN-HE, CN-HL, CN-HN, CN-HU, CN-JL, CN-JS, CN-JX, CN-LN, CN-NM, CN-NX, CN-QH, CN-SA, CN-SC, CN-SD, CN-SH, CN-SX, CN-TJ, CN-XJ, CN-XZ, CN-ZJ
Eurasia	BA, BG, CY, HR, LT, LV, MK, MT, RO, RS, RU, SI, UA
India	IN
Latin America	BR, CL, PE
Middle East	IR, SA
OECD Europe	AT, BE, CH, CZ, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, NL, NO, PL, PT, SE, SK, TR
OECD North America	CA-AB, CA-BC, CA-MB, CA-NB, CA-NF, CA-NS, CA-NT, CA-NU, CA-ON, CA-PE, CA-QC, CA-SK, CA-YK, MX, ASCC, FRCC, HICC, MRO, TRE, WECC, NPCC, SPP, RFC, SERC
OECD Pacific	AU, JP, KR
Other Asia	ID, MY, TH, TW

In a next step, the detailed subtechnologies (e.g., different size classes of onshore wind turbines) of the database have to be mapped to a technology class (e.g., wind onshore) of the global scenario. If all the markets assigned to a scenario region (see Table A1) contain more than three technologies of a group (e.g., lignite power plant), the number of technologies selected is limited to a maximum of three of the same type. This selection is based on the amount of electricity produced annually in the individual markets documented in the ecoinvent database, multiplied by the share of electricity produced by these technologies in these markets. While three are selected to consider inner-regional differences (e.g., in full load hours, emission factors, sub-technology types) within a technology class, the method is open to more representative data sets for a region. If there is no specific technology in the markets assigned to the scenario region, the corresponding Rest-of-the-World (RoW) data set is used as proxy (see Table S4 in the supplementary material for the documentation of the specific technologies per scenario region and the electricity production shares). The markets are parameterized for the scenario years 2015, 2020, 2030, 2040 and 2050. The resulting LCA impacts for the (foreground) technologies between those years are obtained using linear interpolation.

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2.2 Paper 2

Status	**Accepted in:** Energies, Special Issue Life Cycle Assessment of Sustainable Energy System
Title	Considering life-cycle greenhouse gas emissions in power systems expansion planning for Europe and North Africa using multi-objective optimization
Co-Authors	Karl-Kiên Cao, Kim Kira Miskiw, Heidi Hottenroth, Tobias Naegler
Submission year & month	12/2020
Access	- ☒ Gold Open Access ☐ Green Open Access ☐ Closed access
Contributions	☒ Conceptualization ☒ Methodology ☒ Software ☒ Validation ☒ Formal analysis ☒ Investigation ☒ Data curation ☒ Writing: original draft preparation ☒ Writing: review and editing ☐ Supervision ☒ Funding acquisition
Specific objective	Assessment of the trade-offs between system costs and life cycle GHG emissions in future scenarios on the power system in EUNA.
Thesis-overarching objectives	2.a) Implementation a method for multi-objective optimization in large-scale ESOMs 2.b) Parameterization of an ESOM with life cycle impacts 2.c) Analysis of the trade-offs between system costs and life cycle GHG emissions, including ex-post assessment of other life cycle impacts
Methodology	Parameterization of an ESOM with life cycle environmental impacts, multi-objective optimization
Key outcome	More accurate model-based assessments of future scenarios by considering life cycle environmental impacts in ESOMs using multi-objective optimization and environmental ex-post assessment.

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Considering Life-Cycle Greenhouse Gas Emissions in Power System Expansion Planning for Europe and North Africa Using Multi-Objective Optimization

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Abstract: We integrate life-cycle indicators for various technologies of an energy system model with high spatiotemporal detail and a focus on Europe and North Africa. Using multi-objective optimization, we calculate a pareto front that allows us to assess the trade-offs between system costs and life-cycle greenhouse gas (GHG) emissions of future power systems. Furthermore, we perform environmental ex-post assessments of selected solutions using a broad set of life-cycle impact categories. In a system with the least life-cycle GHG emissions, the costs would increase by ~63%, thereby reducing life-cycle GHG emissions by ~82% compared to the cost optimal solution. Power systems mitigating a substantial part of life-cycle GHG emissions with small increases in system costs show a trend towards a deployment of wind onshore, electricity grid and a decline in photovoltaic plants and Li-ion storage. Further reductions are achieved by the deployment of concentrated solar power, wind offshore and nuclear power but lead to considerably higher costs compared to the cost optimal solution. Power systems that mitigate life-cycle GHG emissions also perform better for most impact categories but have higher ionizing radiation, water use and increased fossil fuel demand driven by nuclear power. This study shows that it is crucial to consider upstream GHG emissions in future assessments, as they represent an inheritable part of total emissions in ambitious energy scenarios that so far mainly aim to reduce direct CO_2 emissions.

Keywords: energy system modeling; life-cycle assessment; multi-objective optimization

1. Introduction

As the power sector offers the greatest cost-effective potential for emission reductions compared with other sectors, such as heat and transport, cost-optimized strategies to limit global warming to below 2 °C typically have close to zero emissions in the power sector by the middle of the century [1]. However, energy system optimization models (ESOMs) usually only consider direct on-site CO_2 emissions when assessing the cost-optimized design of infrastructure components of future electricity supply (e.g. power plants, storage facilities, and grids).

Life-cycle assessments (LCAs) quantify the potential impacts of technologies and processes across a comprehensive set of environmental categories, covering entire life-cycle chains, associated emissions, and ecologically relevant extractions from the environment [2]. The LCA literature on renewable energy conversion technologies showed that they are associated with higher upstream energy demand compared to conventional technologies and higher corresponding indirect (i.e. not caused by the combustion of fuels on site) greenhouse gas (GHG) emissions and other environmental impacts per unit of capacity [3]. Thus, concerns have been raised that these may affect the emissions reduction potential of low-carbon technologies and that other environmental stressors may be overlooked [4]. ESOMs with high spatial and temporal resolution analyze cost-optimized, long-term strategies to meet the emission limitations implied by climate targets [5]. However, indirect emissions, especially those related to the energy required for the construction of power plants and the production and transport of fuels and other inputs, are usually not considered in those models. Thus, the inclusion of data on life-cycle impacts in ESOMs is a promising approach in order to overcome the shortcomings of "classical" ESOMs. Due to their complementary nature, the combination of ESOMs and LCAs is an emerging field of research and can guide energy policy to achieve energy systems with improved overall environmental performance.

To date, life-cycle indicators have mostly been linked to model output in order to estimate environmental impacts (also called "ex-post assessment"). For example, Berrill et al. [6] showed that systems largely based on variable renewable energy (VRE) perform better for most impact categories but have larger resource depletion and land occupation impacts than systems based on fossil energy options. Hertwich et al. [7] compared the global BLUE Map and the business-as-usual scenarios from the International Energy Agency (IEA) and found that low-carbon technologies allow for the reduction of pollution-based impacts, while metal demand increases. Xu et al. [8] confirmed the results of the latter two studies for European electricity scenarios, pointing out in particular the high land requirements of photovoltaic (PV) installations. Luderer et al. [9] assessed scenarios from various integrated assessment models (IAMs) and showed that environmental effects largely depend on the choice of technology and that mitigation efforts tend to increase resource and land use impacts in line with the former studies.

While such approaches provide meaningful insights into the environmental performance of given scenarios, they do not take full advantage of the model's capabilities to determine environmentally improved system configurations compared to original model setups (e.g. pure cost optimization with upper limits for direct CO_2 emissions). More specifically, solutions are overlooked that internalize (also called "model-endogenous integration") life-cycle environmental impacts. In the literature, integration efforts are manifold and range from the setting of upper limits for certain indicators to the monetarization of emissions and indicators to multi-objective optimization. For example, Daly et al. [10] set upper limits on both direct and indirect CO_2 emissions in an ESOM for the UK and found that mitigating the total emissions nearly doubles the marginal abatement costs compared to the consideration of direct CO_2 emissions only. McDowall et al. [11] took a similar approach with a focus on Europe and showed that limiting indirect GHG emissions increases the use of wind power, while the expansion of solar PV declines. Algunaibet et al. [12] downscaled the eight planetary boundaries defined by Ryberg et al. [13], which aim to provide a safe space for humanity, to the US power sector and showed that compliance with the upper limits leads to a doubling of system costs compared to the cost-optimal solution. Portugal-Pereira et al. [14] considered a tax on both direct and indirect GHG emissions for part of the energy system studied. This led to a shift towards the use of technologies that did not consider indirect emissions and underlined the importance of integrating indirect emissions for all technologies that can be expanded in an ESOM. Another study by Pehl et al. [15] followed a similar approach but covered GHG emissions for all technologies optimized endogenously. The authors showed that a tax on indirect GHG emissions, as opposed to a tax on direct emissions only, leads to an increased expansion of concentrated solar power (CSP), wind, and nuclear power plants. An aggregated environmental indicator was included in the optimization function by Rauner and Budzinski [16] covering the German electricity supply. Applying multi-objective optimization, the authors showed that an environmentally sustainable system leads to increased deployment of VRE, particularly wind energy, compared to an unconstrained cost-optimal system based mainly on fossil fuels. Multi-objective optimization integrating costs and life-cycle impacts was conducted by Tietze et al. [17] and applied to an exemplary residential quarter. In several model runs that considered different impacts, the authors showed a number of different system configurations resulting from different weightings of environmental impacts and highlighted the importance of including the life-cycle perspective in the design of energy systems. Vandepaer et al. [18] optimized both the system costs and life-cycle impacts and then included predefined system cost constraints in the optimization of environmental impacts for the Swiss energy system. The authors demonstrated that a small increase in costs can result in substantial climate change mitigation. However, this statement is based on only a small selection of solutions explored.

At present, however, the consideration of life-cycle GHG emissions as an additional objective to system costs is still very limited. Furthermore, the ESOMs in most of the latter studies have a low temporal and/or geographical resolution and are therefore not able to fully capture the feed-in of VRE and the resulting impact on auxiliary infrastructures such as storage and grid. We overcome these limitations with the integration of life-cycle impacts into the spatiotemporal high-resolution ESOM "Renewable Energy Mix" (REMix). The model is particularly designed to assess the infrastructural demand for a reliable power supply. We use a comprehensive set of life-cycle inventories (LCIs) of up-to-date electricity supply, distribution, storage, and conversion technologies. The life-cycle indicators generated rely on harmonized LCIs that consider the evolutions in their upstream life-cycles by incorporating the effects of future decarbonization measures in the global electricity sector (such future-oriented applications of LCAs are also known as "prospective LCAs" [19]). To evaluate the effect of the reduction of life-cycle GHG emissions on system costs, we apply multi-objective optimization and calculate a pareto front. This concept was first introduced by Vilfredo Pareto and allows for the systematic assessment of trade-offs between conflicting objectives [20]. In addition, we analyze the occurrence of burden shifts over several life-cycle impacts for the solutions explored. The extended ESOM is applied to Europe and North Africa (EUNA). Specifically, our aim is to answer the following research questions:

- What are the trade-offs between total system costs and life-cycle GHG emissions for the future electricity system in EUNA?
- How does the structure of the power system and the grid change when life-cycle GHG emissions are reduced?
- What are the trade-offs that occur regarding further life-cycle environmental impacts?

Our research is particularly useful for energy and environmental policy makers aiming for cleaner power generation considering the entire upstream supply chain.

This article is structured as follows: Section 2 presents the methodology and the case study, Section 3 illustrates the results of the case study, Section 4 presents the discussions, while Section 5 draws the main conclusions from the work.

2. Materials and Methods

Figure 1 illustrates the workflow of this study and the corresponding sections of the paper in which we provide details on the different steps.

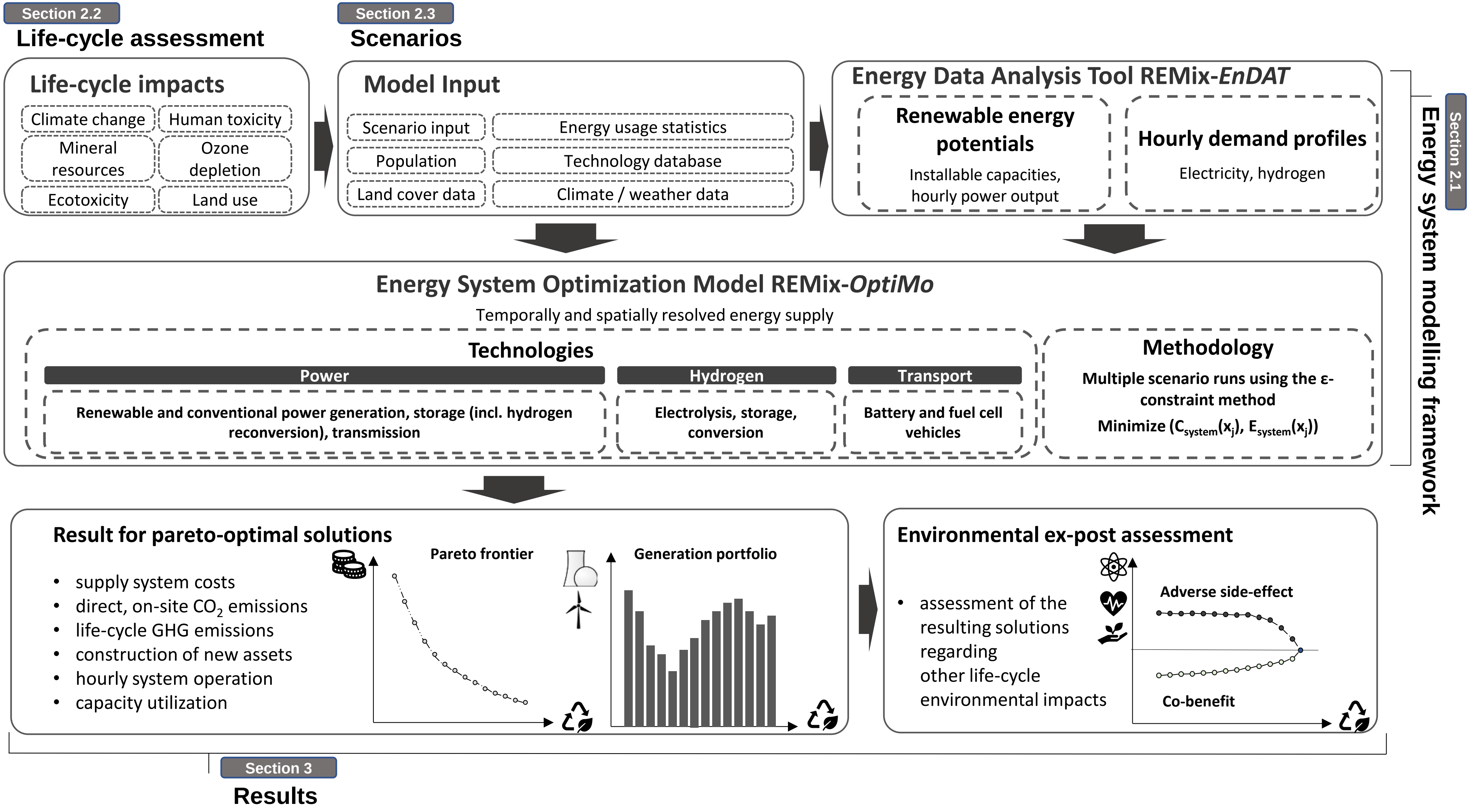

Figure 1. Flowchart of models, methods, and results. Block circles indicate the corresponding sections in the article.

The approach consists of two main parts: ESOM on the one hand and life-cycle impacts for the technologies considered on the other hand. The ESOM used in this study is REMix which is extended by an algorithm that enables multi-objective optimization (see Section 2.1.). The LCI database used provides the technology specific indicators for the ESOM (see Section 2.2.). We use a specific scenario setup for this case study based on earlier work (see Section 2.3.). Then, multi-objective optimization is performed using techno-economic parameters and the life-cycle indicators (in this case study, GHG emissions). In addition, environmental ex-post assessment is conducted for the resulting pareto optimal solutions. Details on the modeling approach developed are described in the next section.

2.1. Extended Energy System Model to Perform Multi-Objective Optimization

In this chapter, we first explain the general structure of the REMix modeling framework and then describe the adjustments necessary to calculate the life-cycle indicators for the power system and to perform multi-objective optimization.

2.1.1. The Traditional REMix Modeling Framework

A comprehensive description of REMix and the corresponding equations are provided in Gils et al. [21]. In short, the model consists of two main elements: the energy data analysis tool (REMix-EnDAT) and the optimization model (REMix-OptiMo) (Figure 1). REMix-EnDAT performs the VRE resource assessment in high spatial and temporal resolution. It provides hourly generation profiles for the main technologies aggregated to user-defined regions. In addition, electricity demand profiles are generated in this part of the model. The supply and demand profiles are used in REMix-OptiMo to determine the most cost-effective operation and expansion of all system components during every hour of the year. REMix-OptiMo is a deterministic linear optimization program in a formulation of a general algebraic modeling system (GAMS). The model is built in a modular structure with a wide range of technology modules (e.g. a module for storage technologies) that are largely independent of each other. In each module, the parameters, variables, equations, and inequalities used to represent the respective technical and economic characteristics are defined. Power generation, storage and grid technologies are represented by their installed and maximum installable capacities, their investment and operating costs, and their efficiencies. All technology modules allow for the operation and expansion of the technologies considered. Additions of power plants, transmission lines or storage capacities can be optimized by the model according to the existing potentials and system requirements. Investments in new capacities consider technology costs, payback periods, and interest rates.

In short, the model:

- Minimizes the total system cost, which consists of investment costs (treated as annuities) and the operating costs of the entire system;
- Decides on the size of energy storage (power capacity, energy capacity), hydrogen storage, grid, and generation technologies;
- Considers a one-year modeling horizon (in our case the year 2050) with full hourly resolution (i.e. 8760 time steps) for which the optimal operation of each technology at each modeling node is determined.

In previous studies, REMix was used to estimate the cost-optimal design of energy systems and has been applied in several studies, ranging from case studies for specific regions [22–27], model comparisons [28] to comprehensive model coupling [29]. The model adaptions necessary to consider LCA-based indicators in the REMix are described in the next section.

2.1.2. Extension of the REMix Modeling Framework

For the purpose of this study, two new modules are introduced to REMix-OptiMo. The first module collects all investment and dispatch variables of the different technologies and calculates the system-wide life-cycle impacts, which can also be used for environmental ex-post assessments. This module also contains the description of the second objective function (Equation (1)) next to systems costs. Note that for the sake of clarity, we simplified the notation (e.g. planning year or technology sets are neglected) compared with that implemented in REMix. In the present study, the second objective function to be minimized summarizes the life-cycle GHG emissions of all technologies considered to the overall life-cycle GHG emissions. It is composed of the GHG emissions of all added capacities $\mathrm{E_{invest}}$ (Equation (2)), with $\mathrm{P_{addedCap}}$ being the endogenous optimization results, $\mathrm{I_{specImp}}$ the corresponding technology specific impacts (e.g. per GW$_{\text{electricity}}$), divided by the calendrical lifetime of the plant $\mathrm{T_{mod}}$ to account for the single year time horizon of the model calculation. Operation dependent life-cycle impacts $\mathrm{E_{operation}}$ (Equation (3)) consist of the sum over each time step t of the hourly generation of added $\mathrm{P_{genAddedCap}(t)}$ as well as existing capacities $\mathrm{P_{genExistCap}(t)}$ multiplied with the corresponding life-cycle impacts related to operation $\mathrm{I_{genSpecImp}(t)}$ (e.g. per GWh$_{\text{electricity}}$). The term is multiplied by the efficiency ratio between the LCI data η_{LCI} and the ESOM η_{mod} to correct for differences in assumptions on efficiencies. Existing capacities can be defined exogenously. In addition, we include a penalty for unsupplied power $\mathrm{E_{unsupplPow}}$.

$$\min\left\{\mathrm{E_{invest}} + \mathrm{E_{operation}} + \mathrm{E_{unsupplPow}}\right\} \tag{1}$$

$$\mathrm{E_{invest}} = \mathrm{P_{addedCap}} \cdot \mathrm{I_{specImp}} \cdot \frac{1}{\mathrm{T_{mod}}} \tag{2}$$

$$\mathrm{E_{operation}} = \sum_{\mathrm{t}} \left(\left(\mathrm{P_{genAddedCap}(t)} + \mathrm{P_{genExistCap}(t)} \right) \cdot \mathrm{I_{genSpecImp}(t)} \cdot \frac{\eta_{\mathrm{LCI}}}{\eta_{\mathrm{mod}}} \right) \tag{3}$$

In the second module, the augmented epsilon-constraint method (ε-CM) described by Mavrotas [30] is implemented to perform multi-objective optimization to assess the trade-offs between system costs and life-cycle GHG emissions. The pareto front covers the solution space between the minimum cost and the least GHG emission-intensive solution. Compared to a weighted objective function, the ε-CM offers the advantages of finding solutions that are not supported by weighting and of avoiding sensitivities to scaling. In addition, it allows for a systematic exploration of pareto-efficient solutions. A description of the approach adopted can be found in Appendix A.

The adaptions of the LCIs necessary to populate the REMix model with life-cycle indicators for the different technologies (i.e. for deriving $\mathrm{I_{specImp}}$ and $\mathrm{I_{genSpecImp}(t)}$) are described in the next section.

2.2. Life-Cycle Assessment

The aim of this study is to quantify life-cycle impacts of meeting the electricity demand of the EUNA region in 2050, considering all upstream activities in the supply chain of energy technologies. For this purpose, we base this study on the Framework for the Assessment of Environmental Impacts of Transformation Scenarios (FRITS) that uses the ecoinvent 3.3 cut-off background LCI database [31]. The framework was developed to assess the life-cycle impacts of existing energy system scenarios on different sectoral and geographical scales and contains the LCI data used in this case study.

2.2.1. Foreground Life Cycle Inventory Data and Technology Mapping

In LCA, LCI data are differentiated into fore- and background data. Foreground data are those that describe the system that is the focus of the analysis; background data are those supporting the modeling of the foreground system. In our case, foreground LCI data represent the technologies in REMix. Therefore, the technologies presented in REMix must be mapped to the appropriate LCI data sets based on the technical specifications described in both sources. The LCI data for energy technologies that are missing in the ecoinvent 3.3 database (e.g. stationary battery storage, high-voltage direct current (HVDC) electricity grid, electrolyzers) were collected from scientific sources and integrated into the LCI database. The full list of technologies and corresponding LCI data sources are listed in Appendix B, Table A2.

2.2.2. Adjustments of Fore- and Background Life-Cycle Inventory Data

In LCAs, operations- and infrastructure-related datasets are usually aggregated into one LCI dataset. We therefore disaggregate the LCI data into operations- and infrastructure-related processes for each technology to match the corresponding decision variables in REMix.

FRITS enables the consideration of regional adjustments of the global background power generation mix. In the present study, the 2 °C scenario by Teske et al. [32] is applied to the background database, which describes region-specific power mixes until 2050. The main feature of renewable energy technologies is that a large proportion of the environmental impact occurs in the upstream supply chain of these technologies. Changes in the electricity system affect the environmental impacts caused, in particular, by the manufacturing processes. Thus, we capture important improvements in the electricity system that provides electricity in the manufacturing of power plants, storage and conversion technologies, and electricity grids.

A challenge in coupling LCA-based environmental impacts to geographically large-scale ESOMs is to avoid double counting of environmental impacts in the background LCI database. More specifically, the LCI for processes in the upstream supply chain (e.g. steel production) may include energy flows from processes that are already within the boundary defined in the ESOM (e.g. electricity production). In this study, we avoid double counting for the electricity sector by matching the markets for electricity generation in ecoinvent with the regions in REMix (see Table S2). Subsequently, we delete all of the input flows (e.g. electricity production by a wind turbine) from these markets. This approach to avoid double counting in the background has already been implemented in the earlier application of FRITS [31], and similar approaches have been used in other work as a possible option to address this challenge [15,33,34].

In addition, double counting also occurs in operation depended foreground data sets (e.g. electricity as input to electrolysis). Thus, these flows are removed from the respective LCI data sets.

2.2.3. Life-Cycle-Based Indicators

In the final step, we generate life-cycle indicators that provide the environmental scores of the different impact categories for the technologies and integrate them as parameters into the model (see Section 2.1.2.).

In this paper, indicators are calculated using the International Reference Life Cycle Data System (ILCD) 2.0 2018 impact assessment method that translates thousands of LCI entries (e.g. NO_X and $PM_{2.5}$) to sixteen mid-point impact categories using a variety of environmental mechanisms [35] (Table 1). The method was selected because it was the most up to date at the time the study was conducted and was developed in a transparent and scientifically sound process. Furthermore, the characterization factors were adapted for the ecoinvent database used.

The technology-specific indicators integrated in REMix are listed in Table S4 of the Supplementary Materials. Life-cycle CO_2 eq emissions represented by the impact category “climate change” are used as an additional objective in the ESOM. The other indicators are applied in environmental ex-post assessment of the different solutions. Note that in the following, life-cycle CO_2 eq emissions, which also include emissions other than carbon dioxide, such as ethane, methane or nitrogen fluoride, are referred to as life-cycle GHG emissions and CO_2 emissions are the direct, ESOM-based emissions (traditional scope of REMix).

Table 1. Mid-point indicators following the International Reference Life Cycle Data System (ILCD) 2.0 2018 methodology [35] used in this study.

Impact Category	Indicators	Units
	For multi-objective optimization	
Climate change	GWP 100a	kg CO_2 eq
	For additional ex-post assessment of environmental co-benefits and adverse side effects	
Ecosystem quality	Freshwater and terrestrial acidification	mol H+ eq
	Freshwater ecotoxicity	CTUe
	Freshwater eutrophication	kg P eq
	Marine eutrophication	kg N eq
	Terrestrial eutrophication	mol N eq
Human health	Non-carcinogenic effects	CTUh
	Carcinogenic effects	CTUh
	Ionizing radiation	kg U235 eq
	Ozone layer depletion	kg CFC-11 eq
	Photochemical ozone creation	kg NMVOC eq
	Respiratory effects, inorganics	disease incidence
Resources	Fossils (including uranium) [1]	MJ
	Land use	points
	Minerals and metals	kg Sb eq
	Dissipated water	m^3 water eq

[1] In the ILCD 2.0 2018 methodology, this indicator was initially named “Fossils” and was renamed to “Fossils (including uranium)” for the sake of clarity.

The information considered in the ESOM for the adjustment of the LCA indicators is efficiency and lifetime to ensure consistency and to allow for the correct consideration of the impacts from construction (see Equations (3) and (4)), in line with earlier integration work [16,18].

2.3. Scenario Setup

Our scenario setup is based on the model parameterization and the “CSP&H2” scenario in combination with the “Trend” scenario for transmission grid expansion defined in Cao et al. [36]. The “Trend” scenario assumes that all major ten-year network development plan (TYNDP) projects [37] are implemented and the current structure of the transmission network will be maintained. New expansion in the high and extra-high voltage network is possible. Note that REMix also allows for the expansion of cables (ground embedded overland cables in combination with submarine cables), which are presented separately from lines (aerial lines in combination with submarine cables) in this work.

A certain part of power plant capacities is defined exogenously. For conventional power plants, the commissioning date from the World Electric Power Plants Data Base (WEPP) [38] is combined with lifetime assumptions to determine the phase-out date. The capacities remaining in the scenario year are assumed model-exogenous for the modeling. Model-exogenous capacities for PV and wind power plants are derived from Reference [37]. Wind power plants are divided into on- and offshore plants and PV into open ground and rooftop plants. The country-specific distribution is done as follows: For wind, one half of the wind power generation capacity given in the data set is divided according to the current onshore–offshore ratio, determined from Reference [39]. The other half is divided according to the ratio of maximum installable generation capacities based on the potential analysis in REMix-EnDAT. PV is allocated exclusively according to the ratio of the maximum installable generation capacities based on the potential analysis. Hydropower plants are differentiated into run of river, pumped storage, and reservoir hydropower plants. For the installed capacities and their geographical allocation, a data set from the Frankfurt Institute for Advanced Studies (FIAS) is used [40]. There is no model-exogenous specification of generation capacities for biomass and geothermal. Note that in the following, the life-cycle-based environmental impacts as well as the system costs are composed of exogenously defined as well as added capacities.

For the sake of simplicity, the heat sector is not considered in the present study. This is the main difference with the scenario setup by Cao et al. [36], who, for example, also considered the additional electricity demand by heat pumps, electric boilers, and the heat demand to be covered by cogeneration.

In short, the scenario setup has the following characteristics:

- **Regions:** European countries (ENTSO-E members), with the exception of Turkey, Iceland, Cyprus, and Ukraine; North African countries: Algeria, Morocco, and Tunisia. Figure 2 illustrates the spatial resolution and the representation of the power grid;
- **Technological and sectoral scope:** Fossil, nuclear, and renewable power generators, energy storage for load balancing, electricity exchange, and hydrogen transport (via H_2 pipelines) among model nodes. Furthermore, we allow direct electricity imports via HVDC lines from North Africa to Europe as specified by Hess [25,26]. Concerning the sectoral scope, we consider the power system as well as additional electricity demands for electric and H_2 vehicles. The hydrogen demand for mobility is specified exogenously, while hydrogen production and storage are optimized endogenously. All assumptions on specific investment, operation, and maintenance costs are listed in Table S1 of the Supplementary Materials;
- **Constraints:** To allow regional flexibility in achieving CO_2 reduction targets on direct emissions of ~95% compared to 1990, we define a CO_2 cap (~60 Mt) for the entire model region. This cap is based on country-specific annual energy balances [41] for electricity generation and fuel-specific CO_2 emission factors [42]. Recall that the renewable potentials derived from REMix-EnDAT (including hydropower plants) constrain the maximum installable capacity of renewable technologies. In addition, nuclear power is restricted to currently installed capacities and projects planned in countries where it is permitted in line with assumptions used in the project "analysis of the European energy system under the aspects of flexibility and technological progress" (REFLEX) and follow-up publications [43–45]. This results in maximal installable capacities of ~131 GW, most of which can be located in France (~63 GW). Furthermore, we distribute the power and hydrogen generation capacities across EUNA by setting country-specific self-supply thresholds of 80% in terms of annual demand (see Equation (A5) in Appendix A).

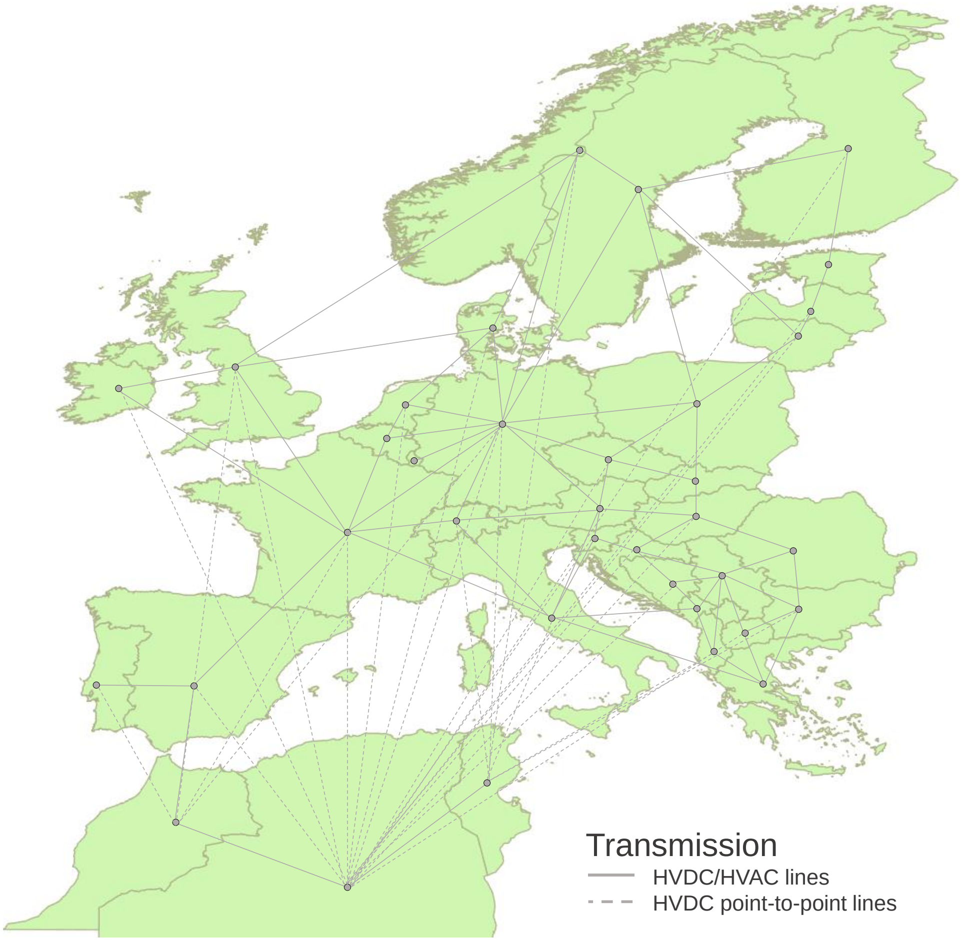

Figure 2. Geographical scope and abstraction of the power transmission grid as used in this study. High-voltage direct current (HVDC) point-to-point transmission options serve to supply electricity from North Africa as studied by Hess [25,26].

