THE ROLES OF CHEMICAL ENERGY CARRIERS IN FUTURE RENEWABLE ENERGY SYSTEMS

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For Suki.

ZUSAMMENFASSUNG

Klimaschutz ist eines der Hauptziele der Energiewende und bedeutet, dass der Einsatz von fossilen Energieträgern und den damit verbundenen Treibhausgasemissionen massiv reduziert werden muss. Um die Lücke, die von den fossilen Energieträgern hinterlassen wird zu schließen, werden erneuerbare Energieerzeugungstechnologien allein jedoch nicht ausreichen. Im Gegensatz zu fossilen Quellen sind erneuerbaren Energiequellen wetterabhängig und benötigen geeignete Flächen. Diese zwei Herausforderungen bei der Nutzung von erneuerbaren Energien können durch Ergänzung mit Speichertechnologien und Reservekapazitäten bewältigt werden, um eine zuverlässige Energieversorgung zu gewährleisten.

Eine zentrale Rolle kann dabei chemischen Energieträgern, synthetisch hergestellt aus erneuerbaren Energien und weiteren nachhaltig gewonnen Rohstoffen, zufallen. Synthetische Energieträger besitzen ähnliche Eigenschaften wie die derzeitig verwendeten, fossilen Energieträger und sind daher potenziell geeignet zur Energiespeicherung, im Transportsektor und als Industriegrundstoff. Die infrage kommenden Energieträger unterscheiden sich untereinander jedoch in ihren chemischen und physikalischen Eigenschaften, sodass davon auszugehen ist, dass sie sich unterschiedlich gut für die spezifischen Aufgaben in künftigen Energiesystemen eignen.

In dieser Arbeit werden die verschiedenen Energieträger mit Hilfe von Energiesystemmodellen untersucht und auf Basis von technoökonomischen Kriterien bewertet. Die Untersuchungen fokussieren sich dabei auf ihre Eignung für den Import als Energieträger und Grundstoff, den Stromtransport über große Entfernungen gegenüber der Nutzung lokaler Nachfrageflexibilitäten, sowie den Einsatz zur langfristigen und strategischen Energiespeicherung. Weiterhin wird ein Softwarepaket zur Modellierung von erneuerbaren Energien für Energiesystemmodelle vorgestellt, sowie die Grundlagen für ein globales, räumlich und zeitlich hochaufgelöstes Energiesystemmodell geschaffen.

Mit ihren Ergebnissen stellt die Arbeit einen Ausgangspunkt für zukünftige Analysen der globalen Rollen von chemischen Energieträgern und deren Wechselwirkungen mit regionalen Energiesystemen dar.

ABSTRACT

With climate change mitigation as one of the key goals of the energy transition, the use of fossil fuels and their connected greenhouse gas emissions has to decline sharply in the future. Renewable generation technologies alone however will be insufficient to fill the gap left by fossil fuels. Other than fossil fuels, renewable energy sources are constrained by their weather dependency and land requirements, making complementing storage and firming technologies necessary to ensure a reliable energy supply. To be successful, the energy transition has to address these key challenges of renewables, regional availability and weather dependency.

Chemical energy carriers are a puzzle piece to the energy transition, expected to address these two challenges. They can be synthetically produced from renewable energy and sustainably sourced feedstocks. With properties similar to currently used chemical energy carriers of fossil origin, they offer attractive characteristics for use in energy storage, transport and as industry feedstock. However, because of their distinct chemical and physical properties, they are expected to be suited differently well to fulfil the various roles in future energy systems.

In this thesis, the potential of candidate chemical energy carriers to fulfil the various roles are investigated. Using bottom-up energy system modelling, their performance and suitability for energy and feedstock imports, long-distance electricity transport as alternatives to demand-side flexibility, and long-term strategic energy storage are evaluated based on techno-economic criteria. The findings are complemented by the introduction of a software package for modelling input data on renewables for energy system models and the foundations for a global energy system model of high temporal and spatial resolution.

With its results, this thesis lays the basis for future, more comprehensive analyses of the global roles of chemical energy carriers and their interactions with regional energy systems.

PUBLICATIONS

PEER-REVIEWED PUBLICATIONS

- F. Hofmann, **J. Hampp**, F. Neumann, T. Brown and J. Hörsch. 'Atlite: A Lightweight Python Package for Calculating Renewable Power Potentials and Time Series'. In: *Journal of Open Source Software* 6.62 (2021), p. 3294. DOI: 10.21105/joss.03294, cited as [1].
- **J. Hampp**, M. Düren and T. Brown. 'Import Options for Chemical Energy Carriers from Renewable Sources to Germany'. In: *PLOS ONE* 18.2 (2023), e0262340. DOI: 10.1371/journal.pone.0281380, cited as [2].
- **J. Hampp**. 'Flexing with Lines or Pipes: Techno-economic Comparison of Renewable Electricity Import Options for European Research Facilities'. In: *PLOS ONE* (accepted for publication). DOI: 10.1371/journal.pone.0292892, cited as [3].
- T. Brown and **J. Hampp**. 'Ultra-Long-Duration Energy Storage Anywhere: Methanol with Carbon Cycling'. In: *Joule* 7.11 (2023), pp. 2414–2420. DOI: 10.1016/j.joule.2023.10.001, cited as [4].
- M. Parzen, H. Abdel-Khalek, E. Fedotova, M. Mahmood, M. M. Frysztacki, **J. Hampp**, L. Franken, L. Schumm, F. Neumann, D. Poli, A. Kiprakis and D. Fioriti. 'PyPSA-Earth. A New Global Open Energy System Optimization Model Demonstrated in Africa'. In: *Applied Energy* 341 (2023), p. 121096. DOI: 10.1016/j.apenergy.2023.121096, cited as [5].

FURTHER PUBLICATIONS WITH CO-AUTHORSHIP

- D. Kirli et al. 'PyPSA Meets Africa: Developing an Open Source Electricity Network Model of the African Continent'. In: *2021 IEEE AFRICON*. 2021 IEEE AFRICON. 2021, pp. 1–6. DOI: 10.1109/AFRICON51333.2021.9570911, cited as [6].
- SustainableHECAP+ Initiative. *Environmental Sustainability in Basic Research: A Perspective from HECAP+*. 2023. URL: https://sustainable-hecap-plus.github.io/ (visited on 13/06/2023), cited as [7].

'Among the residual possibilities of unforeseen events,
it is just possible that some day the sunbeams may be collected,
or that some source of force now unknown may be detected.
But such a discovery would simply destroy our [Britain's]
peculiar industrial supremacy. '

— W. S. Jevons (1866) [8]

ACKNOWLEDGEMENTS

The journey for this thesis was a wild ride. A lot of people shared this journey with me, helping me through the downs and celebrating the ups.

First and foremost, I'd like to thank my supervisor Prof. Michael Düren for him enabling my PhD, guiding and supporting me throughout it. Michael introduced me to the right people and gave me an incredible amount of freedom to explore my own ideas as well as to pursue my own path. Together with Prof. Peter Winker and Dr. Marc Strickert, the three repeatedly provided me with valuable feedback and discussions and reminded me to look at the bigger picture when I was getting lost in the details.

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During the high-time of the Corona pandemic, I was lucky to connect with Max Parzen and start our work on PyPSA-Africa. I'm proud to see it having grown into PyPSA-Earth with the help of many individuals and contributions from all over the world.

I'd also like to thank my former colleagues at ZEU for the interesting discussions, helping me to look at the world from perspectives other than energy. And I want to mention the cakes here; we all now SDG 18 is a serious business.

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ACRONYMS

AIS Automated Identification System.

CBAM Carbon Border Adjustment Mechanism.
CGLC Copernicus Global Land Cover.
CRediT Contributor Roles Taxonomy.
CSP Concentrated Solar Power.

EAC Equivalent Annual Cost.
ECMWF European Centre for Medium-Range Weather Forecasts.
EEZ Exclusive Economic Zone.
EU European Union.

FT fuel Fischer-Tropsch fuel.

GEBCO General Bathymetric Chart of the Oceans.
GIS Geographic Information System.
GSTD Global Shipping Traffic Density.

HVDC High-Voltage Direct Current.

IAM Integrated Assessment Model.
IEA International Energy Agency.

LHV Lower Heating Value.

NZE Net Zero Emissions.

PV Photovoltaics.
PyPSA Python for Power System Analysis.

RES Renewable Energy Source.

TES Thermal Energy Storage.

WDPA World Database on Protected Areas.

CONTENTS

1

INTRODUCTION

Chemical energy carriers in the form of fossil fuels form the basis of today's energy systems. Gas, lignite, coal, and oil are easy to extract, store and transport and have thus been widely adapted in transportation, for electricity and heat generation. Industrial processes have been tuned to rely on them as chemical feedstock, for example as reduction agents for refining iron ore or as hydrogen source for ammonia production. Their fossil origin comes however with significant drawbacks: The usage of these chemical energy carriers leads to the release of additional carbon, previously buried stably underground, into the atmosphere together with other greenhouse gases, thereby accelerating man-made climate change [9]. Having formed millions of years ago, fossil fuels are also a limited resource with regions being reliant on their natural resource endowments. This has led to regions that combine limited economic reserves of fossil fuels with high demand, like the European Union (EU), to become reliant on fossil fuel imports. As of 2021 more than half of the primary energy demand of the EU are imported [10].

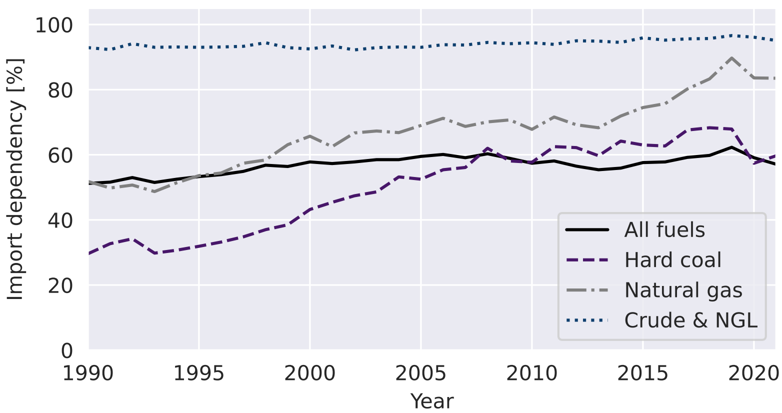

Figure 1.1: Import dependency of the EU for fossil fuels between 1990 to 2021. More than half of the energy demand is imported, with more than 90 % of crude oil originating from outside EU countries. Data from [10].

Energy systems worldwide are currently in a state of transformation [11] away from fossil fuels towards renewable energy sources. Driven by the need for climate change mitigation through greenhouse gas emission reduction and significant cost reductions, renewable energy sources like wind and solar are promising a more sustainable future. Beyond climate change mitigation and economic attractiveness, renewables also allow countries to diversify their energy supply with local resources, enabling them to reduce energy imports and their dependency on foreign countries. The International Energy Agency (IEA) maps out a pathway to net-zero emissions by 2050 in their latest Net Zero Emissions (NZE) 2023 scenario [12]. In the NZE scenario, the IEA sees this shifting trend in the energy mix to continue. By 2050, wind and solar are expected to become the dominant sources of energy in the global energy mix, see Figure 1.2.

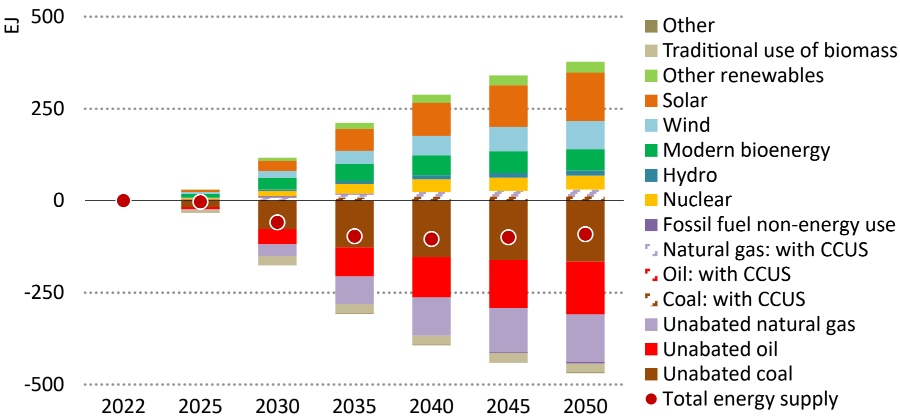

Figure 1.2: Changes in Total Energy Supply in the NZE 2023 scenario by IEA until 2050, showing the anticipated continuing shift from fossil fuels to Renewable Energy Source (RES) in the global energy supply. Figure CC-BY-4.0 IEA from [12].

There are challenges linked to the increasing shares of renewables in energy systems. The times when RES can produce electricity are variable, depending on the local weather and climatic conditions. This variability has to be managed to match supply with demand. Also, the generation potential of renewables is linked to the availability of suitable land areas. Regions with limited land availability or high energy demand are thus expected to face challenges in meeting their energy demand through local renewable resources sustainably and economically. Finally, while for many of today's uses of chemical energy carriers alternative processes can be found, not all processes will be able to switch from fossil fuels to run on RES-based electricity or heat.

Synthetic chemical energy carriers could be a solution to these challenges. Their general basis is formed by hydrogen produced from the electrolysis of water with electricity, combined with carbon, oxygen or nitrogen feedstocks. These synthetic energy carriers can then be made chemically identical or similar to commonly used fossil fuels. With comparable properties to fossil fuels, synthetic energy carriers offer many of the advantages of their fossil counterparts, like high energy density, easy storage and transport, while avoiding their major environmental impacts, if the energy and feedstocks are derived from sustainable sources. Synthetic chemical energy carriers could then be used for storing energy from renewable sources for long periods, enabling the variability of renewables to be managed across seasons or even years. With their high energy density, they could be used for long-distance transport of energy, enabling the trade of energy between regions with high renewable potentials and energy demands. And finally, they would allow for existing processes requiring chemical feedstocks to decouple from fossil fuels.

This thesis explores the potential roles synthetic chemical energy carriers could play in future energy systems. Using bottom-up energy system modelling for synthesizing, transporting, storing and using chemical energy carriers, the techno-economics of different carriers are put under scrutiny. Through comparison and analysing alternatives, we find out which chemical energy carrier is most suitable to fulfil the roles in future energy systems.

OUTLINE

Chapter 2 provides the necessary context for this thesis regarding the representation of RES in energy system models, the potential roles of synthetic chemical energy carriers in the future, techno-economic energy system modelling and the importance of open and FAIR research.

Chapter 3 introduces the publications which form the basis of this thesis. How the publications are linked to each other is shown in Figure 1.3. Starting with Publication 1, the paper describes a software package developed to model renewables input data for energy system models. Publication 2 then compares different chemical energy carriers and their suitability for use in energy and chemical feedstock imports to Germany. It is followed by Publication 3 in which the impacts of the weather-dependent availability of renewables, inflexibilities in demand and their impact on energy imports are analysed. In Publication 4 potential uses of hydrogen and methanol in a closed-carbon loop are studied for long-duration energy storage. Finally, Publication 5 presents a new open-source energy system model with global coverage, which enables better research into the interactions of energy systems and synthetic chemical energy carriers on a global scale.

Chapter 4 closes with a summary of this thesis and provides an outlook on future desirable extensions of the research presented here.

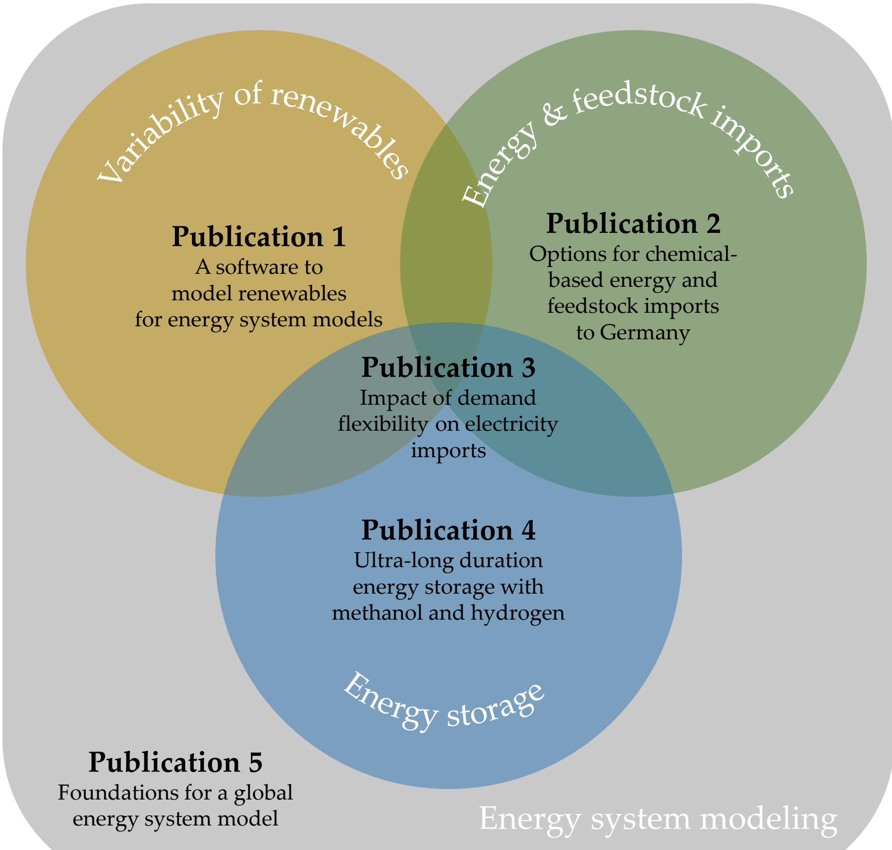

Figure 1.3: Publications of this thesis and their topical overlaps.

2 BACKGROUND

This chapter lays out the methods and concepts used in this thesis. First an introduction to renewables, their challenges to future energy systems and how to represent them in energy system models is given. Then chemical energy carriers with their potential roles in the future are discussed, followed by a short description of energy system modelling and how it can be used to evaluate the potential of chemical energy carriers. The chapter concludes with a note on the importance of FAIRness and openness related to this thesis and the field of energy system modelling in general.