The use of 80% of the self-sufficiency ratio for electricity and hydrogen generation is based on expert judgement deduced in an internal workshop from preliminary model runs.

The annual electricity demand amounts to 3062 TWh for conventional consumers, 263 TWh for electric vehicles and 570 TWh for H_2 vehicles. Note that final inputs for REMix are hourly time series of electricity and hydrogen consumption. The optimization is performed using weather data from the year 2006, which was a year with average capacity factors compared to other available years in REMix-EnDAT. Since it is our goal to investigate a variety of system configurations, we calculate 20 pareto-efficient points for the scenario setup.

3. Results

We first focus on the trade-offs between system costs and life-cycle GHG emissions in Section 3.1. Subsequently, we analyze the structure of the power system and the power grid for the individual solutions on the pareto frontier (Section 3.2.). Co-benefits and adverse side effects with respect to further life-cycle environmental impacts are analyzed in Section 3.3 (ex-post assessment of solutions on the pareto front).

3.1. Trade-Offs between System Costs and Life-Cycle Greenhouse Gas Emissions

The pareto front illustrated in Figure 3 represents the trade-offs between system costs and climate impacts for both life-cycle GHG emissions (green dots) and the share of direct CO_2 emitted due to the energy system operation (blue dots). Each point on the pareto front represents an energy system in the year 2050. According to the implementation of the ε-CM, the solution of the point in the upper left represents the point with least GHG emissions, whereas the point on the very right represents the system with the least costs. Finally, the solutions for the points between these two extrema result from minimizing system costs while constraining life-cycle GHG emissions for a given threshold. Starting at the least cost-intensive solution this threshold is increased in equidistant steps.

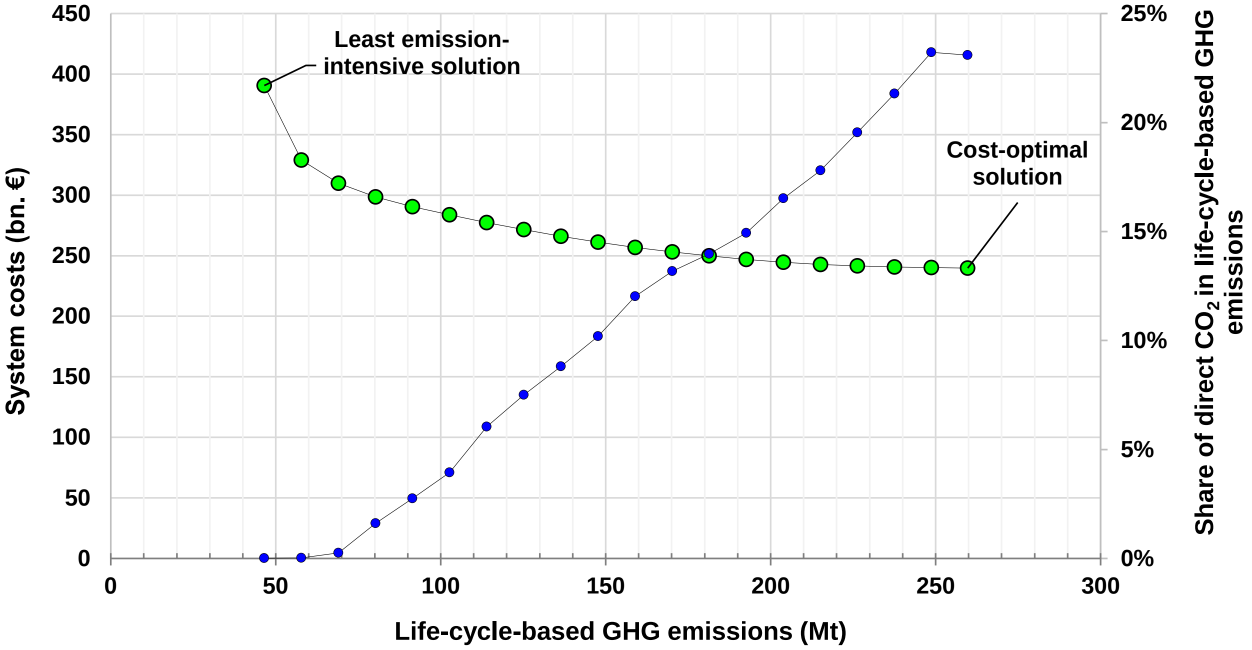

Figure 3. Pareto front to illustrate the trade-offs between system costs (left *y*-axis) and life-cycle GHG emissions (*x*-axis) (green dots). Share of direct CO_2 emissions (right *y*-axis) in total life-cycle GHG emissions for the individual solutions (blue dots); direct CO_2 emissions are based on the REMix output.

Following the pareto front from right to left, we initially see a strong decline in life-cycle GHG emissions in relation to rising system costs. More specifically, 22% (i.e. from 260 Mt to 204 Mt) of life-cycle GHG emissions could be mitigated with an increase in system costs of 2%. This range of solutions could be described as the "low-hanging fruit" of a cost efficient, comprehensive, climate-friendly electricity supply. A reduction in life-cycle GHG emissions by approximately two-thirds (from 260 Mt to 91 Mt) is accompanied by an increase in system costs of 21%. A further reduction is theoretically possible to 18% of the initial emissions. The cost increase in this case is 63% compared to the cost-optimal solution.

In the cost-optimum solution, the carbon footprint of the electricity mix is 67 g CO_2eq/kWh, whereas in the system with least GHG emissions it decreases to 12 g CO_2eq/kWh. Compared to the current electricity mix for Europe (409 g CO_2eq/kWh) [46], this is a reduction of 84% or 97%, respectively.

As expected, the reduction in life-cycle GHG emissions also leads to a reduction in direct CO_2 emissions. With a 6% cost increase compared to the cost optimum, life-cycle GHG emissions reduced by 34% (to 170 Mt) and direct CO_2 emissions by 63% (to 22 Mt). This drop in direct emissions continues and reaches 100% in the last two solutions. As life-cycle GHG emissions are reduced, the relative cost differences between the individual solutions grow. This is particularly evident in the last two points on the pareto front (i.e. the reduction of emissions by 78% (to 58 Mt) and 82% (47 Mt) compared to the cost optimum).

From an LCA perspective, the impacts associated with electricity supply in increasingly ambitious systems are being shifted from operations to the manufacturing of the generation infrastructure: whereas direct CO_2 emissions account for 23% of the total life-cycle GHG emissions in the cost optimum, their share drops to 0% in the solution with least life-cycle GHG emissions. At this point, all GHG emissions are caused by background processes. This highlights the need for full emissions accounting in future assessments of ambitious energy systems. It also shows that technologies with low GHG emissions upstream in the supply chain are crucial for ambitious energy systems, as their direct counterparts can almost be omitted with still moderate cost increases. Note, however, that while the LCI database has been adapted to reflect low carbon future electricity supply, other emission-intensive processes, such as fossil fuel-based heat in industry and freight transport, remain at the current state on the database. Further adjustments in these sectors would reduce upstream GHG emission and thereby increase the share of direct CO_2 emissions in total life-cycle GHG emissions.

To better understand the roles of individual technologies for the solutions on the pareto front, we next analyze the resulting mix of power generators and technologies for temporal and spatial load balancing in the power system.

3.2. Structure of the Power Plant Portfolio

Figure 4 shows the power generation capacities in panel (a) and the difference between the two extremes, the cost optimum, and the least GHG emissions intensive solution, are shown in panel (b).

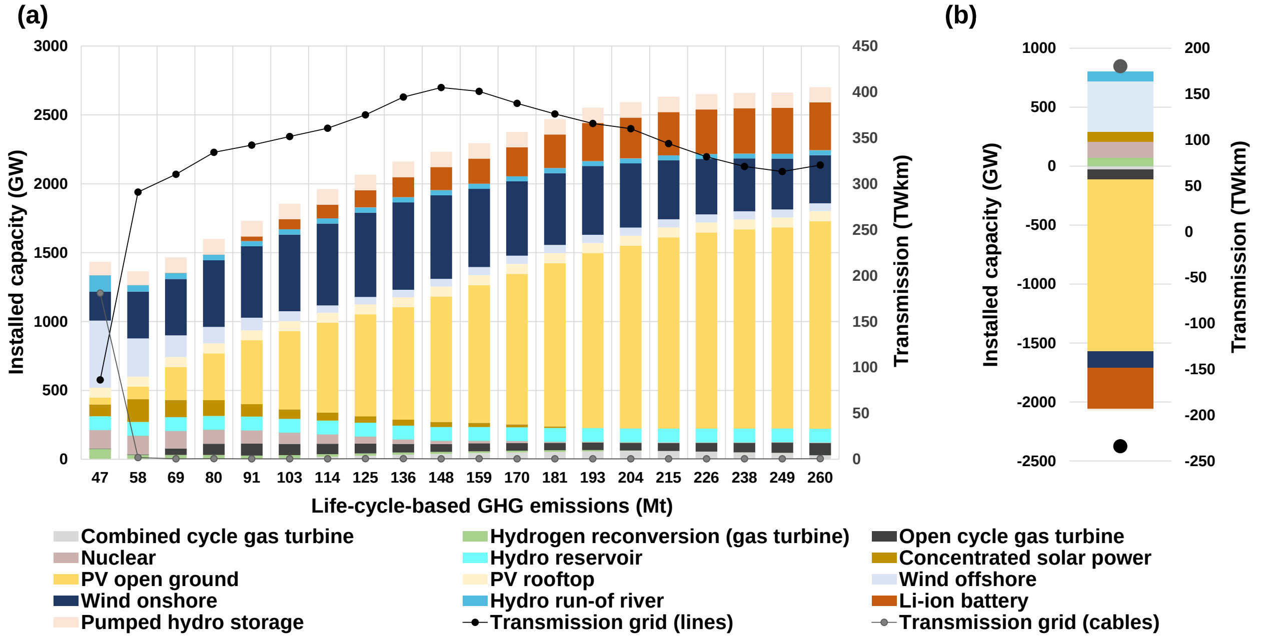

Figure 4. Power plant and power storage portfolio and transmission capacities in the EUNA region. Panel (**a**) shows the power plant and storage portfolio (left y-axis) and the grid installations (right y-axis) for each solution on the pareto front (Figure 3). Panel (**b**) shows the technology specific differences between the cost-optimal solution and the least life-cycle GHG emissions intensive solution for both, power generation and storage capacities and grid. Technologies with less than a 1% share of capacity in any solution are not shown for the sake of clarity.

As shown in panel (a), the cost optimal power system (outer right bars) is dominated by PV open ground and wind onshore. Temporal flexibility is mainly provided by Li-ion batteries and pumped hydro storage, while the grid is expanded to ~320 TWkm, which is in the range of grid expansion needs shown in earlier work with comparable scenario setups [21,36]. Additional flexibility to the system is provided by a small share of combined and open-cycle gas turbines. As shown Figure 5, life-cycle GHG emissions in the cost-optimal system are dominated by PV open ground and gas power plants. For PV, upstream industrial (e.g. flat glass production) and transport processes are responsible for most of the GHG emissions, whereas direct combustion emissions dominate the impact for gas turbines.

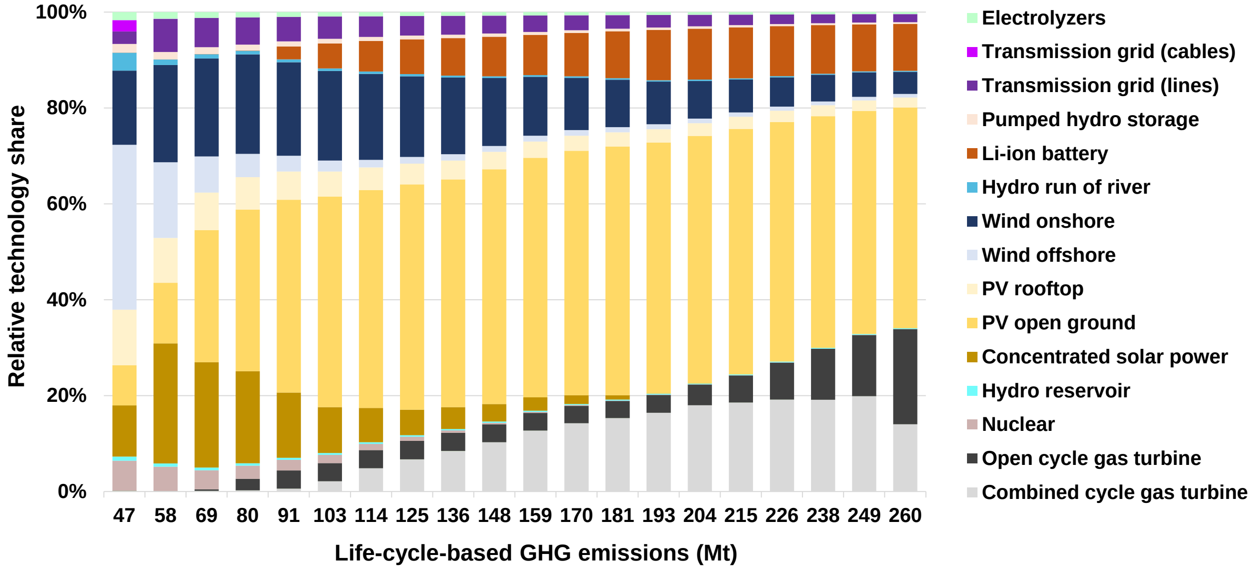

Figure 5. Shares of the different technologies in the life-cycle-based GHG emissions over the pareto frontier (cost-optimal solution: far right, least GHG emissions: far left, compare also with Figure 3). Technologies with less than a 1% share of impact in any solution are not shown for the sake of clarity.

The first 22% of the reduction of life-cycle GHG emissions (from 260 to 204 Mt) is achieved through an expansion of wind onshore and grid, while the share of PV open ground systems and Li-ion batteries is reduced. The correlation between the expansion of the grid with an increasing share of wind power when dispatchable generation is limited has been shown in earlier work [27] and can be observed until life-cycle GHG emissions are reduced to 148 Mt, where the grid expansion reaches a maximum. In addition, the decline of Li-ion battery storage with the reduction of life-cycle GHG emissions contributes to the increasing need for power transmission. Thus, a co-expansion of the grid and wind power can be considered a viable option for a cost-effective reduction of life-cycle GHG emissions. At 148 Mt life-cycle GHG emissions, the system is balanced between PV and wind onshore with small shares of conventional power plants and CSP to provide dispatchable generation. Life-cycle GHG emissions are still dominated by PV open ground (Figure 5).

The need for grid expansion and storage, however, decreases when increasing shares of CSP and nuclear enter the system to further reduce emissions. Until life-cycle GHG emissions are reduced to 69 Mt, open-cycle gas turbines are operated at low capacity factors (<0.01) to meet demand at peak load hours. VREs still make up a considerable share in the overall power plant portfolio with offshore wind becoming a more dominant source of power supply, as it is associated with higher capacity factors and less specific life-cycle GHG emissions per unit of electricity supplied than onshore wind power plants and PV. A reduction of emissions to 58 Mt is accompanied by an increasing share of CSP, wind offshore, with nuclear being deployed to its full capacity (~131 GW) and operating with a high capacity factor (>0.9). At this stage, total life-cycle GHG emissions are no longer dominated by PV technologies but CSP and wind on- and offshore. Moreover, direct emissions are fully mitigated as gas turbines are no longer operated to cover demand in peak load hours.

The system that is the least GHG emission intensive is characterized by a large share of wind off- and onshore, hydro run of river, CSP, and nuclear capacities (Figure 4). As the share of CSP is reduced compared to the previous three solutions, hydrogen reconversion provides additional temporal flexibility to the system. In addition, this is the only system in which electricity transmission is based on copper-based cables that are more climate friendly than aerial lines that rely on aluminum as a conductor. The significantly higher costs of cables compared to aerial lines, however, leads to the deployment of this technology only in the least emission intensive solution. Total grid transfer capacity is almost as high as in the cost optimal solution.

Along the pareto front, the total installed capacity is increasingly reduced. Comparing the two extremes, the cost optimum and the least emission-intensive solution in panel (b) of Figure 4, the reduction of life-cycle GHG emissions to the minimum results in systems with technologies that are characterized by higher capacity factors and lower GHG emissions per power output than the technologies deployed in the cost optimal solution. Although the high share of wind offshore is associated with considerable need for a transmission grid for geographical load balancing, the total grid demand is lower than in the cost optimum.

In summary, it is possible to achieve power systems that are both affordable and sustainable in terms of reducing life-cycle GHG emissions. In this respect, PV is still the dominant technology, but with a higher importance of wind onshore and the expansion of grid transmission capacity compared to the cost minimal system. Further reductions in life-cycle GHG emissions can be achieved through the increased expansion of dispatchable generation but are accompanied by higher increases in system costs. However, for a comprehensive assessment of life-cycle environmental sustainability, a multitude of indicators needs to be analyzed. Therefore, in the following we perform an ex-post assessment of the energy systems presented above using the indicators listed in Table 1.

3.3. Environmental Ex-Post Assessment

In this section, the co-benefits and adverse side-effects of the reduction of life-cycle GHG emissions are analyzed with respect to indicators listed in Table 1. This ex-post assessment of environmental impacts is based on the solutions on the pareto frontier shown above. Figure 6 illustrates the evolution of life-cycle metrics for the different areas of protection over the pareto front.

The majority of indicators shows co-benefits with reduced life-cycle GHG emissions. Only three impact categories increase with the reduction of life-cycle GHG emissions. The co-benefits are mainly induced by the decreasing deployment of PV open ground installations, since this technology dominates nearly all impact categories in the cost optimal system (see the relative share of technologies for each impact category in Figure A1 in Appendix C). Onshore and offshore wind show the highest impacts for the least GHG-emitting system in most categories. The increase in nuclear power is responsible for adverse side-effects.

The strongest adverse side-effect on human health (panel (a)) results from exposure to ionizing radiation caused by nuclear energy, which increases with its use (up to a factor of ~34 compared to the cost-optimal solution). With the exception of ozone depletion, most other indicators show clear trends with decreasing climate impacts. At a reduction of life-cycle GHG emissions to 80 Mt, ozone layer depletion reaches its minimum. At this point, Li-ion battery storage leaves the system, after dominating this indicator in the previous solutions, and the main driver becomes nuclear power plants. The use of nuclear energy is associated with ozone depleting emissions of halogenated hydrocarbons for cooling during uranium production. The evolvement of impacts over the pareto front related to resource depletion are shown in panel (b). Down to 136 Mt GHG emissions we see co-benefits related to reduction of climate impacts. For fossils (including uranium) and dissipated water they turn into adverse side-effects with further emission reduction. In the cost-optimal system, the use of fossils is dominated by electricity generation with gas turbines and the construction of PV plants. As life-cycle GHG emissions are reduced, fossils and water depletion become dominated by nuclear power. For nuclear power, cooling water has a high impact on water depletion. Both, PV and CSP have a high direct land demand. CSP accounts for nearly half of the land use when installed capacity peaks at the reduction of life-cycle GHG emissions to 58 Mt. A further avoidance of life-cycle GHG emissions from 58 Mt to 47 Mt results in a slight increase in minerals and metals as wind offshore and copper-based cables are deployed where the metals used have a higher depletion potential compared to metals used for CSP and aluminum-based aerial lines. The evolvement of impacts over the pareto frontier related to ecosystem quality are shown in panel (c). For all these indicators, we see co-benefits associated with reducing climate impacts. In this group, the contributions of the individual technologies show a similar pattern to that of climate change. Only the electrolyzers have a higher contribution to freshwater and terrestrial acidification, while gas turbines have a lower impact, especially in freshwater ecotoxicity and freshwater eutrophication. As with minerals and metals, the use of transmission cables overcompensates for the reduction in freshwater eutrophication achieved by decreasing PV deployment. Again, the higher impact of copper production is responsible for the increase.

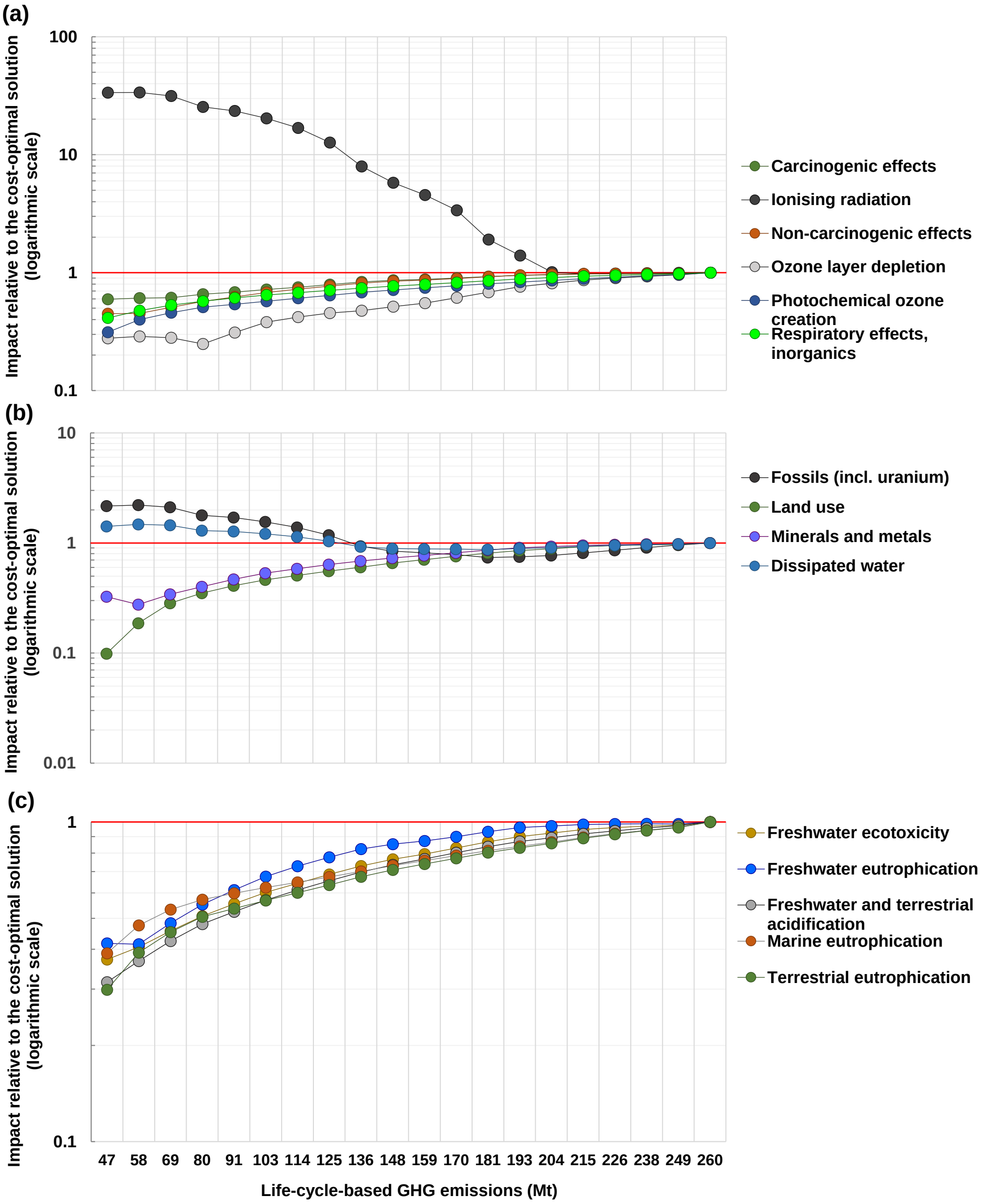

Figure 6. Impact on life-cycle indicators as a function of life-cycle GHG emissions over the pareto frontier. Panel (**a**): indicators related to human health; panel (**b**): indicators related to resource depletion; panel (**c**): indicators related to ecosystem quality. Impacts at the solution with minimal costs are scaled to 1. Reading the graph from right to left, impact values below 1 indicate co-benefits in reducing climate impacts, above 1 show adverse side effects.

The high share of PV in most impact categories is also consistent with findings by Berrill et al. [6], who conducted an LCA of 44 electricity scenarios for Europe in 2050. The authors showed that wind-dominated systems have half as much life-cycle GHG emissions as PV-based systems. Moreover, they found that PV-based systems have a higher environmental impact on indicators that affect human health and ecosystems than wind-dominated systems.

Carcinogenic, non-carcinogenic, and respiratory effects show the lowest reduction over the pareto front. This means that they are least sensible to the technological changes. Most sensible are ionizing radiation, fossils, and dissipated water, although these changes are only due to the expansion and operation of nuclear power.

As illustrated in Figure A2, compared to today's impacts of power supply, land use is likely to increase should the power system have a high share of PV open ground. A similar increase compared to today could be expected in ozone layer depletion in case the system has high shares of Li-ion batteries. Moreover, all systems analyzed in this study could result in higher depletion potential for minerals and metals compared to today's values. Current levels in ionizing radiation could be exceeded if nuclear energy is largely deployed.

4. Discussion

In this section, we first summarize our findings and derive the main implications. We then examine the role of nuclear power and provide an outlook based on the identified needs for further research.

4.1. Summary and Implications of the Results

In this study, the ESOM REMix is populated with environmental impacts of the entire supply chain of the considered technologies, which is achieved through coupling with the elaborated LCA-framework FRITS. Thereby, we conduct the first integration of LCA impacts in an ESOM with high spatiotemporal detail. This enables a comprehensive assessment of the trade-offs of life-cycle GHG emissions and system costs of the electricity sector in EUNA combining the strengths of energy system modeling and LCA approaches. Furthermore, the comprehensive nature of the methodology provides information on a large set of additional environmental co-benefits and adverse side effects, highlighting potential areas of conflict between an increasingly climate friendly electricity supply and other life-cycle impact categories.

The results underline the fact that the most cost-effective decarbonization of the power sector in EUNA leads to emissions that are largely generated in the upstream supply chain. A reduction of life-cycle GHG emissions, which includes all emissions (direct and indirect), strongly reduces direct CO_2 emissions, thereby increasing the relative importance of upstream emissions. Moreover, our results show that different low-carbon power supply options are not equally effective. Rather, they differ significantly in terms of life-cycle GHG emissions, with the result that a reduction in these emissions relies increasingly on wind, CSP, and nuclear with moderate variations in grid expansion. At the same time, the share of PV and Li-ion storage is declining. A study which confirms these observations was published by Pehl et al. [15]. It had a global focus and showed that a tax of 30 US$ per ton of life-cycle GHG emissions leads to an energy system with a larger share of wind power, CSP, and nuclear power compared to a system with a tax on direct GHG emissions only, underlining the life-cycle GHG emission benefits of these technologies. However, since the authors did not perform multi-objective optimization covering the entire solution space of possible system configurations, our study also shows extreme solutions with higher deployment of technologies favorable for reducing life-cycle GHG emissions.

This study focuses exclusively on very ambitious systems regarding the avoidance of direct CO_2 emissions. It is therefore important to note that even if decarbonization of the power sector follows cost optimality, life-cycle GHG emissions can be expected to be low compared to today's levels (see Figure A2).

4.2. The Role of Nuclear Power Generation

Our analysis shows that the reduction of life-cycle GHG emissions largely increases ionizing radiation, water consumption and depletion of fossils (particularly uranium) due to the expansion of nuclear power. The deployment of nuclear to reduce life-cycle GHG emissions also raises several other concerns not captured in LCAs, such as the risk of severe accidents, risks to the environment and local communities and the storage and treatment of nuclear waste. Furthermore, Kim et al. [47] showed that the degree of public acceptance of nuclear power in European countries is highly dependent on perceived potential risks, which could hinder the continuation of nuclear based electricity generation through social opposition (e.g. in case of an accident). In this context, we additionally conducted REMix calculations without nuclear energy (see Figure 7). Corresponding figures regarding the pareto frontier and the development of the other environmental indicators can be found in the Supplementary Materials.

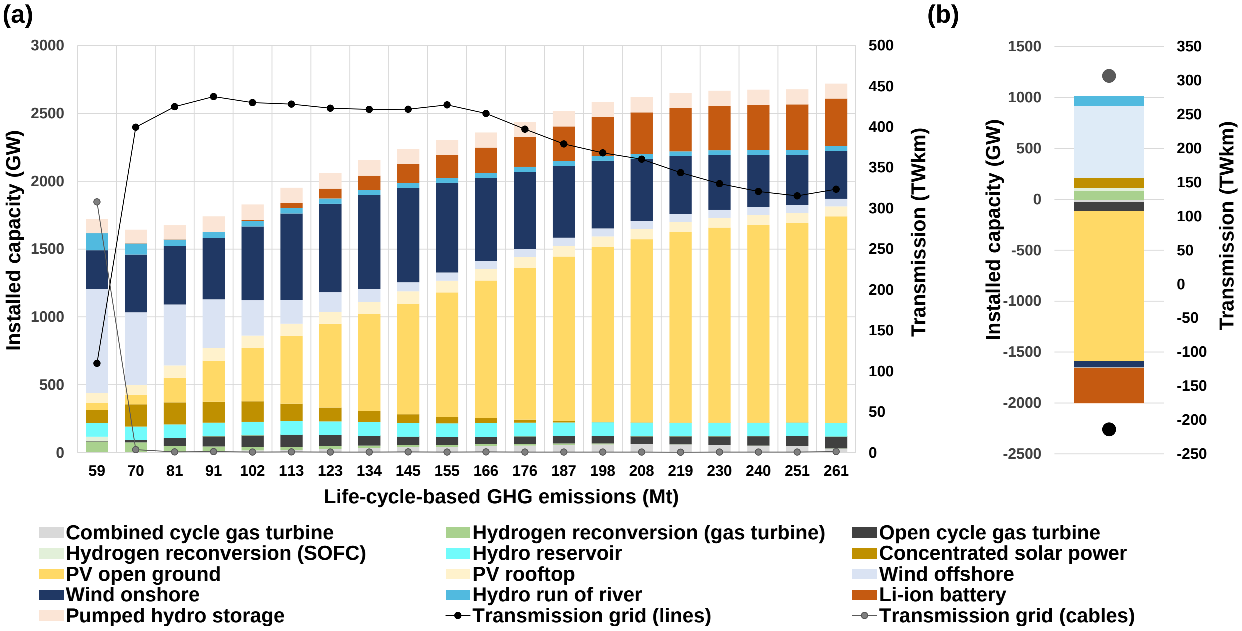

Figure 7. Power plant and power storage portfolio and transmission capacities in the EUNA region in case of a complete phase-out of nuclear power by 2050. Panel (**a**) shows the power plant and storage portfolio (left *y*-axis) and the grid installations (right *y*-axis) for each solution on the pareto front (Figure S1). Panel (**b**) shows the technology specific differences between the cost-optimal solution and the least life-cycle GHG emissions intensive solution for both, power generation and storage capacities and grid. Technologies with less than a 1% share of capacity in any solution are not shown for the sake of clarity.

This results in a reduction in the life-cycle GHG emissions of up to 59 Mt with a simultaneous cost increase to 415 bn. € (Figure S1). Such a system is dominated by wind and CSP and accompanied with higher grid expansion and hydrogen re-conversion for regional and temporal load balancing compared to a system with nuclear power. Furthermore, systems without nuclear power only show co-benefits with regard to other environmental impacts with decreasing life-cycle GHG emissions (see Figure S2).

4.3. Life-Cycle Data Must Become Prospective

This study encounters methodological limitations that need to be considered when interpreting the results.

First, the LCIs are not fully prospective with respect to the fore- and background processes. For example, fossil-based process heat is responsible for a high share of the life-cycle impacts of PV. To better understand how these emissions can be reduced in the future, a comprehensive understanding of potential decarbonization measures in the upstream supply chain of energy technologies and the corresponding integration into life-cycle databases is necessary. Fully decarbonized industrial and transportation processes could largely reduce the upstream emissions and have a significant impact on the results. Combined with prospective foreground LCIs, this could also strengthen the role of PV in reducing life-cycle emissions of ambitious energy systems in future studies. It should be noted, however, that relative differences between technologies are decisive in optimization. Thus, if PV does not improve relative to the other technologies when adjustments are made to fore- and background LCI data, it can be assumed that the technology mix will remain similar as shown here and only the absolute level of environmental impact would be affected.

Second, the classification of technologies for which LCI data are available is not necessarily identical with the rather general classification in the ESOM. For this purpose, we selected representative technologies from the available LCI data and, in the case of PV, relied on sub-technology compositions to capture different technological characteristics. However, future efforts are required to better align the ESOM technology classification with the LCIs on energy technologies. Coping with all these challenges, however, involves uncertain impacts across the different life-cycle phases and requires a significant modeling effort, which in turn calls for joint community action.

4.4. Outlook

Our modeling approach should be used to include further indicators to aim for completeness from the perspective of sustainability, such as societal aspects and other economic and environmental impacts of the energy transition [48]. Options for performing such analyses could include either multi-objective optimization considering a variety of conflicting objectives or ex-post assessment. Parallelizing the ε-CM as performed here could keep computation time manageable when extending the optimization approach to other indicators and more dimensions. However, the calculation of social and economic indicators requires more specific modeling approaches as they are currently not sufficiently covered by LCA.

When interpreting the results of the present study, the limited sectoral resolution must be considered. For example, the expansion and operation of technologies in the heat and transport sectors are not considered. Vandepaer, et al. [18] used a multi-sectoral ESOM for Switzerland and showed, for instance, that in an energy system optimized towards life-cycle GHG emissions, additional power generation capacity is added to deploy a higher proportion of hydrogen-based transportation technologies compared to the cost-optimal solution where transportation is mostly based on battery electric vehicles. Therefore, the sectoral extension of the approach presented in our study is crucial to fully understand the impact of considering life-cycle GHG emissions on the structure and overall environmental performance of the entire energy system.

5. Conclusions

In this study, we included life-cycle environmental impacts in the highly resolved ESOM REMix applied for the assessment of infrastructural demand in low-carbon scenarios. We thereby extended the usually cost-oriented nature of such analyses. The ESOM was applied to assess future configurations of the power system in Europe and North Africa that aims to reduce direct CO_2 emissions by at least 95% compared to 1990. Within this ambitious system, life-cycle GHG emissions were considered in the optimization and systematically reduced to the feasible minimum. Moreover, we provided further insights by quantifying other life-cycle impacts associated with the different system configurations (such as land use, minerals and metals, carcinogenic effects and other impacts). In this way, co-benefits as well as adverse side effects for fifteen mid-point indicators that come along with a reduction of climate impacts were assessed using the ILCD 2.0 2018 impact assessment methodology.

The first half of possible life-cycle GHG emission avoidance can be achieved with comparably small increases in total system costs (compared to the cost-optimal solution for a 95% reduction in direct CO_2 emissions), while a reduction of the last half considerably increases the system costs. Systems where life-cycle GHG emissions are reduced at moderate costs increasingly rely on on-and offshore wind power, grid expansion with reduced shares of Li-ion batteries and PV. Thereby, the deployment of wind turbines and PV panels contribute to the climate impact of electricity generation with up to 70%. The increasing reduction of life-cycle GHG emissions is supported by the deployment of wind offshore, CSP and nuclear power. Nuclear operates as a base-load power plant with high capacity factors (>0.9). However, such systems are associated with considerable cost increases (by up to 63% compared to the minimum cost solution). As life-cycle GHG emissions are reduced, hydrogen re-conversion is used to cover demand in peak load hours.

This research contributes to a better understanding of trends in environmental impact categories other than climate change (e.g. land use). The impacts in most categories are improved in the reduction of life-cycle GHG, i.e. they show co-benefits. Considering the increasing deployment of nuclear power plants which represents an option to reduce the effects of climate change, it also affects other categories such as ionizing radiation, fossils (including uranium) and water use negatively. Moreover, other impacts related to nuclear power and not included in LCA such as the risk of an accident, waste treatment and social acceptance were outside the scope of our assessment. In an additional model calculation, we illustrated that high reductions in life-cycle GHG emissions are also possible without nuclear power. Here, grid expansion for regional load balancing is more important than in a system with nuclear power. Moreover, all life-cycle indicators improve compared to the cost-optimal system.

In summary, the combination of LCA and ESOMs is of great benefit to both methods. Integrated assessments of future energy systems and their impacts on sustainability are expected to become more important due to pending developments in the energy system, such as renewable electrification of transportation, heat and other sectors. Moreover, global supply chains linked to the world’s energy system are becoming increasingly complex and energy system transformations are evolving at different speeds across regions. Informed decisions on the design of the future energy system therefore require the consideration of impacts upstream in the supply chain to avoid major burden shifts.

A potential policy implication from our work is that life-cycle impacts of energy technologies should be considered in the future design of policy instruments, as emissions are increasingly shifted upstream in an ambitious energy system. However, current approaches that combine both modeling worlds in an integrative approach still face several limitations, such as missing aspects regarding prospectivity and high uncertainties of LCI data and should remain a priority research area in the future. This study should therefore be regarded as a further step towards integrated model-based assessment and confirms the call for joint work between researchers in the field of energy system modeling and industrial ecology. For example, it would be of great benefit to develop a system in which a centralized, collaboratively developed, and prospective LCI database is used as a reference with defined criteria to map LCI data to processes in the ESOMs.

Supplementary Materials: The following are available online at www.mdpi.com/xxx/s1, Figure S1: Pareto front to illustrate the trade-offs between system costs and life-cycle GHG emissions for a system without nuclear power, Figure S2: Impact on life-cycle indicators as a function of life-cycle GHG emissions over the pareto front for a system without nuclear power, Table S1: Technology-specific cost assumptions, Table S2: Matching of the regions in REMix with the electricity markets in ecoinvent, Table S3: Electricity mix in 2050 in the background LCI database for Eurasia and OECD Europe, Table S4: Technology-specific life-cycle environmental impacts.

Author Contributions: Conceptualization, T.J., T.N.; methodology, T.J., K.-K.C. and K.K.M.; software, T.J., K.-K.C. and K.K.M.; validation, T.J., H.H.; formal analysis, T.J.; investigation, T.J.; data curation, T.J.; writing—original draft preparation, T.J., H.H.; writing—review and editing, T.J., K.-K.C., K.K.M., H.H. and T.N.; supervision, T.N. All authors have read and agreed to the published version of the manuscript.

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

Glossary

Bn.	Billion
CSP	Concentrated solar power
ENTSO-E	European Network of Transmission System Operators for Electricity
ESOM	Energy system optimization models
EUNA	Europe and North Africa
ε-CM	Epsilon-constraint method
FIAS	Frankfurt Institute for Advanced Studies
FRITS	Framework for the Assessment of Environmental Impacts of Transformation Scenarios
GAMS	General algebraic modeling system
GHG	Greenhouse gas
HVDC	High-voltage direct current
IEA	International Energy Agency
ILCD	The International Reference Life Cycle Data System
LCA	Life-Cycle Assessment
LCI	Life-Cycle Inventory
PV	Photovoltaic
REFLEX	Analysis of the European energy system under the aspects of flexibility and technological progress
REMix	Renewable Energy Mix
REMix-EnDAT	Energy data analysis tool that is part of the REMix framework
REMix-OptiMo	Optimization model that is part of the REMix framework
TYNDP	Ten-year network development plan
VRE	Variable renewable energy
WEPP	World Electric Power Plants Data Base

Appendix A

In the present study, we follow the augmented epsilon-constraint method (ε-CM) described in Mavrotas [30]. The process consists of calculating the payoff table by optimizing on both objectives $f_1(\vec{x})$ (in our case system costs) and $f_2(\vec{x})$ (in our case life-cycle GHG emissions) as presented in Equation (A1), while $\vec{x}_{1opt}$ is the variable vector used for the optimization of $f_1(\vec{x})$ and $\vec{x}_{2opt}$ accordingly for $f_2(\vec{x})$:

$$\text{Pay} - \text{off table} = \begin{bmatrix} f_1(\vec{x}_{1opt}) & f_2(\vec{x}_{1opt}) \\ f_1(\vec{x}_{2opt}) & f_2(\vec{x}_{2opt}) \end{bmatrix} \quad \text{(A1)}$$

From this table, the best and the worst value is used for each objective function. For a problem that is two-dimensional, the best value of a function is achieved when an optimization is performed according to it. Therefore, the worst value is generated, if not optimized towards it. The considered range is therefore between $f_2(\vec{x}_{2opt})$ and $f_2(\vec{x}_{1opt})$. Subsequently, on the basis of the determined range, the epsilon (ε) values are defined, which set the boundary conditions for the optimization. For this purpose, the range is divided into a selected number μ of equidistant intervals, where n represents the elements within the set equidistant interval steps ranging from 0 to μ. Thus μ + 1 ε-values are determined which are one interval step apart from each other, starting with the worst value of the target function. These ε-values are often referred to as grid points. Since in a two-dimensional optimization only one dimension must be converted into a boundary condition, the ε-values for f_2 are defined as shown in Equation (A2). For a minimization problem, it applies that $f_2(\vec{x}_{1opt}) > f_2(\vec{x}_{2opt})$.

$$\varepsilon_n = f_2(\vec{x}_{1opt}) - \left(\frac{f_2(\vec{x}_{1opt}) - f_2(\vec{x}_{2opt})}{\mu}\right) \cdot n \tag{A2}$$

With these determined points of $f_2(\vec{x})$, the so-called epsilon constraints are defined, under which the optimizations of the other objective function then take place in the last step described in Equation (A3).

$$\begin{gathered} \min f_1(\vec{x}) \\ \text{s.t.}\, f_2(\vec{x}) \leq \varepsilon_n \end{gathered} \tag{A3}$$

Consequently, for each of these interval steps the first objective function is optimized under the condition that the predefined value of $f_2(\vec{x})$ is not exceeded. Thus, n solutions are generated, which form the so-called pareto front.

In order to guarantee the efficiency of the grid point solutions found, we use the augmented ε-CM by integrating the second target function into the optimization. This is achieved by minimizing $f_1(\vec{x})$ and maximizing the distance from $f_2(\vec{x})$ to the epsilon value. Accordingly, a point at the same value of $f_1(\vec{x})$, but with a lower value of $f_2(\vec{x})$ would be found. Therefore, the relation formulated in Equation (A3) is rewritten from an inequality by means of the slack variable δ into a binding constraint as shown in Equation (A4). To ensure that this slack is also included in the optimization, it is also written into the function to be minimized. The slack is then divided by the determined range and multiplied by a very small factor, which both ensure a correspondingly low weighting of the slack in the optimization.

$$\begin{gathered} \min f_1(\vec{x}) - 10^{-3} \cdot \frac{\delta}{f_2(\vec{x}_{1opt}) - f_2(\vec{x}_{2opt})} \\ \text{s.t.}\, f_2(\vec{x}) + \delta = \varepsilon_n \end{gathered} \tag{A4}$$

To avoid excessive computation times, we decompose the augmented ε-CM and follow a parallel execution of the grid point calculations after the payoff-table is determined. To reflect a potential cost variance in the GHG optimum, the last grid point corresponding to the GHG optimization in the payout table calculation is recalculated following Equation (A4). For solving the model, a computing cluster is used consisting of eight machines with similar hardware configurations: Intel® Xeon® CPU E5-2697 v4 @ 2.30 GHz. The Solver settings are listed in Table A1.

Table A1. Commercial solver settings for solving the model.

Solver	Cplex 12.10.0.0
Algorithm	Barrier (interior point)
Maximal number of threads	16
Convergence tolerance	1E-5
Cross-over	Disabled
Scaling	Aggressive
Solving the dual problem	Disabled

In order to avoid extreme spatial distributions of technologies across the considered regions r and to ensure a certain degree of self-supply of power and hydrogen generation P_{gen} in each region, we assume self-sufficiency thresholds of 80% in terms of annual (by summation over each time step t) power and hydrogen demand P_{dem} (see Equation (A5)).

$$\sum_{t,\tau} M_{gen}(s,\tau) \cdot P_{gen}(t,r,\tau,s) \leq 0.8 \cdot \sum_{t,\tau} M_{dem}(s,\tau) \cdot P_{dem}(t,r,\tau,s) \tag{A5}$$

The maps M_{gen} and M_{dem} categorize the technologies τ for each sector $s \in [\text{electricity}, \text{hydrogen}]$ into generation and demand technologies, respectively.

Appendix B

The LCI data used and the corresponding mapping to the technologies in REMix are listed in Table B1. For PV rooftop and open ground, we assume a share of 70% single-Si and 30% multi-Si solar cells in line with data on PV installations by cell type for the year 2019 reported by [49]. LCI data for CSP is transferred from ecoinvent v.3.5 to v.3.3.

Table A2. Technology mapping between REMix and available LCI data.

Technology Group	Technology in REMix	Corresponding LCI Data	LCI data Source
Electricity generation	PV open ground	Multi-Si panel Single-Si panel	[50]
	PV rooftop	Multi-Si panel Single-Si panel	[50]
	Concentrated solar power	Concentrated solar power plant (parabolic trough)	[51]
	Wind onshore	Wind onshore (geared)	[51]
	Wind offshore	Wind offshore (geared)	[51]
	Hydro reservoir	Hydro reservoir	[52]
	Hydro run-of-river	Hydro run of river	[51]
	Geothermal	Deep geothermal	[51]
	Nuclear power plant	Nuclear boiling water reactor	[51]
	Biopower	Wood-chip-biomass-fired plant (steam turbine)	LCI data based on [53] with wood-ship supply based on [51]
	Lignite power plant	Lignite power plant	[51]
	Hard coal power plant	Hard coal power plant	[51]
	Open cycle gas turbine	Open cycle gas turbine	[51]
	Combined cycle gas turbine	Combined cycle gas turbine	[51]
Conversion	Electrolyzer	Alkaline water electrolysis (AEL)	[54]
Storage	Hydrogen storage (cavern)	Hydrogen storage in salt caverns	[55]

	Hydrogen storage (tank)	Carbon fiber hydrogen tank	[55]
	Vanadium redox-flow battery	Vanadium redox-flow battery	[56]
	Li-ion battery	Lithium-iron phosphate with lithium-titanate anode (LFP-LTO)	[57]
	SOFC fuel cell (hydrogen)	SOFC fuel cell	[51]
	Pumped hydro	Pumped hydro	[52]
Grid	HVDC line	HVDC overhead line for connections on land, sea cable for connections over water	[58,59]
	HVDC cable	HVDC land cable for connections on land, sea cable for connections over water	[58,59]

The LCI data is disaggregated to match the investment and dispatch variables in REMix. However, it was not always possible to include an LCA score for all cost parameters. For example, we did not match fixed variable costs with LCI data. In addition, most storage technologies in REMix are disaggregated into storage and converter units that can be expanded separately. However, it was not possible to disaggregate the LCI dataset for Li-ion batteries into storage and converter units [60], so the c-rate was fixed at the value assumed in the LCI data (~0.17).

Appendix C

Figure A1 illustrates the relative share of technologies for each impact category shown in Figure 6 across the pareto front.

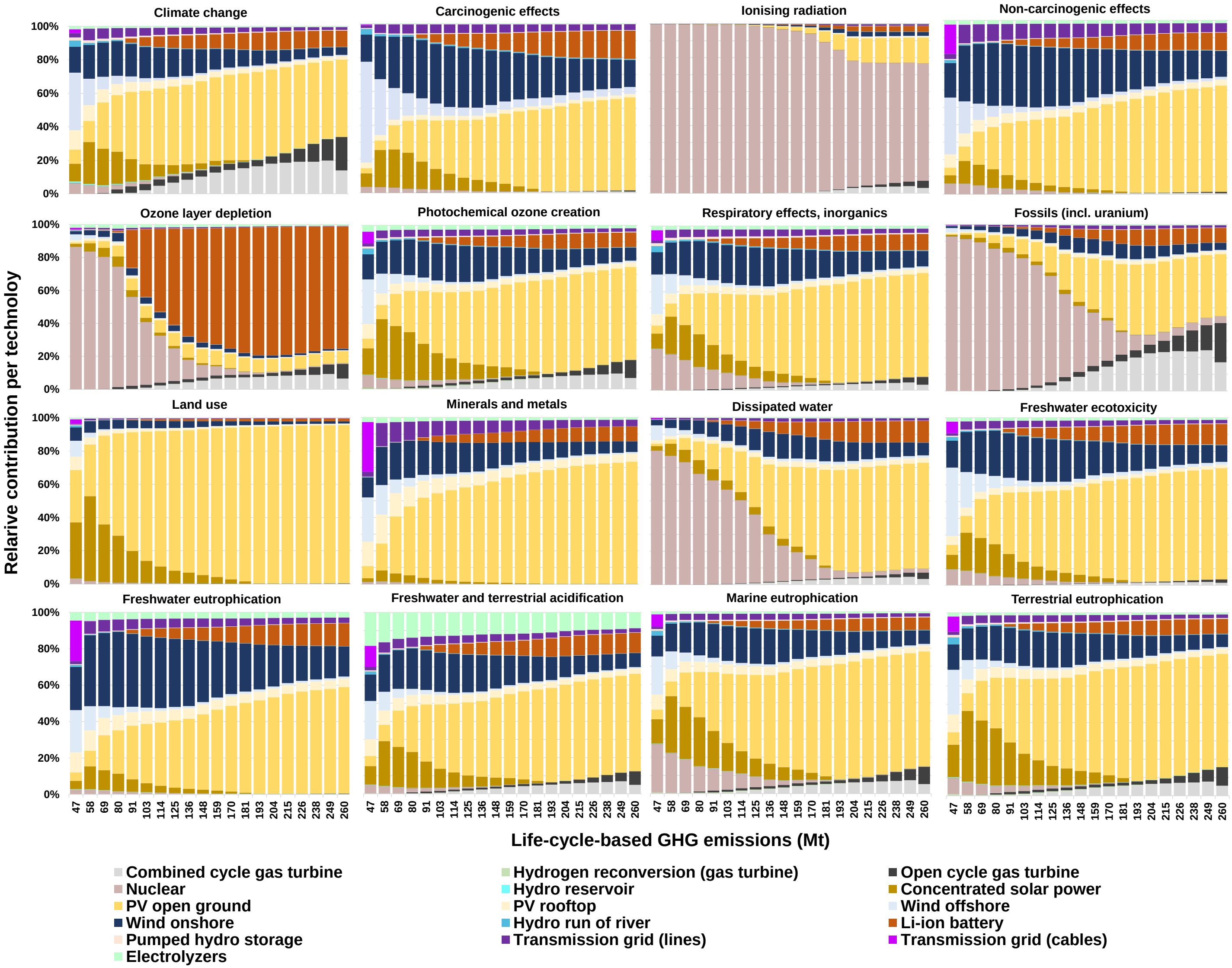

Figure A1. Relative share of technologies for each impact category and each solution on the pareto front. Technologies with a share of less than 1% in any solution and for any indicator are not shown for reasons of clarity.

Figure A2 shows the environmental impacts of the cost-optimal solution and the least emission-intensive solution (see Figure 3) relative to the environmental impacts of today’s electricity mix in Europe as documented in the ecoinvent database [46]. This comparison is based on the environmental impact per kilowatt hour of electricity supplied.

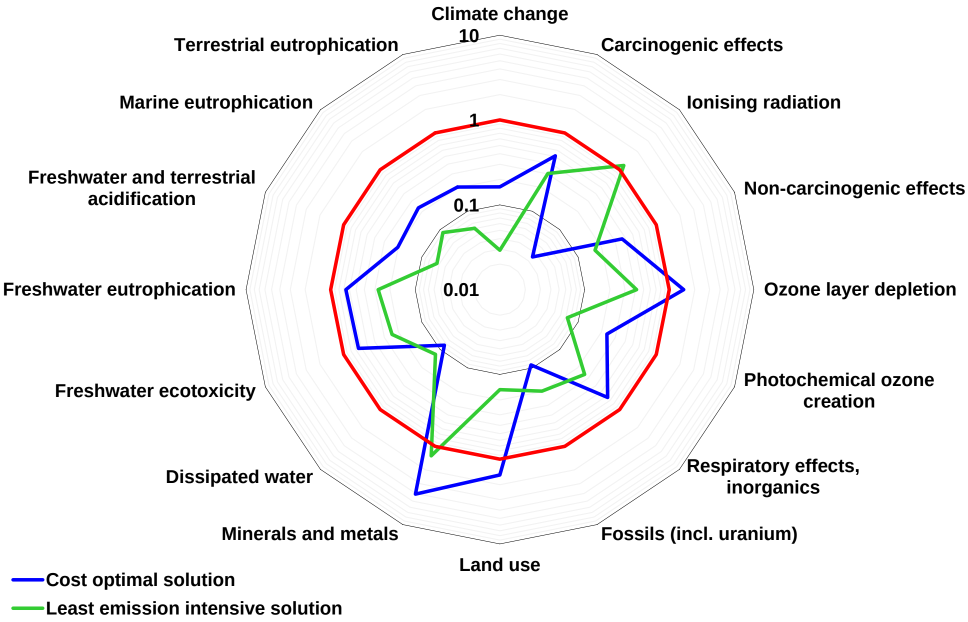

Figure A2. Ratio of impacts of the cost optimal solution (blue line) and the least emission-intensive solution (green line) relative to today’s impacts in Europe [46] (red line) using a logarithmic scale. The red line separates adverse side-effects (increasing impacts, impact ratio > 1) from co-benefits (decreasing impacts, impact ratio < 1). Note that for this comparison, the original data set from ecoinvent v.3.7.1 [46] is used and not further adjusted. Thus, it has a different regional and technological resolution than the present study and is based on the original ecoinvent database. The comparison shown can therefore only indicate trends with regard to the life-cycle indicators.

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2.3 Paper 3

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Specific objective	Quantification of the possible future material demand of global energy scenarios and assessment of potential supply bottlenecks.
Thesis-overarching objectives	2.a) Development of a method to quantify the future material demand for various global energy scenarios 2.b) Assessment of the influence of sub-technology scenarios and variations in specific material demand on the results 2.c) Analysis of potential supply bottlenecks and deviation of future research needs for energy scenario modelers
Methodology	Material flow analysis
Key outcome	Method that enables the quantification of the material demand in global energy scenarios under the consideration of sub-technology scenarios and variations in specific material demand; directions for possible inclusion of potential metal bottlenecks in future scenario studies.

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Critical materials in global low-carbon energy scenarios: The case for neodymium, dysprosium, lithium, and cobalt

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ABSTRACT

The requirements for neodymium, dysprosium, lithium, and cobalt in power generation, storage and transport technologies until 2050 under six global energy scenarios are assessed. We consider plausible developments in the subtechnology markets for lithium-ion batteries, wind power, and electric motors for road transport. Moreover, we include the uncertainties regarding the specific material content of these subtechnologies and the reserve and resource estimates. Furthermore, the development of the material demand in non-energy sectors is considered. The results show that the material requirements increase with the degree of ambition of the scenarios. The maximum annual primary material demand of the scenarios exceeds current extraction volumes by a factor of 3 to 9 (Nd), 7 to 35 (Dy), 12 to 143 (Li), and 2 to 22 (Co). The ratios of cumulative primary material demand to average reserve estimates range from 0.1 to 0.3 (Nd), 0.3 to 1.1 (Dy), 0.7 to 6.5 (Li), and 0.8 to 5.5 (Co). Average resource estimates of Li and Co are exceeded by up to a factor of 2.1 and 1.7, respectively. We recommend that future scenario studies on the energy system transformation consider the influence of possible material bottlenecks on technology prices and substitution technology options.

1. Introduction

Within the energy systems modelling research community, there is a consensus that achieving the goals of the Paris Agreement requires extensive electrification of end-use sectors, such as industry, transport, and households, including a defossilisation of the power sector, which is still dominated by thermal power plants [1]. However, electrification strategies depend on technologies that require significant amounts of metals and make resource scarcity a potential threat that is often overlooked by the energy systems modelling community [2].

Several studies use energy scenarios in combination with dynamic material flow analysis (MFA) to assess future demand for materials needed to deploy technologies such as photovoltaic (PV) modules [3–8], batteries for the transport sector [9–12], wind turbines [13], and a wider range of technologies relevant for the energy transition [14–21]. However, deriving reliable statements about possible material shortages requires the involvement of all energy technologies and non-energy sectors that use these metals. For example, Habib and Wenzel [22] estimate that future demand for rare earth elements (REEs) Nd and Dy will primarily come from non-energy sectors and the manufacturing of battery electric vehicles (BEVs). This estimate agrees with results presented by Hoenderdaal et al. [23], who analyse the demand for Dy and conclude that the wind turbine sector would represent a significant share of total demand only in very ambitious energy scenarios. On the other hand, Ziemann et al. [24] show that future demand for Li from non-energy sectors seems to play only a minor role, driven primarily by the manufacturing of batteries for mobility. Valero et al. [25] depict significant growth in demand for 31 raw materials and show that the relevance of demand in non-energy sectors strongly depends on the material. Capellán-Pérez et al. [26] show the relevance of non-energy sector material demands for possible bottlenecks. Sverdrup [27] uses a systems dynamics (SD) model to assess future supply, market prices and the duration of extractable amounts for Li under different combinations of resource estimates, recycling rates and material requirements for BEVs. Sverdrup [27] shows that future Li demand is mainly driven by BEVs, but that their deployment could be limited due to material price increases.

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Glossary

A	Annum
AG	Asynchronous generator
BEV	Battery electric vehicle
CONT	Continuity subtechnology roadmap
Dy2O3	Dysprosium oxide
EOL-RR	End-of-life recycling rate
[E]R ADV	Greenpeace Energy [R]Evolution 2015—Advanced Energy [R]evolution scenario
ETP B2deg	Energy Technology Perspectives 2017—Beyond 2 °C scenario
FCEV	Fuel cell electric vehicle
GDP	Gross domestic product
HS	High speed
IEA	International Energy Agency
IRENA	International Renewable Energy Agency
IRENA REmap	IRENA Global Energy Transition: A roadmap to 2050—REmap scenario
JAC	Jacobson et al. 100% clean and renewable wind, water, and sunlight all-sector energy roadmaps for 139 countries with an assessment of stationary storage demand
UNFCCC	United Nations Framework Convention on Climate Change
USGS	United States Geological Survey
GHG	Greenhouse gas
HEV	Hybrid electric vehicle
HS	High speed
IND	Scenario on sector-specific growth in non-energy sectors
LDV	Light duty vehicle
LFP	Lithium iron phosphate
LiO_2	Lithium oxygen
LiS_8	Lithium sulphide
LMO	Lithium metal oxide
LUT/EWG	LUT University and Energy Watch Group global energy system based on 100% renewable energy
MEDEAS	Modelling sustainable energy system development under environmental and socioeconomic constraints
MFA	Material flow analysis
MRIO	Multi-regional input-output
MS	Medium speed
NCA	Lithium nickel cobalt aluminium oxide
NdFeB	Neodymium-iron-boron
Nd2O3	Neodymium oxide
NMC	Lithium nickel cobalt manganese oxide
PHEV	Plug-in hybrid electric vehicle
PM	Permanent magnet
PtL	Power-to-liquid
PV	Photovoltaic
RC	Recycled content
REE	Rare earth elements
SD	Systems dynamics
SG	Synchronous generator
TC	Technology change subtechnology roadmap
UNFCCC	United Nations Framework Convention on Climate Change
WEO SDS	World Energy Outlook 2018—Sustainable Development Scenario

De Koning et al. [28] assess demand for eleven metals in energy scenarios implemented in a multi-regional input-output (MRIO) table to capture the metal requirements of the global economy. They report that demand for metals depends not only on the metal and the scenario being analysed but also on the specific material content of the energy technologies.

The technological representation of most energy scenarios is too coarse to derive quantitative implications for material requirements. This causes some authors to draw on detailed, exogenously defined subtechnology scenarios, which may change the estimates by an order of magnitude [29]. Although many papers have analysed future material requirements, to our best understanding, no study has yet addressed the uncertainties that arise from combining different energy scenarios with detailed subtechnology scenarios, and variations in specific material requirements and reserve and resource estimates.

In a recent global criticality assessment by Graedel et al. [30], Nd, Dy, Li, and Co are shown to currently have relatively low criticality, which may lead to the possibility of overlooking these metals from a status-quo perspective. In the context of global energy scenarios, however, these metals have been repeatedly identified to be subject to possible supply bottlenecks as they are included in technologies that may drive future global material demand due to necessary defossilisation efforts. Electric motors are used in BEVs, plug-in hybrid electric vehicles (PHEVs), hybrid electric vehicles (HEVs), and fuel cell electric vehicles (FCEVs) which need neodymium-iron-boron (NdFeB) magnets containing Nd and Dy to increase the coercive field strength and remanence of the materials and to preserve the magnetic properties at high temperatures [31]. In addition, there is an ongoing trend in wind turbines towards increasing hub height, rotor diameter, and nominal capacity, so the number of wind turbines using NdFeB magnets is expected to increase because of weight savings and lower maintenance requirements [32]. Furthermore, mobile batteries and storage technologies that balance the variability of renewable energy sources are likely to be Li-ion batteries, which may require significant amounts of Li and Co. Therefore, we focus this analysis on Nd and Dy (in certain types of wind turbines and electric motors) and Li and Co (in certain types of mobile and stationary batteries).

The amount of work required, particularly regarding the derivation of subtechnology scenarios, the subsequent collection of estimates of specific material content and the estimation of demand in non-energy sectors, allows us to focus only on the aforementioned materials and technologies. It should therefore be noted that there are several other technologies (e.g. PV and CSP) outside the scope of this paper that are pivotal to the energy transition and whose metals could be subject to potential scarcity.

We aim to make three contributions to the literature with this paper: (1) We explicitly assess uncertainties arising from subtechnology market shares, specific material content and material availability for Li, Co, Nd and Dy. (2) We include six current, high-impact energy scenarios as examples to discuss the extent of material demand and potential bottlenecks in different defossilisation strategies. (3) We discuss the implications of this analysis from the perspective of energy system modelling.

We do not offer predictions, but aim to motivate the energy system modelling community to meet the challenges of certain technologies and the metals they consume by including effects such as rising market prices for technologies due to material scarcity and their effects on techno-economic data and changes in consumer behaviour in future assessments.

2. Materials and methods

An overview of the data, assumptions and methods is given in Fig. 1. Energy scenarios are selected, and the information contained therein (e.g., the installed capacities) is collected. Subsequently, subtechnology scenarios are derived from the literature and supplemented with assumptions where data is scarce. Material demand for non-energy sectors is combined with information about the metal composition of energy technologies to calculate the annual material demand and the primary material demand using dynamic MFA. In the following, the term 'material demand' refers to the total demand of society, while 'primary material demand' is the part of this demand that has to be covered from mines. Further details on the methods and data used are given in the following subchapters.

2.1. *Choice of energy scenarios for the assessment of technology development*

The following six different global energy scenarios are selected for detailed analysis in this study:

- Greenpeace Energy [R]Evolution 2015—Advanced Energy [R]evolution scenario [33] ([E]R ADV)
- International Renewable Energy Agency (IRENA) Global Energy Transition: A roadmap to 2050—REmap scenario [34] (IRENA REmap)
- International Energy Agency (IEA) World Energy Outlook 2018—Sustainable Development Scenario [35] (WEO SDS)
- IEA Energy Technology Perspectives 2017—Beyond 2 °C Scenario [36] (ETP B2deg)
- Jacobson et al. 100% clean and renewable wind, water, and sunlight all-sector energy roadmaps for 139 countries [37] with an assessment of stationary storage demand [38] (JAC)
- LUT University and Energy Watch Group global energy system based on 100% renewable energy [39] (LUT/EWG)

Each scenario chosen meets the following criteria: (1) has global coverage, (2) is a recent study, published no earlier than 2015; (3) has relevance to international discussion, not only among scientists but also non-scientific stakeholders; (4) describes transition pathways for power, heat, and transport sectors; (5) aims at a significant reduction in energy-related CO_2 emissions (at least 50%, base year 2005).

The diversity of estimates on the future energy system is illustrated by Fig. 2 and Fig. 3. Fig. 2 illustrates the different degrees of GHG emission reduction (right y-axis) and respective installed capacities (left y-axis) in the power sector. Please note that in some passages we summarise the scenarios that show a 100% CO_2 reduction by 2050 as 'highly ambitious', while the others are characterized as 'less ambitious'.

The energy carriers in transport of the scenarios considered are shown in Fig. 3. Global installed power generation capacities as well as energy carrier demand in transport differ significantly because they depend on different CO_2 emission reduction targets, projections of global gross domestic product (GDP), population growth, the standard of living and individual behaviour, and technical efficiency, different estimates of direct and indirect electrification of the heat and transport sectors, and different portfolios for renewable power generation.