2.1 REPRESENTING RENEWABLES IN ENERGY SYSTEM MODELS

RES are expected to provide the majority of primary energy supply in the future. Technologies like solar Photovoltaics (PV) and wind turbines have seen significant technological improvements and cost reductions in the past decades. With significantly lower specific greenhouse gas emissions and environmental impacts compared to fossil fuels, renewables are compelling technologies to base more sustainable energy systems on. For today's energy systems, which have been purpose-built around the use of fossil fuels, the transition to a renewables-dominated system faces two major challenges, weather dependency and land requirements. In the following we discuss these two challenges and how they are modelled to adequately represent them in energy system models.

Challenge 1: Weather-dependent availability

The times during which RES technologies are available to provide electricity and other energy services are dependent on the current weather conditions. This is in contrast to energy technologies based on fossil fuels, which are considered dispatchable, i.e. available to provide their energy services upon demand. The weather dependency of RES technologies means that the energy system incorporating them has to be able to accommodate their variability from daily, seasonal and multi-year weather variations. Commonly discussed methods to accommodate the variability are on the supply side the use of energy storage, transmission infrastructure across weather regimes and building overcapacity of RES in combination with curtailment. In addition on the demand side, demand-side flexibility to shift demand to an earlier or later point in time is available as an option. While solutions for implementing these measures exist and are already in use in today's energy systems, their capacity and operational modes are not set up for use in RES-dominated energy systems.

To determine the needs of future energy systems to accommodate RES, they need to be properly represented with their weather-dependent availability in energy system models. Most accurately this can be done using measured data from existing RES installations, but this approach is limited to locations with available data on existing installations with their technical specification as well as to past weather conditions. However large-scale energy system models used for capacity expansion and future scenarios studies need to be able to represent RES availability for locations without existing installations and for both past and possible future weather conditions. For this reason, the use of synthetic time series for RES availability has been widely adopted. These time series are derived from high-resolution weather data in combination with detailed technological models for specific RES technologies.

For this purpose, reanalysis weather datasets are often used. These are derived from a combination of satellite-based observations, measurements and calibrated climate models, providing consistent datasets over wide areas with high spatial and temporal resolution. Through backcasting these datasets can be expanded long into the past and can thus cover very long periods. This is important for capturing rare extreme weather events like cold spells or multi-year low wind periods. Figure 2.1 exemplifies daily and seasonal variations experienced by solar PV.

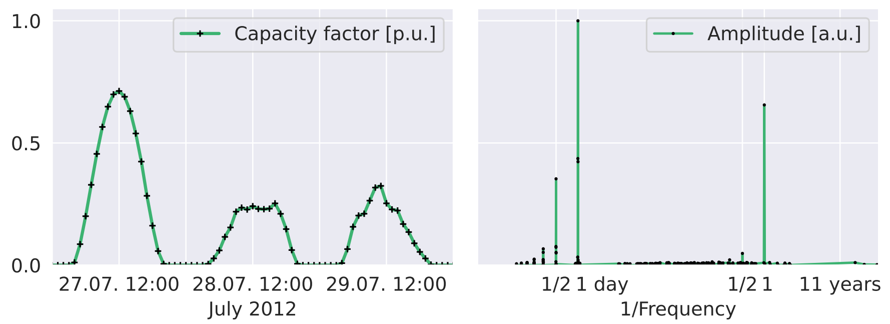

Figure 2.1: Examples of a synthetic time-series for solar PV in Germany covering 71-year by [13]. (left) Hourly capacity factor for three selected, consecutive days during summer, demonstrating typical daily variations and reduced availability due to cloud cover, (right) Fourier transform of the full 71-year time series, showing how solar PV availability is dominated by daily and seasonal cycles.

In this thesis, the reanalysis dataset ERA5 [14] by the European Centre for Medium-Range Weather Forecasts (ECMWF) was used. The dataset offers solar radiation, temperature and wind speed variables at a spatial grid resolution of $0.25° \times 0.25°$ and an hourly temporal resolution with global coverage from 1940 until the present day. Qualitywise the dataset is known to be inferior to specialized datasets for solar [15] and wind variables [16]. The advantages of ERA5 as opposed to these specialised datasets are its global coverage, the long period it covers and that it offers consistent data for modelling a mix of wind and solar technologies.

Different models are then used to derive the synthetic RES availability time series from the weather data variables. For solar PV, solar irradiation, panel orientation and temperature in combination with semi-empirical technology-specific parameters are used to determine the specific power output [17, 18]. Wind turbine power output can be determined from hub-height-adjusted wind speeds and manufacturer-provided power curves detailing their specific power output at a given wind speed.

The synthetic time series have the native resolution of the used weather dataset which leads to high computational complexity when used directly in energy system models. For this reason, aggregation of time series to lower spatial and temporal resolutions is therefore common, like the hourly profiles aggregated to country-level by Bloomfield et al. [13] or regional level used in [5, 6]. To reduce the temporal resolution aggregation or selection of representative weather days [19] can be used. Time series can also be grouped into quality classes based on yield estimated like in Mattsson et al. [20], Publication 2 and 3. Applying any of these methods is a trade-off between computational complexity and model accuracy and needs to consider the purpose of the model: For Publication 2 and 3 region-level aggregate time-series with an hourly resolution for a single representative weather year are sufficient to capture the principal suitability for energy export of the investigated regions. On the other hand Publication 4 analyses ultra-long-term energy storage conceptually, which requires hourly temporal resolution and multi-year time-period coverage to capture short-term as well as long-term variability, climatic cycles and extreme events. Complex models like Publication 5 are limited in their time horizon and spatial resolution by computational complexity, with solving times often taking hours or days, such that chosen resolutions become a trade-off between model resolution and solving time.

Challenge 2: Land requirements

While fossil fuels are the result of an integrated solar energy influx over hundreds of thousands of years which has led to the formation of highly concentrated deposits of oil, gas and coal, RES technologies make use only of the current influx of solar and wind energy. With this influx being comparatively low, RES technologies have much higher land requirements to provide the same amount of energy as with the extraction of fossil fuels. Further complicating is that RES technologies compete to some extent with other uses of land and not all locations are equally suitable for a specific RES technology. An area's availability depends on its current land use and land type as well as competing uses, like agriculture, urban areas or nature reserves. An area's suitability is affected by aspects like local topology, proximity to infrastructure and local weather conditions. Regions across the world vary in their areas available and suitable for RES technologies, resulting in different potentials for RES technologies and a maximum of capacities that can be installed in a region.

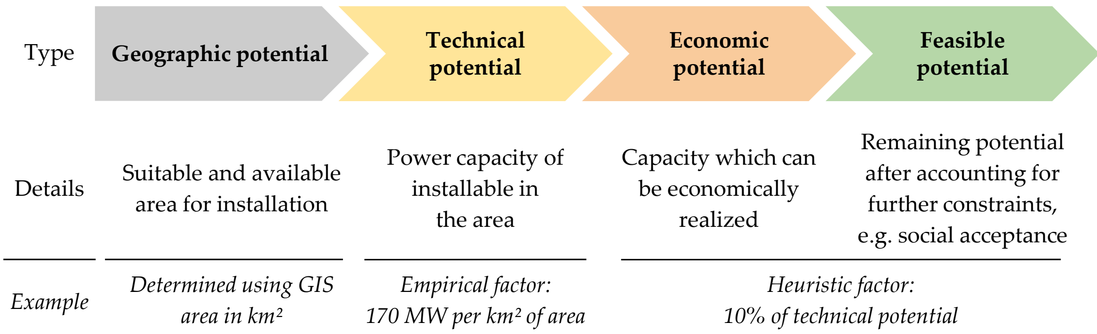

Figure 2.2: Overview of the different types of potentials of RES capacities that are distinguished in energy system models, loosely based on [21]. The provided example is based on the methodology used in Publication 3 for utility-scale PV.

These maximum potentials are important for energy system models, as they determine the maximum amount of RES-sourced energy a region can provide. Thus they represent a region's ability to meet its own energy demand and export surplus energy to other regions or require energy imports. To assess the potentials of a region to be used in energy system models, Geographic Information System (GIS)-based methods are first used to determine available and suitable areas within a region. This can involve a combination of spatially-resolved datasets, Table 2.1 show example criteria used in Publication 3 for inclusion and exclusion of potential areas. The eligible areas represent a region's geographical potential. From there using assumptions on the technical power density and heuristic factors to account for economic and social constraints, the feasible potential of a region can be estimated, see Figure 2.2 for more details.

The feasible potential is generally calculated at the native resolution of the used datasets. Depending on the research question, potentials can then be aggregated to a lower spatial resolution. For example, in Publication 2 and 3 the potentials are aggregated to region-level and distinguished by technology and quality class such that they are consistently aligned with the representation of RES availability time series. In Publication 4, RES potentials are not looked into at all, as they are not relevant to the research question discussed there. Publication 5 also aligns the spatial resolution of potentials

Table 2.1: Inclusion and exclusion criteria for evaluating the geographic potential for RES in a region as used in Publication 3 for solar PV, onshore and offshore wind.

Exclusion criteria	Elevation (GEBCO)	Water depth (GEBCO)	Slope (GEBCO)	Land use and type (CGLC)	Protected areas (WDPA)	Shipping routes (GSTD)	Economic zones (EEZ)
solar PV	Any	✗	✗	low-height vegetation, farm land, urban areas	Excluded	N/A	N/A
Onshore wind	$< 2000\,\mathrm{m}$	✗	$30\,\%$	low-height vegetation, farm land, forests	Excluded	N/A	N/A
Offshore wind	N/A	$> -60\,\mathrm{m}$	N/A	Lakes, open sea	Excluded	< 400 AIS contacts/h	✓
Description	Wind power density wanes with air density	Fixed-pole wind turbines need shallow waters	Steep slopes block turbine installation	Determined from satellite data	Reserves and nature-protected areas	AIS contacts as proxy for ship activity and traffic	Exclusive offshore areas for economic usage

with availability time-series for each RES technology but does not distinguish between different quality classes.

Correctly determining the potentials of a region relative to its energy demand is essential to determine a region's ability for energy autarky and energy trade, leading to a continuous improvement of methods for determining potentials and datasets, see e.g. [22, 23].

2.2 CHEMICAL ENERGY CARRIERS: FUTURE POTENTIAL ROLES

Today, fossil fuels and their derivatives, are chemical energy carriers of fossil origin and the backbone of most energy systems [24]. They have high energy densities (cf. Figure 2.3) and many are liquid or solid and stable under ambient conditions, like oil and coal, making them well-suited for transport and storage. Since they are of fossil origin, however, extraction, refining and use come with adverse environmental impacts. Prominently the burning of fossil fuels leads to the emission of additional fossil carbon into the atmosphere, which is the main driver of man-made climate change.

Synthetic chemical energy carriers can reduce the adverse environmental impacts of fossil fuels. From a chemical perspective, fossil-sourced and synthetic alternatives are similar, allowing synthetic carriers to substitute fossil ones in many applications. As shown in Figure 2.4, their synthesis requires hydrogen, carbon dioxide or nitrogen feedstocks, together with heat and electricity. When the feedstocks are sustainably sourced, e. g. extracted from the atmosphere using

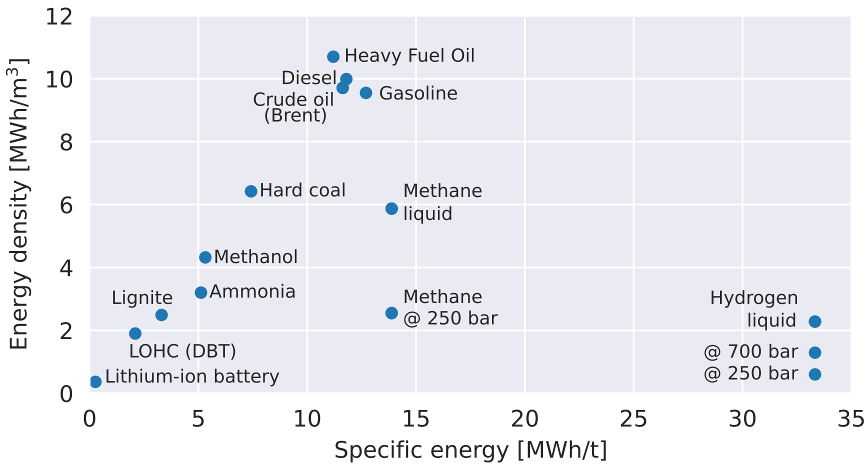

Figure 2.3: Energy densities and specific energy (in LHV) of chemical energy carriers and Lithium-ion batteries, showing how efficiently chemical energy carriers can store energy compared to batteries.

electricity and heat from sustainable sources, much of the negative environmental impact found in fossil fuel counterparts is prevented. The amount of energy required for feedstock sourcing and synthesis depends on the specific energy carrier and synthesis process. The simplest chemical energy carrier, hydrogen, can be produced through water electrolysis. Its low energy density and physical properties however make it difficult to store, transport and use. More complex energy carriers like methanol and Fischer-Tropsch fuels (FT fuels) have higher energy densities and are liquid at ambient conditions, making them easier to handle, but their synthesis is more energy intensive and requires carbon dioxide as additional feedstock.

In future energy systems, synthetic chemical energy carriers may play increasingly important roles as fossil fuels are being phased out. For industrial processes and sectors that are hard to electrify, as well as in the chemical industry, where fossil fuels are currently used as feedstocks for their carbon and hydrogen content, fossil fuels can be substituted with synthetic alternatives. Synthetic chemical energy carriers can further address the two major challenges of RES, weather-dependency and land requirements.

With them being easier to store than electricity, they can be used to store energy for managing the variability of RES availability. Their high energy densities and better transportability make them suitable for long-distance transport and energy export from regions with high RES potentials to regions with lower potentials and high demand.

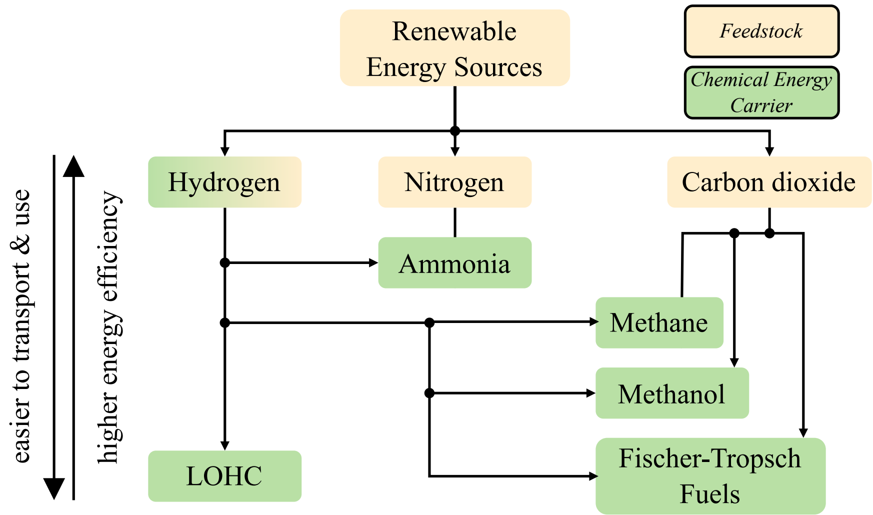

Figure 2.4: Required feedstocks for the synthesis of different chemical energy carriers. More complex carriers with higher energy densities are easier to handle, with the trade-off of their synthesis requiring more energy.

2.3 ENERGY SYSTEM MODELS: BASIC CONCEPTS AND METHODS

The trade-offs between synthetic chemical energy carriers and their suitability for specific applications can be evaluated using energy system models. These models create insight into the infrastructure and energy requirements, costs and utilization of equipment. For example, the authors in [25, 26] modelled costs for providing baseload electricity, hydrogen and ammonia around the world. Taking into account best production locations and transport costs, Runge et al. [27] compared synthetic fuels specifically for road transport against electrification. Regional differences in the quality and potentials of RES can incentivize trade [28, 29], or lead to the relocation of industries reliant on energy or energy-intensive feedstocks [30, 31].

Energy system models became widely adopted after the oil crisis in 1973 to describe and further energy systems understanding [32]. Since then, they have evolved into multi-purpose tools for system planning, scenario exploration and evaluation of energy policies. Initially used by governments, they have been adopted by academia, industry and civil society. Along with their wider use, different methodologies and levels of detail were developed; a good overview of the classification of energy system models is provided by Hall and Buckley [33].

In this thesis, techno-economic bottom-up capacity-expansion optimization models are used. Such models combine detailed representations of technologies with their technical and economic properties to model energy and material flows in an energy system. The models then determine the necessary capacities of included technologies required to meet a given energy demand, optimized for the lowest total system costs. The models we use in this thesis consider on the economic side the total system costs for installing, maintaining and operating the technology capacities. Given varying technical lifetimes of technologies, the economic assumptions need to be harmonized and aligned with the modelling horizon, in our case using the Equivalent Annual Cost (EAC) method assuming a technology-independent discount rate. The technical perspective of the models focuses on their conversion efficiencies between material and energy flows, the efficiency of transport, standing losses for storage technologies and restrictions to the use of specific technologies. Such restrictions are for example the weather-dependent availability of RES or part-load and ramping restrictions on synthesis processes. Figure 2.5 shows the assumptions used in Publication 4 for the synthesis process of methanol.