This selection of scenarios is not intended to give a complete overview of defossilisation strategies for global energy systems in the literature, but to illustrate the diversity of defossilisation levels and strategies among the broad variety of existing scenarios. Please

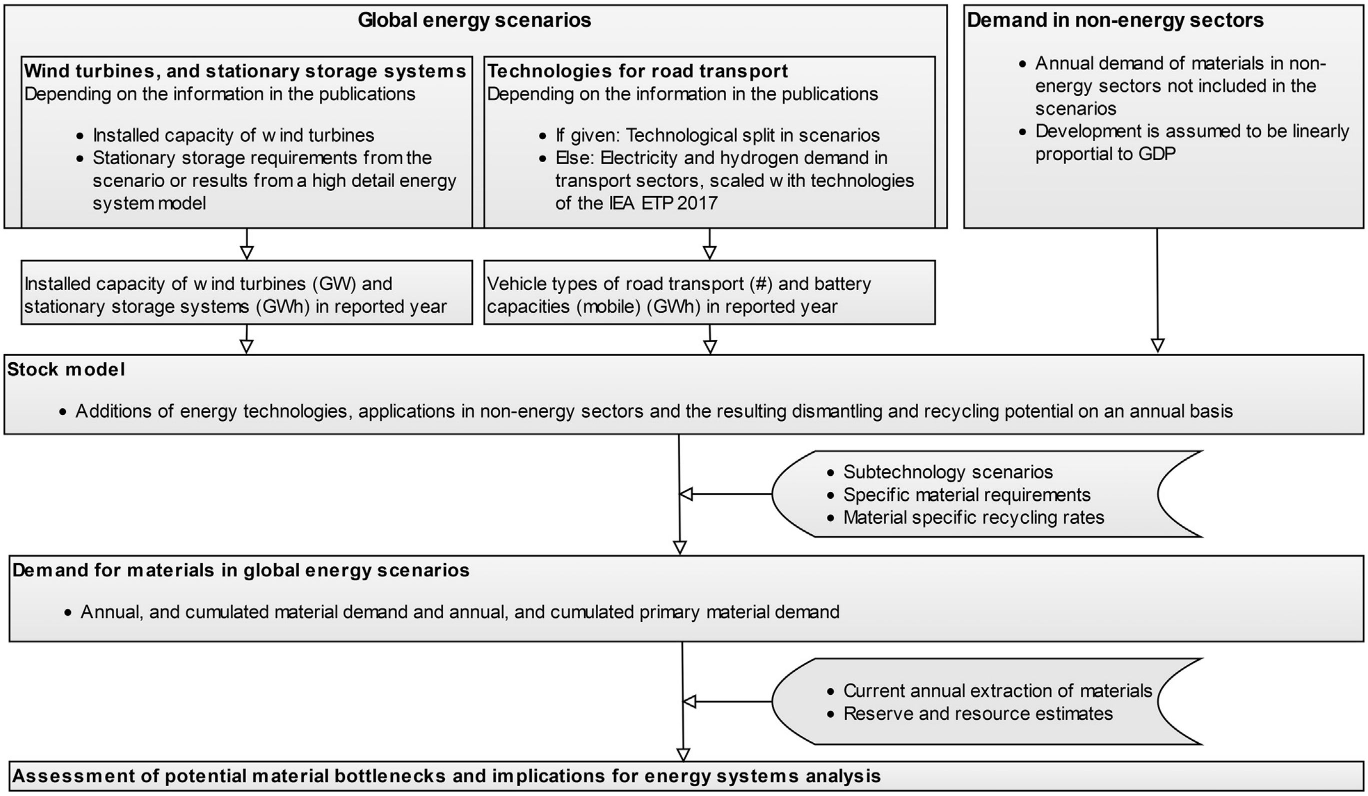

Fig. 1. Overview of the workflow of this study.

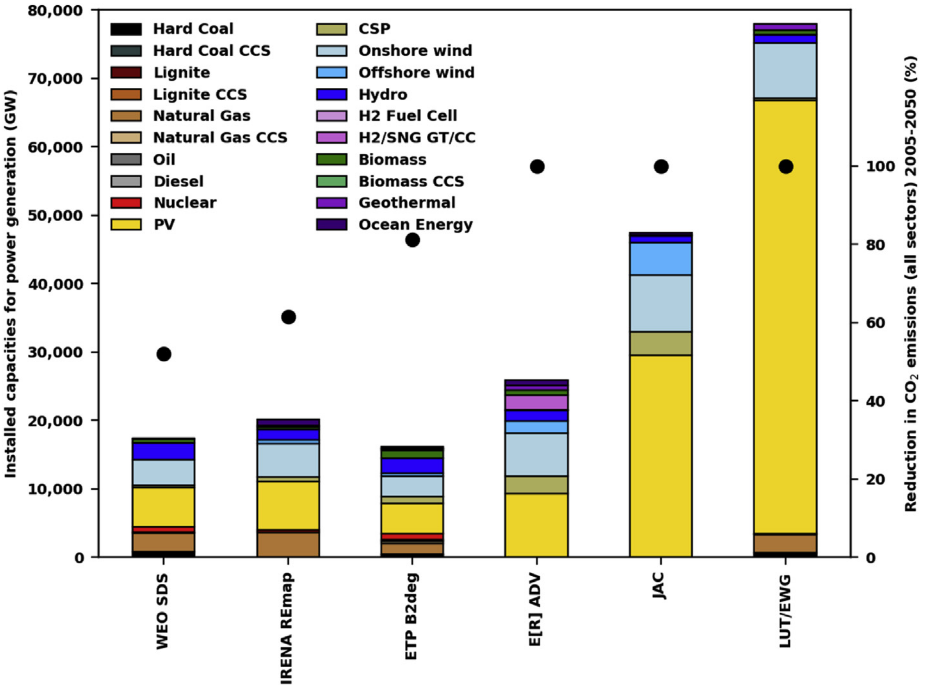

Fig. 2. Global installed capacity for power generation in 2050 in the selected scenarios (in GW, left scale) and reduction in global energy-related CO_2 emissions between 2005 and 2050 (all sectors, black dots, right scale).

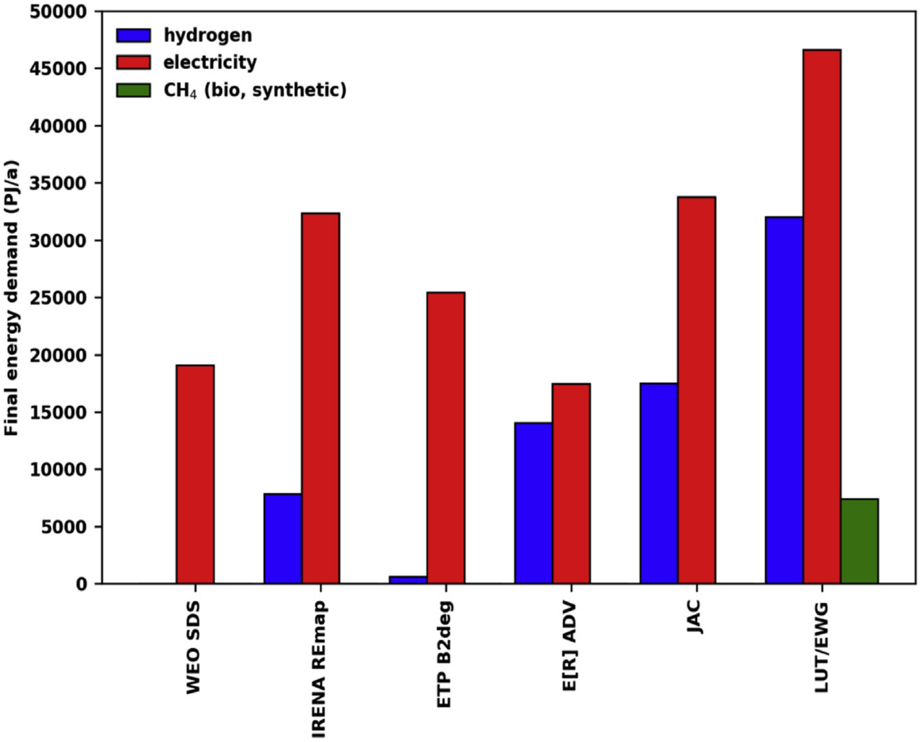

Fig. 3. Final energy demand of renewable energy carriers in 2050 in the transport sector (in PJ/a).

note that for the purpose of this study, the original scenario data had to be adapted moderately (see the supplementary material for details).

2.2. Energy technology roadmaps

Because the future development of market shares for each energy technology is uncertain [40], we draw from a review of the literature to establish technology roadmaps for each technology class, thereby addressing major uncertainties in market developments.

We distinguish between the ‘continuity’ (CONT) and ‘technological change’ (TC) roadmaps for each technology class. The CONT roadmap extrapolates current market trends and assumes that in the future, currently mature technologies that are capable of being installed at a large scale will be used. In the TC roadmap, technologies may not yet have reached maturity in all cases; however, they are predicted in the scientific literature to achieve market penetration. The ten subtechnology roadmaps are shown in Fig. 4 (see supplementary material for more details).

2.3. Specific material content

Results of a literature review of the specific material content of Dy and Nd in wind power technologies and electric motors, as well as of Co and Li in stationary and mobile batteries for the considered subtechnologies are shown in Table 1.

The complete dataset is included in the supplementary material.

2.4. Data on annual extraction, reserves, resources and further specifications

Our analysis focuses on potential material shortages worldwide;

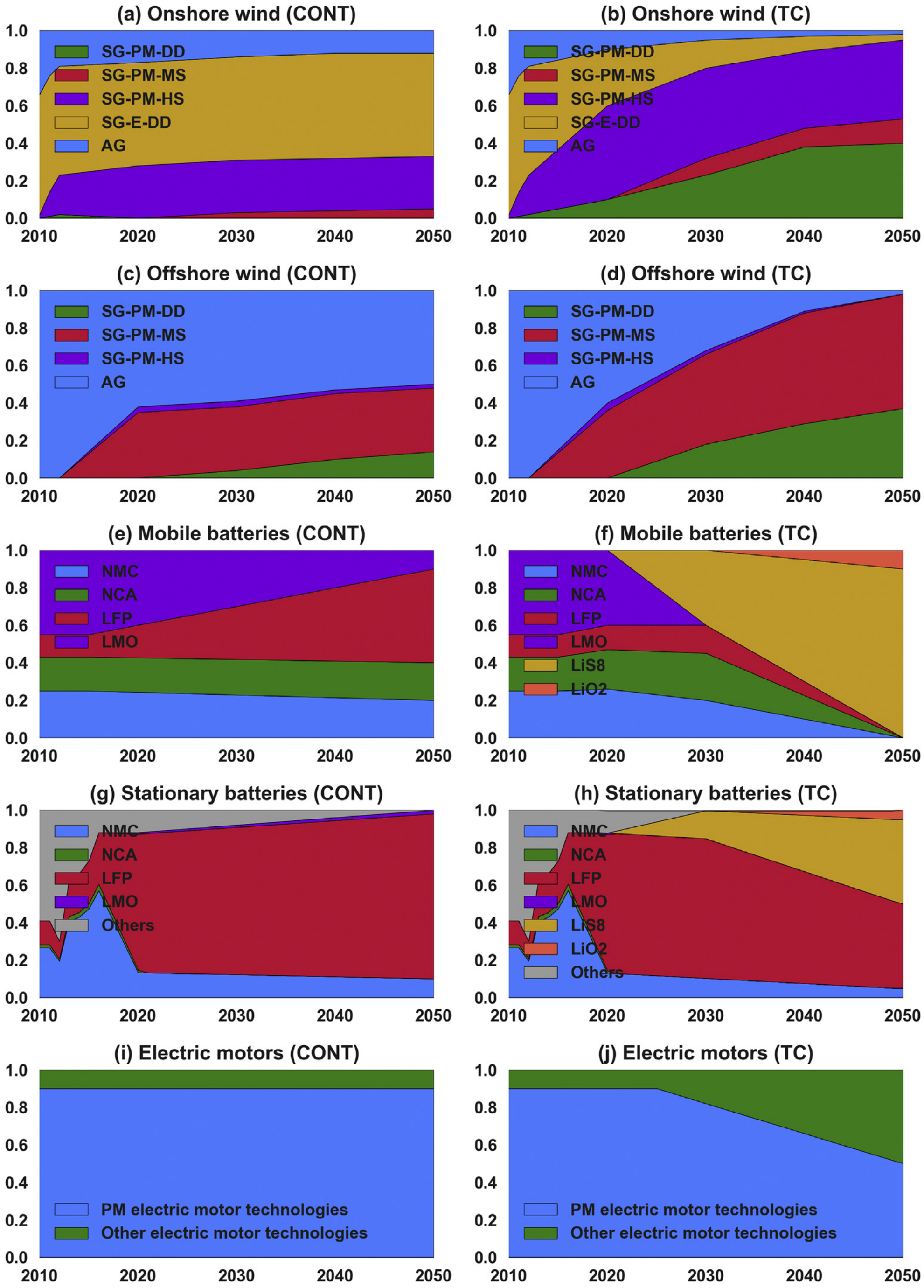

Fig. 4. Market shares of subtechnologies within a technology class.

Table 1
Mean values and uncertainties (Unc.) of the specific material content (Nd, Dy, Li, Co) in wind power plants, batteries, and electric motors. Uncertainties are based on the minimum and maximum values available in the literature. Numbers are rounded according to the uncertainty listed. Technologies that are part of a subtechnology roadmap but do not have specific material content that is relevant to this study are listed for the sake of completeness.

	Unit	Dy	Unc. (%)	Nd	Unc. (%)	Co	Unc. (%)	Li	Unc. (%)
Wind power									
SG-PM-HS	kg/MW	3	−45 +36	21	−12 +21				
SG-PM-MS	kg/MW	4	−34 +28	30	−41 +55				
SG-PM-DD	kg/MW	20	−29 +63	170	−41 +27				
SG-E-DD	kg/MW	0		0					
AG	kg/MW	0		0					
Electric motors									
With PM	kg/MW	2	−98 +78	10	−64 +247				
Without PM	kg/MW	0		0					
Stationary and mobile batteries									
NMC	kg/MWh					300	−67 +69	140	−19 +17
NCA	kg/MWh					200	−32 +47	160	−30 +40
LFP	kg/MWh					0		170	−51 +97
LMO[a]	kg/MWh					500	−100 +100	113	−0 +0
LiS_8	kg/MWh					0		410	−20 +20
LiO_2	kg/MWh					0		150	−20 +20
Others	kg/MWh					0		0	

[a] LMO: lithium metal oxide, where the metal can be either Mn or Co. We consider one value each. Because there is no Co content for cathode materials using Mn, the average between both values is half of the Co cathode chemistry value with an uncertainty of 100%.

therefore global resources, reserves and annual extraction are included. Reserves are a subset of resources that can currently be economically extracted [41]. To consider the uncertainty connected to the estimation of reserves and resources, we include a range of estimates from different studies as well as the mean value of these estimates. Current extraction volumes are based on the most recent data reported by the USGS [42] (see Table 2).

A literature overview of Li and Co reserve and resources is provided in Sverdrup [27] and Sverdrup et al. [43]. Sources provided in the project ‘Modelling sustainable Energy system Development under Environmental And Socioeconomic constraints’ (MEDEAS) were also consulted [44]. For Dy and Nd, apart from the estimates in the literature, we conduct a resources estimate based on information about specific mines (see supplementary material for details).

In the literature, a distinction is made between the terms recycled content (RC) and end-of-life recycling rate (EOL-RR) [45]. RC refers to the proportion of recycled metals in relation to the total metal input. The EOL-RR describes the share of metal that can be recovered at the end of a product’s life. In a dynamic environment where the metals markets show high growth rates, RC is lower than EOL-RR and material input may still be dominated by primary material extraction. Since our approach does not capture the stocks of metals in the economy, we assume that only the materials that are recovered by EOL-RR within our technological/sectoral scope are reused and the rest has to be provided by primary material extraction.

The assumptions on current recycling rates are taken from Sverdrup et al. [46]. In order to show what effects an ambitious recycling strategy has on the primary material demand, we assume a target EOL-RR of 80% in 2050 for all metals. Although this target rate is at the lower end of the assumptions for improved recycling made in other studies [17,21,26,47], it is based on the premise that a recycling infrastructure is established and that currently not commercially available recycling processes become economically viable and/or new processes are developed. To account for a dynamic behaviour of the recycling rates, we assume that the current rates are valid until 2020 and increase linearly until 2050.

The material demand in non-energy sectors is subdivided into subsectors for which the market shares for the year 2015 are estimated from the literature. Based on a regression analysis for Li, Co and REE, we assume that demand in these sectors is linearly proportional to global GDP projections from Refs. [33] (see supplementary material for further details).

Table 2
Annual extraction, reserves, and resources and current recycling rates of the metals assessed.

Material	Extraction (t/a)	Sources	Range (and average) of Reserves (Mt)	Range (and average) of Resources (Mt)	Current recycling rate (%)	Source
Nd	28730	[42], neodymium oxide (Nd_2O_3) content from [48]	8-23 (16)	17-74 (46)	15	[46]
Dy	1490	[42], dysprosium oxide (Dy_2O_3) content from [48]	0.32−1.30 (0.85)	3 (3)	15	[46]
Li	77000	[42]	15-29 (21)	28-116 (64)	10	[46]
Co	140000	[42]	7-16 (12)	25-66 (38)	40	[46]

3. Results

The average annual growth rates of material requirements for 2015–2050 for a single technology class are obtained by combining the subtechnology roadmaps and the specific material content (see Table 3). In addition, an analysis of the variation of the specific material requirement for each subtechnology is included in this chapter.

Unless otherwise stated, the results discussed are calculated using the average specific material requirements from Table 1. The annual primary material demand is compared with the annual extraction and the cumulative primary material demand with the reserves and resources listed in Table 2.

3.1. *Annual material demand*

3.1.1. *Neodymium*

The maximum annual material demand is between ~135 kt/a (ETP B2deg TC) and ~258 kt/a (LUT/EWG CONT). These values are the sum of the coloured areas of the bar plots in Fig. 5 (a). The estimates for the CONT and TC roadmaps differ among scenarios, ranging between ~0% (JAC) and ~27% (WEO SDS). In the TC roadmap, the possibility of replacing electric motors that rely on NdFeB magnets with other technologies and wind turbines that mostly use asynchronous generators is illustrated. Because demand is primarily driven by electric vehicles, the effect of substitution becomes more dominant in the TC roadmap. However, demand is still mainly driven by road transport. Furthermore, those scenarios that show comparably low demand for Nd are also less ambitious.

Using the minimum values of specific Nd requirements in subtechnologies in the year of the maximum annual material demand, total demand decreases to ~89 kt/a (ETP B2deg TC). If the maximum values are used, then demand increases to ~745 kt/a (LUT/EWG CONT). Assuming the lowest specific material content, total demand becomes also driven by demand from non-energy sectors. Uncertainties in specific material requirements cause the results to vary greatly at the overall scenario level. Using maximum values, the estimates are ~99% (IRENA REmap TC) to ~189% (LUT/EWG CONT) higher than estimates calculated with average values. Using minimum values, the estimates are ~31% (IRENA REmap TC) to ~49% (LUT/EWG CONT) lower.

By assuming recycling, the maximum annual primary material demand is between ~77 kt/a (WEO SDS TC) and ~155 kt/a (LUT/EWG CONT) (see the red dots and the years below in Fig. 5 (a)). Thus, annual primary material demand for Nd increases 3- to 5-fold compared to current extraction. Furthermore, it occurs at an earlier point in time than maximum material demand in most cases.

Table 3
Effects of sub-technology scenarios in combination with the average values of specific material contents.

Technology	Roadmap	Average annual growth rate of specific material content 2015–2050 (%)			
		Nd	Dy	Co	Li
Wind onshore	CONT	0.1	0.2		
	TC	4.9	4.5		
Wind offshore	CONT	5.8	5.8		
	TC	8.4	8.2		
Electric motors for EVs	CONT	0.0	0.0		
	TC	−1.5	−1.5		
Batteries for electric mobility	CONT			−2.2	0.4
	TC			N/A*	3.1
Stationary batteries	CONT			−3.7	1.2
	TC			−6.3	2.7

*Co demand for mobile batteries is assumed to be zero in 2050.

3.1.2. *Dysprosium*

The maximum annual material demand is between ~17 kt/a (ETP B2deg TC) and ~52 kt/a (LUT/EWG CONT) (Fig. 5 (b)). The estimates for the CONT and TC roadmaps differ among scenarios, ranging between ~29% (JAC) and ~60% (WEO SDS). These ranges are larger than those for Nd demand because electric vehicles in the CONT roadmap require comparatively more Dy than wind turbines in the TC roadmap. As with Nd, Dy demand is dominated by road transport in both subtechnology roadmaps.

Assuming minimum values of specific Dy requirements, total demand decreases to ~2.4 kt/a (IRENA REmap CONT). If the maximum values are used, total demand increases to ~90 kt/a (LUT/EWG CONT). Uncertainties in specific material requirements cause the results to vary at the overall scenario level. Using maximum values, the estimates are ~69% (IRENA REmap TC) to ~75% (LUT/EWG CONT) higher than estimates calculated with average values. Using minimum values, the estimates are ~93% (LUT/EWG CONT) to ~73% (JAC TC) lower.

The maximum primary material demand is between ~11 kt/a (IRENA REmap TC) and ~33 kt/a (LUT/EWG CONT) and, in most cases, occurs at an earlier point in time than maximum material demand. Thus, annual primary demand for Dy increases 7- to 22-fold compared with current extraction.

3.1.3. *Lithium*

The minimum annual demand of ~1698 kt/a is in the CONT roadmap of the WEO SDS scenario (see Fig. 5 (c)). The maximum annual demand of ~11511 kt/a occurs in the TC roadmap of the LUT/EWG scenario. The influence of subtechnology roadmaps on variations in material demand within a scenario is notably stronger for Li than for Nd or Dy. However, the variation between the scenarios is not as high (ranging from ~55% in LUT/EWG to ~58% in ETP B2deg). In all cases, the batteries for BEVs and stationary storage systems (especially in the highly ambitious scenarios) are the largest consumer of Li. The dominance of BEVs results from the comparatively low battery capacity of the other vehicle types.

Minimum values of specific Li demand in subtechnologies imply a decrease in total demand to ~1093 kt/a (WEO SDS CONT). Using maximum values, total demand increases to ~14366 kt/a (LUT/EWG TC). In contrast to Nd and Dy, uncertainties due to specific material requirements for Li are not quite as high. Using maximum values, the estimates are ~20% (ETP B2deg TC) to ~77% (LUT/EWG CONT) higher than estimates calculated with average values. Using minimum values, the estimates are ~20% (ETP B2deg TC) to ~40% (LUT/EWG CONT) lower.

The maximum primary material demand for Li is between ~938 kt/a (IRENA REmap CONT) and ~6811 kt/a (LUT/EWG TC) and occurs at an earlier point in time than material demand in only some cases. Thus, current global annual Li extraction must increase 12- to 88-fold.

3.1.4. *Cobalt*

The minimum annual material demand of ~715 kt/a is in the TC roadmap of the WEO SDS scenario (Fig. 5 (d)). The maximum annual demand of ~4471 kt/a is in the CONT roadmap of the LUT/EWG scenario. The influence of subtechnology roadmaps on variation in demand within a scenario is the highest for Co and varies largely between the scenarios (ranging from ~59% in E[R] ADV to ~67% in LUT/EWG). In both subtechology roadmaps, material demand is mainly driven by BEVs as stationary storage systems mostly rely on Co-free batteries.

Using the minimum values of the specific Co demand of subtechnologies, total demand decreases to ~364 kt/a (JAC TC). Assuming the maximum values, total demand increases to ~7412 kt/a (LUT/EWG CONT). In the most optimistic case of specific

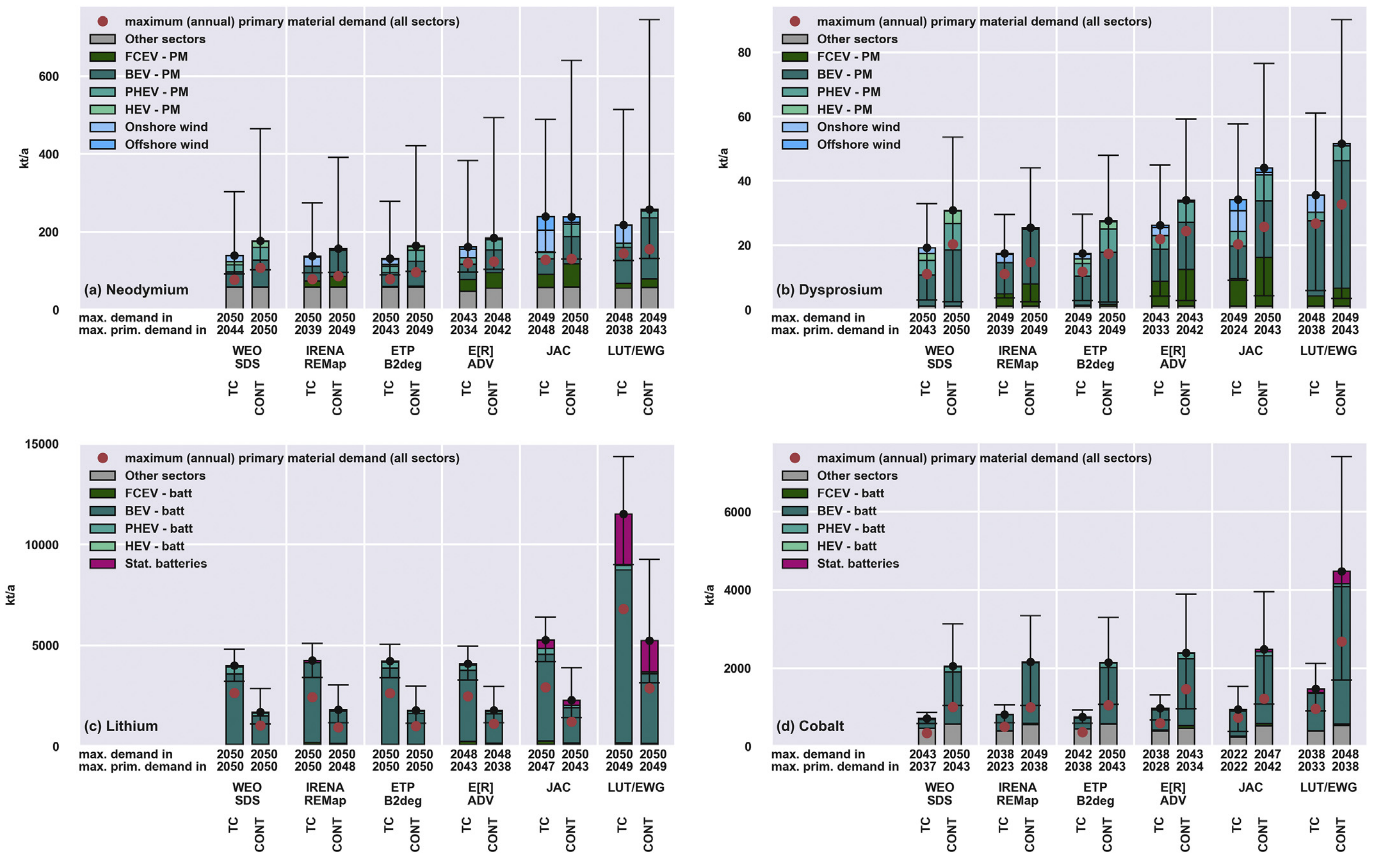

Fig. 5. Maximum annual material demand (sum of coloured areas in the stacked bars) with the respective year for each scenario/subtechnology roadmap. Values are calculated using average values for the specific material content. Error bars are calculated using the high and low estimates of the specific material content at a subtechnology level for the year with the highest material demand. Maximum primary material demand (red dots) and the respective year are calculated using the average values for the specific material content. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

material content and subtechnology development, the material consumption from non-energy sectors becomes dominant in most scenarios. Uncertainties in specific material requirements cause the results for Co to vary within a magnitude similar to that of Li: Using maximum values, the estimates are ~21% (WEO SDS TC) to ~66% (LUT/EWG CONT) higher than estimates calculated with average values. Using minimum values, estimates are ~17% (WEO SDS TC) to ~60% (JAC TC) lower. In the most optimistic case of specific material content and subtechnology roadmap, material demand from non-energy sectors has a share of ~43% and above in all scenarios.

Maximum primary material demand is between ~337 kt/a (WEO SDS TC) and ~2675 kt/a (LUT/EWG CONT) and, in all cases, occurs earlier than the maximum material demand. Thus, current global annual Co extraction would have to increase 2- to 19-fold even when an ambitious recycling strategy is implemented.

3.2. Cumulative material demand

3.2.1. Neodymium

Cumulative Nd demand ranges from ~2.7 Mt (WEO SDS TC) to ~4.7 Mt (JAC TC) (Fig. 6 (a)). Differences in the material requirements within individual scenarios due to applying the TC or CONT roadmap are relatively small; the differences are between ~2% (IRENA REmap) and ~8% (ETP B2deg). Higher demand for Nd in the TC roadmap of the JAC scenario results from the high proportion of offshore wind turbines. Thus, demand from the wind turbine sector outweighs the reduction in electric motors equipped with NdFeB magnets. In all scenarios and both subtechnology roadmaps, demand from the energy sector is mainly driven by road transport.

Using the minimum values of Nd demand for specific material content in subtechnologies, the cumulative material demand decreases to ~1.9 Mt (ETP B2deg TC). If the maximum values are used, then cumulative demand increases to ~12.8 Mt (LUT/EWG CONT).

The cumulative primary material demand decreases to between ~2.0 Mt (ETP B2Deg TC) and ~3.6 Mt (LUT/EWG CONT). Notably, the primary material demand does not exceed current estimates of reserves or resources in any case.

3.2.2. Dysprosium

Cumulative demand ranges from ~0.4 Mt (WEO SDS TC) to ~0.9 Mt (LUT/EWG CONT) (Fig. 6 (b)). For individual scenarios, estimates for CONT and TC roadmaps differ by ~14% (JAC) to ~23% (ETP B2deg). As with Nd, Dy demand is dominated by road transport.

Assuming the minimum values of Dy demand for specific material content in subtechnologies, cumulative material demand decreases to ~0.06 Mt (WEO SDS CONT). If the maximum values are used, then demand increases to ~1.5 Mt (LUT/EWG CONT).

The TC roadmap of the WEO SDS and the CONT roadmap of the LUT/EWG scenario have a cumulative primary material demand of ~0.3 and ~0.7 Mt, respectively. Thus, ambitious recycling prevents the average reserve estimate from being exceeded in all scenarios. Furthermore, exceeding the lower limit of reserve estimates in the TC roadmap of the less ambitious scenarios is avoided.