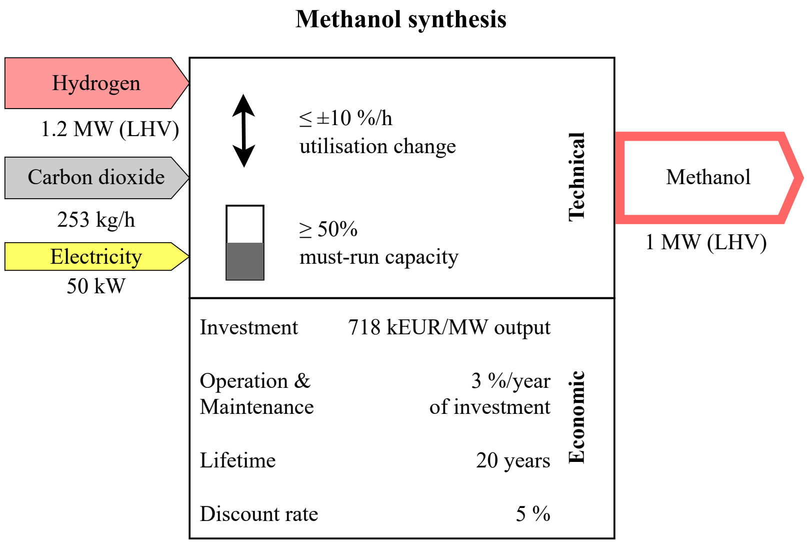

Figure 2.5: Techno-economic assumptions used to model the methanol synthesis process in Publication 4 for synthesizing methanol from hydrogen, carbon dioxide and electricity.

The models we use in this thesis are based on the open-source energy system modelling framework Python for Power System Analysis (PyPSA) [34], which is a Python package for building and optimizing energy system models. The framework uses a component-based approach, dividing an energy system model into individual components which are then linked together through their energy and material flows. From these interlinked components PyPSA builds the mathematical model for a linear program, which in turn is then solved with Gurobi [35] or a similar solver to determine the optimal solution. A detailed description of the modelling framework can be found in Brown et al. [34].

2.4 FAIRNESS AND OPENNESS IN ENERGY SYSTEM MODELLING

Openness and following the four principles of FAIRness — Findable, Accessible, Interoperable and Reusable — is considered good scientific practice by many, including the Deutsche Forschungsgemeinschaft [36].

In the field of energy system modelling, it is unfortunately still not yet standard practice with publications missing the data and models used in their preparation. Lack of access to data and models creates 'black boxes', models which are intransparent and not verifiable by others [37], reducing the credibility of results. It also creates inefficiencies, as data preparation and model development have to be repeated all over, even for small projects where only updates to a previous study are intended. The advancement of the field as a whole is thus slowed down, as similar tasks have to be continuously done from scratch.

Aiming to address this issue, members of the Open Energy Modelling Initiative (openmod) have called for more openness in energy system modelling from individuals [37] as well as institutions like the IEA [38].

Not only does openness benefit the field itself, it also allows actors without the necessary resources to build and maintain a model of their own, to participate in energy system modelling and research. This benefits especially researchers from the global south and civil society organizations and enables them to introduce their perspectives into the field from which they have been excluded before. While energy system modelling is no crystal ball into the future, openness thereby helps to reduce biases and improve the quality of the field [39].

Following these arguments, we considered it essential to have as much of the research related to this thesis open as possible:

- All datasets used are publicly accessible and mostly open
- All models and results have been published under open licenses
- All publications have been published open-access or free-access

This thesis would not have been possible without the prior work of others who developed countless open-source software packages that were used. During this thesis, we were also able to contribute back to some of these software projects. Table 2.2 gives an overview of the contributions made to open-source software projects during this thesis.

Table 2.2: Contributions made to open-source projects during this thesis.

Project name	Maintainer	Features	Issues and Bug fixes	Usability and Documentation	Related to	GitHub Repository
Advanced Nuclear	✓	✓	✓	✓	Reproduction of [40].	euronion/advanced_nuclear_reproduction_study
atlite	✓	✓	✓	✓	Publication 1, 3, 4 and 5.	PyPSA/atlite
GlobalEnergyGIS			✓	✓	Publication 2 and 5.	niclasmattsson/GlobalEnergyGIS
PyPSA			✓	✓	Publication 2, 3, 4, 5 and [6].	PyPSA/PyPSA
PyPSA-Eur	✓	✓	✓	✓	Publication 5 and [6].	PyPSA/PyPSA-Eur
PyPSA-Earth	✓	✓	✓	✓	Publication 5 and [6].	PyPSA-meets-earth/PyPSA-Earth
snakemake		✓	✓		Publication 2, 3, 4, 5, and [6].	snakemake/snakemake
synde	✓	✓	✓	✓	Publication 5 and [6].	euronion/synde
technology-data	✓	✓	✓	✓	Publication 2, 3, 4, 5 and [6].	PyPSA/technology-data
trace	✓	✓	✓	✓	Publication 2 and 3.	euronion/trace

3 PUBLICATIONS

3.1 A SOFTWARE FOR MODELLING RENEWABLE ENERGY SOURCES

This section refers to Publication 1 by Hofmann et al. [1] in Appendix A.

Representing RES is a critical challenge for energy system models. Determining their weather-dependent variable availability and location-specific potentials requires processing of large weather datasets in combination with technology-specific models. Commonly this task was reiterated for every new study, causing work duplication, risking errors in the implementation of models and hindering comparability between studies.

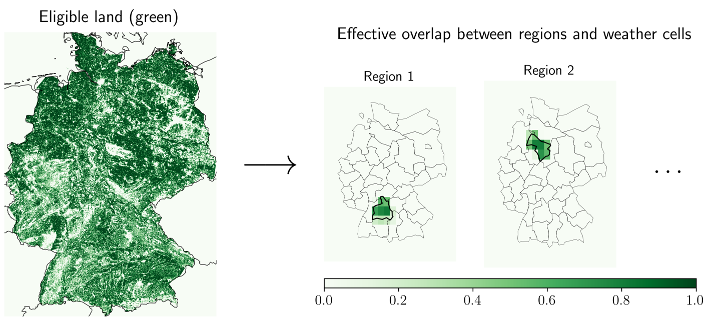

Figure 3.1: Evaluating land use to determine eligible areas for renewables is one of the core capabilities of *atlite*, demonstrated here on a NUTS-3 level for Germany excluding forest and urban areas shown in white. Figure CC-BY-4.0 from [1].

In this publication, we address these issues by presenting a software package for these common tasks encountered in modelling renewable energy sources for energy system models. The package is designed to handle weather datasets in a harmonized data format. It incorporates a library of commonly used technology models for, among others, solar PV, Concentrated Solar Power (CSP), onshore and offshore wind, and hydroelectricity, to be used in conjunction with the harmonized weather data. The library can handle geospatial datasets to evaluate the land availability for determining RES potentials based on land-use and land-cover data, demonstrated in Figure 3.1.

A key feature of the software is its scalability purpose-built to efficiently process very large datasets even with limited computing resources. The harmonized data format allows for easy adaption of new weather data and technology models making it suited for current and future research questions.

3.2 OPTIONS FOR CHEMICAL-BASED ENERGY IMPORTS TO GERMANY

This section refers to Publication 2 by Hampp et al. [2] in Appendix B.

Imports of chemical energy carriers from fossil sources are a cornerstone of today's German and European energy systems. As energy systems transition away from fossil fuels towards renewable energy sources, these fossil energy imports will have to be replaced. To some extent, energy imports can be substituted with domestically sourced renewable energy. A full switch to domestic renewable energy sources however is unlikely, as limited land availability and renewable resources are most likely insufficient to meet the high energy demand of Europe. Other reasons for continuing to import some of Europe's energy demand from outside can be found in economic, geopolitical or energy security considerations. These residual imports would then also need to transition away from fossil to more sustainable energy sources.

A range of chemical energy carriers can be sustainably produced from renewable energy sources. They differ in their properties, e.g. their simplicity of production and use, their transportability or their storability. Hydrogen for example is easy to produce but difficult to store, whilst more complex molecules like synthetic Fischer-Tropsch fuels require more complex and energy-intensive production processes with the advantage of being easier to transport, store and use.

In this publication, we compare options for chemical energy carrier imports to Germany. For the most prominently discussed energy carriers, we model the energy supply chain, starting with the production in an exporting country, to conditioning, storage and transport into Germany, considering the different techno-economics of each energy carrier.

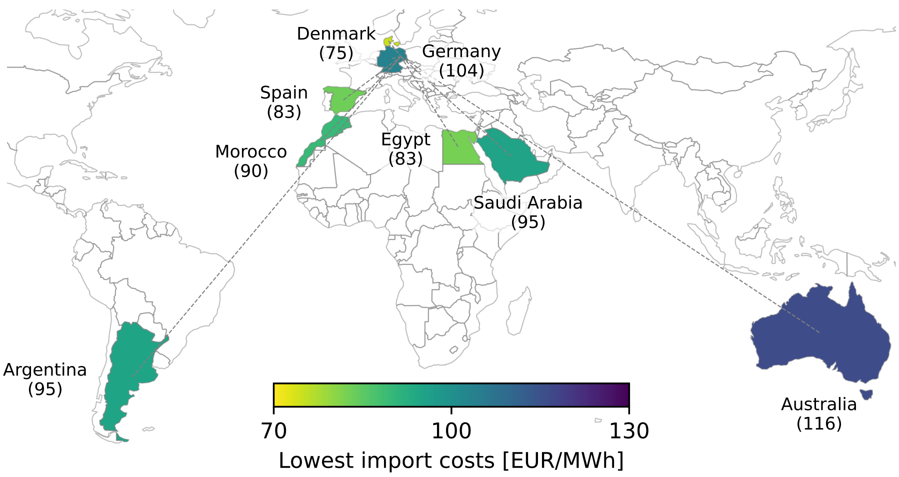

Figure 3.2: Map of the lowest costs for energy exports to Germany in 2030 from any of the evaluated energy carriers.

We find that for every investigated energy carrier there is a potential exporter able to export to Germany at lower costs compared to domestic production in Germany. For all energy carriers there exist multiple potential exporters with similar economic attractiveness, as Figure 3.2 illustrates by showing the lowest cost export option per country to Germany in 2030. Overall our results show that in the absence of stark economic advantages of a specific energy carrier or exporter, decisions on energy imports and infrastructure can be made based on criteria other than costs or energy efficiency.

3.3 impact of demand flexibility on energy imports

This section refers to Publication 3 by Hampp [3] in Appendix C.

As the share of renewable electricity generation in the European electricity mix rises, matching the variability of renewables with electricity demand becomes increasingly challenging. While in fossil-based electricity generation, fossil fuels can be stored and used to produce electricity when needed, the weather-dependency of RES makes storing their energy a necessity. Options are for example in pumped hydro storage, batteries, hydrogen or methanol. Alternatively, electricity can be imported over long distances from regions with uncorrelated weather or demand patterns, or with higher RES availability due to more favourable climate conditions. A third option is to make demand more flexible and to make it follow the variable availability of RES.

In this publication, we investigate long-distance electricity imports, measures to match demand with the variable supply of electricity from renewable sources and their effects on total system configurations. In multiple scenarios, electricity imports from Morocco and Tunisia to Central Europe, directly by High-Voltage Direct Current (HVDC) lines or indirectly by hydrogen pipelines with subsequent conversion to electricity are modelled. For supply-side measures, we consider battery and hydrogen storage, as well as CSP with integrated Thermal Energy Storage (TES). On the demand side, flexibility in the time of consumption is considered.

Our results, summarised in Figure 3.2, show that costs for direct electricity imports are generally a third to half lower than for indirect imports using hydrogen. This is due to the higher efficiencies for direct electricity transmission and the additional infrastructure needed for hydrogen. Morocco and Tunisia are both similarly attractive export locations for electricity exports to Central Europe. Both offer high potential for solar-based electricity generation with low intra-annual variability. Demand-side flexibility and CSP with integrated TES both offer distinct advantages for matching renewable electricity supply with demand by reducing the infrastructure needs and costs for electricity imports.

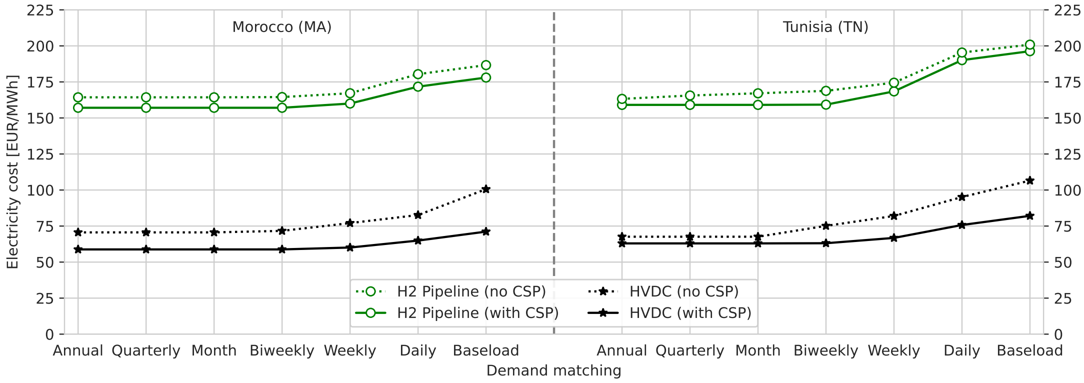

Figure 3.3: Costs for importing electricity from Morocco and Tunisia to Central Europe depend on whether imports are by electricity or hydrogen pipeline and on the available options for demand-side flexibility and CSP with TES. Figure CC-BY-4.0 from [3].

Studies evaluating the costs of energy imports often neglect the effects of demand-side flexibility and the need for temporal matching of supply and demand. With this study, we provide insight into the effects on system costs of systematically varying demand-side flexibility for electricity and hydrogen-based imports.

3.4 ULTRA-LONG DURATION ENERGY STORAGE WITH METHANOL

This section refers to Publication 4 by Brown and Hampp [4] in Appendix D.

Energy systems that rely only on wind and solar power need energy storage to balance weekly, seasonal and annual variations in the availability of renewable energy supply. While short-term storage can be provided by batteries, solutions for long-term storage are more challenging. Hydrogen in salt caverns is often considered because of its low cost, but requires suitable salt deposits which may be far from renewable sites and would thus need long-distance transport of electricity or hydrogen, adding additional costs and efficiency losses.

In this publication, we explore methanol storage as a promising alternative to hydrogen for long-duration energy storage. Methanol is liquid under ambient conditions and can be easily stored in tanks, which can be built anywhere, making it independent of geological conditions. Storage facilities can be built with small and medium capacities and methanol can also be easily transported. As such it could also serve as a strategic reserve and ultra-long duration energy storage for cases of extreme weather events, natural catastrophes or energy-infrastructure disruptions.

We compare methanol storage with hydrogen storage in simulations of a stylized renewable energy system over 71 weather years for multiple European countries. The methanol storage system is designed with a net-zero carbon footprint. The carbon dioxide used for methanol synthesis is either obtained using direct air capture, closing the carbon loop via the atmosphere, or captured during the oxyfuel combustion in an Allam-cycle turbine.

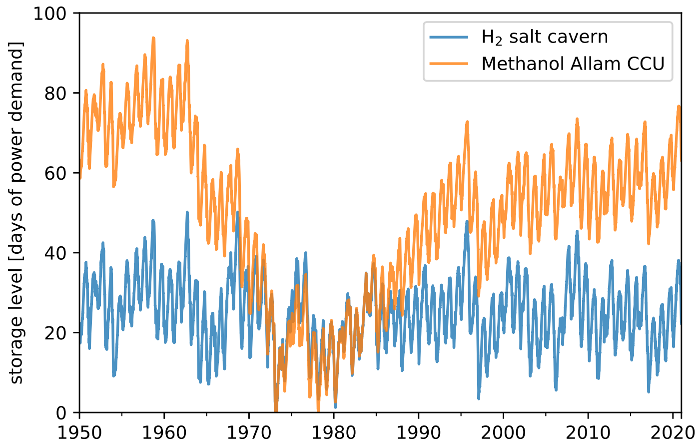

Figure 3.4: Storage filling levels measured in days of electricity demand that can be met across 71 weather years for hydrogen (blue) and methanol (orange) in cost-optimal system configurations. Figure © 2023 Elsevier Inc. from [4].

Results show that methanol storage leads to systems with lower electricity costs compared to hydrogen storage in steel pressure vessels and higher costs compared to hydrogen storage in salt caverns if long-distance transport infrastructure costs can be neglected. The storage filling levels of one modelled scenario are shown in Figure 3.4, highlighting how hydrogen storage is used to cover primarily intra-annual variations, while methanol storage is also used to cover inter-annual variations. From the analysis of the system cost components, we identify opportunities for cost reductions.

With this publication, we show that methanol storage could be an attractive alternative to hydrogen storage for long-duration and ultra-long energy storage, especially for regions without access to salt deposits. Methanol storage could also be used as a strategic reserve to increase the resilience of energy systems. By showing the techno-economic attractiveness of methanol storage with carbon-cycling we want to bring attention to this technology option and encourage its simultaneous development as an alternative to hydrogen storage, mitigating the risks in technology development and deployment.

3.5 FOUNDATIONS FOR A GLOBAL ENERGY SYSTEM MODEL

This section refers to Publication 5 by Parzen et al. [5] in Appendix E.

In the previous sections, export, import and energy storage using synthetic chemical energy carriers were investigated stand-alone. In reality, they will be embedded and interacting with the surrounding energy system. To investigate any effects of their interaction, a model of the surrounding energy system is needed. For regions like the European continent or North America, detailed energy system models already exist that could be used for this purpose. For other regions of the world, publicly accessible and extendable energy system models are lacking. This concerns not only developing countries, but also e. g. Australia which is an potential energy exporter due to its high renewable energy potentials.

With this publication, we aim to establish an energy system model generator, which can be used to create detailed energy system models for any country or region of the world. The basis for this model are open and publicly available data sources. It follows the learnings and structure of an established energy system model for Europe, PyPSA-Eur [41]. The model generator is designed to be extendable and made available under open licenses to allow reuse and future extensions by anyone.

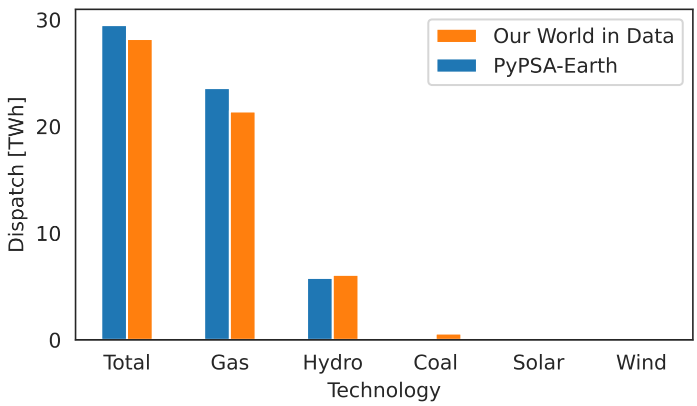

Figure 3.5: Electricity mix in Nigeria in 2020 as reported by *Our World in Data* compared to the results obtained from the PyPSA-Earth model, showing the good agreement between the two.

Validation against third-party data sources for the African continent shows good agreement and confirms the methodology used. A case study for Nigeria demonstrates the ability of the model to reproduce historic results (cf. Figure 3.5) and to explore future scenarios.

With the model generator, we enable future studies in regions that have until now been neglected in energy planning studies. By creating a community around the model generator and providing capacity building, we empower researchers and civil society local to these regions to use advanced energy system models in their work.

4 CONCLUSIONS AND OUTLOOK

Energy systems around the globe are transforming away from fossil fuels towards more sustainable energy sources. In future systems with high shares of RES, synthetic chemical energy carriers could play important roles previously held by fossil fuels. Using energy system modelling, this thesis explored the suitability of chemical energy carriers to fulfil these roles.

In Publication 1 a software package for modelling RES for energy system models was outlined. Its extendible and modular design allows it to be adapted for different RES technologies and enables modelling their weather-dependent availability. The software package was central to Publication 3 and 5.

In Publication 2 multiple options for importing energy to Germany from seven potential exporting regions using synthetic chemical energy carriers were compared. The results show a range of options for Germany to import energy as well as feedstock hydrogen at prices well below domestically produced hydrogen. This shows the potential for synthetic chemical energy carriers to enable in their role large-scale energy trade in future energy systems as fossil fuels are phased out.

In Publication 3 a closer look into the effects of weather-dependent availability of RES on energy imports was taken. Imports of electricity from RES directly by cable and indirectly via hydrogen were compared and the effects of variability management using storage and demand-side flexibility were analysed. The variability and management measures were found to have significant effects on the costs of both direct and indirect electricity imports. Demand-side flexibility as well as low-cost storage options like CSP-integrated TES were found to be able to reduce the costs of electricity imports. Overall direct electricity imports showed favourable properties compared to the import of hydrogen with subsequent conversion to electricity, suggesting hydrogen being at a disadvantage in the role of long-distance electricity transport.

In Publication 4 options for seasonal and inter-annual energy storage for energy systems were investigated. Using multi-weather year modelling, methanol was found to be a viable alternative to hydrogen for long-duration energy storage. Methanol can be stored independently of geological conditions and its carbon emissions can be kept in a closed carbon cycle, making it a suitable option for the role of ultra-long-duration energy storage in future energy systems.

In Publication 5 a new open-source energy system model was presented. Using publicly accessible and open data sources, this model builds upon the learnings of an existing European energy system model and extends it to a global scope. The capabilities of the model were demonstrated on a continental level for Africa and a national level for Nigeria. With its high spatial and temporal resolution, the model is suitable for exploring the potential roles of chemical energy carriers and their interactions with other technologies in future energy systems in greater detail than previously possible.

OUTLOOK ON FUTURE WORK

Methods for representing and modelling renewables are being continuously improved. These improvements can be expected to propagate into the field of energy system modelling, where they will address some of the known and yet-unknown shortcomings of the research detailed here. For the representation of renewables, expected improvements include refinements to existing and adaptation of new weather datasets, including higher spatial [42] and temporal resolution [43, 44], as well as validated downscaled datasets [45]. Synthetic weather datasets will allow future scenarios under changing climate conditions and extreme events to be explored [46, 47]. Using satellite-based imagery and machine learning techniques [48], more refined methods for resource assessment [22, 23] are expected to enable more accurate estimates of RES potentials.

Beyond the opportunities for future research outlined in the individual publications, there are research gaps that can be addressed by integrating the individual strains of research presented here.

In Publication 2 to 4, the prospective roles of synthetic chemical energy carriers were examined in isolation. Within real energy systems, however, they would be interacting with other technologies and processes, leading to synergies, competition and trade-offs [49]. Modelling and representing these interactions requires sector-coupled energy system models and expanding energy flows to also include energy-intensive commodities like iron [50], steel [51], high-value chemicals [52] as well as carbon [53, 54]. The methodology used in Publication 2 and 3 with their stylized representation of exporting regions' energy systems could serve as a starting point for such an analysis. An European perspective could be formulated by coupling the two models to a detailed European energy system model like PyPSA-Eur [55] and expanding them to include energy-intensive commodities. Such a one-sided coupling would create a more detailed insight into the effects of energy imports on the importing, here European, energy system and its energy-intensive industries.

Going beyond a one-sided model improvement does require a detailed representation of the exporting regions' energy systems as well. The groundwork for this was laid with the PyPSA-Earth model shown in Publication 5. This enables studies of the effects of energy trade on any of the world's regions in far greater detail than existing studies relying on simplified modelling approaches like [28, 29, 56, 57].

As the trade of renewable-based energy carriers and commodities intensifies, differences in RES potentials and subsequently costs could lead to a restructuring of industrial production. Energy-intensive industries for which costs of energy and feedstock are a significant share of their total costs could be incentivized to relocate to different regions and instead export their products. This 'green pull' effect has recently attracted attention in the literature [30, 58] and in related policy discussions on Carbon Border Adjustment Mechanisms (CBAMs) to prevent carbon leakage, industry relocation due to carbon and energy price differentials [59, 60]. Representation of such industry migration in energy system models would require a detailed representation of the specific industries and relocation opportunities. Considering the distance of these questions from the core competencies of energy system models, different modelling approaches and structures could be more appropriate for this task. Collaborations with other modelling communities like Integrated Assessment Model (IAM) models to inform and couple their models with energy system models [61] could be an avenue into approaching more profound economic and distributional challenges related to the energy transition.

A PUBLICATION 1

This chapter has been published as

- F. Hofmann, **J. Hampp**, F. Neumann, T. Brown and J. Hörsch. 'Atlite: A Lightweight Python Package for Calculating Renewable Power Potentials and Time Series'. In: *Journal of Open Source Software* 6.62 (2021), p. 3294. DOI: 10.21105/joss.03294

Contributions to the publication (CRediT):

J.H. Conceptualization, Writing – Original Draft, Writing – Review and Editing.

Individual contributions to software packages under active development and maintenance are difficult to assess using the established CRediT. Contributions by J. H. to the software package include: General code development, documentation, maintenance, project management, improvement of methodology, implementation of new features.

The Journal of Open Source Software

atlite: A Lightweight Python Package for Calculating Renewable Power Potentials and Time Series

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Summary

Renewable energy sources are likely to build the backbone of the future global energy system. One important key to a successful energy transition is to analyse the weather-dependent energy outputs of existing and eligible renewable resources. `atlite` is an open Python software package for retrieving global historical weather data and converting it to power generation potentials and time series for renewable energy technologies like wind turbines or solar photovoltaic panels based on detailed mathematical models. It further provides weather-dependent output on the demand side like building heating demand and heat pump performance. The software is optimized to aggregate data over multiple large regions with user-defined weightings based on land use or energy yield.

Statement of need

Deriving weather-based time series and maximum capacity potentials for renewables over large regions is a common problem in energy system modelling. Websites with exposed open APIs such as renewables.ninja (Pfenninger & Staffell, 2016; Staffell & Pfenninger, 2016) exist for such purpose but are difficult to use for local execution, e.g. in cluster environments, and restricted to non-commercial use. Further, by design, they neither expose the underlying datasets nor methods for deriving time series, here referred to as conversion functions/methods. This makes them unsuited for utilizing different weather datasets or exploring alternative conversion functions. The pvlib (Holmgren et al., 2018) is suited for local execution and allows interchangeable input data but is specialized to PV systems only and intended for single location modelling. Other packages like the Danish REatlas (Andresen et al., 2015) face obstacles with accessibility, are based on proprietary code, miss documentation and are restricted in flexibility regarding their inputs.

The purpose of `atlite` is to fill this gap and provide an open, community-driven library. `atlite` was initially built as a lightweight alternative to REatlas and has evolved further to contain multiple additional features. `atlite` is designed with extensibility in mind for new renewable technologies and conversion methods. An abstraction layer for weather datasets enables interchangability of the underlying datasets. By leveraging the Python packages xarray (Hoyer & Hamman, 2017), dask (Dask Development Team, 2016) and rasterio (Gillies & others, 2021), `atlite` makes use of parallelization and memory efficient backends thus performing well even on large datasets.

Basic Concept

The starting point of most `atlite` functionalities is the `atlite.Cutout` class. It serves as a container for a spatio-temporal subset of one or more topology and weather datasets. Since such datasets are typically global and span multiple decades, the Cutout class allows `atlite` to reduce the scope to a more manageable size. As illustrated in Figure 1, a typical workflow consists of three steps: Cutout creation, Cutout preparation and Cutout conversion.

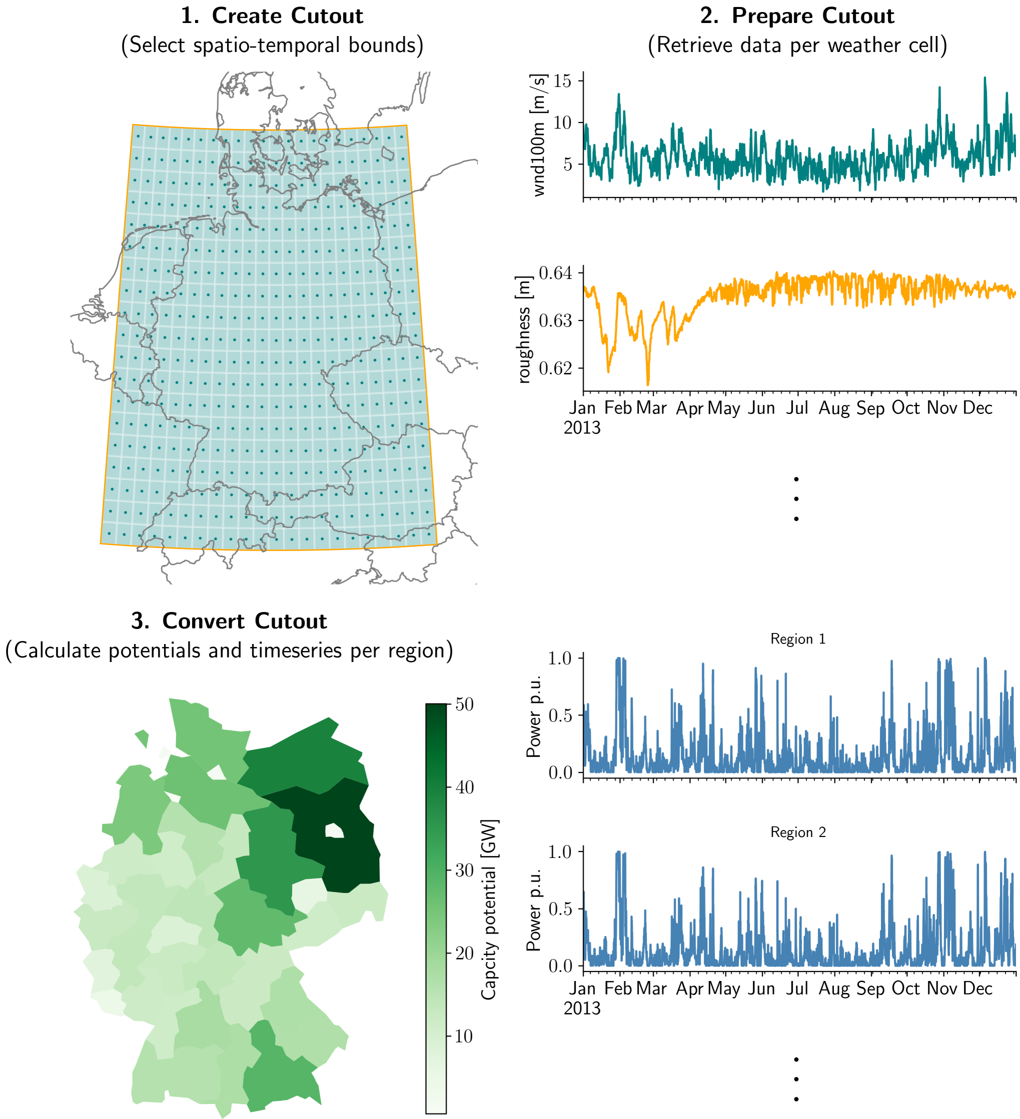

Figure 1: A typical workflow in `atlite` consists of the three steps: 1. Cutout creation, 2. Preparation, 3. Conversion.

Cutout Creation and Preparation

The Cutout creation requires specifications of the geographical and temporal bounds, the path of the associated `netcdf` file to be created and the data source referred to as *module*.

Optionally, the temporal and spatial resolution may be adjusted. The default is set to 1 hour and 0.25° latitude times 0.25° longitude. So far, `atlite` supports three different *modules*:

1. ECMWF Reanalysis v5 (ERA5) provides various weather-related variables in an hourly resolution from 1950 onward on a spatial grid with a 0.25° x 0.25° resolution, most of which is reanalysis data. `atlite` automatically retrieves the raw data using the Climate Data Store (CDS) API after the initial set up by the user. When the requested data points diverge from the original grid, the API retrieves interpolated values based on the original grid data.
2. Heliosat (SARAH-2) provides satellite-based solar data in a 30 min resolution from 1983 to 2015 on a spatial grid ranging from -65° to +65° longitude/latitude with a resolution of 0.05° x 0.05°. In case of a diverging Cutout grid, a resampling function provided by `atlite` projects the data accordingly. The full dataset cannot be automatically retrieved and must be downloaded by the user beforehand.
3. GEBCO is a bathymetric dataset covering terrain heights on a 15 arc-second resolved spatial grid. Using an averaging resampling method, the data is projected to the Cutout resolution. The full dataset cannot be automatically retrieved and must be downloaded by the user beforehand.

Creating a Cutout triggers the program to initialize the grid cells and the coordinate system on which the data will lay. As indicated in Figure 1, the shapes of the grid cells are created such that their coordinates are centered in the middle. As soon as the Cutout preparation is executed, `atlite` retrieves/loads data variables, adds them to the Cutout and finally stores the Cutout in a `netcdf` file. `atlite` groups weather variables into *features*, which can be used as front-end keys for preparing a subset of the available weather variables. The following table shows the variable groups for all datasets.

feature	ERA5 variables	SARAH-2 variables	GEBCO variables
height	height		height
wind	wnd100m, roughness		
influx	influx_toa, influx_direct, influx_diffuse, albedo	influx_direct, influx_diffuse	
temperature	temperature, soil_temperature		
runoff	runoff		

A Cutout may combine features from different sources, e.g. 'height' from GEBCO and 'runoff' from ERA5. Future versions of atlite will likely introduce the possibility to retrieve explicit weather variables from the CDS API. Further, the climate projection dataset CORDEX, for which support was dropped with the latest release `v0.2` due to compatibility issues, is likely to be reintroduced.

Conversion Functions

`atlite` currently offers conversion functions for deriving time series and static potentials from Cutouts for the following types of renewables:

- **Solar photovoltaic** – Two alternative solar panel models are provided based on Huld et al. (2010) and Beyer et al. (2004), both of which use the clear sky model from Reindl et al. (1990) and a solar azimuth and altitude position tracking based on Kalogirou (2009), Michalsky (1988) and Sproul (2007) combined with a surface orientation algorithm following Sproul (2007). Optionally, optimal latitude heuristics from Landau (2017) are supported.

- **Solar thermal collector** – Low-temperature heat for space or district heating is implemented based on the formulation in Henning & Palzer (2014), which combines average global radiation with storage losses dependent on the current outside temperature.
- **Wind turbine** – The wind turbine power output is calculated from down-scaled wind speeds at hub height using either a custom power curve, one of 16 predefined wind turbine configurations, or any of those listed in the OEP Wind Turbine Library. Optionally, convolution with a Gaussian kernel for region-specific calibration given real-world reference data as presented by Andresen et al. (2015) is supported.
- **Hydro run-off power** – A heuristic approach uses surface run-off weather data (e.g. from rainfall or melting snow) which is normalized to match reported energy production figures by the EIA. The resulting time series are optionally weighted by the height of the run-off location and may be smoothed for a more realistic representation.
- **Hydro reservoir and dam power** – Following Liu et al. (2019) and Lehner & Grill (2013), run-off data is aggregated to and collected in basins which are obtained and estimated in their size with the help of the HydroSHEDS dataset.
- **Heating demand** – Space heating demand is obtained with a simple degree-day approximation where the difference between outside ground-level temperature and a reference temperature scaled by a linear factor yields the desired estimate.

The conversion functions are highly flexible and allow the user to calculate different types of outputs, which arise from the set of input arguments. In energy system models, network nodes are often associated with geographical regions which serve as catchment areas for electric loads, renewable energy potentials and more. As indicated in the third step of Figure 1, `atlite`'s conversion functions allow projecting renewable time series on a set of regions. Therefore, `atlite` internally computes the Indicator Matrix **I** with values $I_{r,x,y}$ representing the per-unit overlap between region r and the grid cell at (x, y). Then, the resulting time series $\varphi_r(t)$ for region r is given by

$$\varphi_r(t) = \sum_{x,y} I_{r,x,y}\, \varphi_{x,y}(t),$$

where $\varphi_{x,y}(t)$ is the converted time series of grid cell (x, y). Further, the user may define custom weightings $\lambda_{x,y}$ of the grid cells, referred to as layout, representing, for instance, the spatial distribution of installed capacities within a region, which modifies the above equation to

$$\varphi_r(t) = \sum_{x,y} I_{r,x,y}\, \lambda_{x,y}\, \varphi_{x,y}(t).$$

The conversion functions may optionally return the per-unit time series $\tilde{\varphi}_r(t) = \varphi_r(t)/c_r$ where c_r is the installed capacity per region given by

$$c_r = \sum_{x,y} I_{r,x,y}\, \lambda_{x,y},$$

which may be returned as an output as well.

The Journal of Open Source Software

Land-Use Restrictions

Land-use restrictions limit the deployment of renewables infrastructure. Wind turbines, for example, may only be placed in eligible places which have to fulfill general and country-specific requirements, e.g. being outside of protected areas or at a sufficient distance to residential areas.