3.2.3. Lithium

The lowest cumulative demand of ~20.5 Mt results from the

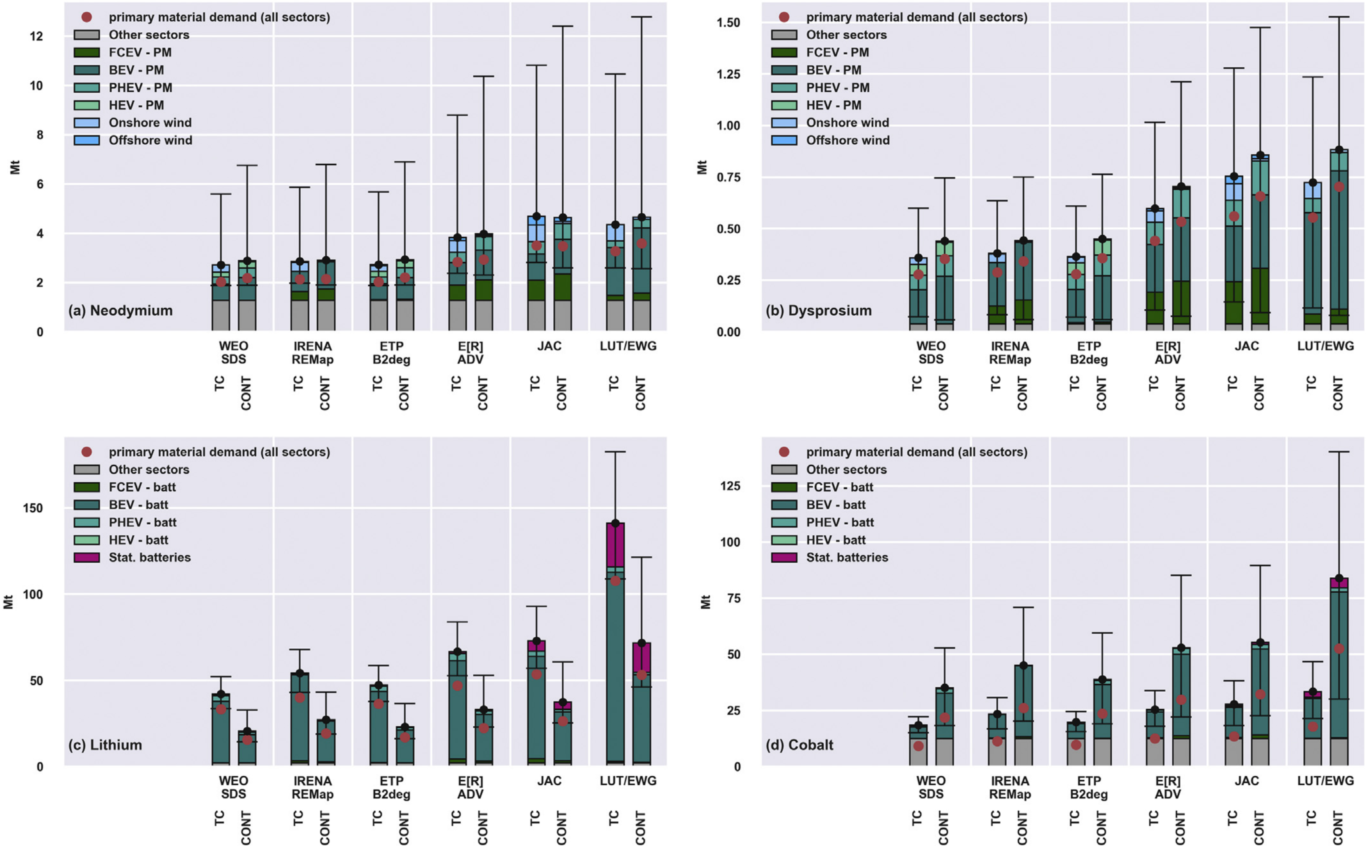

Fig. 6. Cumulative material demand 2015–2050 (sum of coloured areas in the stacked bars) for each scenario/subtechnology roadmap. Values are calculated using average values for the specific material content at a subtechnology level. Error bars are calculated using the high and low estimates of the specific material content. Cumulative primary material demand (red dots) is calculated using the average values for the specific material content. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

CONT roadmap of the WEO SDS scenario (Fig. 6 (c)). The highest demand of ~141.2 Mt results from the TC roadmap of the LUT/EWG scenario. Differences in cumulative demand within a scenario due to applying the TC or CONT roadmap are between ~49% (JAC) and ~51% (ETP B2deg) and are higher than for Nd and Dy.

Assuming minimum values of Li demand for specific material content in subtechnologies, the cumulative material demand decreases to ~14.3 Mt (WEO SDS CONT). If maximum values are used, the demand increases to ~182.6 Mt (LUT/EWG TC).

The cumulative primary material demand lies between ~15.5 Mt (WEO SDS CONT) and ~107.8 Mt (LUT/EWG TC). Thus, for the TC roadmap and in all scenarios, primary material demand exceeds upper bound reserve estimates and is higher than the lower bound of resource estimates. Average resource estimates are exceeded by ~68% in the LUT/EWG scenario. In the CONT roadmap, primary demand is below average reserve estimates for the less ambitious scenarios. However, in all scenarios the primary material demand exceeds lower bound reserve estimates. In the E[R] ADV and the JAC scenarios, average reserve estimates are exceeded. In the LUT/EWG scenario, both, the upper bound reserve estimates and the lower bound resource estimates are exceeded.

3.2.4. Cobalt

The lowest cumulative material demand of ~18.4 Mt results from the TC roadmap of the WEO SDS scenario (Fig. 6 (d)). The highest demand of ~83.9 Mt results from the CONT roadmap of the LUT/EWG scenario. Consequently, technologies that are expected to gain high market share in the TC roadmap reduce Co demand, but they significantly increase demand for Li (Fig. 6 (c)). Demand from the non-energy sectors is almost equal to the average reserve estimates, since current annual consumption is already high in relation to reserves. Differences in cumulative demand within a scenario due to applying the TC or CONT roadmap are between ~91% (WEO SDS) and ~151% (LUT/EWG).

Assuming minimum values of Co demand for specific material content in subtechnologies, cumulative demand decreases to ~15.0 Mt (WEO SDS TC). If the maximum values are used, then cumulative demand increases to ~140.2 Mt (LUT/EWG CONT).

The cumulative primary material demand is between ~9.1 Mt (WEO SDS TC) and ~52.5 Mt (LUT/EWG CONT). In the TC roadmap, primary material demand remains below average reserve estimates in the less ambitious scenarios. The upper bound of reserve estimates are exceeded in the LUT/EWG scenario. Subtechnology deployment according to the CONT roadmap leads to the exceedance of upper bound reserve estimates in all scenarios. The lower bound of resource estimates is exceeded in the IRENA Remap scenario and in all highly ambitious scenarios. In the LUT/EWG scenario, average resource estimates are exceeded by ~38%.

4. Discussion

In the following we discuss the results with regard to their broader implications, the results in the literature, the most important uncertainties and their significance for future scenario studies. In section 4.3 we present the sensitivity of the results with respect to the assumptions of recycling rates and material demand in the non-energy sectors.

4.1. Implications of the results

Although it is difficult to isolate the driving factors for material demand due to different assumptions and scopes of the scenarios, our results confirm that high ambitions to reduce CO_2 emissions and high direct electrification drive material demand.

We assume ambitious recycling to assess the maximum annual and cumulative primary material demand. Although no depletion of reserves is expected for Nd, in most scenarios, primary demand for Dy exceeds lower bound reserve estimates and could be vulnerable to supply bottlenecks. Li and Co demands exceed lower bound reserve estimates for both metals in all scenarios. The current resource estimates may motivate the switch to low-Li batteries as a priority, so that the lower bound of resources is only exceeded in one scenario. However, our study also reveals the dilemma that could arise from this switch, as low-Li batteries generally require higher amounts of Co, which in most scenarios lead to at least the lower limit of Co resource estimates being exceeded.

Recycling can only mitigate short-term increases in demand to a limited extent, as the recycling potential is highly dependent on the lifetime of the technologies. Long-lived technologies, such as wind turbines, contribute little to the recycling potential within the time horizon of the analysis. A significant increase in primary annual extraction volume must take place for each material in all scenarios. The need for an increase is strongest for Li. The proposed strategy for low-Li batteries necessitates the expansion of annual Co extraction by a factor of 7–19, well before 2050.

It is important to note that key factors in primary material supply include not only the amount of the resource but also the rate and efficiency with which the target materials are extracted and processed. Should these factors be unable to keep pace with increasingly difficult extraction conditions due to high demand from energy system transformations, metal shortages and price increases are to be expected, which in turn could significantly impact technology prices (see chapter 4.4 for further elaboration). Moreover, because Nd, Dy, and Co are not mined as main products, but as by- or co-products, extraction capacity is not primarily determined by an increase in demand for these metals [49].

4.2. Results in the context of other studies

We limit the comparison of our results to studies that have a global focus, a time horizon until at least 2050, and also include the material demand from non-energy sectors. Results are compared with regard to the maximum annual material demand and, if provided by the studies, cumulative demand until 2050 (Table 4).

Habib and Wenzel [22] use three scenarios from the IEA ETP 2010 and an additional scenario that assumes 100% renewables in 2050 and combine these with varying penetration rates of direct-drive wind turbines. For all non-energy sectors, the authors assume an annual growth rate of 3–4% depending on the degree of ambition of the respective scenario. Upper bound values correspond to our results for the less ambitious scenarios and are mainly driven by the deployment of BEVs. Hoenderdaal et al. [23] use scenarios which combine low and high expansion scenarios for wind turbines with low and high assumptions on the market penetration of direct-drive wind turbines. The growth rates of non-energy sectors are assumed to be sector-specific. As in Ref. [22], the material demand is mainly driven by BEVs. Although the results in Hoenderdaal et al. [23] are in the range of material demand in the our study, they assume a lower degree of ambition of the analysed scenarios (i.e. lower installed capacities of wind power, less electric vehicles) which is compensated by a higher specific material content of the energy technologies.

Hache et al. [50] assess the Li demand in road transport using scenario results from the TIMES Integrated Assessment Model. Demand from non-energy sectors is assumed to be sector specific, with particularly high growth in batteries expected for the near future. Hache et al. [50] consider only NMC batteries, which have a comparably low specific Li demand. In their 2 °C scenario, the demand for materials is therefore slightly below the demand of the less ambitious scenarios in combination with the CONT roadmap of our study. The lower bound of the material demand results from a less ambitious scenario with low demand for mobility. Harvey [51] does not use specific energy scenarios to predict the future demand for light duty vehicles (LDVs), but assumes that the number increases with GDP per capita and demand from non-energy sectors increases with GDP. The upper bound of the material requirements is lower compared to the scenarios of our study, because the authors assume a late market entry of BEVs (3–6% in 2030) which reduces the early demand for large battery capacities. This is also reflected in the primary material demands, which are similarly low for Co in our study only in the less ambitious scenarios in combination with the TC roadmap. Similar to Harvey, Kushnir and Sandén [11] do not rely on energy scenarios but assume different vehicle demand scenarios per capita. Growth of the non-energy sectors is assumed to be sector-specific and recycling is at a constant rate of 80%. The upper bound of primary Li demand is in line with the primary demand of the less ambitious scenarios in combination with the CONT roadmap of our study. The lower bound of primary demand is based on the assumption that only PHEVs are deployed and therefore significantly lower.

Valero et al. [25] use sector-specific (e.g. transport only) results from several scenario studies, most of which were published by the IEA in 2014. The authors assume constant proportions of wind turbines with (75%) and without (25%) gearboxes. Both, demand from non-energy sectors and recycling rates remain at current levels. The cumulative primary material requirement for Dy is significantly lower, mainly because the specific material requirement in electric motors for BEVs and PHEVs is ~80% below our assumptions. Estimates of annual primary demand are in the range of the less ambitious energy scenarios of our study. Watari et al. [52] assess the demand in the ETP 2017 scenarios from the IEA. Similar to our study, demand in non-energy sectors is assumed to increase proportional to GDP. The assumed lower Dy content in electric motors compared to our study is the main reason for the lower demand for this material. The demand for Nd, Li and Co is in line with the present study. Assuming a constant recycling rate of 90%, the primary material demand is significantly lower compared to all scenarios in our study.

Ziemann et al. [24] assess the Li demand by LDVs in the IEA Blue map scenario published in 2009. The authors assume the deployment of either NMC, NCA or LiS_8 batteries. Demand in non-energy sectors corresponds to current annual extraction and is scaled at an annual growth rate of 5%. The upper bound of the annual demand is due to the deployment of LiS_8 batteries. Even though the use of Li rich batteries corresponds closely to our TC roadmap, the demand is lower. The lower bound of material demand is based on the sole use of NMC batteries and is lower than the demand of all our scenarios. This can be attributed in particular to the significantly lower assumed battery capacities of 25 kWh in BEVs and the narrower technological scope in Ref. [24].

In de Koning et al. [28], the demand is at the lower end of our estimates. This is mainly due to the less ambitious scenarios (4 °C pathways) in their study. In addition, the authors assume a reduction of 80% of the current Dy requirement in NdFeB magnets until 2050, which explains the comparably low demand for this material.

Table 4
Methods, material demands, recycling assumptions and references/limitations in other studies compared to our study. Maximum values in top row, minimum values in bottom row per source. The average specific material content values are used for our results.

Study	Method	Maximum annual (and cumulative) demand until 2050 (kt/a, Mt)				Recycling[a]	Comparatie values/limitations
		Dy	Nd	Li	Co		
De Koning et al. [28]	MRIO	5	125	1628	–	–	Extraction, reserves
		3	58	1230	–	–	
Habib and Wenzel [22]	MFA	32 (0.4)	242 (4)	–	–	–	Extraction, reserves
		11 (0.2)	100 (2)	–	–	–	
Hache et al. [50]	MFA	–	–	1200 (25)	–	–	Extraction, reserves
		–	–	300 (7)	–	–	
Harvey [51]	MFA	–	–	400	800	–	Extraction, resources
		–	–	230	480	✓ (I)	
Hoenderdaal [23]	MFA	50 (0.8)	–	–	–	–	Extraction, reserves
		9 (0.3)	–	–	–	✓ (I)	
Kushnir and Sandén [11]	MFA	–	–	1470 (26)	–	✓ (I)	Extraction, resources
		–	–	210 (3)	–	✓ (I)	
Sverdrup [27]	SD	–	–	500 (7)	–	–	Extraction, reserves, resources
		–	–	450 (6)	–	✓ (I)	
Sverdrup et al. [43]	SD	–	–	–	400 (15)	–	Extraction, reserves, resources
		–	–	–	225 (10)	✓ (I)	
Valero et al. [25]	MFA	9 (0.02)	70 (2)	950 (27)	420 (9)	✓ (C)	Extraction, reserves, resources
Watari et al. [52]	MFA	13 (0.5)	110 (4)	1300 (20)	950 (25)	–	Extraction, reserves, resources
		6	50	450 (12)	300	✓ (I)	
Ziemann et al. [24]	MFA	–	–	1630	–	–	–
		–	–	570	–	–	
This study	MFA	52 (0.9)	258 (5)	11511 (141)	4471 (84)	–	Extraction, reserves, resources
		11 (0.3)	77 (2)	938 (16)	337 (9)	✓ (I)	

[a] Recycling rates correspond to the reported values, 'I': Improved recycling rates compared to current levels; 'C': Recycling rates based on current values.

Finally, Sverdrup [27] assesses the global supply dynamics of Li with various combinations of resources from 34 to 116 Mt and recycling rates ranging from 50 to 85%. The main drivers of Li demand are assumed to be batteries in electric vehicles and in other applications. Demand from non-battery applications is assumed to grow with population size. In the base case (resources of 73 Mt and specific demand of 10kg/BEV), the material demand and the primary material demand is lower compared to our study. Sverdrup et al. [43] assess the demand for Co assuming sector specific growth. In the base case (resources of 76 Mt), material demand and primary material demand are in line with the demand of the TC roadmap of the less ambitious scenarios. Note that the comparison of results from SD models with results from MFA is challenging as the former accounts for market dynamics that may prevent the deployment of certain technologies. For example, Sverdrup [27] concludes for the base case that the possible fleet size of BEVs is between 400 and 1000 million, which is significantly lower than those in the present scenarios.

This study confirms the significant increase in metal demand for a low-carbon transition from (road) transport and wind power supply, as reported by others. However, especially the scope of the technologies considered and the methods used to estimate demand, have a significant impact on the results. Furthermore, studies with a time horizon until 2100 and longer such as [11,27,43,51] regard resource estimates as a limiting factor rather than reserves or annual extraction. Our assessment is based on some very ambitious energy scenarios (e.g. LUT/EWG) that have not yet been assessed in the previous literature and show a high growth in demand compared to the estimates in other studies. Further differences mainly result from different assumptions on battery capacity, engine power, penetration rates of certain subtechnologies, specific material requirements, recycling rates and growth rates of non-energy sectors.

4.3. Scope, methods and uncertainties

The scenario/roadmap combinations illustrate the large spread in future material demand that arises from possible market developments at the technology and subtechnology levels. Note that the combination of the TC roadmap for wind with the CONT roadmap for electric motors leads to higher demand for Dy and Nd. For example, the cumulative material demand for Dy and Nd in the JAC scenario would increase to ~0.9 Mt (~10% more than in JAC CONT) and ~5.4 Mt (~16% more than in JAC TC), respectively.

The target recycling rate of 80% by 2050 assumed in this study is a rough assumption to illustrate what could be achieved with very ambitious measures. Furthermore, it should be noted that achieving high recycling rates is an issue that needs to be addressed at the design stage of the technologies and is therefore not only a policy whose measures promote the development of efficient recycling systems and changes in citizens' behaviour [45]. The assumption that the global demand for minerals in non-energy sectors is linearly dependent on GDP growth is a rough estimate, especially due to the lack of robustness of the data underlying the regression [26]. It could be assumed that, for example, the material demand for batteries in non-energy sectors will continue to grow faster than economic growth, while demand in other sectors continues to decline (as e.g. shown by Fu et al. [53] for Co).

In the following, we briefly assess the influence of sector-specific growth on the results assuming ambitious and status quo recycling rates (see Table 2). Sector-specific growth rates for Nd and Dy originate from Schulze and Buchert [54], for Li from Martin et al. [55] and for Co from Fu et al. [53]. However, the strong exponential growth of some sectors assumed in these studies are mostly valid until 2030 and do not seem to be realistic up to 2050, so that from 2030 we expect growth proportional to GDP (see supplementary material for further details). Fig. 7 shows that sector-specific growth leads to an increase in cumulative and annual primary

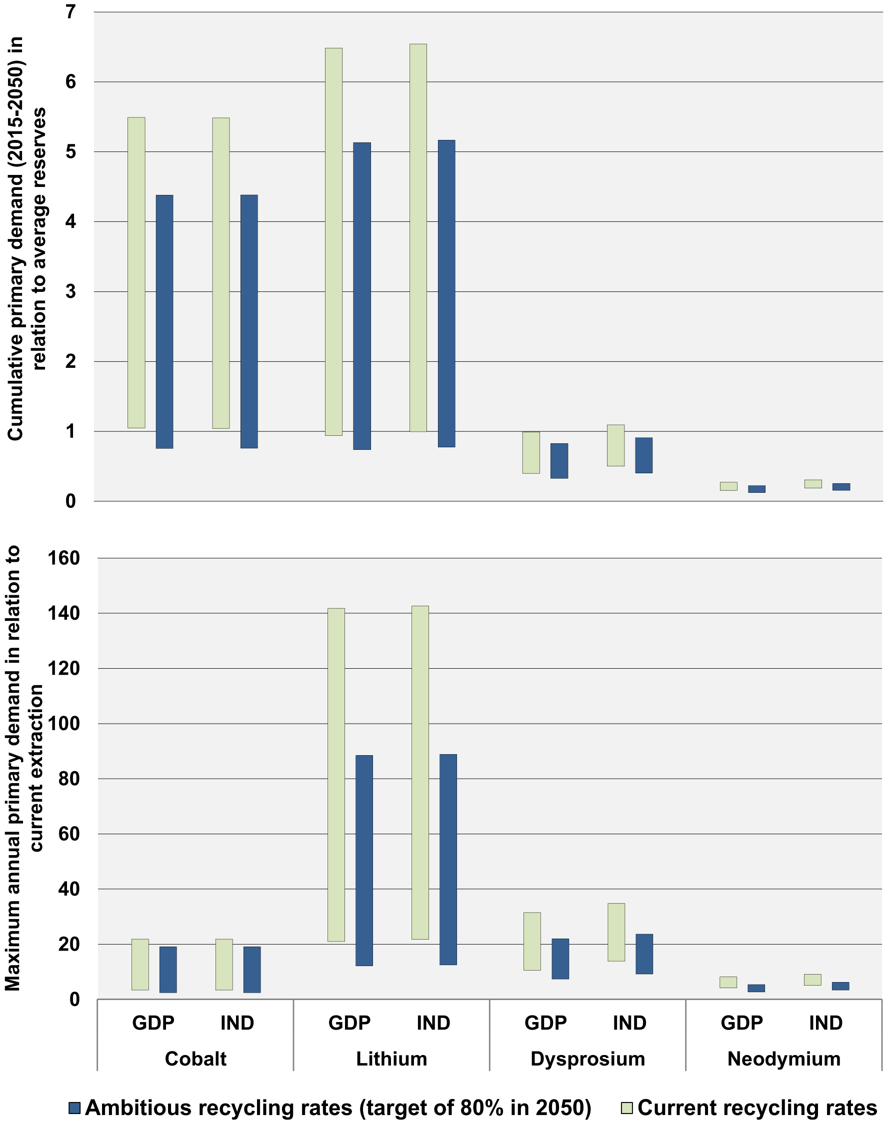

Fig. 7. Influence of different assumptions on growth rates in non-energy sectors and on recycling rates on primary material demand. 'GDP' shows the results for which growth in non-energy sectors was assumed according to GDP. 'IND' shows results with sector-specific growth. The upper panel illustrates the results range of the cumulative primary demand across all scenario roadmap combinations in relation to average reserve estimates. The lower panel shows the maximum annual primary demand relative to current extraction. Results are based on the average material requirements for the subtechnologies.

material demand for Dy, Nd and Li. The highest impact occurs for Nd in the case of ambitious recycling with an increase of 13% of both, upper bound cumulative and maximum annual primary demand. The demand for Co decreases slightly, because although strong growth is expected for batteries, demand in many of the other sectors is expected to decline. The impact of applying current recycling rates on implications for metal scarcity is large and shows similarly strong effects in both assumptions on growth in non-energy sectors. Average resource estimates of Li and Co are exceeded by up to a factor of 2.1 and 1.7, respectively (not shown in Fig. 7). Scenario-specific results can be found in the supplementary material (Excel format).

Due to the magnitude of uncertainty and lack of data concerning specific material content for promising new technologies, the present analysis considers only technologies or technology components for which market readiness already exists or is expected shortly. Although average values of specific material content for each subtechnology is used to calculate the primary demand, it cannot be assumed that those values are more probable than others found in the literature. Additional uncertainty about material demand lies in upstream losses [56], neglected in this analysis, that increase demand for primary materials in the subtechnologies. However, these losses are strongly dependent on the mine (e.g., ore grade and composition, mining technologies) and subtechnology manufacturing processes; therefore, they are difficult to estimate [57]. Further research is needed to expand our database of specific material content in terms of the expected technology-specific material efficiency, the scale of material demand with higher performance/capacity, and material losses in the upstream supply chain.

Furthermore, it should be noted that different subtechnologies differ in their technical characteristics, which may have an impact on properties such as lifetime and performance. This applies in particular to Li-ion batteries, since the lifetimes of the various battery chemistries depend to different degrees on parameters such as the number of charging cycles, operating temperature, depth of discharge and use frequencies [58]. The assessment of the impact of subtechnology-specific lifetimes on demand and supply dynamics remains a topic for future research.

The subtechnologies considered may impose demands for materials not included here (e.g., Fe in LFP, Mn and Ni in NMC and Ni in NCA batteries). Additional uncertainty arises from the inclusion of LiS_8 and LiO_2 batteries, which have not yet reached market maturity and whose properties are still unknown for large-scale applications [59]. Furthermore, we did not consider solar power (PV and CSP), technologies related to hydrogen supply and use, and other infrastructure components that may result in a substantial increase in demand for other relevant materials (e.g., Ag in CSP and silicon based PV; Ca, Ga, In, Se and Te in thin film PV; Zr, Pd, Ni, Pt, or Y in electrolysers and/or fuel cells; Cu as a substitute for Ag in silicon based PV, in the electricity grid, EVs and EV chargers). Thus, the potential subtechnology projections and the focus on a limited number of metals in this study are therefore by no means evidence that an ambitious, climate-friendly transformation of the global energy system is possible.

The material requirements in the scenarios for which the number of road transport technologies had to be estimated in whole or in part must be considered as first approximations. More valid calculations require that future scenario studies document the scope of the model (e.g., depth of modelling of transport modes and resolution of technologies and sectors), assumptions about technological characteristics at the subtechnology level, and technology-specific development in terms of installed capacities.

4.4. Implications for energy scenario modelling

Even if we assume high recycling rates, a significant low-cost, direct electrification of global transport as proposed by many studies seems possible only through the development of efficient and affordable low-Li and preferably Co-free batteries or through the development of new battery technologies for mobile applications.

However, currently promising battery technologies, such as dual systems that combine Zn-air with Li-ion batteries, as proposed by Li and Lu [60], are expected to be more expensive and complex to operate [61]. Other reduction possibilities, such as dynamic wireless power transmission for charging on motorways, are associated with increased ranges and decreased battery capacities of up to 20% for BEVs [62] but generate increased demand for other materials (e.g., Cu for the coils) and incur higher infrastructure costs.

Another technical solution for reducing the demand for Li and Co could be a shift towards a high share of FCEVs in future vehicle markets, as the electrical storage capacity of FCEVs is significantly lower than that of BEVs or PHEVs. However, technology-for-technology substitution has a larger implementation threshold than component-for-component or metal-for-metal substitutions because such substitutions often require a different set of knowledge and manufacturing processes and therefore usually take longer to implement, as shown by Curtius [63] for the case of building-integrated PV. Metal-for-metal substitution on a large scale, however, is only possible with a metal that is produced in larger quantities than the one it is intended to replace [64], as for example Sverdrup and Olafsdottir [65] illustrate for the substitution of Ni by Co, Mo, Ta or Va in stainless steel manufacturing. Furthermore, if the substitution material is scarce in its own supply, substantial substitution may lead to price increases which further aggravate scarcity [66]. Therefore, metal-for-metal substitution is rarely suitable for reducing potential material shortages.

To analyse the roles of multiple hypothetical substitutions efficiently, energy system modellers need techno-economic parameters and material inventories not only for the technology class (e.g., Li-ion batteries) but also for the subtechnology level and substitution options to facilitate estimating the material requirements and accounting for technology shifts driven by material bottlenecks. Such increases in detail are considered challenges not only in terms of acquiring representative data but also in terms of model calculation times. Nevertheless, if properly implemented in the models, material bottlenecks are expected to have a significant impact on the resulting model-based transition paths. One option would be to set upper limits for material requirements of the energy system (comparable to CO_2 limits). However, these only appear to be meaningfully integrated if assumptions are made about material use in non-energy sectors. In addition, upper limits for all relevant materials of all technologies must be integrated into such models; otherwise, system configurations whose material criticality is not fully captured may occur. The integration of global reserve caps seems to be more appropriate than the use of resource limits, as exceeding them may increase the price of materials and the associated technologies. If the geographical framework for the analysis is less than global, budgeting must be conducted (e.g., by allocating reserves via population shares or GDP [29]). However, budgeting is prone to subjectivity and difficult to justify scientifically. Moreover, budgeting approaches do not reveal the price effects of material shortages on the technologies that are relevant to energy system models.

As illustrated by Creutzig et al. [67], non-technical measures to decrease the demand for transport are the avoidance of travel and shifting modes by incentivising behavioural change. Wynes and Nicholas [68] show that such measures may have a greater impact on emission reductions than technical solutions. According to the scenario reports, such measures are included in the WEO, the ETP and the E[R] scenarios and are combined with assumptions on efficiency improvements and fuel switching. Among the scenarios, LUT/EWG assumes the strongest increase for transport demand and mostly relies on fuel switching and efficiency gains. Potentially resulting material price increases may destruct consumer behaviour and lead to behavioural change in line with the ‘avoid’ and ‘shift’ measures. Such measures, however, are not associated with potential material scarcity in current scenario studies. The WORLD6 model developed by Sverdrup and Olafsdottir [69] is a reality-based metal price model that allows price estimation from market fundamentals within the model with feedback on mining, demand and recycling. Therefore, the coupling of such a model with energy system models and/or models to assess transport demand has a large potential to account for the effects of material scarcity on technology prices in energy scenario development. However, to the authors’ best knowledge, such combinations do not yet exist and should be pursued.

5. Conclusions and outlook

This study improves our understanding of future criticality by showing the extent to which different energy scenarios are within the range of currently known reserves and resources and indicating which primary material extraction capacities have to increase. The results show that demand for Nd, Dy, Li, and Co does not depend only on the energy scenario but is also driven by specific subtechnologies and variations in the specific material content documented in the literature.

Among the materials analysed, demand for Li by stationary and mobile battery manufacturing is likely to cause central bottlenecks for the defossilisation of global energy systems. This demand must be countered by reductions in specific material content by increasing material efficiency and conducting research on Li recycling and substitution. However, the more specific the function of a material in an application, the less likely is the substitution of that material [70], and technological substitution becomes necessary. Furthermore, it has to be assured that substitution material is not scarce in its own supply [66]. Another option would be to strongly promote synthetic fuels such as hydrogen for FCEVs as complementary and backup solutions, although costs and energy losses may be considerably higher.

When interpreting the results presented, it must be considered that neither reserves nor resources are static. Experts estimate that the amount of even rare elements in continental and oceanic crusts and in seawater is virtually inexhaustible. In addition, experience to date has shown that the introduction of new, more efficient techniques for identifying, extracting, and processing ores can, in principle, offset potential costs of lower quality or mining under more difficult conditions [71].

Nevertheless, strong dynamics are associated with the necessary extraction increases in very ambitious scenarios. The fact that reserve and resource estimates may be exceeded suggests that material shortages may greatly affect prices. Ideally, model-based assessments would address possible solutions to material bottlenecks, by increasing the cost of investment in technologies due to material bottlenecks and by explicitly including techno-economic parameters of substitution technologies with a lower specific demand for critical materials. Because specific cost assumptions are pivotal to obtaining meaningful results from cost-optimising models, future transformation scenarios may differ significantly from current scenarios that neglect constraints on material availability. For more accurate ex-post assessment of materials that are deemed critical, scenario modellers should include detailed information on subtechnology-specific expansion dynamics and transparently document assumptions. In addition, the expected high demand for the metals studied raises geopolitical issues related to the uneven global distribution of material reserves and resources, which are often overlooked in energy scenario studies and require interdisciplinary research approaches.

Credit author statement

Tobias Junne, Conceptualization, Investigation, Methodology, Software, Formal analysis, Data curation, Writing - original draft, Writing - review & editing, Visualization. Niklas Wulff, Conceptualization, Data curation, Writing - review & editing, Visualization, Christian Breyer, Writing - review & editing. Tobias Naegler, Conceptualization, Methodology, Software, Writing - review & editing, Visualization

Declaration of competing interest

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

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Appendix A. Supplementary data

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2.4 Paper 4

Status	**Published in:** Energy Strategy Reviews, 26:100380, Special Issue Energy Scenarios: Construction, Assessment, and Impact
Title	How to assess the quality and transparency of energy scenarios: Results of a case study
Co-Authors	Mengzhu Xiao, Lei Xu, Zongfei Wang, Patrick Jochem, Thomas Pregger
Submission year & month	2019
Access	https://doi.org/10.1016/j.esr.2019.100380 ☒ Gold Open Access ☐ Green Open Access ☐ Closed access
Contributions	☒ Conceptualization ☒ Methodology ☐ Software ☒ Validation ☒ Formal analysis ☒ Investigation ☒ Data curation ☒ Writing: original draft preparation ☒ Writing: review and editing ☐ Supervision ☐ Funding acquisition
Specific objective	Application of a transparency checklist for energy scenario studies to three scenarios.
Thesis-overarching objectives	2.a) Review energy scenario studies according to their compliance with pre-defined criteria of transparency 2.b) Specific focus on the objectives, methods, data used, results obtained and traceability of energy scenario studies 2.c) Offer advice for energy scenario developers on how to ensure transparency and traceability in future energy scenario studies
Methodology	Systematic classification of information provided in the scenario studies
Key outcome	First-time application of a transparency checklist for various energy scenario studies. Guidance for scenario modelers to increase impacts of energy scenarios on society, policy and economy.

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How to assess the quality and transparency of energy scenarios: Results of a case study

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ABSTRACT

The exploration and evaluation of strategies for decarbonizing the energy system is the subject of a series of national and international studies conducted by governmental, industrial and independent stakeholders. These studies play an important role in the energy policy debate on understanding and assessing different transformation paths of the energy system, technology options and their implications. They support strategic decisions on the type and scale of investments in the energy system under uncertain future conditions. However, in recent years the increasing complexity of these studies lead to a decreasing transparency even though their transparency and traceability is important for society, politics, research, and industry.

In this article, three energy scenarios at different regional scales are reviewed according to their compliance with our pre-defined criteria of transparency. They are analysed in detail with regard to their objectives, methods, data used, results obtained and traceability. Our comparison shows that the results are often presented sufficiently in order to inform decision makers. However, the underlying model-based methods lack information on data exchange between the models, the transparent description of model couplings and a discussion on the rationality of method selection and the strengths and weaknesses of the applied approaches. Based on our findings, we present some general advice for energy scenario developers on how to ensure transparency and traceability in future energy scenario studies.