`atlite` provides a performant, parallelized implementation to calculate land-use availabilities within all grid cells of a Cutout. As illustrated in Figure 2, the entries $A_{r,x,y}$ of an Availability Matrix **A** indicate the overlap of the eligible area of region r with grid cell at (x, y). Note that this is analogous to the Indicator Matrix **I** but with reduced area. The user can exclude geometric shapes or geographic rasters of arbitrary projection, like specific codes of the Corine Land Cover (CLC) database. To determine capacity expansion potentials per region, `atlite` does not use an explicit placement algorithm (e.g. for wind turbines), but the product of available area and allowed deployment density. The implementation is inspired by the GLAES (Ryberg et al., 2018) software package, which itself is no longer maintained and incompatible with newer versions of the underlying GDAL software.

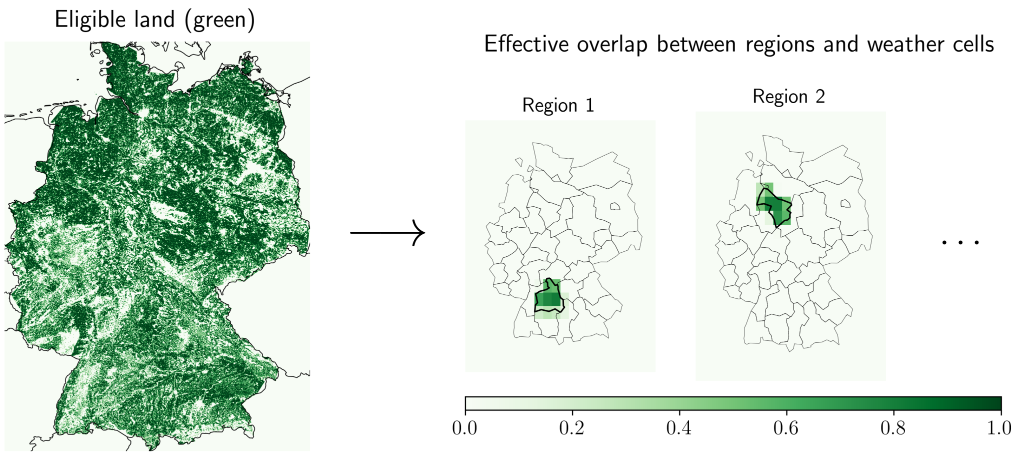

Figure 2: Example of a land-use restrictions calculated with `atlite`. The left side shows a highly-resolved raster with available areas in green. In this example all urban and forest-like sites are excluded areas, drawn in white. The right side visualizes exemplary entries per region r of the resulting Availability Matrix **A**.

Related Research

`atlite` is used by several research projects and groups. The PyPSA-Eur workflow (Hörsch et al., 2018) is an open model dataset of the European power system which exploits the full potential of `atlite` including Cutout preparation and conversion to wind, solar and hydro reservoir time series with restricted land-use availabilities. The sector-coupled extension PyPSA-Eur-sec (Brown et al., 2018) calculates heat-demand profiles as well as heat pump coefficients with `atlite`. The Euro Calliope studied in Tröndle et al. (2020) uses `atlite` to generate hydroelectricity time series from reservoirs. The interactive tool model.energy also employs the `atlite` libary.

Availability

Stable versions of the `atlite` package are available for Linux, MacOS and Windows via `pip` in the Python Package Index (PyPI) and for `conda` on conda-forge. Upstream versions and development branches are available in the projects GitHub repository. Documentation including examples are available on Read the Docs. The `atlite` package is released under GPLv3 and welcomes contributions via the project's GitHub repository.

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RESEARCH ARTICLE

Import options for chemical energy carriers from renewable sources to Germany

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Abstract

Import and export of fossil energy carriers are cornerstones of energy systems world-wide. If energy systems are to become climate neutral and sustainable, fossil carriers need to be substituted with carbon neutral alternatives or electrified if possible. We investigate synthetic chemical energy carriers, hydrogen, methane, methanol, ammonia and Fischer-Tropsch fuels, produced using electricity from Renewable Energy Source (RES) as fossil substitutes. RES potentials are obtained from GIS-analysis and hourly resolved time-series are derived using reanalysis weather data. We model the sourcing of feedstock chemicals, synthesis and transport along nine different Energy Supply Chains to Germany and compare import options for seven locations around the world against each other and with domestically sourced alternatives on the basis of their respective cost per unit of hydrogen and energy delivered. We find that for each type of chemical energy carrier, there is an import option with lower costs compared to domestic production in Germany. No single exporting country or energy carrier has a unique cost advantage, since for each energy carrier and country there are cost-competitive alternatives. This allows exporter and infrastructure decisions to be made based on other criteria than energy and cost. The lowest cost means for importing of energy and hydrogen are by hydrogen pipeline from Denmark, Spain and Western Asia and Northern Africa starting at 36 EUR/MWh_{LHV} to 42 EUR/MWh_{LHV} or 1.0 EUR/kg_{H2} to 1.3 EUR/kg_{H2} (in 2050, assuming 5% p.a. capital cost). For complex energy carriers derived from hydrogen like methane, ammonia, methanol or Fischer-Tropsch fuels, imports from Argentina by ship to Germany are lower cost than closer exporters in the European Union or Western Asia and Northern Africa. For meeting hydrogen demand, direct hydrogen imports are more attractive than indirect routes using methane, methanol or ammonia imports and subsequent decomposition to hydrogen because of high capital investment costs and energetic losses of the indirect routes. We make our model and data available under open licenses for adaptation and reuse.

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github.com/euronion/trace/releases/tag/2022.11.07 as well as the underlying technology cost assumptions https://github.com/pypsa/technology-data/tree/v0.4.0.

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Abbreviations: AE, alkaline electrolysis; **AR**, Argentina; **ASU**, air separation unit; **AU**, Australia; **CAPEX**, Capital Expenditures; **CC**, carbon capture; **CF**, Capacity Factor; **DAC**, Direct Air Capture; **DBT**, dibenzyltoluene; **DE**, Germany; **DK**, Denmark; **EAC**, Equivalent Annual Cost; **EG**, Egypt; **ES**, Spain; **ESC**, Energy Supply Chain; **ESF**, energy surplus factor; **EU**, European Union; **FOM**, Fixed Operation & Maintenance; **FT fuel**, Fischer-Tropsch fuel; **FTD**, Fischer-Tropsch-Diesel; **GDP**, gross domestic product; **GEGIS**, GlobalEnergyGIS; **GIS**, geographic information system; **GWA**, Global Wind Atlas; **GWP**, global warming potential; **HVDC**, High-Voltage Direct Current; **IRENA**, International Renewable Energy Agency; **LCoE**, Levelised Cost of Energy; **LCoH**, Levelised Cost of Hydrogen; **LHV**, Lower Heating Value; **LNG**, liquefied natural gas; **LOHC**, Liquid Organic Hydrogen Carrier; **MA**, Morocco; **MCoE**, Marginal Cost of Energy; **MSR**, methanol steam reforming; **OECD**, Organisation for Economic Co-operation and Development; **PEM**, proton exchange membrane; **PV**, photovoltaics; **RES**, Renewable Energy Source; **SA**, Saudi Arabia; **SMR**, steam methane reforming; **SNG**, synthetic natural gas; **USA**, United States of America; **WACC**, Weighted Average Cost of Capital; **WANA**, Western Asia and Northern Africa.

Introduction

Climate change mitigation efforts are driving energy transitions across the world. In these efforts alternatives for established fossil energy carriers are being sought. These aspirations gained additional traction with the plans of major international players like China, the European Union (EU) and United States of America (USA) to become climate neutral by the middle of this century. With technologies for the electricity sector already existing, these plans require a shift of focus to the industrial, heating and mobility sectors. Today's and tomorrow's energy demand of these sectors will have to be met with climate neutral and sustainable alternatives. The same requirements also hold for industrial feedstock which have to be de-fossilised. For some countries producing chemical energy carriers and feedstock from domestic RES or other near-zero-carbon energy sources may be an option. For other countries this will prove challenging due to geographical, sociological or technological restrictions. Germany can be considered such a country where limited potentials for domestic energy generation will presumably be insufficient to to meet energy demand for chemical energy carriers. Nowadays Germany strongly relies on energy imports, which made up more than 76% (approximately 13.5 EJ) of Germany's domestically handled energy in 2018 [1]. Despite a high population density and mediocre RES potentials in a world-wide comparison, Germany has commited itself to RES as a future source of energy. With these limitations the continued import of energy should be investigated, where fossil carriers are substituted by synthetic chemical energy carriers produced from RES.

Compared to electrical or heat energy, chemical energy carriers are easy to transport and store, making them a preferred option for energy exports. Aided by pre-existing infrastructure and experience from handling of fossil energy carriers, extensive use and significant trade volumes of synthetic chemical energy carriers from RES can be expected by 2050. One option, hydrogen, is currently receiving renewed world-wide attention with an increasing number of nations adopting hydrogen strategies. A convergence to a system with one single predominant chemical energy carrier might not be ideal: Depending on the end use the adaptation of processes to a different chemical, e.g. hydrogen, will have to be weighed against substituting fossil chemicals with synthetic drop-in alternatives. Adding to the complexity of this decision are the different chemical and energy carrier specific properties which influence the conditions and behaviour of a chemical during transport and storage. It therefore becomes important to gain insight into the costs, composition and interaction of steps inside potential future chemical Energy Supply Chains (ESCs).

Previous works have already analysed possible schemes for sourcing chemical energy carriers. Fasihi et al. [2] conducted a world-wide analysis on how renewable energy sources may be combined with other technologies to locally provide electricity and hydrogen at baseload quality and determined possible cost developments for 2020 to 2050. With a focus on synthetic fuels another study by Fasihi et al. [3] analysed an ESC for Fischer-Tropsch-Diesel (FTD) and synthetic natural gas (SNG) (methane) from the Maghreb region to Europe. Watanabe et al. [4] and later Heuser et al. [5] modelled green liquefied hydrogen production and transport from Patagonia to Japan. Ishimoto et al. [6] analysed the cost for transporting hydrogen and ammonia from Norway to Japan and compared it with transport to the Port of Rotterdam in Europe. Lanphen [7] also looked into ship-based supply chain options for importing liquid hydrogen, ammonia and methylcyclohexane from various exporting ports to the Port of Rotterdam. Niermann et al. [8] explored the transport of hydrogen using a variety of Liquid Organic Hydrogen Carriers (LOHCs) and compared their results against a hydrogen gas pipeline system to supply the energy carrier over a distance of 5000 km to Germany (DE). Schorn et al. [9] compared shipping of methanol with shipping of H_2 (l) from Saudi Arabia (SA) to DE and the economic viability depending on H_2 and CO_2 feedstock costs. More recently a number of global studies and analysis for importing hydrogen and other energy carriers from various regions around the world to DE have been released [10–13]. With a stronger focus on downstream infrastructure and energy distribution to end users, Runge et al. [14] compared the costs for transport fuels in a well-to-wheel analysis for mobility services in Germany. A global view on international hydrogen trade was taken by Heuser et al. [15] who modelled transport by pipeline and ship to determine optimal global supply costs. Later, International Renewable Energy Agency (IRENA) [16] gave an outlook on global energy trade scenarios for RES-based hydrogen and additionally ammonia.

While each case study provides important insights, it is difficult to compare these studies due to their different system boundaries, limited subsets of overlapping technologies, different energy carriers and regions investigated.

With this study we add several novel features to the existing literature. First we provide a comprehensive comparison of multiple ESCs from several different countries based on uniform assumptions and system boundaries. Secondly we deduct local electricity demand from the renewable resource availability in exporting countries, so that the best resources may be used locally. Thirdly we design our ESCs to work as islanded systems and be energy self-sufficient. Fourthly we make our data and model available under open licenses to allow for reproduction, adaptation and reuse.

Materials and methods

In this section we first describe how our ESCs are structured. The investment optimisation problem is outlined followed by a description of the assumed technologies and a motivation for the countries selected. We then illustrate how RES potentials and feed-in are derived domestic demand is considered. We end this section by motivating our choice of Weighted Average Cost of Capital (WACC) and an overview of the technical model structure. The most important equations on which this model builds are given in S3 Appendix.

Design of Energy Supply Chains

We model and investigate ESCs for chemical energy carriers starting at the energy source in an exporting country until the energy carriers are available in the importing country, in this analysis choosen to be DE. The ESCs considered in this study are export of a.) electricity by High-Voltage Direct Current (HVDC) with conversion to hydrogen in DE, b.) hydrogen gas by pipeline, c.) methane gas by pipeline, d.) liquid hydrogen by ship, e.) liquid methane by ship, f.) liquid ammonia by ship, g.) liquid methanol by ship, h.) hydrogen bound to LOHC dibenzyltoluene (DBT) [8] by ship, i.) liquid Fischer-Tropsch fuels (FT fuels) (kerosene-like) by ship. Fig 1 shows a schematic representation of all ESCs. For ESCs transporting ammonia, methane and methanol, an optional cracking step to hydrogen is further included for the case that the consumer needs pure hydrogen. Key properties of the chemical energy carriers are listed in Table 1.

The basic idea of the ESCs is shown in Fig 1. Detailed representations for all components, energy and chemical flows considered in each ESC are included in S1 Fig. In each ESC we consider

a.) sourcing of energy as electricity from RES,

b.) sourcing of the major chemical feedstock for synthesis i.e. water from seawater desalination, carbon-dioxide (CO_2) using Direct Air Capture (DAC) and nitrogen (N_2) using an air separation unit (ASU) from ambient air,

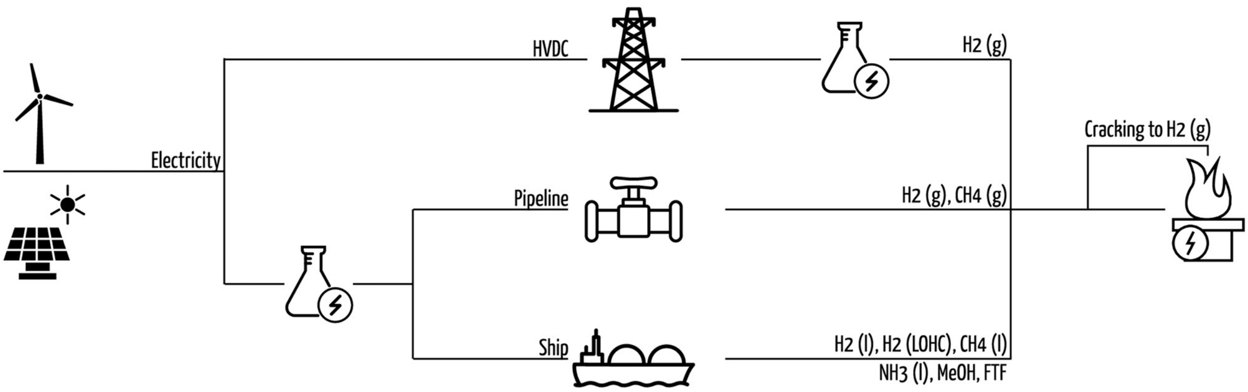

Fig 1. Schematic representation of ESCs considered in this study. ESCs cover electricity generation from RES, intermediary buffer storage for electricity and chemicals, conversion to chemical energy carriers, conditioning and transport from exporter to importer. Each ESCs delivers one out of five chemical energy carriers. Detailed representations of each ESC and all involved technologies are included in S1 Fig. License for icons: CC-BY-3.0 [17–21] and CC-0.

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c.) electrolysis of hydrogen and optional synthesis (hydrogenation) of the chemical energy carrier,

d.) necessary conversion of the energy carriers for transport, e.g. compression or liquefaction,

e.) back-conversion into the energy carriers' usable form at ambient conditions, e.g. relaxation or evaporation.

If downstream processes require energy as input in addition to chemical feedstock, then this energy is provided from within the ESC. Either electricity is used for processes on the exporter side or the currently available chemical energy carrier is used, e.g. the propulsion energy for shipping is provided using the energy carrier transported by the ship and LOHC dehydrogenation uses part of the transported hydrogen. We exclude the transport within the exporting and importing country and storage in the importing country, i.e. excluded is

1. transport of electricity, feedstocks and chemical energy carriers between facilities and to the export terminal

Table 1. Energy content of chemical energy carriers considered.

Energy carrier	State of matter (normal conditions)	Specific energy[a] [MWh/t]	Hydrogen content [wt. %]
Hydrogen H_2 (g) / (l)	Gas / Liquid (cryogenic)	33.33	100
LOHC (DBT)[b]	Liquid	1.87[c]	5.6[d]
Methane CH_4 (g) / (l)	Gas / Liquid (cryogenic)	13.89	25
Ammonia NH_3	Gas / Liquid (cryogenic)	5.17	17
Methanol MeOH (CH_3OH)	Liquid	5.54	12.5
FT fuel	Liquid	11.95	- (var.)

Values based on [22].

[a] All values represent the LHV.

[b] LOHC chemical is not consumed and reused, hydrogen is the chemical energy carrier delivered to the importer.

[c] H_2 share.

[d] DBT can hold up to 6.2% H_2, a depth-of-discharge for cycling at 90% is favourable for (de-)hydrogenation [14].

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2. short-term or long-term storage at the importer in DE
3. distribution and end use of chemical energy carriers within DE

We exclude these steps because the range of possible options, such as the time patterns of the demand, would create too many scenarios and detract from the generality of our analysis. Such scenarios are better suited for investigation in specific case studies.

The ESCs are generally designed to not interact with any systems outside the ESCs. This design decision excludes the possibility for use of secondary products such as process heat and cooling services from cryogenic carriers, the sale of chemical by-products such as O_2. Also excluded are possible synergies by sector-coupling to heat and electricity systems on the exporter's and importer's sides, e.g. of industrial waste heat into the ESCs. Integration with other processes and commercial use of secondary products may provide grounds for business cases and lower market prices for chemical energy carriers.

Investment optimisation problem

We model and optimise for least-cost investment of the essential components of ESCs to supply an annual energy demand. The ESCs components include electricity generators and generation based on historic weather data, conversion processes, buffer storage and transport between countries. The ESCs with their components, energy and mass flows are modelled using the open source modelling framework PyPSA [23]. We use a greenfield approach for our model and disregard existing infrastructure. We justify this modelling decision as a comparable scale of infrastructure described by the ESCs does not yet exist anywhere. Minimum annual investment costs are determined for each ESC based on the annualised cost c_i of every single component i. The annualised cost represent cost for investment Capital Expenditures (CAPEX) C_i and Fixed Operation & Maintenance (FOM) and are annualised using the Equivalent Annual Cost (EAC) method:

$$c_i = C_i \cdot (\mathrm{A}_i + \mathrm{FOM}_i) \tag{1}$$

where the component-specific annuity factor A_i is

$$\mathrm{A}_i = \frac{(1+r)^{\mathrm{lifetime}(i)} \cdot r}{(1+r)^{\mathrm{lifetime}(i)} - 1} \tag{2}$$

The annual interest rate r is assumed equal to the selected WACC discussed below. The objective function to be optimised for minimal investment is

$$\min\left\{ \sum_{i\in\mathrm{Generators}} c_i \cdot G_i + \sum_{i\in\mathrm{Converters}} c_i \cdot F_i + \sum_{i\in\mathrm{Storage}} c_i \cdot H_i \right\} \tag{3}$$

where generators (e.g. photovoltaics (PV)) are considered with their nominal capacities G_i (e.g. MW), converters (e.g. compressors, electrolysers) with their throughput capacity F_i (e.g. tonne per hour t/h, MW) and storage components (e.g. batteries, tanks) with their storage capacity H_i (e.g. MWh, m^3). The optimisation is subject to constraints which ensure conservation of energy and mass flow and runs at hourly resolution. Most components may be freely dispatched without restrictions on ramping rates and minimum must-run capacities, as most technologies are usually flexible within a below hourly time-scale. Must-run capacities are only enforced for the synthesis of methane, ammonia, methanol and FT fuel, see the discussion in the technologies section. RES electricity feed-in is limited to the individual modelled time-series and excess electricity may be freely curtailed.

RES capacities may only be extended to the maximum potentials of their respective technology and resource quality class determined through geographic information system (GIS)-analysis, see the section on electricity supply below for details. The nominal capacities of all other components may be freely extended without limit. Capital costs for all components scale linearly with their capacity representing a situation where capacity expansion requires new facilities rather than extending existing ones. The used capital costs and FOM already assume large scale facilities with respective economies of scale applied as well as exogenous learning rates for cost reductions between 2030 to 2050. Process efficiencies are assumed constant for all years (see S4 Table) due to the difficulty of making well-founded estimates for future technological developments and improvements. One exception is made for hydrogen electrolysis where efficiency is expected to increase across all available technology options [24, 25], an improvement which would affect all ESCs presented here. Thus the electricity-to-hydrogen (Lower Heating Value (LHV)) efficiency for electrolysis is assumed to improve from 68% in 2030 to 71.5% in 2040 and 75% in 2050.

Choice of technologies and energy carriers

The following section discusses the chemical energy carriers listed in Table 1 and their simplified production pathways. For most production pathways, alternative methods and integrated technologies with potential for efficiency improvement exist. Integrated technologies and alternative technology options are beyond the scope of our investigation and not discussed further.

Renewable energy sources. We select utility PV, on-shore and off-shore wind as the only sources of energy for our model. We consider these technologies the only available ones with sufficient modularity and possibility for quick build up to high capacities while delivering near-zero carbon electricity necessary for a sustainable deployment. We consider the following other sources of energy unsuitable (with selected reasons):

a.) hydro power (prioritised for domestic demand, limited geographical locations, significant environmental impact, poor modularity and scalability),

b.) concentrated solar power (limited to specific geographical locations, low modularity and scalability),

c.) conventional nuclear fission (intransparent cost, unmodular and difficult deployment, sustainability issues with fuel and waste streams),

d.) nuclear fusion and unconventional nuclear fission (insufficient technology readiness level with unclear techno-economic prospects).

Hydrogen. In all ESCs electricity is converted to the simplest chemical energy carrier, hydrogen, via alkaline electrolysis (AE). Compared to alternatives like proton exchange membrane (PEM) electrolysers, AEs electrolysers were historically considered to be less suitable to provide grid services due to their slow start-up times in the range of minutes [25]. For large scale operations in chemical energy carrier production the slow start-up time may be neglected because the electrolysis here does not need to provide grid services and the variability of RES feed-in can be managed using for example battery storage. The main advantages of AEs are that it is a well established technology which has in comparison to PEMs lower costs and does not require rare-earth-metals or platinum which may become bottlenecks for massive deployments in the future. In the case of large-scale hydrogen production and hydrogen-derived chemical energy carriers investigated here, we expect installations to run at high utilisation factors with a large number of modular units that can combine into a large unit to create virtual flexibility, thus negating the main weakness of AE. The necessary water for electrolysis is produced through desalination of seawater via reverse osmosis to achieve the required purity and conserve existing, potentially scarce fresh water resources.

Hydrogen as a chemical energy carrier is versatile and may also be used as a feedstock for chemical synthesis. The physical properties of hydrogen make it difficult to transport as a gas due to its low energy density and as a cryogenic liquid due to the very low temperature required and high energy demand for liquefaction (0.203 MWh/MWh_{LHV}).

Methane. Methane is an alternative gaseous energy carrier to hydrogen and is synthesised in established production processes through catalytic reaction of CO_2 with H_2 via the reverse water gas shift reaction:

$$CO_2 + 4\,H_2 \rightleftarrows CH_4 + 2\,H_2O \quad (4)$$

The synthesis is accompanied by adverse side reactions but can be run at high selectivity [26]. Transport of methane is well established and infrastructure for pipeline transport or transport as liquefied natural gas (LNG) already exists on large scales were synthetic methane may be used as drop-in replacement. Downsides are the emissions of CO_2 from combustion and methane during handling (leakage, slippage) and the high global warming potential (GWP) of methane. Liquefaction of methane requires less energy (0.036 MWh/MWh_{LHV}) than liquefaction of hydrogen and handling of cryogenic LNG is less complex and better established compared to liquefied hydrogen.

Ammonia. Ammonia is another option for an gaseous energy carrier and was already used as energy carrier in past applications. Ammonia is synthesised by hydrogenation of nitrogen in the Haber-Bosch reaction:

$$N_2 + 3\,H_2 \rightleftarrows 2\,NH_3 \quad (5)$$

Feedstock nitrogen gas N_2 is available through extraction from the atmosphere via e.g. cryogenic ASUs. The ammonia synthesis process is well-established and an increasing focus in research for direct energetic applications of ammonia can be seen. In comparison to H_2 or CH_4, NH_3 has a lower specific energy but a high boiling point at −33˚C, making it easier to handle as a liquid with a high volumetric energy density. In addition industry has long-standing experience of transporting and handling ammonia in its various forms, with around 10% of the global 183 Mt annual ammonia production being traded [27]. Direct energetic use of ammonia is possible but poses a range of challenges including suppression of NO_x emissions [28]. Alternatively ammonia may be used as hydrogen carrier where the dehydrogenation of NH_3 happens through thermal decomposition. The dehydrogenation process has high energy requirements ($>$ 25% of LHV [29]) and the technology is not yet fully commercially mature. Large specialised ammonia crackers are already in operation for the production of heavy water [27].

Methanol (MeOH). Methanol (MeOH) is a liquid organic compound with favourable properties for transport, storage and energetic use. It is obtained by hydrogenation of CO_2:

$$2\,CO_2 + 6\,H_2 \rightleftarrows 2\,CH_3OH + 2\,H_2O \quad (6)$$

either in a direct catalytic methanolisation reaction or by an indirect route using a reverse water gas shift reactor to obtain syngas [30]. With an annual production volume of ca. 100 Mt [31] methanol synthesis is a well-established process with industry experience in handling, storage and transport. Methanol is used either as a industrial feedstock, for power and heat generation, as a mobility fuel [32, 33] and also be considered a member the LOHC family with the dehydrogenated form being CO_2 [8]. Methanol-to-hydrogen cracking (steam methanol reforming) is mature on small industrial scales [34] and practical where methanol logistics are easier than logistics for alternative hydrogen feedstocks like e.g. natural gas.

Fischer-Tropsch fuels (FT fuels). Liquid fuels like Fischer-Tropsch-Diesel or kerosene can be produced from CO_2 and H_2 via Fischer-Tropsch synthesis. These fuels can be used as drop-in replacements for today's fossil based fuels and are simple to transport and store due to their liquid nature. The catalytic Fischer-Tropsch synthesis is not very selective and yields a mixture of hydrocarbon products, requiring post-processing to yield FT fuels [35]. We neglect gaseous outputs like fuel gases which constitute approximately 20% of the output [25] in our analysis and assume the products to have an average LHV of 11.95 MWh_{th}/t which is similar to regular diesel and aviation kerosene. Fischer-Tropsch synthesis is well established process using fossil syngas and infrastructure as well as experience from fossil hydrocarbon handling can be directly applied to FT fuels.

Liquid Organic Hydrogen Carrier (LOHC). LOHC is the last chemical energy carrier we consider which allows for piggyback transport of hydrogen. We choose DBT as a representative of the variety of LOHCs available [8]. Between its dehydrogenated ('unloaded', H0DBT) and hydrogenated ('loaded', H18DBT) form it may be loaded with up to 9 H_2:

$$9\,H_2 + C_{21}\,H_{20} \rightleftarrows C_{21}H_{38} \tag{7}$$

For repetitive cycling and favourable (de-) hydrogenation a depth of discharge of 90% is more favourable [14] corresponding to 5.6 wt. % H_2. One significant advantage of DBT is that its properties do not change significantly between its hydrogenated and dehydrogenated form, allowing for the same infrastructure to be reused to achieve a closed LOHC cycle. The cost for the LOHC chemical DBT is assumed to be 2264 EUR_{2015}/t. The LOHC can be easily handled and stored with infrastructure similar to that of commonly traded liquid carbohydrates. To access the hydrogen stored it has to be dehydrogenated which requires about 28% of the hydrogen content as energy [8] as we assume the necessary heat has to be provided by the ESC itself and is not provided from an external source.

CO_2 feedstock. Methane, methanol and FT fuels require carbon dioxide (CO_2) as feedstock for synthesis. In our model all CO_2 feedstock is sourced from atmospheric CO_2 using DAC, thus creating a closed carbon cycle via the atmosphere between energy carrier synthesis and use. We do not consider the alternative approach of carbon capture (CC) at the location of use and back-transport of pure CO_2 to the location of energy carrier synthesis via a dedicated CO_2 infrastructure. This approach would require guaranteed capture of CO_2 from all use cases, which will prove complicated for applications where concentrated point sources are not available, like in aviation and individual mobility. Another obstacle to a perfect carbon cycle via CC is carbon leakage from imperfect CC which would need to be compensated through DAC infrastructure to ensure atmospheric carbon neutrality. Finally the infrastructure for recirculation of CO_2 would for most ESCs require additional dedicated infrastructure for CO_2 transport, incurring additional costs and complexity. While the costs of carbon capture at the location of use and back-transport may not be prohibitive, but such closed carbon cycles would require detailed analysis that is out of the scope of this paper. For the LOHC ESC recirculation is considered here as the infrastructure for recirculation of DBT in the LOHC ESC is the same as required for delivery of the hydrogen-loaded energy-carrying LOHC.

Battery and chemical storage. Storage technologies are essential for balancing the variable nature of RES electricity, buffering chemical feedstock and storing chemical energy carriers before export. Storage technologies smoothen the utilisation of downstream processes by buffering variable upstream processes like RES or hydrogen production in RES-follow mode. Storage capacity expansion is an alternative way to increase process capacities by additionally increasing downstream utilisation rates and thus leading to lower Levelised Cost of Energy (LCoE) if the investment into storage capacity is lower than into process capacity expansion. In our model electricity from RES may be stored in a battery buffer storage. CO_2 as a feedstock gas may be stored in liquefied form. Hydrogen and methane may be stored for short term buffer storage in a compressed form as their liquefaction process is energy and capital intensive. Larger amounts of any chemical are only stored in liquid form to reduce the necessary storage volume. For hydrogen and methane this requires energy intensive and well insulated tanks to store both liquids at cryogenic temperatures. Underground storage like salt caverns for gases are not considered to keep our ESCs independent of location and geological conditions. In comparison ammonia liquefaction and storage is significantly easier as its boiling point is only −33˚C and thus ammonia may be stored in liquefied form. Storage tanks for methanol, LOHC and FT fuel are straightforward as they correspond to today's technologies used for light and heavy hydrocarbons. The storage technology options available for each ESC are as shown in S1 Fig. Storage capacities are endogenously determined by the model and represent optimal capacities under the given constraints minimising the objective function.

Flexibility of synthesis processes. In addition to the economic perspective of operating synthesis processes at a high utilisation rate, some synthesis processes may be designed for continuous operation from a chemical process point of view [25, 26] and not be suited for flexible operation or standby. We consider this by assuming a must-run capacity for the methanation and ammonia synthesis processes of 30% each, based on what could potentially be feasible for the methanation [26] and Haber-Bosch [25] processes. Methanol and FT fuel synthesis are assumed to run at a minimum of 94.25% capacity corresponding to a maximum of 3 weeks downtime for e.g. maintenance per year. The must-run capacity is assumed for the aggregated availability factor of the whole respective process plant, e.g. a must-run capacity of 94.25% translates to a maximum of 5.75% of the facilities capacities being unavailable for maintenance or other reasons at the same time (see S3 Appendix).

Transport: Transmission lines, pipelines and ships. Transfer of the energy between exporting and importing country plays a significant role due to the different characteristics between transport modes. HVDC transmission lines for transfer of electricity and pipelines for hydrogen and methane gas are already deployed technologies. These technologies allow for a continuous export-import supply stream. We consider here average costs, energy demand and distance-related losses for HVDC transformers, transmission lines, pipelines and pipeline compressors for above-ground if geographically possible. For imports from Argentina (AR) and Australia (AU) subsea connectors are unavoidable and we consider average subsea HVDC transmission line and subsea pipeline costs. The pipeline compressor costs in these few cases are the same as for above-ground pipelines due to a lack of reference numbers for long-distance deep-sea pipeline connectors. The numbers may thus prospectively underestimate real compressor costs. Shipping is the third class of transport modes considered and characterised by a non-continuous and delayed transfer of the energy carrier. We take this shipping characteristics into account by not allowing for concurrent use of loading and unloading infrastructure by different (groups of) ships at the same time. Rather than having ships travel at their (maximum) average cruise speeds and wait for the (un-) loading terminals to become available we create ex ante shipping schedules with lowered cruise speeds such that the arrival and departure of (groups of) ships does not overlap. The shipping distance along sea routes affect the shipping duration in the shipping schedules and the energy demands for propulsion, optional onboard refrigeration of boil-off gases and finally the necessary number of ships.

Countries investigated

In our study we investigate large scale energy imports to Germany (DE) from the various countries shown in Fig 2. Germany as a country is interesting, as it heavily relies on energy imports today, is phasing out nuclear power and has less abundant renewable energy resources compared to other countries. We assume an energy import volume of 120 TWh based on the estimated hydrogen energy demand (LHV) for 2030 in the German Hydrogen Strategy [36]. On the one hand this number may seem ambitious given the high German fossil energy imports today and that its hydrogen production currently is mostly captive or merchant hydrogen from fossil sources without carbon capture. On the other hand we also presume an increase of this volume by 2040 and 2050 as not only fossil energy carriers but also industrial feedstock will have to be substituted by hydrogen or other chemicals. The import volume in our model is considered as annual demand since hydrogen uses and their demand patterns are yet to be known. This way it is decoupled from a specific demand pattern such with constant baseload or seasonally changing hydrogen demand and their case-specific buffer storage needs. As a reference we model and include chemical energy carriers produced from domestic resources in DE. The other countries included in our study are:

a.) Spain (ES), an EU country with high solar potentials,

b.) Denmark (DK), an EU country in close proximity to DE with high wind potentials,

c.) Morocco (MA), Egypt (EG) and Saudi Arabia (SA), representative countries in relative proximity to the EU with low population densities and high renewable potentials,

d.) Argentina (AR), a country repeatedly investigated by similar studies for exports of hydrogen to Japan,

e.) Australia (AU), a country discussed for energy exports to DE and as a possible future powerhouse for Asian countries.

The distance of an export-import route ESC influences the associated costs. With increasing distance investment costs, transportation energy demand, losses and duration (for shipping)

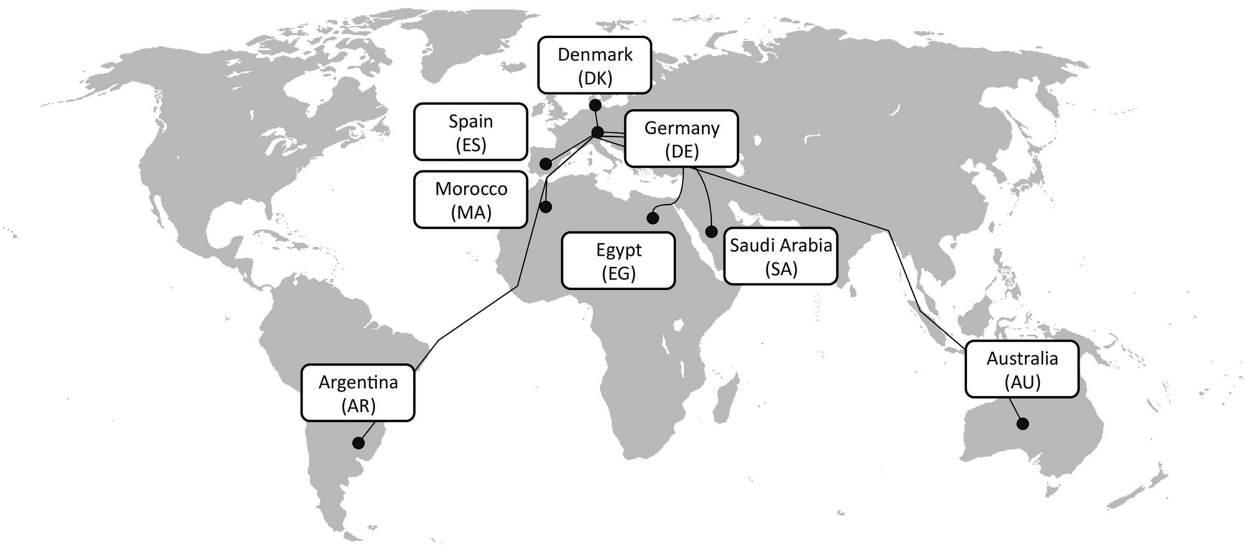

Fig 2. Countries considered for export. Exports of chemical energy carriers from countries shown to Germany (DE) are modelled and investigated for nine different Energy Supply Chains (ESCs).