1. Introduction

During the last decades, the complexity of energy system modelling and scenario studies regarding the energy transition increased significantly. While most scenario studies during the 1990's and in the beginning of the 2000s used bottom-up models on a national and annual scale and focused on the potentials and fundamental role of renewable energy sources (RES; e.g. the analysis of the German energy system in Ref. [1]), current scenario studies are more international and on a higher level with respect to the technological, temporal, as well as regional detail. Furthermore, they also consider interactions between the power, heat/gas, and transport sectors (sector coupling) by applying several interlinked, sophisticated models to derive further insights into the grid constraints, storage demand, or environmental implications. Using these complex approaches, scenarios provide important insights into techno-economic, societal, and political options for energy system transformation and their various impacts. Therefore, they are often used to guide and influence decision makers and to motivate or justify policy interventions and developments. Energy scenarios have received much attention by the media, public, and politicians [2–4]. Ideally, published information originates from scenario studies that focus on a broad range of possible conditions and available options and provide transparent and robust results and conclusions. Such studies must have a holistic view and integrate substantial state-of-the-art background knowledge such as information about current policies, sectoral and technological development, potentials and constraints of future market developments, or ecologic and economic effects of certain pathways [5]. Furthermore, accurate and reliable

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Abbreviations: CPS, Climate Protection Scenario 2050; ERS, EU Reference Scenario; REF, reference scenario; WEO, World Energy Outlook; EMS, Existing Measures Scenario; CP, Current Policies Scenario; NP, New Policies Scenario; CS 80, Climate Protection Scenario with 80% GHG reduction; CS 95, Climate Protection Scenario with 95% GHG reduction; EEG, Renewable Energy Sources Act; WEM, World Energy Model; EU-ETS, European Union Emissions Trading System; ESD, Effort Sharing Decision; PRIMES, Price-Induced Market Equilibrium System; EUMENA, Europe, Middle East and North Africa; NP, not provided; LRMC, long-run marginal costs; ESMs, energy system models; LULUCF, land use, land use change and forestry

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energy data are necessary to generate plausible and comparable results.

In the scientific, political, and industrial context, scenario data are used as an orientation framework or even for model parametrisation in scientific analyses of economic, ecologic, or societal drivers and impacts. Advanced energy system modelling approaches consider a multitude of interrelations between energy demand and supply options and involve a variety of assumptions to represent those in models. Therefore, model-based scenario building often leads to results that are not fully transparent and understandable for scientists, stakeholders, and other interested individuals. This lack of transparency can give rise to the assumption of deliberate manipulation of the future of energy supply. For example, scientists frequently find traces of a systematic bias, such as the conservative predilection by the World Energy Outlook (WEO) of the International Energy Agency (IEA), based on which the role of fossil fuels is substantiated and the dynamics of the RES progress are repressed, which seems to be consistent with the interests of IEA member countries [6,28].

In addition, the use of complex models or even model coupling is associated with a large number of uncertain and influencing assumptions regarding their parametrisation such that their overall quality and consistency are unclear [7,34,35]. To grasp the complexity of models with regard to the applicability of various modelling techniques, Börjeson et al. [8,9] presented classifications of energy system models (ESMs) and scenario clustering according to aspects such as planning tasks (e.g. international or national policy advice, sector-specific analyses) and model types (e.g. top-down and bottom-up models). However, Sullivan et al. [10] and Nursimulu [11] emphasised that a complete understanding of scenario analysis and its results can only be achieved through the greatest possible transparency and comprehensibility of the applied data and models despite the classification of the models. One recent study by Cao et al. [29] provided modelers with a fully operational transparency checklist focusing on scenario studies that examine energy systems. Hülk et al. [12] already applied this transparency checklist methodology to evaluate the degree of transparency of their own modelling work. In addition to many other researchers (e.g. Refs. [36,38]), they derived the idea of an open source and open data community from the political desire for more public transparency and comprehensibility of scenario studies. The systematic literature review and qualitative evaluation by Wiese et al. [30] revealed that the main challenges regarding open energy modelling frameworks are the complexity, scientific standards, utilisation, interdisciplinary modelling, and uncertainty. A high scientific standard of the models as tool for scenario building does not guarantee that robust statements are made. Instead, the approaches must be comprehensively evaluated, from the narratives and assumptions, data sources, and model approaches to the data evaluations and derivation of conclusions.

The extent to which scenario analyses can be evaluated based on published scenario studies is the subject of this article. In the following analysis, we systematically examine three exemplary scenario studies that result from the application of complex models and the use, exchange, and generation of a wide variety of data regarding their transparency and comprehensibility. The studies are systematically described according to various criteria suitable for model and scenario evaluation presented in the scientific literature. The points raised are essential for the understanding of scenario analyses and should be comprehensively addressed and presented in future scenario studies. This article has the following structure. We describe our methods in Chapter 2 and provide and discuss our results by comparing the most important assumptions and applied models in Chapter 3. The implications and recommendations for scenario developers and our final conclusions are provided in Chapters 4 and 5, respectively.

2. Methodology and concept

We focus our analysis on the Climate Protection Scenario 2050 (CPS) [23] for Germany, European Union (EU) Reference Scenario (ERS) [13] for Europe, and World Energy Outlook (WEO) [21] for the world and its modelled regions. All three scenario studies represent important and current quantitative bases for guidance regarding energy politics as well as investment decisions of businesses and discussions in the society. These studies are currently the most relevant published scenarios for the corresponding geographical areas, which were developed using advanced modelling approaches. The overlapping geographical scopes of the three selected studies make it possible to compare the model-based scenario results. However, because this analysis is limited to the three scenarios, which each have a different geographical focus, the statements made in this article cannot be generalised but are intended to demonstrate how modelers can assess the presentation of their work. In addition, we advise interested individuals on how they can evaluate the studies presented to them in terms of the transparency criteria and traceability. Furthermore, the selection of a limited number of studies and the documentation of the results in a comprehensive table enable the reader to follow the points criticised here for each of the reports. This would not be possible if many scenario studies would be included, because of the high documentation effort, and is beyond the scope of this case study.

Each of the selected scenarios is conducted at a different regional level: 1) at the national level: the CPS for the energy transition in Germany, 2) at the supranational level: the ERS for the energy future in Europe, and 3) at the global level: the WEO for long-term scenarios according to different world regions. We outline their differences with a special focus on the traceability of the model approaches and model linkages and the ability to understand and access input and output data.

Table 1
Sources included in this assessment.

Scenario study	Information gathered	Source	Comments
ERS ‘16	Main study	[13]	The main study report only provides results in the main text and supplementary sheets. Study-specific supplementary model documents are available online. However, additional efforts are needed to interpret the model input and output and model linkages related to the supported scenario analysis.
	Supplementary, on the energy system	[14]	
	Supplementary, on transport	[15]	
	Supplementary, on biomass	[16]	
	Supplementary, on the air pollution and climate change simulation tool	[17]	
	Supplementary, on the computable general equilibrium model used for value-added projections by branch of activity	[18]	
	Supplementary, on the global forest model	[19]	
	Supplementary, on agricultural activity projections	[20]	
IEA WEO ‘16	Main study	[21]	The main study includes the objective and results, while the supplementary information contains the description of the model and data sources.
	Supplementary, on the methodological description	[22]	
CPS ‘15	Main study	[23]	The main study provides the results and background information about the models and the model linkages. There are no further study-specific supplements.

Table 2
List of the analysed categories for each of the three studies.

Category	Analysis points, collected for each study
Scope & purpose of the analysis	Indication of authors and institutions Aim and funding of the study Indication of geographical scope Indication of time horizon Scenario names and aims (normative/explorative?) Storyline behind the scenarios Assumptions about socioeconomic development
Data	Main empirical data sources used (e.g. economic data, price data) Data requirements (e.g. level of aggregation on the demand side, temporal resolution, spatial resolution) Input and output data access Main neglected relevant aspects and significant implicit assumptions
Applied methods & models	Applied models and purpose (e.g. forecast or impact analysis of policies) Model structure (internal and external assumptions of the model) Analytical approach and methodology (e.g. top-down/ bottom-up; optimisation, simulation, accounting, economic equilibrium, game-theoretic or agent-based) How can these models consider the future energy system (decentral, flexible, new technologies)? Technological resolution on the supply side Model validation Uncertainty treatment in the model and reporting Model documentation
Further aspects	Other relevant exogenous assumptions Inconsistencies in the approach Inconsistencies of the input data

We only use publicly available information such as the main study and study-related supplementary documents because we require study authors to present the data and models in a form that is comprehensible to the reader within the study itself (see Table 1 for used documents). Therefore, the analysis of cited secondary literature (such as peer-reviewed papers as well as grey literature) is beyond the scope of this study.

Our analysis contains the following main methodological steps:

1. We define a suitable list of categories and indicators for the study evaluation based on the literature and our own consideration from modeler and user perspectives.
2. We gather and describe data relevant for the three selected scenario studies in a systematic and comparative way.
3. We identify the main differences of the scenarios regarding defined transparency indicators.
4. We evaluate how far the applied models and further assumptions of the scenario analysis are traceable, if input and output data are understandable and reliable, and if relevant information is accessible.

Table 2 shows the selection of the categories used as evaluation criteria, which is mainly based on [29]. The main categories are basic information about the study (‘Scope & purpose of analysis’), specification of data used and generated (‘Quantitative assumptions & results’), information on the analytical approach (‘Applied methods & models’), and other issues such as implicit assumptions and inconsistencies (‘Further aspects’). We partly modify the evaluation criteria and adjust them to our purpose to understand and compare the scenario building of the studies. While Cao et al. [29] take the perspective of the modeler and formulate a systematic manual for transparent documentation, we also look for information that allows the greatest possible understanding of the work that was carried out, the data used, and the results obtained. Hence, in addition to the checklist from Cao et al. [29], we use the model classification method from Van Beeck et al. [24] and our own considerations to define a list of categories that is well suited to analyse the studies from an external perspective. This first step in our analysis was necessary to adapt the categories to the information available from scenario reports and documentation.

Detailed results of the systematic and comparative analysis for all three studies are provided in the Supplementary material. The comparison is presented in a structured table including a description of the data structures, the analytical approach, methods used, and comments on how the studies cope with our evaluation criteria. The main aspects according to the four evaluation categories are further discussed in Chapter 3. In addition, we provide a concise graphical overview (Fig. 2) that shows the typical structure of scenario analyses including the analysed sectors and components and the underlying model types and accessibility of input–output data.

3. Scenario characterisation and discussion

In this section, we discuss the evaluation results according to the criteria defined in Table 2 (for further details regarding the results, see the tables in the Excel data sheets provided as Supplementary material). In the following sections, we will discuss the most important aspects for which we gained interesting insights.

3.1. Scope and purpose of the analysis

As indicated in Table 2, the category ‘scope and purpose of the analysis’ is measured by seven evaluation criteria. In the three studies, the background information about the authors, participating institutions, aims and funding of the studies, geographical scope, and time horizons is described in a comprehensible way. The German and European studies were each funded by governmental institutions, while the IEA and its studies are generally funded by the Organisation for Economic Co-operation and Development (OECD) member states. The aims of the studies are very similar and clearly defined: 1) to inform policy makers where current policies and policy ambitions may lead the energy sector, and 2) which policies and measures are needed to achieve specific climate targets. Naturally, the WEO addresses the global objectives of controlling global warming (in the case of <2 °C above preindustrial levels), while the other two reports deal with country- or EU-specific climate targets. The WEO also claims to be carrying out a first comprehensive study of the new era launched by the Paris Agreement. The German study is carried out until 2050, while the WEO analyses the transformation paths until 2040. Among the seven scenarios in the ERS, only the reference scenario (REF) has a time horizon until 2050, while all other six policy scenarios only cover the period until 2030. This makes it difficult to allow for a comprehensive assessment of different long-term measures and impacts of possible strategies in line with specific global objectives (e.g. the <2 °C target). The CPS and WEO explicitly examine explorative scenarios, whereby the Existing Measures Scenario (EMS) for Germany corresponds to the current policies scenario (CP) of the worldwide analysis. For both scenarios, it is assumed that the current legislation will be continued and that no new legislative proposals or efforts will enter into force or will be implemented. In the New Policies Scenario (NP) of the WEO, the implementation of the political announcements and plans up to 2040 is assumed (current goals, targets, and intentions such as available nationally determined contributions for the Paris Agreement). The WEO also analyses a normative scenario based on which the 2 °C target would be met. The normative goal of avoiding global climate change is implemented in the CPS and ERS in two (CS 80, CS 95) and six scenarios (EUCO27, EUCO30, EUCO + 33, EUCO + 35, EUCO + 40, and EUCO3030), respectively, using greenhouse gas reduction targets, efficiency measures, and share of RES in the gross final energy consumption or other specific targets for RES deployment in the power, heat, and transport sectors. The main quantitative drivers, their differences, and the composition of the primary energy demand as well as

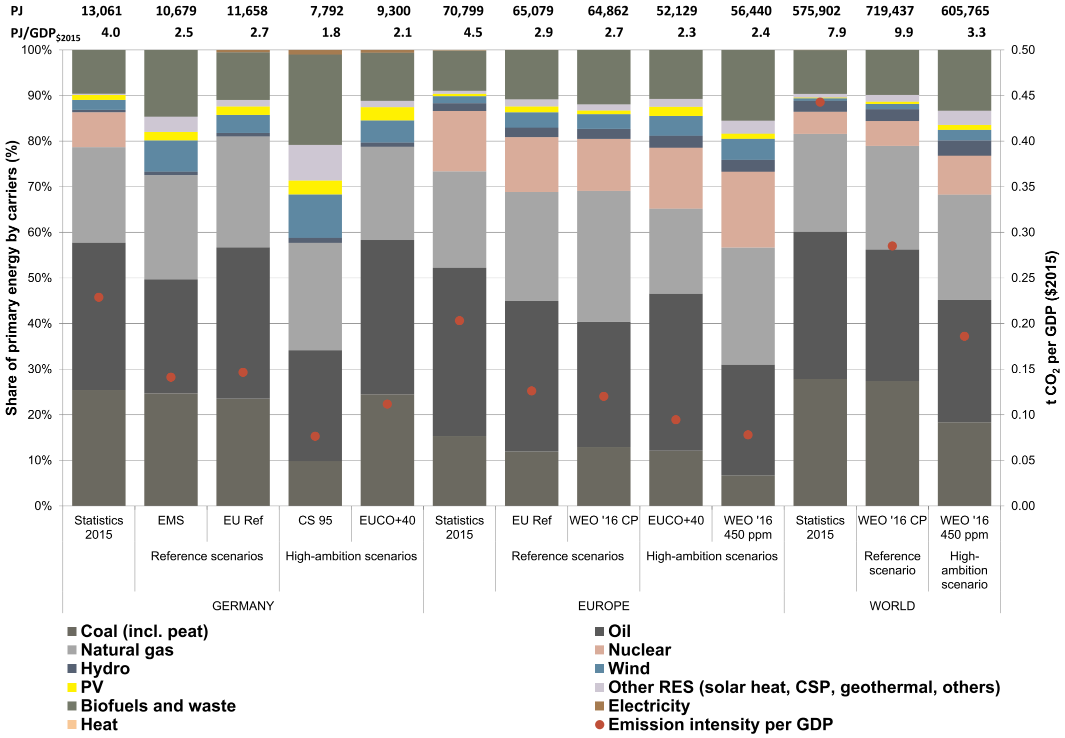

Fig. 1. Primary energy demand by energy type and energy-related CO_2 intensity in the reviewed energy scenario studies for the year 2030 differentiated by baseline scenarios and most ambitious scenarios for Germany, Europe, and the world. For the ERS and CPS, the category 'Solar' in the datasheets of the power generation is assumed to be only photovoltaic (PV) generation due to the lack of information.

the CO_2 intensity per Gross Domestic Product (GDP) in the different studies are described in the next section.

3.2. Results and traceability of the main assumptions

In general, assumptions and/or modelling results on region-specific population development and economic growth coupled with assumptions and/or modelling results on efficiency improvements represent the main drivers of the demand development in scenario analysis and may have a great influence on the supply structure and potential depth of sector coupling. Thus, in this section we focus on the main quantifiable assumptions and characteristics of the three studies, such as economic and population trends, energy demand, differences in electricity generation (i.e. share of RES, fossil fuels, nuclear power, and biomass), technological development, fuel and CO_2 prices and point to transparencies regarding these assumptions, which would require more comprehensive clarification in the scenario studies to be understandable to the reader.

3.2.1. Key differences of the scenario results

To understand the degree of ambition of the scenarios and to identify the most important energy sources and technologies, we present the structure of the primary energy supply and CO_2 emissions per GDP in 2030 (Fig. 1). The overlapping geographical analysis frameworks of the studies allow for a comparison of the CPS and ERS for Germany and the ERS and WEO for the EU28 scenario. The selection of the year 2030 is due to the limited analysis horizon of the ERS scenarios. Thus, the figure indicates the mid-term transformation perspectives of different scenarios. For each overlapping geographical area, we present the reference and most ambitious scenarios in terms of emission reduction and additionally compare the values (also for the world average in the WEO) with the 2015 statistics from Ref. [25].

The comparison shows that the studies significantly differ in the reference and most ambitious scenarios regarding their primary energy supply structures and CO_2 efficiencies per GDP. When comparing the CPS and ERS scenarios for Germany, the latter study shows fundamentally lower renewable shares. However, the ERS REF and all scenarios for Germany derived in the European study do not consider the target of the German Energy Concept 2010/2011 (Renewable Energy Sources Act, EEG) to achieve a share of renewable energies in the total primary energy demand of 30% by 2030 and 60% by 2050. It remains unclear whether the German national goal was deliberately not considered or ignored. A comparison of the EU28 scenarios based on the ERS and WEO shows a higher use of natural gas in the reference scenario of the global study. With respect to the ambitious scenarios, the WEO shows a higher use of renewable energy, especially biomass, but also nuclear power.

3.2.2. GDP and population development

All studies assume the same population development and GDP growth in their reference and transformation scenarios. For Germany, the CPS and ERS expect a GDP growth of 50.5% and 61.5%, respectively, with population expectations ranging from −10.0% and −9.3% from 2015 to 2050. The ERS and WEO expect the GDP for the EU28 scenario to increase by 65.4% and 71.2%, respectively, between 2015 and 2040. The population of the EU28 is assumed to slightly grow by 2.5% (ERS) and 0.6% (WEO) from 2015 to 2040. The WEO estimates a global GDP and population growth of ~150% and ~25%, respectively, between 2015 and 2040. The main reasons for the high global GDP growth compared with the EU28 are the assumed strong developments in Asia, the Middle East, and Africa. The latter two countries also have the highest population growth rates. The analysis and comparison of the key quantitative assumptions and drivers (GDP and population) for scenario analysis suggests that no disruptive assumptions were made and that the differences between the studies are small. The assumptions behind these two drivers are provided to the reader in a clear and understandable way.

3.2.3. Differences in the electricity generation with a focus on the roles of carbon capture and storage and nuclear energy

The future electricity demand per GDP for the same regions differs in the individual scenarios (depending on the degree of ambition) of the studies as well as between the studies themselves. This is mainly due to different (regionally specific) assumptions about energy efficiency policy, efficiency development and electrification rates in the sectors heat, transport and industry in the scenario studies (and respective scenarios). It is noticeable that only the EUCO + 40 and EUCO3030 scenarios for Germany are in line with the 50% target (share of electricity produced from renewable energy sources in the gross electricity consumption) set by the German Energy Concept. However, it remains unclear why the target is violated in the other scenarios of the ERS.

Regarding the role of the much-discussed carbon capture and storage (CCS) technology in the CPS, it would only be used in the CS 95 scenario for industry and biomass combustion starting in 2030. The capture rate is assumed to be far below 50 Mt CO_2/yr in all scenario years of the CS 95 (~6% of the German CO_2 emissions in 2015). Based on the ERS, fossil fuel combustion with CCS would be implemented in the EU28 in 2020 but not in Germany. The installed capacity equipped with CCS for the energy conversion of solid fossil fuels would reach up to 17 GW (66% of the solid fuel based generation and ~3.4% of the total generation capacity) by 2050 for the EU28. In contrast to the targets for renewable energies with respect to electricity generation, the ERS study is corresponds to the current legislation in Germany but does not justify the assumed installation rates of CCS technology in Europe. In the WEO 450 ppm scenario, CCS would start to play a relevant role in 2025 because 4% of the global power plants are equipped with CCS technology and 60% of them are coal-fired. In the 450 ppm scenario, the share of coal power plants would only account for 7% of the total installed capacity in 2040, while 70% of them would be fitted with CCS technology (260 GW, mostly in China and the United States) globally. The possible effects associated with CCS, such as large CO_2 leakages and social barriers (see e.g. Wennersten et al. [26] for the characterisation of the various types of risks), are quantitatively included in the ERS via risk premiums (i.e. the technology becomes more expensive). The CPS qualitatively refers to the risk of CO_2 leakages, while the WEO only refers to the intensive water use of the technology and assumes that it can be installed in regions in which the technology is politically accepted.

Nuclear power would start to phase out in Germany in 2025, while the share of nuclear power in the installed power capacity would reach 7% by 2050 in the EU28. In the WEO, a renaissance of nuclear energy occurs in all scenarios with shares of 9% (CP), 12% (NP), and 18% (450 ppm) in the global power generation, while fluctuating RES only play a minor role. Thus, the WEO assumes that nuclear energy will play an increasingly important role and will be socially accepted by the public in the future. This seems to be highly questionable regarding recent acceptance surveys about nuclear power (see e.g. Siegrist and Visschers [27]). The ERS and WEO deal with nuclear power in similar ways to CCS technology (risk premiums in the ERS, qualitative discussion of water consumption, as well as installation where politically accepted in the WEO).

3.2.4. Development of fuel and CO_2 prices

The fuel prices are subject to a high degree of uncertainty due to the availability of resources, demand projections, and global climate policies. In the CPS, no differentiation is made among the scenarios and the prices increase between 2015 and 2050. The ERS also does not differentiate between scenarios and EU28 countries. In contrast to the former two studies, the prices of natural gas and steam coal are differentiated in the WEO by regions and scenarios for the main import regions or countries. The prices of crude oil are only differentiated by scenarios because of the existence of a global market. The 450 ppm scenario has the lowest expectations with respect to the growth of future fossil fuel prices, followed by the NP and CP scenarios. Thus, it can be stated that only the WEO incorporates the interdependencies between fossil raw material prices and scenarios. This may be justified based on the fact that the pure price taker approach does not apply to a global analysis (e.g. an analysis for Germany in the CPS). On the other hand, at least for Europe, it could be expected that the scenarios aimed at a high CO_2 reduction will have an influence on global market prices (see e.g. Zhang and Sun [50]). Such interactions or uncertainty analyses based on sensitivity estimates are not considered in the CPS or ERS and might substantially influence the results (e.g. the choice between hydrogen and fossil fuels in industrial processes and potentially induced necessary reduction measures in other sectors in both normative and explorative scenarios).

Other influential policy variations among the scenarios are the scope and level of carbon pricing, which have a major impact on the relative costs of the use of different fuels. In general, surcharges on the fossil fuel prices have a strong incentive effect on emission reductions, which must be addressed when developing climate protection strategies. While the CO_2 prices are differentiated between the scenarios in the CPS and WEO (also by regions in the WEO), the carbon prices among the scenarios are not differentiated in the ERS (at least, they are not reported). The ERS scenarios only focus on the policies for efficiency improvement, GHG emission reduction, and RES share increase without discussing the influence of higher carbon prices (although the Price-Induced Market Equilibrium System, PRIMES, simulates emission reductions in the European Union Emissions Trading System, EU-ETS, sectors as a response to current and future EU-ETS prices). Even in the most ambitious EUCO + 40 scenario, the energy-related CO_2 emissions in 2030 (2132 t) do not nearly match those of the WEO 450 ppm scenario (1844 t), which targets a global temperature increase of $< 2\,^{\circ}C$. Thus scenarios that only have a short-to medium-term perspective, such as the ERS, carry the risk that they will not be consistent with the global long-term climate goals or will discard the potentially higher regional transition costs after 2030.

3.2.5. Technological development and the role of disruptive technologies

The CPS deals with the penetration of new and more efficient technologies in sectors on the demand side (buildings, households, industry, tertiary sector, and transport). The documentation of the assumed technological progress and the consideration of new technologies in the individual models used in the CPS widely vary but do not allow for a comprehensive technology description. In the transformation sector (heat and power generation), new technologies that are currently not mature enough for the market are not included in the study. Learning curves are provided as input to all models of the transformation sector, but no further information on decreasing costs and/or increasing efficiencies is given. It can therefore only be assumed that potential efficiency gains and decreasing technology prices are included as assumptions in all models, but no feedback loops regarding the installation rates and cost effects are incorporated in the analysis. However, this limitation seems to be acceptable for a study focusing on Germany because the influence on the market prices of globally traded energy generation technologies (e.g. PV) may be marginal. Feedback loops are more important for technologies that are subject to high local value creation such as wind turbines. In addition to techno-economic aspects, the choice of technologies seems to be essentially driven by the normative policy objectives of the study. The ERS more explicitly describes the penetration and choice of new technologies considered in the PRIMES model. In contrast to the CPS, the ERS REF also provides the levelised cost of electricity (LCOE) development of the power generation both of RES and non-RES technologies until 2050 and learning curves for demand-side technologies, which reflect the decreasing costs and increasing performances as a function of the cumulative production. The EUCO policy scenarios follow more stringent ecodesign standards, but different cost assumptions for technologies are not well documented. Technology learning curves are scenario-specific in most of the applied models in the ERS but only documented for the

REF scenario. Similarly, the process of learning and cost reduction for the WEO scenarios is fully incorporated in the World Energy Model (WEM), both on the demand and supply sides, and applies to technologies in use today and those approaching commercialisation. The 450 ppm scenario assumes a higher cost reduction than the NP and CP scenarios because it is assumed that the more a technology is used, the faster is the cost reduction. This is also differentiated by country/region.

In conclusion, it can be argued that the influence of the scenario specific expansion of technologies on the techno-economic parameters is not explicitly modelled (technology price as a function of deployment) in the three studies but is taken into account in the scenarios via exogenous, scenario-specific assumptions in the ERS and WEO. In contrast, the same technology cost parameters are assumed in all scenarios of the CPS. The implications of such assumptions should be better highlighted in future studies because they may have a significant impact on the development (especially in cost optimisation models) of technology portfolios and the resulting policy advice.

3.3. Applied methods and models

In the following sections, the core methodological aspects of the three scenario studies are compared using the table provided in the Supplementary material in combination with specific findings about the applied models and the transparency of the provided input and output data. All three studies follow an advanced scenario building approach but differ in many aspects. However, it remains difficult to assess the methodological robustness of the three studies because of the limited transparency regarding the applied models and model coupling and associated input–output data.

3.3.1. Analytical approach and methodology

We systematically characterise the traceability of the studies and their analytical approaches with respect to framework assumptions, resource supply, fuel processing and supply, energy conversion, network and flexibility options, end-use sectors, and emissions and pollutants. Using this representation of model-based scenario analysis, we graphically capture the main components regarding the applied methodology (e.g. top-down or bottom-up approaches) and the transparency and presentation of the input and output data (input data: database, statistics, or literature; output data: results of general calculations/data processing of the applied models). To represent the complexity of the scenario studies in a well-structured figure, we define several acronyms with clear rules for the classification of the model parts:

Assessment methods

- We mark aspects of the studies as not available (**N/A**) if the study mentions certain components of the modelling framework and considers them in the analysis; based on this, the modelling/underlying assumptions of the analysis are insufficiently described (e.g. only mentions them qualitatively).
- We mark modules of the study as available (**A**) when the input data are directly used without significant processing.
- We mark data/results that come from internal model-based assessments (**M**). A component not included in a study (e.g. due to the different scope of a study) is marked with '/'.

Data

- We highlight the naming of the source for the individually used input data (**I**); otherwise, we define it to be not provided (**NP**). This also holds true for data exchanges in model coupling (see Fig. 2).
- The clear naming and representation of output data/processed data are marked as well illustrated output (**O**); otherwise, we define it to be **NP** (see Fig. 2).

Note that the resulting figure does not describe internal model links (e.g. between different models in studies with model coupling).

Fig. 3 presents our evaluation results in a condensed format (more information regarding technological resolutions and model structures can be found in the Supplementary material). The following sections provide an in-depth discussion of significant methodological aspects of the scenario construction in the three studies.

3.3.2. Applied models and purpose

A critical aspect regarding scenario transparency is the documentation of methods and models applied for the scenario studies. The CPS describes the models shortly, without citing further literature for more detailed information, while the ERS and WEO include comprehensive model reports and documentation online, for example, for the PRIMES and WEM models, respectively (see Table 1).

General framework assumptions, such as normative objectives, are usually not based on model results but are derived from other studies and official policy objectives or are defined within the consortium. Quantitative scenario drivers, such as fuel prices and macroeconomic and demographic development, are either determined by assumptions or model-based calculations. The development of fuel prices in the CPS is taken from other studies, while it is calculated using models in the ERS and WEO. The ERS study uses a global partial equilibrium ESM that endogenously derives consistent price trajectories for oil, natural gas, and coal based on the evolution of the global energy demand, resources and reserves, extraction costs, and bilateral trade between regions. The WEO uses a top-down economic equilibrium approach to calculate the output of coal, gas, and oil that is stimulated under the given price trajectory. Feedback loops between the demand and supply take place until the equilibrium is attained. In the CPS and ERS, macroeconomic data (sectoral developments aggregated to the GDP) are derived based on top-down equilibrium models, while the WEO uses assumptions for the GDP development based on forecasts from International Monetary Fund (IMF), World Bank, and IEA databases and analyses. In addition, the demographic development in the CPS study is calculated by a top-down model with input–output tables at its core. However, the study does not explain how this model is used to calculate demographic trends. In contrast, the ERS and WEO use assumptions derived from secondary literature for this scenario driver. In general, the use of models to quantify the scenario drivers within the consortium may enable potential model interactions between the scenario analysis framework and price sensitive models, which in principle can improve the internal consistency (e.g. by considering to which extent the results of macroeconomic models are affected by the level of energy demand, implemented technologies, or electricity prices of the individual transformation paths). However, this does not seem to be considered in any of the studies of the macroeconomic and demographic developments (the CPS only carries out an ex-post assessment of the scenarios regarding these variables). An exception regarding the commodity prices is the WEO, which assumes scenario-dependent price paths.

Electricity as a resource in an imported form is only relevant for analyses of limited geographical areas (as it is only the case in the CPS). In the CPS, these are calculated using an additional supranational bottom-up optimisation model for Europe, the Middle East, and North Africa (EUMENA). The ERS applies bottom-up optimisation models to study the internal electricity market of the EU (no electricity exchange with countries/regions outside the EU28), while the power generation module in the WEO ensures that enough electricity is generated to meet the annual demand volume in each region (thus, no electricity exchange is considered for each modelled region). While the fossil fuel mining and import are not modelled in the CPS (Germany as a price taker), the ERS uses a gas supply module, which calculates the gas import by country of origin, transport means (liquefied natural gas (LNG) or pipeline), and route as well as the wholesale gas prices for the EU member states. However, the WEO contains detailed modules for oil and gas to project the levels of production and trade and a module for

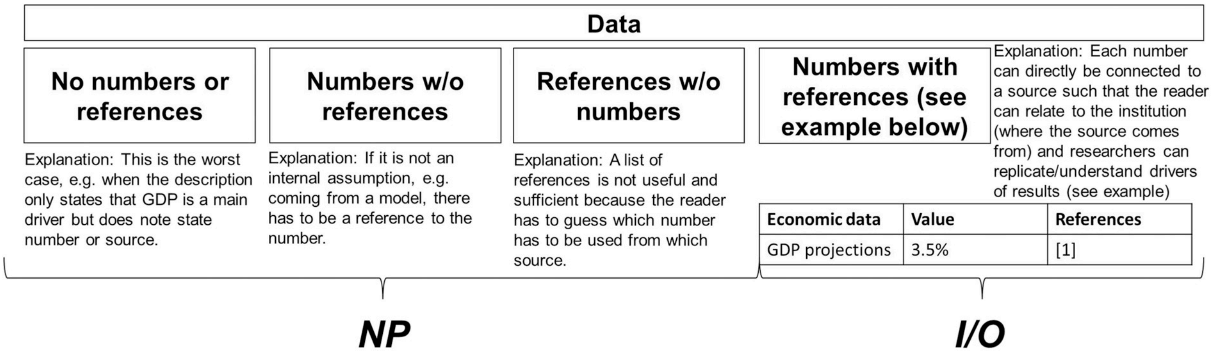

Fig. 2. Background information on the figure: rules for the sufficient description of input and output data.

coal to assess the remaining recoverable resources in the modelled regions. Renewable energy potentials for wind and PV plants are calculated bottom-up in the CPS using a geographical information system (GIS). However, these renewable potentials with the corresponding feed-in profiles only appear to be taken into account in the supranational model for electricity import and export modelling. In the ERS, the renewable potentials are based on various sources, while the WEO has a submodule for RES to calculate dynamic cost-potential curves including technological learning for electricity supply from RES (such as bioenergy; hydropower; PV; concentrated solar power, CSP; geothermal electricity; wind; and marine energy). The use of energy crops and agricultural residues is not modelled in the CPS and ERS but is based on various other sources and databases providing constraints on potentials and certain sectoral allocation methods (e.g. by defining market shares). In contrast, the WEO uses a bioenergy supply module which enables the calculation of the biomass feedstock supply by region. Therefore, the modelling of fossil primary energy carriers is only conducted if, for example, the individual regions also have a potential influence on the global demand and prices. The smaller the geographical area is, the smaller is the potential effect on the world market and the more likely it is to use assumptions from global projections. On the other hand, the higher the regional resolution of the models is, the higher are the potential exchange of electricity between regions and the associated need to model these energy flows.