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Table 2. Distances between exporting countries and DE assumed for each ESC.

From	Code[a]	Distance[b] [km]	HVDC line[c] [km]	Pipeline[d] [km]	Ship[e] [km]
Argentina	AR	12 280 (3000)	14 736 (3600)	17192 (4200)	13 056
Australia	AU	14 450 (3000)	17 340 (3600)	20 230 (4200)	20 284
Denmark	DK	580 (0)	696 (0)	812 (0)	812
Egypt	EG	3220 (0)	3864 (0)	4508 (0)	6605
Germany	DE	0 (0)	0 (0)	0 (0)	0
Morocco	MA	3330 (0)	3996 (0)	4662 (0)	2938
Saudi Arabia	SA	4240 (0)	5088 (0)	5936 (0)	12174
Spain	ES	1600 (0)	1920 (0)	2240 (0)	3587

Bracketed values indicate the share of submarine distances considered.

[a] Based on ISO 3166–1 alpha-2.

[b] As-the-crow-flies distance between region centres [38], measured in Google Maps.

[c] Distance times a detour factor 1.2, own estimate.

[d] Distance times a detour factor 1.4, based on [39].

[e] Shortest sea route, determined with [37].

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increase. The lengths of pipelines and transmission lines are based on the as-the-crow-flies distances between the country centres scaled by different detour factors for transmission lines (1.2) and pipelines (1.4). For AR and AU a land-only connection is not possible. We therefore estimate the share of distance to be traversed with submarine technologies based on the shortest cross-continental distances and scale them with the same detour factors as for land connections. A comparable approach with detour factors does not work for shipping routes as it does not account for land and water bodies. Instead we opt to use a freely available data source [37] to measure the shortest shipping routes. All resulting distances used are shown in Table 2.

Electricity supply, demand and supply curves

For each country we model RES potentials and time-series based on results from a GIS-analysis and historical weather data using the GlobalEnergyGIS (GEGIS) model [40]. Eligible areas for PV and wind installations are determined on a 1 km^2 grid resolution by exclusion of protected areas, unsuitable land types and areas of high population density. Areas not within a 400 km radius of a gross domestic product (GDP) density of 100 000 USD/km^2 are further excluded where the threshold serves as a proxy to grid access and location accessibility. For a detailed description we refer to [40], for maps of the resulting eligible area see S4 Fig. Annual capacity factors are determined for all eligible grid cells and types of RES using ERA5 reanalysis weather data and data from the Global Wind Atlas (GWA) for 2013 as representative weather year. Grid cells are then categorised into one of 100 quality classes (0% to 100% Capacity Factor (CF)) for each RES technology based on their annual capacity factor. From the categorisation the potential of each quality class for each of the three RES technologies is calculated assuming a deployable potential of 1.45 MW/km^2 (PV) and 3 MW/km^2 (on-shore and off-shore wind). This potential is a compromise between technical potential, accessible potentials and social acceptance used in another study for the European electricity grid [41]. For PV these potentials may be conservative for less population dense regions and closer to the equator where others consider 75 MW/km^2 (PV) and 8.4 MW/km^2 (wind) feasible [2]. For large continuous wind farms power densities may need to artificially be reduced to lessen wake effect penalties [42]. These influences become more relevant for exporters with already high potentials and flat supply curves and therefore should therefore not contribute a major influence on this studies' supply side.

In addition to the potentials we derive hourly generation time-series for each technology and quality class, resulting in a total of up to 300 independent RES time-series for each exporter.

From the annual generation for each quality class we can calculate each classes respective LCoE following

$$\mathrm{LCoE(RES)} = \frac{\text{Annualised cost}}{\text{Annual generation}} = \frac{\mathrm{CAPEX}}{G(2013)} \cdot \left[\mathrm{FOM} + \frac{r}{1-(1+r)^{-t}}\right] \quad (8)$$

assuming technology specific parameters (Table 3), as well as r = WACC and the modelled annual electricity generation G in 2013. By ordering the class potentials based on their LCoE we obtain country specific electricity supply curves. Fig 3 shows examples using 10% p.a. WACC and technology (cost) assumptions for 2030.

Using the supply curve we account for projected domestic electricity demand: We generate electricity demand projections with a machine learning approach implemented by GEGIS [40]. The demand projections are based on global datasets for GDP, calendar days, temperature from ERA5 and the SSP2-34 'Middle of the Road' scenario [44] for 2050. This approach extrapolates past demand into the future and cannot account for structural changes like increasing demand through electrification. The projections are thus to be considered conservative estimates for electricity demand. The projected demands are shown in Table 4.

We consider the domestic electricity demand by removing the equivalent volume and RES with the lowest cost RES supply from our model. This corresponds to reserving the capacities with lowest expected LCoE for domestic use. The respective volumes are marked in the supply curves by the black dashed lines for the shown example 2030 and 10% p.a. WACC. Changes to the RES technology costs (year assumption) and WACC assumption affect the order of RES and therefore change RES with associated time-series available for export. Considering the shape of the supply curves in Fig 3, this approach noticeably affects the Marginal Costs of Energy (MCoEs) for DE and Denmark (DK).

Choice of WACC

The choice of the costs of capital influences all cost calculations and is therefore crucial for meaningful results. [46] showed how configurations of a cost-optimised European electricity system change significantly from changes to WACC assumptions, especially non-homogeneous, country-specific assumptions. At the same time we are aware of the possible bias this might introduce, cf. [47].

Table 3. Main technology assumptions for RES and electrolysis.

Technology 2030/2040/2050	Lifetime [years]	CAPEX [$\mathrm{EUR_{2015}}$/kW]	FOM [% p.a.]	Density [$\mathrm{MW/km^2}$]	Efficiency [%]
PV (utility)	40/40/40	376/329/302	1.9/2/2.1	1.45	—
wind onshore	30/30/30	1035/978/963	1.2/1.2/1.2	3	—
wind offshore	30/30/30	1573/1447/1416	2.3/2.3/2.3	3	—
electrolysis	30/32/35	450/330/250	2/2/2	—	68/71.5/75

Assumptions based on [25, 43] used for 2030, 2040 and 2050. CAPEX reflects the engineering, procurement and construction price. A full list of all technology assumptions is included in S2 Table.

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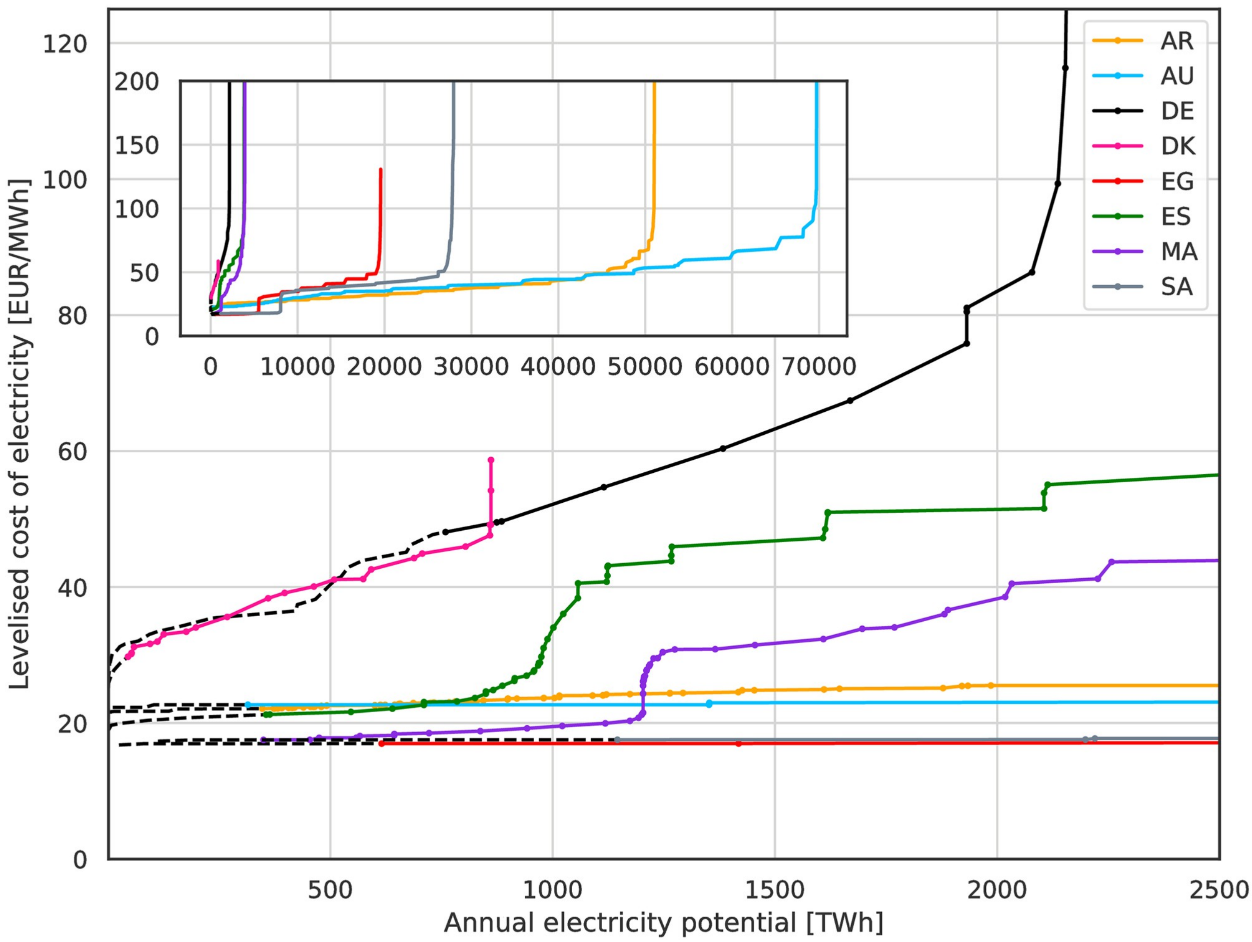

Fig 3. Modelled electricity supply curves for 2030 at 10% p.a. WACC. Dashed black parts are reserved for meeting domestic electricity demand and unavailable for export. The inlet contains the same plot on a larger scale. The visible step-wise increase in LCoE for ES and MA is where the cheapest electricity potentials from low cost PV are exhausted and the onshore and offshore wind enter the supply curve.

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Table 4. Used future (2050, projected) electricity demand and actual (2018) for reference.

Country	demand 2018 (actual)[a] [GWh]	demand used 2050 (projected) [GWh]
Argentina (AR)	125 030	346 904
Australia (AU)	234 278	314 389
Denmark (DK)	32 865	44 854
Egypt (EG)	150 579	615 351
Germany (DE)	533 177	759 065
Morocco (MA)	29 678	122 419
Saudi Arabia (SA)	322 373	1 145 638
Spain (ES)	245 426	355 416

[a] Source: [45].

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To retain comparability we assume time and technology independent WACC. We further choose to assume 10% p.a. WACC for all investments within all ESCs independent of the exporting country. This choice is founded on the assumptions used by IRENA, where the authors used inhomogeneous WACC assumptions of 10% p.a. for non-OECD countries and 7.5% p.a. for OECD countries and China in [48]. WACC for local RES projects usually depend on the technologies used and on individual project as well as country-specific risks [49]. It will therefore be interesting to see how WACC will develop for highly vertically integrated, multi-national and mixed-technology ESCs as presented here.

Technical model structure

We use a multi-step workflow hard-linked using snakemake [50]. In the first part of the work-flow we utilise GEGIS [40] to determine potentials for RES, RES generation time-series and predict electricity demand. In the second part of the workflow we implement the ESCs in PyPSA [23] and combine them with the RES potentials, RES time-series and demand predictions into one dedicated PyPSA model for each combination of ESC and exporting country. The structure is also visualised in S2 Appendix.

Results

Results are compared with a focus on their Levelised Cost of Energy and Levelised Cost of Hydrogen. The LCoE represent the costs for delivering 1 MWh of energy in the form of the energy carrier of the respective ESC, i.e. H_2 (g), CH_4 (g), NH_3 (g), methanol or FT fuel. For the Levelised Cost of Hydrogen (LCoH), costs are compared for delivering 1 MWh of H_2 (g) to the importer.

We first present LCoE for all ESCs and exporting countries for 2030. Then we show the development of LCoE based on technology cost projections up to 2050. Cost compositions for the ESCs are examined and main cost drivers discussed. We then continue by looking at the LCoH and by discussing sensitivities of the ESCs based on an sensitivity analysis for two selected scenarios. The sensitivity analysis shows an expected strong dependence to the choice of WACC on two selected ESCs from Spain (ES) to DE. We therefore also present LCoE and LCoH for 2030 to 2050 under a more optimistic choice for WACC of 5% p.a.. Additional results focusing on supply chain efficiency, curtailment rates and installed RES capacities are discussed in the S1 Appendix and S2 Fig. Presented results for LCoE and LCoH are included as tabular form in S1 and S2 Tables.

Energy import costs for 2030 to 2050

LCoE, i.e. total system cost per MWh_{th} delivered to DE, are shown in Fig 4 for 2030, 10% p.a. WACC and all exporting countries. The lowest cost options for import are by H_2 pipeline from DK at 75 EUR/MWh_{LHV} and at 83 EUR/MWh_{LHV} from Egypt (EG) and ES. All three ESCs take advantage of the low losses and investments associated with H_2 pipelines as static transport option and the short to medium transport distances to DE. With costs of 104 EUR/MWh_{LHV} domestic H_2 production in DE is less attractive than these imports. CH_4 imports by pipeline are the least cost attractive option of the three (HVDC to H_2, H_2 & CH_4 pipeline) static transport connection ESCs. Methane in particular may be imported at lower costs as CH_4 (l) by ship rather than by CH_4 (g) pipeline. Cost performances of the shipping ESCs for H_2 (l), LOHC and NH_3 (l) are similar to those for CH_4 (l). They are followed by ship-based imports of methanol and finally imports of FT fuel by ship. There are some outliers for AR and AU for the static HVDC and pipeline connection ESCs. Reasons are the long transport

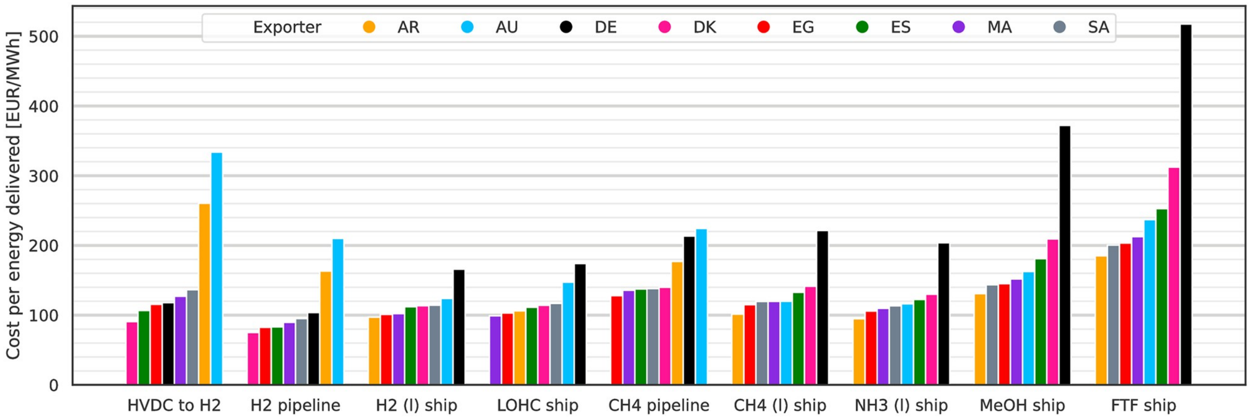

Fig 4. LCoE in 2030 assuming 10% p.a. WACC by ESC and exporter. LCoE are per MWh_{th} delivered to DE. Lowest cost options are imports via HVDC with subsequent electrolysis in DE and H2 pipelines. For more complex and energy intensive ESCs on the right the order of preference is different compared to the static import options with imports from AR in all but one case being the cheapest.

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distances for both exporters and the related high investment required for the HVDC and pipeline infrastructure.

An order of preference for the exporting countries can be identified: For statically connected ESCs short and mid-distanced exporters like DK, ES and EG are preferable. For ship-based ESCs, AR offers the lowest cost imports of energy to DE, making use of its good-quality RES, followed by imports from EG again. The least favourable position is taken by domestic production in DE: Generally for each ESC exists an alternative where the same energy carrier can be sourced for 75% of the cost of domestic production in DE. This development is driven by the low quality RES with high electricity costs and the approach we used to reserve RES capacities for domestic electricity demand. The approach reserved all PV potentials and only left wind resources for chemical production (cf. S2 Fig). Wind energy in Germany suffers from low output between June and September which the model compensates by over expanding wind capacities to keep supplying the synthesis processes. This is cheaper than using storage by batteries, which are not economical for storing more than a few hours worth of electricity demand, and there is no longer term electricity storage in the model. The remaining time of the year excess electricity is curtailed, causing high curtailment rates (cf. S1 Appendix) for DE. This leads to domestic production in DE to be competitive with imports only if H2 is produced without further processing. Under this condition the absence of need to transport chemicals internationally can compensate for the higher production cost in DE.