The fuel processing and supply and refineries and other conversion plants (e.g. biofuel production, other refining plants) are modelled independently in the power generation sector on an annual basis in the CPS. However, the modelling approach lacks a detailed description and cannot be compared with approaches applied in other studies. In the ERS, an oil supply model is used to project the domestic components of the petroleum prices, refining activities, and refinery capacity expansion. The biomass and biogas provision are not based on a model in the CPS but derived from the potential of energy crops and agricultural residues. In the ERS, a biomass model is used to transform the biomass feedstock (primary energy) into bioenergy commodities (secondary or final form) used as input for the energy system (e.g. for power plants, heating boilers, or as fuel for transportation). In the WEO, a bioenergy supply module is included to assess the ability of the WEO regions to meet their demand of bioenergy for power generation and biofuels with domestic resources. It also enables the international trade of solid biomass and biofuels between world regions. Such modelling of the international trade of biomass and biofuels is not considered in the CPS and ERS.

The hydrogen production and other process chains (such as methanation) are modelled in the CPS using the pure increase in the electricity demand, whereas a hydrogen supply submodel is used in the ERS to incorporate many technologies for the hydrogen production, storage, distribution, and end use. The inclusion of infrastructure costs in the large-scale use of hydrogen (or derivatives) in the transport, industry, and power generation sectors can significantly influence the model results. In the WEO, the production of hydrogen is not specifically considered and modelled.

Regarding the energy conversion, flexibility, and infrastructure, a model group of three models is used in the CPS; one is used for the import and export modelling of electricity between Germany and the EUMENA region in which the potential expansions of the grid transfer capacity and energy storage are also considered. The expansion and operation of power plants and the flexibility in Germany are separately modelled; one model simulates the expansion of the power plants and another model optimises the economic dispatch in hourly resolution (including combined heat and power (CHP) plants), whereby the flexibility options (such as flexible hydrogen production and storage systems) are also mapped (the capacities are exogenously given). However, the grid infrastructure of Germany is not modelled (Germany is modelled as a ‘copper plate’). The ERS uses a bottom-up optimisation of the energy supply that simulates the energy market equilibrium in the EU and each of its member states in five-year steps with a sectorial optimisation for the heat and power sectors. The model calculates the infrastructural needs in terms of electricity transmission and distribution grids, heat/steam distribution grids, and energy storage systems including hydrogen generation. The power and steam/heat markets are simultaneously simulated to capture trade-offs between cogeneration/CHP and condensing power plants and between the self-production and distribution of steam/heat. The transmission grid is modelled as entire system of interconnectors in Europe and as Alternating Current (AC) and Direct Current (DC) line extension including optional remote connections with offshore wind power in the North Sea and with North Africa and the Middle East. Highly distributed generation at consumer premises is also included and is considered when calculating the transmission/distribution losses and costs. The WEM uses a combined approach whose principle is very similar to that used in the CPS. The type of new generating capacity to meet the demand is calculated with a simulation model, which uses the regional long-run marginal costs (LRMCs) as a decision variable for investments in conventional (including CHP) and renewable power plants. Investments into the transmission grid are a function of the demand increase and additional transmission network costs are derived from specific renewable grid integration costs. An hourly bottom-up dispatch (no expansion) model provides further insights into the operation of power systems with high shares of fluctuating RES. The analytical approach considers the need for storage and demand-side management (DSM) measures but excludes the expansion of power grids within the regions. Mini- and off-grid power systems are also integrated into the WEM model by choosing available technologies based on their regional long-run marginal costs.

It can be inferred that the electricity transmission grids and energy storage systems are all modelled in the studies as methodological extension of scenario analysis. However, the modelling of the electricity grid and the generation of results and analytical statements clearly differ. While the CPS does not model the grid congestion and related costs within Germany, the costs for grids are integrated in the WEO

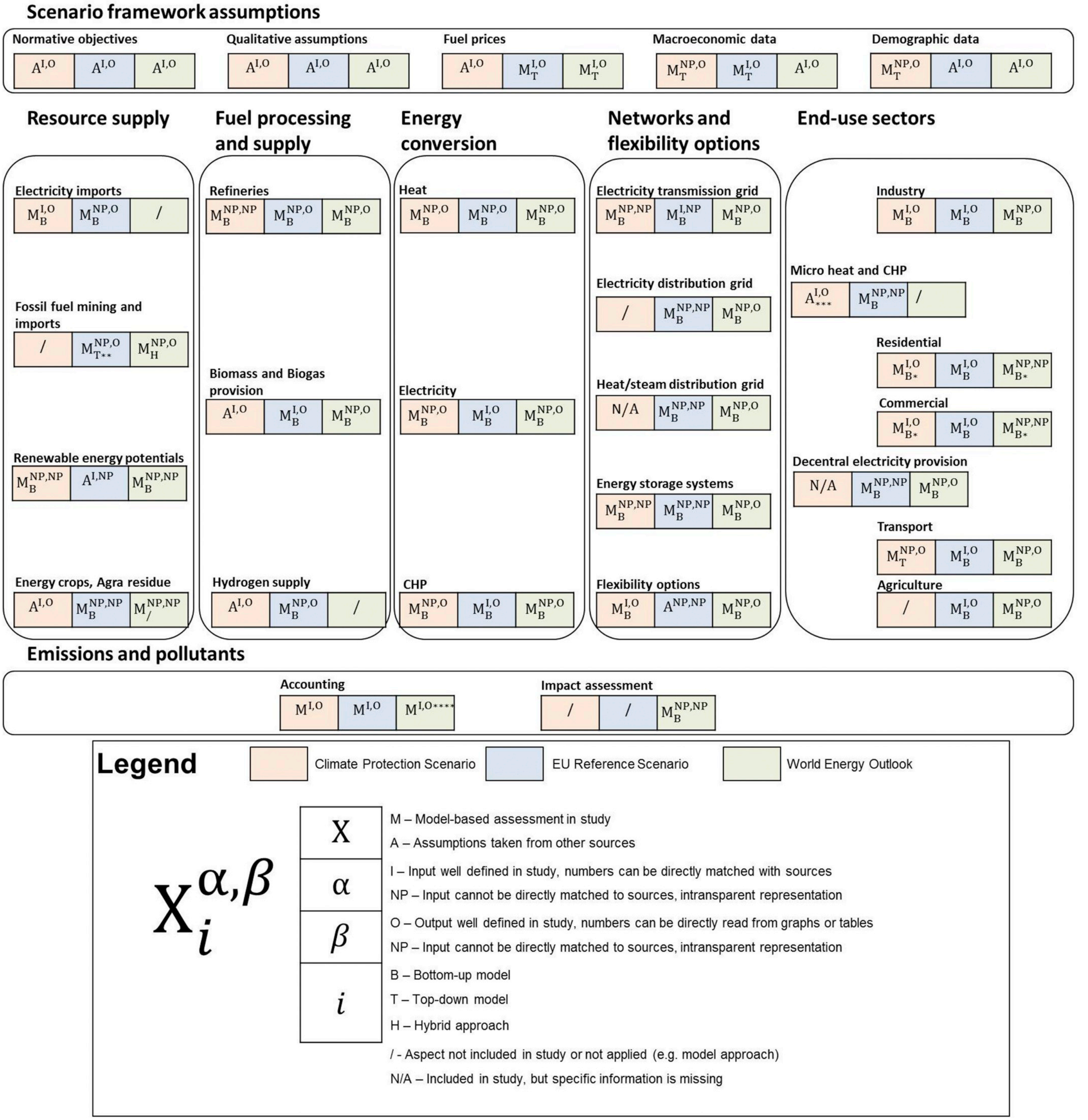

Fig. 3. Graphical representation of the traceability assessment for the three scenarios. Indication of the consideration of partial aspects: *Aggregated as building sector, **Gas sector only, ***Provided for heat pumps only, and ****CO_2 emissions only.

using a heuristic approach. In addition, there is no cost-optimal network expansion. On the other hand, the grid expansion of the network infrastructure between the individual countries is cost-optimal in the ERS. However, all three studies lack an in-depth analysis of the security of the supply under transformation scenario conditions (e.g. under extreme weather conditions).

3.3.3. Model coupling and model structures

All study reports provide graphical overviews of the involved models/modules, general interplay, and assignment to partial components of the energy system. However, note that such a representation never fully captures the interaction between the models for the reader. In all three studies, hybrid modelling approaches are applied for specific sectors or intersectoral analysis. Examples of sector-specific model coupling are the transport models in the ERS and the three-step approach (separate capacity expansion and dispatch models) for the electricity sector in the CPS. The former combines econometric and engineering approaches to derive the transport activity by transport mode and the model interactions seem to make sense from a scientific point of view. However, the three-step approach for the electricity sector in the CPS study is conducted in such a way that the electricity import to Germany (including capacity expansion planning) is derived from one specific model including the EUMENA region, while the capacity expansion and dispatch for Germany is calculated by two other specific models. It seems very difficult to achieve consistency with such a modelling approach and comprehensible explanations are missing. Furthermore, the model coupling of different sectors, especially power–heat, power–gas, and power–transport, must be considered to deal with fluctuating RES and multi-sector electrification, especially in deep defossilisation scenarios. However, the linkage of the models in terms of the model-based input and output and external assumptions is not always clearly stated in the studies. From a scientific point of view, satisfactory reasons for the inclusion of the models are often missing.

An example of model coupling between naturally largely independent model types is the integration of macroeconomic data derived from top-down models in the calculation of driver variables such as the GDP growth or population development. However, the model linkage (e.g. soft- or hard-linked) in terms of the input and output data and the harmonisation of assumptions are mostly poorly described in the three studies and supplementary model documents. Furthermore, information about iterations among the models, which may be pivotal for the resulting policy advice, is insufficiently presented. For example, it can be assumed that the integration of modelled future electricity prices into macroeconomic modelling has a major influence on the relevant drivers of economic growth, which affects the demand for, for example, energy and transport related activities (included as ex-post assessment in the CPS). However, only the ERS provides information on model iterations. This analysis suggests that efforts to achieve consistent model coupling in terms of the data and iterations may also heavily depend on whether the models originate from one institution/group or whether the data must be exchanged between numerous institutions/groups.

3.3.4. Data requirements and input–output data access

Requirements for the model parametrisation and definition of scenario input data strongly depend on the sectoral, technical, spatial, and temporal resolution of the studies. While the analysis of the CPS is only carried out at the national level, the ERS and WEO provide energy balances for 28 EU member states and 25 world regions and countries, respectively. However, the resolution of the demand sectors of the CPS is mostly higher, for example, regarding the building sector or the consideration of industrial processes. The study only occasionally provides information on the spatial resolution of the models and to what extent regionally differentiated information is incorporated. The WEM, as a large-scale simulation model, also states to have a considerable sectoral and technological resolution, but the data requirements and input data for submodels are mostly not provided. In the cases where data information is provided, the granularity is usually not sufficiently represented to be able to derive insights into the model. The ERS also uses models, which considerably differentiate the processes on the demand and supply sides. The study mentions the resolution of the data, but the detailed use must be identified using additional model documents (see Table 1).

The listing of data sources in the text or tables that are sometimes provided for certain numeric input data (in particular in the CPS and WEO) forces the reader to search any cited source using the corresponding number or, in case of doubt, to choose between numbers with the same information content. The ERS describes the input data using developed storylines and models. Some sources explaining the input data are available, but a more detailed database must be used for model-specific documents (e.g. for the PRIMES model). In the WEO, the input data are also not fully provided. Similar to the CPS, multiple sources are often listed for a certain parameter such that readers cannot track specific data values. Furthermore, some input data stem from their own IEA database (with links provided), but further guidance on how to use the database might be necessary for the readers. In all three studies, the main results are always provided in tables or figures, which contribute to the understanding of the reader. However, the data are not available in the maximum resolution of the modelling results according to the model descriptions.

From a scientific point of view, researchers would benefit from scenario reports for future research if the input–output data of the studies would be clearly presented. This especially holds true for the level of data aggregation and the temporal and spatial resolution of the data, which are often unavailable for the reader. By publishing detailed information on the input and output data (e.g. in the Supplementary material or open data platforms), scientists could be compensated for the partial lack of information about the applied models because the structure and functionality of the models can be partially derived from the details on the applied data.

3.3.5. Model validation

Model validation is generally based on the detailed discussion of the model strengths and weaknesses (e.g. parameters, variables, and formulation) and comparison of the model results with real-world data. The idea of validation is to verify if the model performance is as expected and if the models are in line with their objectives. Validation tests to check the model output can be performed internally (self-validation included in the study) and externally (feedback from other researchers). In addition, researchers can make the scenarios available to newspapers and other media (e.g. Twitter) and monitor the reactions to the articles and contributions. The reactions can then be considered in future scenarios. However, none of the three scenario studies state how the models are validated. Only limited output data were internally calibrated using similar studies. For example, the ERS validates the forest harvest removals by calibrating them using the most recent Food and Agriculture Organisation Corporate Statistical Database (FAOSTAT) data from 2015. Furthermore, the economic and transport activity projections are validated by typical indicators such as the GDP or activity per capita. External validation is often reflected by the scientific and public perception, which is outside the scope of our analysis. Although the scenarios of the three studies are used as basis for other researchers in academia and the WEO is positively cited by public media, some criticism exists. For instance Ref. [28], reviewed the methodology of the IEA WEO studies and critically assessed the key assumptions and projections. The authors argued that the IEA may introduce a conservative bias by neglecting the dynamics and interlinkage in the energy and economy nexus. In general, the authors of the three studies should have provided more reasons for making assumptions, selecting data, building and applying models, defining scenarios, and testing against real-world data. These efforts would contribute to internal validation. The public perception, as external validation, should be considered for future research.

3.3.6. Uncertainty treatment in the model and reporting

All three studies present and analyse scenario variants that show different possible developments. However, the uncertainties in the various assumptions and use of models to answer the research questions are not explicitly discussed. In addition, the presented pathways only represent a very narrow selection of possible future developments, for example, regarding the development of the economy, mobility, and society as a whole. On one hand, this is due to the defined narratives and implicit socioeconomic assumptions; on the other hand, this is based on the cost-optimizing approaches of the models in which the cost effects dominate and steer the developments. Assumptions of disruptive factors and elements and thus the possibility to check the robustness of the model results, conclusions, and derived policy recommendations are missing to a large extent. Regarding the different modelling approaches, there is a lack of documented sensitivity analyses showing the effects of variations on the model parametrisation. In general, the studies do not provide qualitative or quantitative uncertainties or explicit sensitivity analysis of individual scenarios but only contain general comments on the uncertainties mentioned in the model descriptions.

3.4. Further aspects

From a societal perspective, all studies neglect several relevant aspects and do not consider nor document significant implicit assumptions. In the case of the former, this concerns the definition of only one single path for the key economic and social drivers, as mentioned above. Significant other aspects include the lack of feedback loops from the change in the energy use and generation to the economy as well as the lack of consideration of possible disruptive developments. Only the CPS carries out an ex-post assessment of the change in the GDP and employment between the EMS and CS 80 scenarios.

In the case of implicit assumptions, this concerns the assessment of the relevance of social factors and risks or the development of technologies and their market implementation as well as required investment incentives for relevant participants. Assumptions or prerequisites regarding the development of political framework conditions are also insufficiently discussed and not integrated into the scenario context, for example, regarding the stronger national, European, or even global integration of the energy policy or possible effects of increasing isolation and confrontation on foreign policies. These aspects may lead to inconsistencies in the methodologies and input data. Regarding the development of technologies and their costs, the studies largely avoid speculative assumptions. As far as the considered technological innovations are documented and traceable, they represent today's achievable state of the art. However, rather speculative assumptions include, for example, assumptions about the future consumption by the population, renaissance of nuclear power, or possible impact of political measures.

The publication of the studies in the form of final reports also clearly differs with respect to, for example, the information available to the public via press releases and events and the suitability of the publications either to inform the interested public or as basis for further scientific scenario analyses. All studies lack parallel scientifically relevant publications in peer-reviewed journals and thus scientific discussions of the scenario construction. In most cases, however, this is the case for the methods and models used. Nevertheless, all studies are used as framework scenarios for scientific studies or expert opinions and are therefore often cited by media and in academia.

4. Recommendations and implications for scenarios developers

Based on our assessment of the three scenario studies, several recommendations can be made, which extend the more theoretical transparency checklist by Cao et al. [29].

4.1. Further improvements of the model transparency

4.1.1. Provide supplementary documents with well-documented input–output data

As discussed above, the input–output data are not completely and transparently documented. One reason might be that the core problem of energy data is that they are generally strictly protected. However, a more precise description of which data are used might improve the reproducibility and transparency of the models and resulting scenarios. An option could be the publication of simulated/artificial data with the main characteristics of the original data but ‘blurred’ critical information such as business-relevant information. The validation of this artificial data is however crucial and complex. For example, Wiese et al. [30] provided a unique open power system dataset for Europe, which can be used as a reference input to ESMs to improve the comparability of their results. Hirth et al. [31] also argued for an open data access and a recent tool allows the evaluation of the quality of input data [32].

4.1.2. Explain the model linkage and data exchange

Model coupling with either the same focus on one sector or different foci across the sectors is widely applied in large-scale energy system scenario studies. Our analysis shows that the description of the model-exogenous input data and their processing and exchange are in most cases insufficient because the data integration into the models is hardly comprehensible for outsiders. This is especially true for studies with model coupling, which transfer comprehensive data volumes between the different models (e.g. the ERS and CPS). Therefore, a description of the data flow in combination with the corresponding model architecture could be helpful for the research community to fully understand the results of the study. Furthermore, the information whether the models are soft- (i.e. manual data transfer between models) or hard-linked (i.e. direct data transfer between models) improves the understanding of the complexity and error-proneness of the coupling. However, the knowledge of the model coupling approach and data exchange is not enough. Lessons-learned publications for all coupling efforts with detailed descriptions of the used approaches, data exchange within these approaches, and difficulties would be helpful for future work [33].

4.1.3. Provide full open source and well-documented model codes

All three reviewed studies do not provide open source model codes. The demand for well-documented model codes was reported by Laugs and Moll in 2012 [34,35]. In the following years, several other contributions were made. For example, Morrison [36] viewed open source models as core aspects of publicly transparent and scientifically reproducible energy system modelling. The author focused on the legal aspects of existing open access models. Pfenninger et al. [37] provided a comprehensive overview of current open source ESMs focusing on open data. The authors indicated that the current trend is overwhelming, although the energy sector seems to lag behind other computer model societies. This optimistic perspective is supported by current grassroots developments such as openmod-initiative.org. The main advances of open source codes in addition to the reproducibility and transparency are the easy comparability of the scenarios and the higher efficiency in developing highly sophisticated and broadly approved ESMs [38,39]. The hope is that the provision of source codes and data might significantly speed up the developing processes. Another positive side effect is the broader acceptability in the scientific community.

4.2. Further improvements of the scenario consistency and robustness

4.2.1. Societal context scenarios

An important weakness of most techno-economic energy scenarios is the lack of uncertainty and complexity in the social context. Several social factors that influence the development of the energy supply and demand are generally not explicitly addressed in scenario reports, for example, the cultural impacts on the acceptance of change processes or politics and state specifics with respect to the change processes and their effects on the interest groups. The combination of explicit, qualitative and quantitative context storylines and energy modelling in a consistent and transparent way could significantly help to improve the robustness of the scenario results and conclusions (see e.g. Ref. [40]). This may lead to the construction of comprehensive sociotechnical scenarios considering crucial aspects of the energy transition such as disruptive elements attributable to societal risks or opportunities [41]. Based on the construction of sociotechnical scenarios as ‘hybrid’ scenarios, the perspectives and methodologies can be combined in the future to create a truly interdisciplinary modelling approach [42].

4.2.2. Stakeholder integration

Stakeholders can be involved in the scenario development process or, subsequently, by commenting on the results (e.g. scientific publications, reports, or media articles). However, they were not included during the scenario creation in any of the reviewed studies. In the last decades, stakeholders were only partially included in the scenario design, for example, to discuss specific parameters of power plants with utilities or to publicly participate in local or regional government planning. Today, arguments about the inclusion of more stakeholders and even consumers become more important [43]. The inclusion of stakeholder opinions can be 'measured' in workshops [44], while the inclusion of consumers usually requires surveys [45]. Most of the energy scenarios and policies are derived from complex techno-economic analyses but rarely consider other types of relevant societal values and interests [46,47]. In this context, public perspectives can provide insights into potential societal opportunities and limitations of energy pathways and, in particular, answer the question regarding which aspects and configurations of the system change will provide a socially acceptable level of affordability, energy security, and environmental protection.

4.2.3. *Uncertainty analysis of the key input data*

The three reviewed policy-oriented scenario analyses did not provide uncertainty analyses of the key input data, which considerably reduces the robustness of the derived results. In principal, relevant uncertainties can be identified using sensitivity analysis, which is intended to derive the key driving forces. A stochastic approach is a way to include small (and well-understood) uncertainties of input data, for example, by Monte Carlo simulations, if the computing times allow multiple model runs. More unknown and significant uncertainties might be considered by different scenario variants. Recent studies showed that sensitivity analysis is widely used to analyse macroeconomic parameters (e.g. Ref. [48]) and energy technology costs, as prerequisites to determine investments (e.g. Ref. [49]), and technical parameters related to multiple research questions (e.g. Ref. [49]). The stochastic approach is mostly used for renewable energy system optimisation, for example, for multi-criteria system design [50], or to deal with the uncertainty in the availability of renewable resources [51].

4.2.4. *Common model structures and open data*

It is rather difficult to compare and assess scenario studies, which is mainly due to the different storylines, applied approaches, model structures, and related data. Different foci of ESMs used for similar tasks could lead to different outcomes and conclusions. On the one hand, model diversity can help us to understand the energy system transformation; on the other hand, it makes it difficult to understand and compare the results. Non-transparent data sources and model descriptions add additional difficulties in assessing the analysis and quality of the derived policy recommendations. A joint definition of common model and data structures could improve this situation and provide advanced, open source reference methods and parametrisations. Such a task could be regulated by an international organisation but requires multinational financing and the wide participation of the academic community and other stakeholders in providing data and sharing experience and perspectives.

5. Conclusions

Although our study is limited to three case studies, we can compare the scenario results with overlapping geographical scopes and perform a systematic analysis of the narratives, assumptions, and applied methods and models. We provide a comprehensive approach to evaluate and compare the quality of scenario studies with a focus on the transparency within and beyond applied modelling approaches for a deep understanding of the scenario results. This analysis demonstrates that fulfilling the criteria of transparency, comprehensibility, and traceability requires a clear concept and certain documentation effort as well as a feasible way of providing detailed data and information. By means of a graphical and tabular summary of the studies and further discussion and evaluation, we report the essential aspects of the studies.

The results confirm that each model-based scenario study has strengths and weaknesses and significantly varies regarding the use of methods and models. Scenario studies often neglect aspects that can hardly be quantified, such as societal and environmental risks and opportunities, or only reflect a restricted spectrum of possible developments, for example, regarding the drivers of the energy demand. Furthermore, it is difficult or even impossible to evaluate the scenarios and their methodological background based on the final report only. All three studies refer to background material, that is, documentation of the models used, or to studies from which the results are used as assumptions for model parametrisation. Notable weaknesses of the studies include the weak transparency with respect to the model coupling and data access. The effort required to obtain a clear picture is unacceptable for people interested in these reports. Although the studies present graphs to visualise the applied models and their results, they often insufficiently describe the model interfaces, data exchange, harmonisation of assumptions, and iteration loops between the models. Furthermore, little information is provided on the model validation and a comprehensive uncertainty analysis of the key assumptions is missing. Thus, the necessity and suitability of the model usage regarding the research questions remain largely unclear to the reader. Therefore, more well-documented open source and open data studies are needed in the field of energy system analysis. Moreover, the authors of scenario study publications must pay more attention to reporting results comprehensible to the general public and to openly discussing the robustness and uncertainties of derived conclusions and policy implications.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.esr.2019.100380.

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3 Discussion

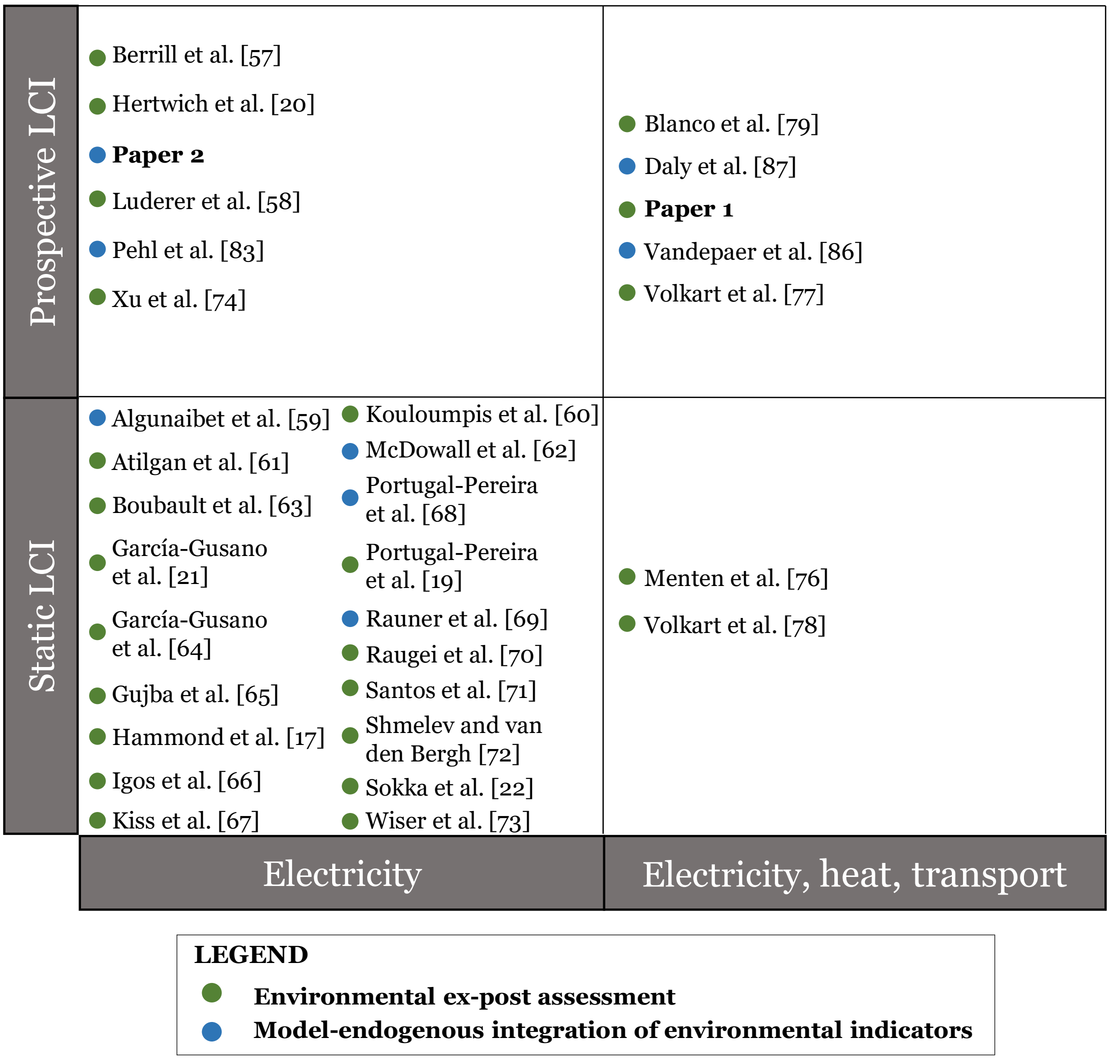
The aim of this work was to contribute to the improvement of the life path of energy scenarios as defined in Grunwald [55]. To do so, the focus was first on the ‘construction’ phase by analyzing the life cycle environmental impacts and material requirements of energy scenarios. These analyses can be viewed as complements to and extensions of conventional analytical frameworks for constructing energy scenarios. Moreover, this dissertation also contributed to the ‘users’ evaluation’ phase by providing an analytical framework that allows the assessment of the quality and transparency of energy scenarios against existing criteria and aims to improve future scenario analysis.

Specifically, the dissertation aimed (1) to provide an analytical framework for the life cycle-based environmental ex-post assessment of multi-sectoral energy scenarios, (2) to use this analytical framework to calculate life cycle environmental impacts of the energy technologies represented in an ESOM and to analyze the interactions of climate impacts and system costs using multi-objective optimization, (3) to analyze the material demands of energy scenarios for a selection of metals and derive implications for scenario modeling, and (4) to help make future scenario analyses more understandable to society, policy makers, and industry by analyzing the quality and transparency of selected scenarios. Towards these goals, four contributions were prepared, which are summarized in Chapter 2.

The respective scientific findings and potentials for further development are presented in the Subchapters 3.1 to 3.3. The discussion is divided into three categories, which are characterized by the methods used: Coupling life cycle-based indicators with ESMs (Chapter 3.1), estimation of the material requirements and potential bottlenecks that may arise from the energy transition (Chapter 3.2) and systematic analysis of the transparency and comprehensibility of scenario studies (Chapter 3.3).

3.1 Coupling of life cycle environmental impacts with energy system models

Recent studies that coupled LCI data with ESMs or scenarios are listed in Figure 2. Studies marked with a green dot conducted ex-post assessments only. A blue dot indicates that the indicators were integrated into the ESM and somehow influenced the model result. Whenever LCI data in the studies have been adjusted for potentially occurring future conditions (e.g. by integrating future scenarios into the background LCI database), they are placed in the ‘prospective LCI’ category. Studies in which the LCI data are based on present-day conditions are placed in the ‘static LCI’ category. Furthermore, a distinction is made between studies that focus exclusively on coupling LCI data with foreground scenarios on the electricity sector and others that assess multi-sector energy scenarios (i.e. electricity, heat and transport).



	Electricity	Electricity, heat, transport
Prospective LCI	🟢 Berrill et al. [57] 🟢 Hertwich et al. [20] 🔵 **Paper 2** 🟢 Luderer et al. [58] 🔵 Pehl et al. [83] 🟢 Xu et al. [74]	🟢 Blanco et al. [79] 🔵 Daly et al. [87] 🟢 **Paper 1** 🔵 Vandepaer et al. [86] 🟢 Volkart et al. [77]
Static LCI	🔵 Algunaibet et al. [59] 🟢 Atilgan et al. [61] 🟢 Boubault et al. [63] 🟢 García-Gusano et al. [21] 🟢 García-Gusano et al. [64] 🟢 Gujba et al. [65] 🟢 Hammond et al. [17] 🟢 Igos et al. [66] 🟢 Kiss et al. [67] 🟢 Kouloumpis et al. [60] 🔵 McDowall et al. [62] 🔵 Portugal-Pereira et al. [68] 🟢 Portugal-Pereira et al. [19] 🔵 Rauner et al. [69] 🟢 Raugei et al. [70] 🟢 Santos et al. [71] 🟢 Shmelev and van den Bergh [72] 🟢 Sokka et al. [22] 🟢 Wiser et al. [73]	🟢 Menten et al. [76] 🟢 Volkart et al. [78]

LEGEND

🟢 **Environmental ex-post assessment**

🔵 **Model-endogenous integration of environmental indicators**

Figure 2. Overview of studies that couple LCI data with ESMs and that have the geographic focus on a country or a wider area (e.g. global).

3.1.1 Environmental ex-post assessment

The first research objective of this dissertation was to develop a framework that enables the life cycle-based environmental ex-post assessment of multi-sectoral energy scenarios by linking the ESSM MESAP [7] to LCI data. This was achieved by developing the 'Framework for the Assessment of Environmental Impacts of Transformation Scenarios' (FRITS) in Paper 1.

The coupling of LCI data with ESMs and energy scenarios has become the focus of various research projects in recent years. By the end of 2015, Hertwich et al. [20] were the first to perform a LCA of different global energy scenarios using the technology hybridized environmental-economic model with integrated scenarios (THEMIS). A major innovation of the model was the adjusted global electricity mix in the background LCI database. Moreover, the authors disaggregated the life cycle phases of power generating technologies (e.g. construction of a power plant) in order to assign the environmental impacts to the correct points in time in the scenarios. To date, THEMIS has also been used to account for future impacts of electricity generation with a focus on storage and grid [57] and has been coupled to various global IAMs for ex-post assessment [58]. While most other studies that performed power sector assessments mainly relied on static LCIs [17, 19, 21, 22, 59-73], Xu et al. [74] adapted the LCI database's electricity mix for Europe to a scenario.

The study by Hertwich et al. [20] greatly inspired the development of the Framework for the Assessment of Environmental Impacts of Transformation Scenarios (FRITS) [75] (Paper 1) and the extension of such assessments to the heat and transport sectors. Other studies that had been published at the start of this thesis, such as a study by Menten et al. [76], did not sufficiently describe the methods used, i.e. the manipulations of the foreground LCI data, and did not adapt the LCI database to future conditions. However, since the beginning of the work on FRITS, other studies on the assessment of multi-sectoral energy systems have been published. For example, Volkart et al. [77] adapted the background electricity mix to a scenario for Europe and performed an assessment of the Swiss energy system. Afterwards, Volkart et al. [78] also assessed global energy scenarios. As in FRITS, both studies relied exclusively on the ecoinvent database to ensure consistency in the background LCI data that were used to model life cycle impacts. Another study by Blanco et al. [79] conducted an ex-post assessment of European scenarios focusing on the introduction of power-to-methane (PtM) technologies. Prospective LCIs were incorporated to the extent that for some of the technologies considered, the authors used LCIs from the LCI database developed in the project on new energy externalities developments for sustainability (NEEDS) [80].

Since there are large differences at the process level and in the system boundaries of the applied ESMs in Refs. [77-79], the comparison of the case study results of Paper 1 with results from the aforementioned studies can only be conducted in terms of general trends. For example, the provision of fossil fuels and materials is outside the system boundary of the MESAP model, whereas these processes are part of the system boundary in most ESMs based on 'The Integrated Markal Efom System' (TIMES) [81]. Moreover, there are differences between the technologies considered in the ESMs and/or the mappings of LCI data to those technologies. Furthermore, the comparability of the results also depends on their presentation (e.g. only at the level of the overall scenario or only presenting relative shares of processes and technologies for an indicator). For example, given the system boundaries of the TIMES model of the Joint Research Center (JRC-TIMES) applied in Blanco et al., impacts of the heat and transport sectors only comprised the construction phase of the technologies. Other impacts that could be associated with these sectors, such as the fossil fuel supply to these sectors, were allocated to other sectors of the ESM (e.g. to the fuel supply sector). This contrasts with the approach in Paper 1, in which impacts of fossil fuel supply for heat and transport as well as the operation of heat and transport technologies are also allocated to the heat and transport sectors, respectively. Thus, assignments of LCI data to processes or technologies in the ESMs strongly depend on the model structure and on the sectoral subdivisions made in the model. In principle, there is no right or wrong in assigning life cycle environmental impacts to processes or technologies in the ESMs, as long as the environmental impacts associated with the transformation of the energy system are included as comprehensively as possible at the overall scenario level. However, such model differences make technological and sectoral comparisons between studies difficult.

Nonetheless, an agreement with existing literature can be found with regard to the adverse side effects arising from the energy transition in the increasing use of minerals and metals as well as in land use compared to business-as-usual scenarios and the current energy system. The results of Paper 1 confirm the strong influence of energy crop cultivation on land use at the overall scenario level that was also highlighted in Refs. [77, 78]. Blanco et al. only showed relative contributions of processes or technologies per sector but also emphasized the large impact of bioenergy supply on land use in the fuel supply sector. The increases in abiotic resource depletion in the power sector in ambitious energy scenarios that are highlighted in Paper 1 confirm the results by Volkart et al. [77] and of studies that focused on the power system only (left half of the Figure 2). In line with other studies, Paper 1 shows that significant co-benefits could be achieved by phasing out fossil-fuel-based power generation (especially lignite) (see e.g. Refs. [20, 74]). Moreover, Paper 1 shows that direct and indirect electrification of passenger transport leads to a decrease in human health impacts associated with $PM_{2.5}$ emissions.

FRITS is being used for life cycle environmental assessments of various energy system transformation scenarios in ongoing scientific projects[1]. Important further improvements will be the integration of prospective elements in the background database (such as the adjustment of heat and transport structures to global energy scenarios) as well as the refinement of the LCIs used for the foreground technologies. Current limitations and further research required in the coupling of LCI data with ESMs are outlined below in Section 3.1.3.

3.1.2 Model-endogenous integration of life cycle environmental impacts

The second research objective of this dissertation was the enhancement of an ESOM to enable the integration of additional environmental indicators into the objective function and into the ex-post assessment of the results. In Paper 2, FRITS was used as a basis for parametrizing the REMix model [82] with environmental indicators for the energy technologies that are explicitly

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[1] Such as the Helmholtz Climate Initiative and the project on the ‘Integrated sustainability assessment and optimization of energy systems’ (InNOSys) funded by the Federal Ministry for Economic Affairs and Energy.

considered in the REMix model. The application of multi-objective optimization enabled the systematic assessment of trade-offs between system costs and life cycle GHG emissions.

Integration efforts of life cycle indicators in ESOMs in the literature are diverse and range from the setting of upper limits for certain indicators, the monetarization of emissions and indicators, to multi-objective optimization on certain emissions and indicators. Studies differ not only in the approaches used to account for life cycle impacts in ESMs, but also in the choice of sectoral and technological resolutions. The technological resolution for electricity generation used in Paper 2 is similar only to the resolution used in a study by Pehl et al. [83], who included a tax on life cycle GHG emissions in the 'REgional Model of Investment and Development' (REMIND). Paper 2 confirms the trends found by Pehl et al. in the structure of power supply when aiming at a mitigation of life cycle GHG emissions: a decrease in PV installations and an increased share of wind power, CSP and nuclear power plants.

The finding of Paper 2 is particularly important in light of four recent studies that advocated the increased use of wind energy and, in some cases, the decreasing deployment of PV when accounting for life cycle environmental impacts: Portugal-Pereira et al. [68] who, similar to Pehl et al., included a tax on indirect GHG emissions in a TIMES model with a focus on the energy system in Brazil showed that wind power is increasingly deployed compared to a system with a tax on direct emissions only. Rauner and Budzinski [69] applied a similar method as in Paper 2 to the electricity system in Germany and illustrated that an increasingly environmentally sustainable system requires an increased use of variable renewables, especially wind, compared to an unconstrained cost-optimal system based mainly on fossil fuels. Similarly, McDowall et al. [62] included upper limits on life cycle GHG emissions in a TIMES model focusing on Europe and showed that respecting these upper limits requires increased deployment of wind energy and decreased deployment of PV compared to systems where upper limits apply only to direct emissions. Likewise, Algunaibet et al. [59] downscaled the eight planetary boundaries defined by Ryberg et al. [84], which aim to provide a safe space for humanity as a whole, to the US power sector and showed that compliance with the upper limits leads to a significantly higher deployment of wind on- and offshore compared to a solution that is in line with the Paris Agreement and only considers GHG emissions. Moreover, Algunaibet et al. demonstrated that respecting the planetary boundaries implies the need to prevent the deployment of PV, which highlights the large upstream environmental impacts of this technology compared to other power generating technologies.

In summary, the trends illustrated in Paper 2 regarding the development of the power generation portfolio when reducing life cycle environmental impacts are in line with the findings of previous studies. However, compared to these previous studies, Paper 2 applies the spatiotemporal high resolution ESOM REMix, which allows more robust statements about the flexibility demand (storage and grids) [85] than the approaches used in the aforementioned studies, which either work with time slices such as REMIND or TIMES and/or do not consider the electricity grid in their assessments. Consequently, Paper 2 closed an important research gap by showing that a reduction in life cycle GHG emissions to a certain level is also associated with increasing grid expansion and decreasing use of Li-ion batteries. In turn, the expansion of dispatchable electricity generation such as CSP and nuclear reduces grid expansion to a certain extent. In summary, the expansion of the electricity grid for regional load balancing is proving to be an important factor in reducing life cycle GHG emissions, even if the shares of dispatchable generation are increasing. In the case of significant reductions in life cycle GHG emissions compared to the cost-optimal solution, hydrogen reconversion can replace the use of Li-ion batteries and gas-fired power plants to cover peak demand.

It should be noted, however, that when interpreting the results of Paper 2, one must consider the limited sectoral resolution, which does not reveal opportunities of sectoral linkages to reduce the environmental impacts at the level of the entire energy system (including heat and transport, as in Refs. [86, 87]). Future studies with REMix should therefore aim to expand the sectoral scope.

3.1.3 Limitations of current coupling attempts and outlook on further research needs

N.B.: This section includes parts of a Paper that I co-authored, 'The integration of life-cycle assessment into energy system models: best practices, current challenges and aim for the next decade' [1] (submitted to 'Renewable and Sustainable Energy Reviews'). Specifically, it includes parts of Chapter 3 of that Paper, entitled 'Discussion and aims for the next decade', which I initiated, structured, and substantially co-authored.

The coupling of ESMs and LCI data has gained momentum in recent years and offers new perspectives for planning the evolution of future energy systems and envisioning configurations with improved environmental performance. However, there are still important modeling challenges that need to be addressed in future research:

- Increased level of integration of LCA and ESMs
- Better technology mapping and consistent technological representations
- Prospectivity of LCIs in line with the temporal scope of ESMs
- Disaggregation of LCIs in phases harmonized with ESMs
- Avoiding double counting of environmental flows
- Sectoral scope and rationality behind ESMs

- Transparency of the modeling approach and of the data to facilitate a collaborative effort

Table 2 lists the key modeling aspects that require attention when coupling the two methods, summarizes the corresponding current practices, and defines aims for the next decade with respect to these practices.

Table 2. Key steps, current practices, and aims for the next decade when combining ESMs and LCA

Steps for combining LCA and ESMs	**Current practices**	**Aims for the next decade**
1. Increased level of integration of LCA and ESMs	Approaches are dominated by ex-post assessment with an increasing trend towards model-endogenous integration of LCA coefficients.	• Development of integrative, hard-linked, and fully endogenized ESMs and LCA models realizing the full potential of the combinations of both methods in terms of the following: o A broad range of solutions provided o Capture of the feedbacks between the system represented by the LCA and the ESM o Increased spatial and temporal resolution
2. Better technology mapping and consistent technological representations	The LCIs of energy processes that are available to the authors are used as proxies and assigned to the technology represented in an ESM based on their name similarities.	• Technologies with their underlying techno-economic assumptions of the ESM have to be closely mapped and harmonized with the corresponding LCI • Development of a common classification between ESMs and LCA for an accurate mapping process and a collaborative effort to facilitate the harmonization of LCI with the different ESMs • Creation of additional LCIs for the integration of technologies into ESMs to allow for more environmentally favorable substitution options
3. Prospectivity of LCIs in line with the temporal scope of ESMs	Studies rarely include LCIs that reflect future technological developments of energy. Moreover, the background database is only partially adjusted to future changes in the upstream supply chains.	• Comprehensive and transparent publication of LCIs for emerging technologies and background processes such as material extraction and industrial processes • Creation of shared routines for LCI database manipulation • Publication of prospective LCA coefficients

Continuation of Table 2. Key steps, current practices, and aims for the next decade when combining ESMs and LCA

Steps for combining LCA and ESMs	Current practices	Aims for the next decade
4. Disaggregation of the LCI in phases harmonized to the ESM	The LCI used to calculate the LCA coefficient generally aggregates the life cycle phases. Certain studies separate the infrastructure and operation in the LCI data used. However, in the current modeling of LCIs, it is not always possible to separate the end-of-life processes.	• Modular modeling of the LCI, which allows a separation of the phases similar to ESMs • Additional data collection to represent the end-of-life processes of energy technologies in future LCA studies
5. Avoiding double counting of environmental flows	Most studies do not consider double counting in the background database. Various approaches have been used in a small set of studies but without any consensus.	• Consensus on an approach to avoid double counting and create shared programming routines that can be adjusted easily to the different ESMs • Harmonized geographical and sectoral classifications between the LCI database and the ESM to consistently avoid double counting before calculating the life cycle indicators
6. Sectoral scope and rationality behind the ESM	Studies cover one specific energy sector (mostly electricity) and only some cover multi-sector energy systems. Approaches are dominated by optimization rationality.	• Extension of the scope to other sectors to capture interactions and include additional rationality to describe the technology selection made by the ESM
7. Transparency of the modeling approach and of the data to facilitate a collaborative effort	In most cases, modeling is only partially documented and seldom reproducible. Code is rarely published.	• Fully transparent coupling of the models integrated in a collaborative effort. • Pre-calculated LCA coefficients or web-based service to easily calculate indicators tailored to multiple ESMs

1. As illustrated in Figure 2, most studies, including the study presented in Paper 1, use LCA impacts for environmental ex-post assessment of energy scenarios. However, the endogenization of LCA coefficients within ESMs allows for a better consideration of the environmental dimension at an early stage of the future energy system design process, as has been shown in a few studies, including Paper 2. Nevertheless, current integration approaches of environmental impacts in ESMs can still be classified as soft-linking due to the absence of a fully formalized and automatized bidirectional connection between the LCA and ESM frameworks. Future studies could aim for a hard-linking approach, where the ESM and LCA models interact without being manually controlled by the modeler. There is a strong interrelationship between the energy system represented by ESMs and the broader life cycle of energy

technologies represented by LCA, and actions in one part of the system will often reverberate in the other part through positive or negative feedback. The development of hard-linked LCA and ESM frameworks would allow the capture of these interdependencies, thereby achieving more accurate representations. Furthermore, hard-linked LCA and ESM frameworks would further unlock the synergies that can be obtained from combining LCA and ESMs. For example, environmental performance in the energy system will often be dependent on local and temporal conditions. A high spatial and temporal resolution is often missing from current LCA models as the underlying data aggregates the time and space dimensions [88-90]. Spatially and temporally differentiated information is available in ESMs and can be used as a source of information to improve the practice of LCA.

2. Technologies represented in ESMs are often mapped to LCI datasets without any other substantiation than noting their name resemblance. This loose approach to technology mapping partly results from the absence of a common taxonomy of energy-related products and technologies. The adoption of a common classification would facilitate the mapping process as well as the general interoperability of both methods. Furthermore, a linear relationship is often assumed between the capacity of a technology and its specific environmental impact (e.g. that a 2 MW wind turbine has the same specific environmental impact as a 6 MW wind turbine), but these assumptions have not been confirmed in upscaling studies of emerging technologies [91, 92]. Assumptions regarding the LCI could be better harmonized with the technology characteristics behind the techno-economic data in the ESMs by considering methods used in prospective LCA models, in which material efficiency is related to technical characteristics [93, 94].

Finally, it is necessary to extend the scope of technologies covered in LCA and ESMs. Given the retrospective nature of current LCI databases, they generally do not sufficiently represent emerging technologies, which will be deployed in future energy systems [95]. In ESMs, the technology coverage remains determined by the objectives served by the pre-existing model, which has not been combined with LCA before. Since coupling LCA and ESMs gives more relevance to environmental dimensions, it is relevant to allow technology substitution based on their environmental performance. This is particularly important for the model-endogenous integration of life cycle impacts as performed in Paper 2, since the model result is influenced by the technology-specific impacts. Otherwise, the range of explored solutions remains limited, which hampers the search for configurations with the least environmental impacts.

3. Most of the LCA coefficients that are incorporated into ESMs are based on current technologies, and future changes are usually accounted for, if at all,

by adjusting energy efficiencies. However, it is expected that even for existing technologies, changes will occur in material inputs and emission factors that are not related to efficiency. For existing technologies using new types of fuel inputs as well as for future technologies, databases have to be extended through additional prospective LCI data collection efforts. Furthermore, future global changes in production schemes in the background database are seldom adapted, and if so, the adaptations are limited to electricity mix evolutions. However, achieving a fully decarbonized economy will also require fundamental changes in the heating and transportation mix and in industrial or material extraction processes. This means that the prospective adaptation of background databases is a complex task that requires specialized knowledge in many different areas. Therefore, in addition to the transparent publication of source codes on the manipulation of LCI databases, it would be an important step forward to develop service platforms that automate these database manipulations.

4. Ex-post assessments in which a single year is analyzed are usually based on aggregated LCA coefficients for the functional unit of energy supply. However, this level of aggregation is also partly applied to the evaluation of transition pathways, even though here, a separation of the LCA phases would be more appropriate (see e.g. Refs. [21, 60, 64]). The separation of operation- and infrastructure-related LCA coefficients in the foreground LCI is usually straightforward, but the processes for decommissioning are often modeled inconsistently and at different levels of the process chains. Thus, LCA coefficients related to operation, construction, and dismantling/recycling are rarely separated in studies analyzing a large number of technologies and sectors (see e.g. Refs. [75, 78, 86]). The separation of these phases could be simplified through a modular approach to LCI modeling in which the different elements are labeled and structured according to uniform classifications and guidelines. Finally, more details about the technologies should be added to the foreground LCI, such as repowering and maintenance operations.

5. In FRITS, an attempt is made to avoid double counting in the background LCI database for the electricity sector by matching the regions under study with the corresponding electricity markets in the database and then deleting the corresponding supplier processes (e.g. electricity generation of a gas turbine) from these markets. Thus, in the corresponding LCI databases, electricity from the electricity market Germany (Paper 1) or from electricity markets that are part of the EUNA region defined in REMix (Paper 2) is free of environmental impacts. However, this approach is based on the simplifying assumption that electricity in the markets of the LCI database serves the same sectors as electricity in the ESM. Moreover, this approach is only suitable for avoiding double counting of the electricity sector, since the electricity markets in ecoinvent have a sufficiently high regional resolution (country scale or

higher). Another option would be to completely match flows between the LCI database and the ESM and then delete identical flows in the LCI database to avoid double counting. In this way, in theory, all double counting could be avoided, also, for instance for heat generation and transport processes.

However, for certain flows, correcting for double counting is hampered by several elements. Firstly, there is no common classification of energy products and services, which has also already been identified as an obstacle to accurate mapping. Thus, flagging duplicated flows relies on name similarity and is prone to errors. Secondly, the correction requires an adequate matching between geographies of the ESM and the LCA data. Thus, algorithms are needed to regroup and disaggregate regions. This function has yet to be generalized, but open source tools, such as the wurst python package, are available to achieve the aggregation and disaggregation step [96]. Thirdly, a complete avoidance of double counting would require a bidirectional link between LCA and ESMs, which has not yet been operationalized.

6. Another limitation is the missing representation of non-energy sectors (e.g. industry, agriculture, and the service sector) in the ESMs applied [76]. It would be relevant to extend the scope of ESMs to these external entities to obtain more representative models and to consider their numerous interrelations. To extend the scope of ESMs can either be achieved by extending and enriching the ESM under consideration into fully integrated frameworks or, more progressively, by coupling them with other sector-specific models or general equilibrium models [66, 83]. Furthermore, the analytical frameworks underlying ESMs are generally dominated by optimization approaches, which forces the model dynamics considered to follow cost optimality [97]. Considering other rationalities besides cost optimality is a necessity to gain a better understanding of the possible future developments of energy systems and to identify suitable strategies to influence the transformation process. In this regard, relevant insights could be provided by different modeling approaches, such as technology diffusion, system dynamics, or agent-based modeling [98-100].

7. Very few studies publish data and codes that can be used by other authors. One reason may be that many of the studies presented in Figure 2 did not use codable methods for their LCI data manipulations and LCIA calculations but relied on software tools such as openLCA (as used for FRITS) or SimaPro. However, coupling of ESMs and LCA has the potential to be reproduced and reused, as it could be fully operated with scriptable procedures. To facilitate reuse, future studies should explicitly license the published data, if possible, with open licenses such as creative commons. If data cannot be provided with the studies, data manipulations should at least be scripted, so the results can be reproduced by anyone who has access to the same data. As

discussed in point 4 of this section, researchers could also publish ready-to-use LCA scores for energy processes represented in ESMs or create web-based applications to enable a more tailored calculation of the coefficients without prior programming knowledge.

3.2 Metal demand of energy scenarios

Currently, energy scenarios mostly neglect the material foundation associated with the transitions outlined. Possible development paths of the demand for metals related to the energy technologies deployed in energy scenarios can be quantitatively modeled with MFA. Such an analysis can also be used as a complement to LCIA methods, as it provides an approach to quantify the future demand for metals while it also identifies potential shortages. Furthermore, it allows the derivation of implications of demand growth and the outlook on possible demand and supply system responses, thus also contributing to the assessment of the criticality of metals.

In Paper 3, possible developments of the total material demand as well as the primary material demand for Li, Co, Nd and Dy were quantified in six different global energy scenarios. In addition, the Paper provides a rough estimation of the demand for these metals from non-energy applications outside the scope of the scenario. The analysis showed that the overall demand for the analyzed metals increases significantly due to the deployment of electromobility in road transport and the expansion of wind turbines. However, Paper 3 also revealed that the primary metal demand could be strongly reduced by high recycling efforts and sub-technology selection. Potential material bottlenecks could arise particularly in the case of Li and Co, as the demand for these metals is driven by the strong expansion of battery-electric road transport as well as stationary storage. To reduce the demand pressure on these metals, it is important to reduce the specific Li and Co demand for Li-ion batteries as soon as possible, but also to deploy other technologies, such as fuel cell vehicles and other stationary energy storage technologies. In addition, metal demand can also be reduced through non-technical measures, such as switching from car ownership to car sharing and thus reducing the absolute number of vehicles needed to satisfy transport demand.

Paper 3 also revealed that there are large differences in demand estimates between studies (see Paper 3, section 4.2. for a detailed quantitative comparison of the results with those of other studies). This is on the one hand due to the different scenarios analyzed, but on the other hand it is also due to differences in the assumptions on battery capacity, engine power, penetration rates of certain sub-technologies, specific material requirements, recycling rates and growth rates of non-energy sectors. Although Paper 3 makes an important contribution to a better understanding of the influence of such assumptions on the results, future research should aim to identify best-fit data on specific material requirements of energy technologies and their future development, as well as consider further sub-technology scenarios. Moreover, as Paper 3 only quantifies the material demand of selected metals, it is important to extend the approach to other metals used in technologies that are widely deployed in energy scenarios. In general, future research on these topics could be significantly supported by collaboration with technology developers.

To identify possible supply shortages, Paper 3 compares primary cumulative material demand with current estimates of reserves and resources. However, these estimates may vary widely and change over time. For example, Jowitt et al. [101] showed that global reserves for most metals have not declined significantly over time relative to production, so that depletion of reserves could not be the main source of risk to metal supply in the coming decades. While exceeding reserves and/or resources is used in most studies as an indication of potential material shortages (see table 4 of Paper 3), future studies should try to better understand supply-side adjustments as demand increases.

Currently, the material basis associated with the outlined transitions is neglected in the construction phase of energy scenarios. In future scenario studies, the material requirements should be published together with energy scenarios in order to highlight high demand increases and point to potential supply bottlenecks. Another possibility would be to integrate upper limits on the use of certain metals by deployed energy technologies in the ESM. However, such approaches only seem reasonable if all potentially critical metals are included in the ESM, as otherwise the system could switch to technologies that use metals which are disregarded.

In addition, the challenge lies in the reasonable definition of upper limits on the use of materials in the energy system. One possible approach could be the disaggregation of global reserves to the region under study (e.g. Germany) as well as to the sector analyzed (e.g. the power sector). Such disaggregation could be proportional to the population or economic power of the analyzed region and/or sector. For example, Viebahn et al. [30] identified critical materials in energy scenarios for Germany by dividing global reserves by population and assuming that 10 % of the reserves are available for the deployment of energy technologies, resulting in a share of 0.1 % of global reserves for the energy transition in Germany.

Paper 3 also emphasized that possible material shortages could also lead to rising metal prices in order to be able to undertake the necessary adjustments in the supply system of the analyzed metals and to meet the increasing demand. Since cost assumptions are a key driver of ESOM outcomes, it would be a large step forward to link these assumptions to metal price models, such as those presented in Glöser-Chahoud et al. [102] or Sverdrup and Olafsdottir [103]. These models can derive metal price estimates as a function of demand and other factors, which in turn could influence energy technology prices and, consequently, ESOM results. For example, Sverdrup et al. [104] showed that the deployment of battery electric vehicles could be constrained by Li price increases. It is important to note that in all approaches in which material demand might have an impact on the scenario outcome, the technological resolution of the ESMs needs to be extended to consider technological substitution options.

An increase in metal demand could also lead to increasing environmental impacts of metal mining operations. For example, Van der Voet et al. [105] estimated that future declines in ore grade may not be offset by more efficient mining operations, and thus the specific GHG emissions of some metals may increase. Increasing environmental burdens of resource provision could even render the implementation of a technology void if that technology was ultimately promoted because of an expected environmental benefit, while this benefit would be cancelled out in the future by higher environmental burdens at the level of resource provision.

This potential counterproductive effect highlights the importance of another future research area for the coupling of MFA and LCA methods with energy scenarios: the integration of dynamic effects such as the effect of the development of material demand on ore grades and the associated increase in specific environmental impacts. As shown in Paper 1, the integration of ambitious electricity scenarios into the background LCI database has a reducing influence on most of the environmental impacts of the foreground scenarios. This suggests that most of the environmental impacts of energy technologies and thus of energy scenarios could be even further reduced by further adjusting the heat and transport mixes as well as the industrial processes in the LCI databases to energy scenarios, a task which was highlighted in chapter 3.1.3 as an important focus for future research. However, it has not yet been comprehensively investigated to what extent such positive effects would be counteracted by decreasing ore grades due to strongly increasing demand.

3.3 Transparency and comprehensibility of energy scenarios to increase their impact on the economy, politics and society

Energy scenarios are usually constructed through the coupling of various models within a larger modeling framework. The knowledge gained in this way is used to develop political measures and possibly even legislation, which means that it has a significant impact on society. Therefore, it is important to disclose the input data and assumptions that were used, to explain the rationale behind the methods and models chosen and to communicate the results. Cao et al. [48] published a transparency checklist, i.e. a collection of necessary attributes for the transparent construction of energy scenarios. In Paper 4, this checklist was be applied to three energy scenario studies to assess to what extent these studies are comprehensible and transparently presented and fulfil the requirements of the transparency checklist.

The analysis in Paper 4 was based on a newly developed scheme that breaks down the construction process into different parts, such as scenario framework assumptions, resource supply, energy conversion, and end-use sectors. This division provides a structure for analyzing the traceability of energy scenarios despite the high complexity of the modeling approaches. This approach made it possible to systematically record and evaluate the models and assumptions used in scenario construction, as well as to verify the input and output data for essential elements. The analysis revealed that while model results are often adequately presented, there is a deficiency of information on the underlying methods. In addition, there often is little or no information on data exchange between models, no transparent description of model couplings and no discussion of the rationality of the choice of methods nor of the strengths and weaknesses of the approaches used. In this regard, the study reported in Paper 4 was the first to apply the transparency checklist of Cao et al. to different energy scenarios and to derive guidance for authors of future scenario studies using 'real world examples'. However, in order to derive more robust recommendations, future analyses should examine more published scenario studies and classify the details accordingly (e.g. following Figure 3, Paper 4). To assess the quality of the individual scenario studies, it is also advisable to evaluate studies with the same geographical focus, as this enables a better comparison of the data sources and modeling approaches used.

Hülk et al. [106] applied the transparency checklist to a scenario study they themselves had conducted and concluded that many of the transparency and reproducibility criteria could be met by the open-access models. The high relevance of open-access models was also emphasized in Paper 4 as indispensable for fully understanding the functionality as well as the data exchange between models. However, it is important to note that the decision to develop open-access models must be made at the very beginning of model development, ideally together with computer scientists who aim for codes that are sustainable in the long term. In addition, basic software training for researchers and better funding for open source software must become standard to ensure the successful development of well-structured, easily accessible model codes [107].

A remaining challenge is the evaluation of the pre-processed data that is incorporated into the models, since it is difficult to capture manual manipulations of pre-processed data [106]. Furthermore, other issues, such as communicating uncertainty, the rationality behind model selection, and the discussion of results in the scientific context, cannot be resolved with open-access models. In evaluating open-access model frameworks, Wiese et al. [108] concluded that while they help address problems of interdisciplinary modeling and improve transparency, the usage (see Figure 1) of the scenario studies depends heavily on communication and organizational structures. Therefore, in addition to providing open-access models, energy scenario modelers must seek to present and communicate scenario results in a way that is understandable to experts but also non-experts.

4 Conclusions

Considering both life cycle environmental impacts and the abiotic resource base is an important step in deriving increasingly robust, science-based decision support for a sustainable transformation of the energy system. In particular, life cycle assessment can help capture environmental impacts that lie beyond the traditional system boundaries of energy system models (ESMs), which typically only include on-site carbon emissions during operation of the energy technologies considered. By calculating the future development of demand and comparing it with estimates of current production, reserves and resources, it is possible to estimate the pressure on the supply system for abiotic resources and to determine whether material shortages may occur.

The framework for the assessment of environmental impacts of transformation scenarios (FRITS) that was developed and applied in Paper 1 can provide policy makers and stakeholders with additional information on environmental co-benefits and adverse side-effects of the energy transition. By combining life cycle impacts with the ESM MESAP, it is possible to look at the entire energy system and not just at individual energy sectors. In a case study for Germany, Paper 1 showed that ambitious scenarios are associated with a significant increase in abiotic resource depletion potential and land use and could increase some negative impacts on human health and the ecosystem compared to the current system and less ambitious transformation pathways. In addition, most of the environmental impacts are outside the typical system boundaries of ESM, i.e. they cannot be assessed by looking at direct emissions only. FRITS is also transferable to the results of other ESMs, which have a different technological and regional scope than the MESAP model. It can thus constitute the basis for future assessments of different mitigation strategies.

However, such ex-post assessments do not fully exploit the model's capabilities to explore system configurations that are more environmentally friendly than the original, mostly cost-driven model configurations. Therefore, in Paper 2, the life cycle impacts of the different technologies included in the REMix model were integrated as additional parameters. The focus was on the power system for Europe and North Africa in 2050. Using multi-objective optimization that included system costs and life cycle greenhouse gas emissions, it was found that an increasingly climate-friendly system is associated with a reduction in photovoltaic and Li-ion storage and an increased expansion of wind (onshore and offshore), concentrated solar power and nuclear. It was also shown that grid expansion is a robust cost-effective and low-emission measure. However, to increase the robustness of the conclusions to be drawn in future studies, future versions of FRITS require further adjustments to the background life cycle inventory (LCI) database and improvements in the quality and prospectivity of the LCI data representing the foreground technologies.

In Paper 3, material flow analysis was used to reveal the extent to which the material demand for Dy, Nd, Li and Co in different energy scenarios lies within the range of currently known reserves and resources, and which capacities of primary material extraction need to be increased. Among the materials analyzed, a key bottleneck for decarbonizing global energy systems could be the demand for Li and Co for stationary and mobile battery manufacturing. To account for an increasing demand for materials, future model-based assessments could either include upper limits on the use of materials in the models or, and this would be preferable, account for the influence of material bottlenecks on the costs of investments in technologies. For both approaches, the models should represent a broader technological spectrum in order to better account for the role of substitute technologies.

In order to achieve an appropriate impact of energy scenario studies on the economy, politics and society, the comprehensibility and transparency of the construction of scenarios is essential. Paper 4 addressed the question of the extent to which current scenario studies meet the quality and transparency criteria defined in the scientific literature. The results showed that the underlying model-based methods often lack information about the data exchange between the models as well as a transparent description of the model couplings and a discussion about the rationality of the choice of methods and about the strengths and weaknesses of the approaches used. Openly accessible modeling code for individual models but also for model couplings should be strived for in the future to ensure transparency and reproducibility. In addition, energy scenario modelers must seek to improve the communication of uncertainty and of the rationality behind the model selection as well as the discussion of results in a scientific context.

In summary, the publications included in this dissertation contribute to a more robust construction of energy scenarios as well as to their increased effectivity in economy, politics and society. These contributions are in particular the consideration of environmental impacts beyond the traditional system boundaries of ESMs, the consideration of the resource base when planning the transformation of the energy system, and the derivation of recommendations for modelers to increase the comprehensibility and transparency of future scenario studies.

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6 Declaration of authorship

I hereby certify that the dissertation entitled

“Constructing and evaluating energy futures – life cycle environmental impacts, material demand and transparency of energy scenarios”

is entirely my own work except where otherwise indicated. Passages and ideas from other sources have been clearly quoted.

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