In Fig 5 the LCoE are shown declining in accordance with decreasing technology cost by 2050. Some of the projected LCoE decrease more strongly than others, most notable for methanol and FT fuel. While CH_4 (l) transport is cost competitive with CH_4 pipeline transport due to technological developments in the LNG industry over the past decades, for hydrogen the more complex of the transport chain and higher energy demands for liquefaction continue to make H_2 pipelines the preferred option for H_2 imports in the future. Noteworthy are the spreads between different ESCs and years. Neglecting domestic production in DE, the spread of LCoE for H_2 (l) or LOHC ship imports is low compared to the spread of methanol and FT fuel imports. It is also worth noting that the exporting country preference order does not change much between the years. Highest and lowest cost exporters stay the same and only some reordering in the cost mid-field can be seen where some countries benefit from anticipated cost developments more than others, see the mid-field options for methanol or NH_3

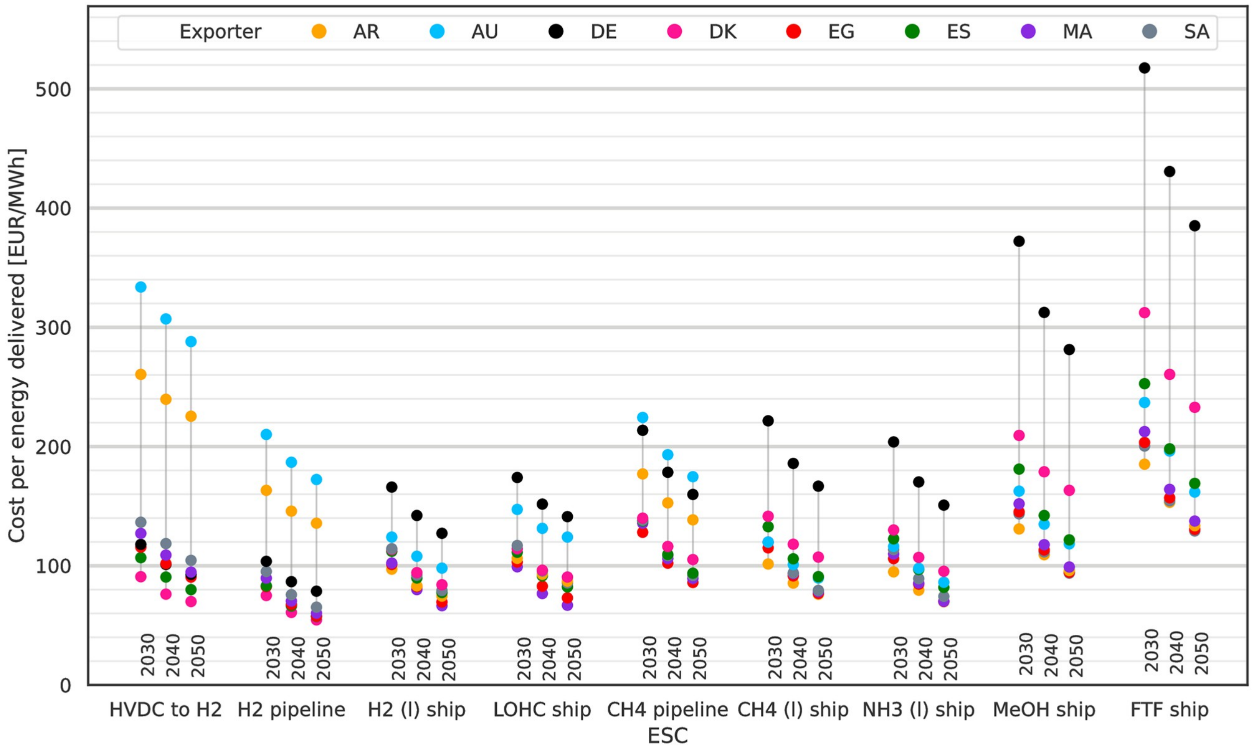

Fig 5. LCoE in 2030 to 2050 assuming 10% p.a. WACC by ESC and exporter. LCoE are per MWh_{th} delivered to DE. The lowest cost import options are H_2 (g) imported by pipeline and electricity imports by HVDC with subsequent electrolysis. Methanol and FT fuel imports experience the strongest cost decrease linked to the anticipated cost reduction for synthesis and DAC.

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shipping. This observation translates to no significant changes in the cost compositions of the ESCs, but rather just a general more or less homogeneous decrease of the total costs due to the cost technology reductions and electrolysis efficiency gains by 2050.

Cost composition and drivers

Cost drivers can be individually identified for all ESCs by investigating their cost compositions. Fig 6 shows the cost compositions for three selected countries, comparing exports from AR and ES with domestic production in DE. Additionally a tenth ESC is included where ammonia is decomposed back into hydrogen for investigating hydrogen import costs discussed in the next section. The costs shown are the annualised cost per component. Energy costs are not attributed to the components and instead cause higher upstream investments for conversion steps or RES capacities to keep the ESCs self-sufficient.

RES generally make the single largest cost contribution between 39% to 55% (interquartile distance). The specific cost contribution depends on the ESC, exporter, the local energy demand and conversion processes involved. Electrolysis plays only a minor role with on average 5% of the costs in the shown cases. The costs for synthesis or liquefaction processes and DAC (for CO2-based ESCs) have a higher contribution than electrolysis. Related to the synthesis processes is the necessity for chemical feedstock storage required to operate the synthesis processes at and above their must-run capacities. The contribution from H_2 and CO_2 feedstock above-ground steel tank storage is higher for most ESCs than the contribution from electrolysis. Some feedstock storage is also deployed for domestic provisioning of H_2 (l) in DE but it

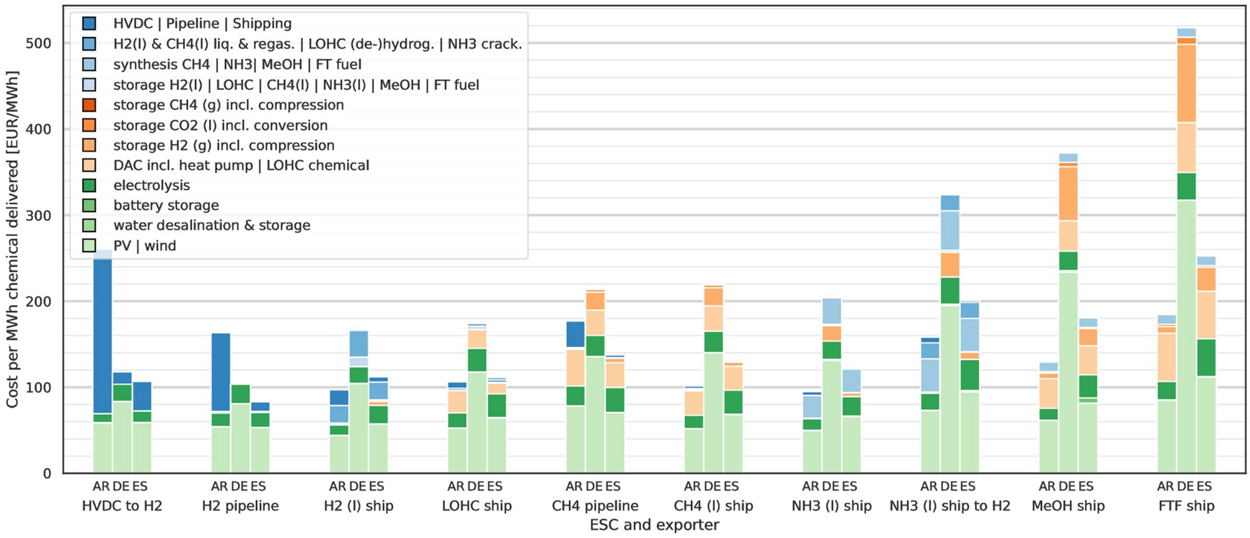

Fig 6. Cost composition of selected ESCs for 2030 at 10% p.a. WACC. Simpler, less energy intensive ESCs are favourable for short distances, e.g. domestic sourcing from DE and imports from ES, where low costs associated with transport can compensate high RES costs. More complex, energy intensive ESCs allow long distances exports, e.g. from AR, to become cost competitive due to lower RES costs and trading more complex molecules with higher energy intensity for lower transport cost.

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cannot be seen for all H_2 (l) ESCs. The costs associated with shipping are negligible in comparison to HVDC and pipeline costs.

From Fig 6 we can also identify cost drivers for the bad performance of AR as an exporter with the static pipeline and HVDC to H_2 ESCs: The HVDC and H_2 pipeline connections have high investment costs due to the long distance between AR and DE. For the CH_4 pipeline connection the investment costs are only a third of the H_2 pipeline, but the LCoE is driven by energy demand of the CH_4 pipeline which is assumed to use the transported CH_4 (g) as energy source. This energy demand for transport requires additional capacities for CH_4 synthesis, H_2 electrolysis and CO_2 capture as well as RES capacities, thus making pipeline transport less attractive across medium and long distances compared to H_2 and CH_4 shipping. For the LOHC ESC the long shipping distance increases shipping time and thus makes larger volumes of the LOHC chemical necessary which is reflected in the share of cost of the LOHC chemical. In comparison to ES as an exporter the necessary LOHC chemical investment volume is 2 times higher for AR as exporter. Despite this the LCoE for imports from AR by LOHC are lower than from ES due to the country-specific differences in available RES: While the LOHC investment volume for ES is lower compared to AR, the LCoE in the electricity supply curve are higher for ES than for AR. For domestic production in DE the LCoE for electricity from RES are driving the ESCs LCoE even higher.

Furthermore the lower CF of RES in DE lead to higher capacities for electrolysis needed during peak production but with lower overall utilisation rate. The case of LOHC is the only ship-based ESC where imports from AR do not offer the lowest LCoE. Comparing the LOHC ESC and the other carbon-based shipping ESCs with the NH_3 (l) ESC shows the advantages of an energy carrier with low investment costs on the synthesis molecule (N_2) compared to the high cost for the LOHC chemical and CO_2 sourcing and handling. Inflexibilities in the synthesis processes do not directly become apparent from the cost composition figure but show up indirectly by the need for increased buffer storage capacities and overcapacities of components upstream in the ESCs, e.g. RES. A good example for this are the FT fuel and CH_4 (l) ESCs where the more inflexible FT fuel synthesis leads to higher RES investments per MWh with higher curtailment and a different mix of RES capacities (see Fig 12 in S1 Appendix).

Battery storage is usually only deployed with limited capacities, able to sustain the ESC only for a few hours. In a few cases larger capacities of battery storage are deployed with a notable influence on the LCoE. Battery deployment can mainly be seen for HVDC, methanol and FT fuel-based ESCs, e.g. the HVDC to H_2 ESC for ES in 2040 (see S3 Fig). Investment into battery storage in the model coincides with higher shares of PV in the generation mix to increase the utilisation factor of downstream infrastructure, e.g. HVDC links, and to provide continuous electricity supply for must-run methanol and FT fuel synthesis processes. While sea water desalination is an important aspect for ensuring a sustainable production environment its costs and electricity needs do not contribute in a significant way to the final energy carrier cost.

Leverages for decreasing overall costs lie in reduction of storage costs by either direct reduction of the investment costs or usage of different technologies, e.g. cavern storage instead of steel-tank storage for H_2. An indirect leverage is the flexibility of synthesis processes as the must-run processes drive the storage volumes in our results, something which was shown for methanol by [51]. Increasing flexibility of processes and enabling lower must-run capacities as well as hot-standby would decrease the required storage volumes. Simultaneously it would increase the cost share of the synthesis process, such that cost improvements of the said processes could have a higher impact in lowering total product costs.

Hydrogen import costs for 2030 to 2050

In addition to comparing the costs of energy delivered, we can also compare the ESCs based on their import costs for delivering hydrogen. For this we calculate the levelised cost of delivering 1 MWh H_2 (g) using adapted versions of the previously discussed ESCs. Comparing the cost of hydrogen rather than the cost of energy is useful for applications which either require pure hydrogen like hydrogen fuel cells or processes requiring hydrogen as an industrial feedstock.

The ESCs used are identical where the ESCs already delivered H_2 (g). The CH_4, NH_3 and MeOH ESCs are extended by cracking processes for converting the energy carrier to H_2 (g) with their respective energy demand and investment costs. The additional cracking processes are steam methane reforming (SMR), methanol steam reforming (MSR) and ammonia cracking. Additional water demand of the cracking processes is neglected. The extra process steps and their location in the ESCs are shown in S1 Fig. We exclude cracking of FT fuel as methanol can be considered an equivalent choice for the purpose of being a liquid, carbon-based hydrogen carrier under ambient conditions but with easier synthesis. FT fuels are better suited as drop-in fuel replacements.

Resulting LCoH for 2030 to 2050 are shown in Fig 7. There is a clear cost advantage for the four ESCs which import hydrogen directly (left side) compared to the four ESCs requiring an additional cracking step (right side). Lowest cost imports are from DK by H_2 (g) pipeline at 2.5 EUR/kg_{H2} in 2030 and 1.8 EUR/kg_{H2} in 2050. Other exporters located in close proximity, i.e. ES and the Western Asia and Northern Africa (WANA) countries, offer hydrogen at only slightly higher LCoH and can thus be considered comparable alternatives. For non-static imports via ship H_2 (l) and LOHC ESCs exports from AR and to some extent from AU are also attractive. By 2050 as most exporting countries show similar LCoH the question of exporter makes no big difference from a techno-economic point of view as there does not seem to be an inherent advantage to a specific exporter. For the remaining non-H_2-based ESCs the additional conversion steps required for CO_2-based and the NH_3 ESCs drive their energy demand

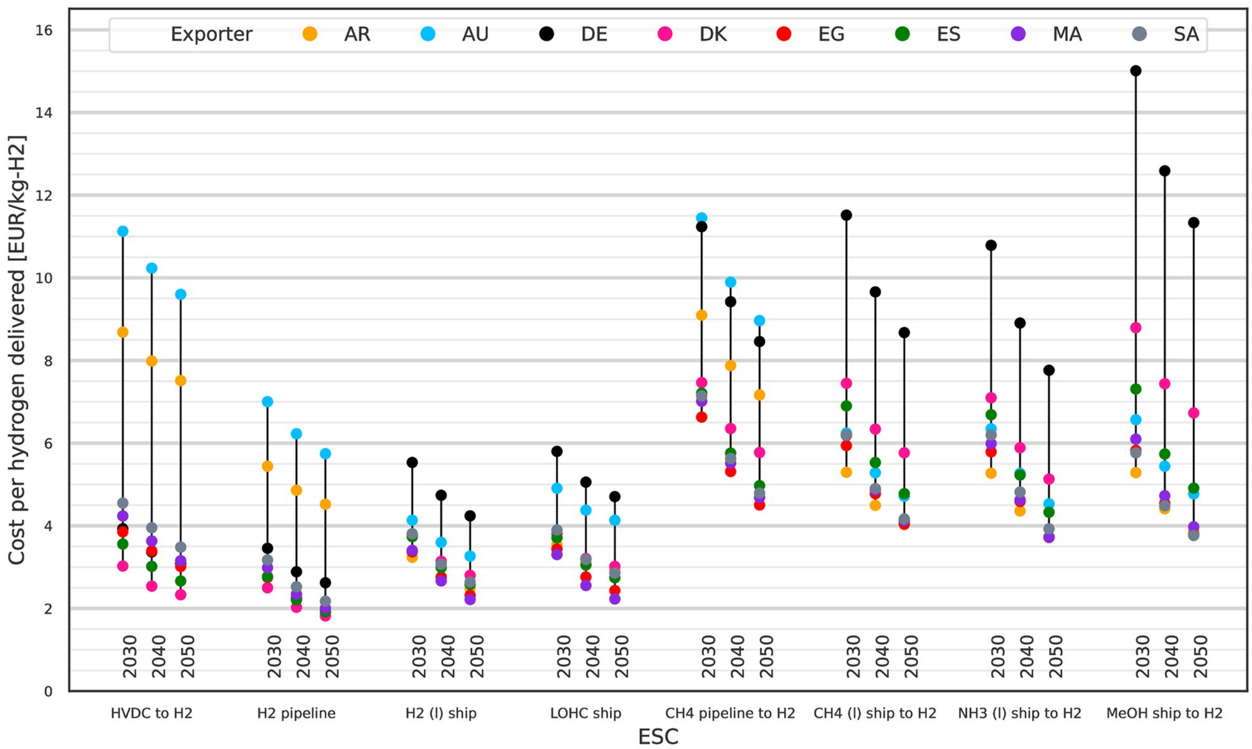

Fig 7. Levelised Cost of Hydrogen (LCoH) for 2030 to 2050 using extended ESCs. Direct hydrogen imports have lower LCoH than the alternative ESCs using methane, methanol or ammonia as energy carrier. The extended ESCs include extra process steps for cracking of the energy carrier to deliver hydrogen. All costs assuming 10% p.a. WACC.

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and investment costs, leading to less attractive LCoH starting at 5.3 EUR/kg$_{H2}$ in 2030 decreasing to 3.7 EUR/kg$_{H2}$ in 2050 from various exporters via NH_3 and methanol.

If long-term storage were additionally taken into account, the ammonia and methanol ESCs would have an advantage over the CH_4-based ESCs due to easier long-term bulk storage. This advantage would translate into lower LCoH in comparison to the other ESCs with the advantage increasing with the storage duration. Examining the results for alternative exporter options, it shows that in general for each lowest cost option of an ESC an alternative exporter with similar or slightly higher LCoH exists. Neglecting the extreme outliers for AR, AU and DE, the spreads for pipeline based and direct hydrogen imports are lower than for ship based NH_3, CH_4 (l) and methanol imports. The higher spreads translate to a higher uncertainty of hydrogen import costs when trade relations change and a switch in exporting country become necessary. Choosing a chemical energy carrier and ESC for scale up based on lower spreads in LCoH and existing low cost exporter alternatives ensures the opportunity for increased competition and potential exporter substitution in the future.

Sensitivity analysis

The sensitivities to exogenous parameter changes are visualised in Fig 8. Sensitivities are dependent on the scenario (year, ESC, exporter) by model design. We present quantified results for two selected scenarios of imports from ES to DE in 2030, by H_2 (g) pipeline and shipping of methanol. The exogenous parameters to be considered in the sensitivity analysis were pre-selected based on which parameters were expected to have the highest influence

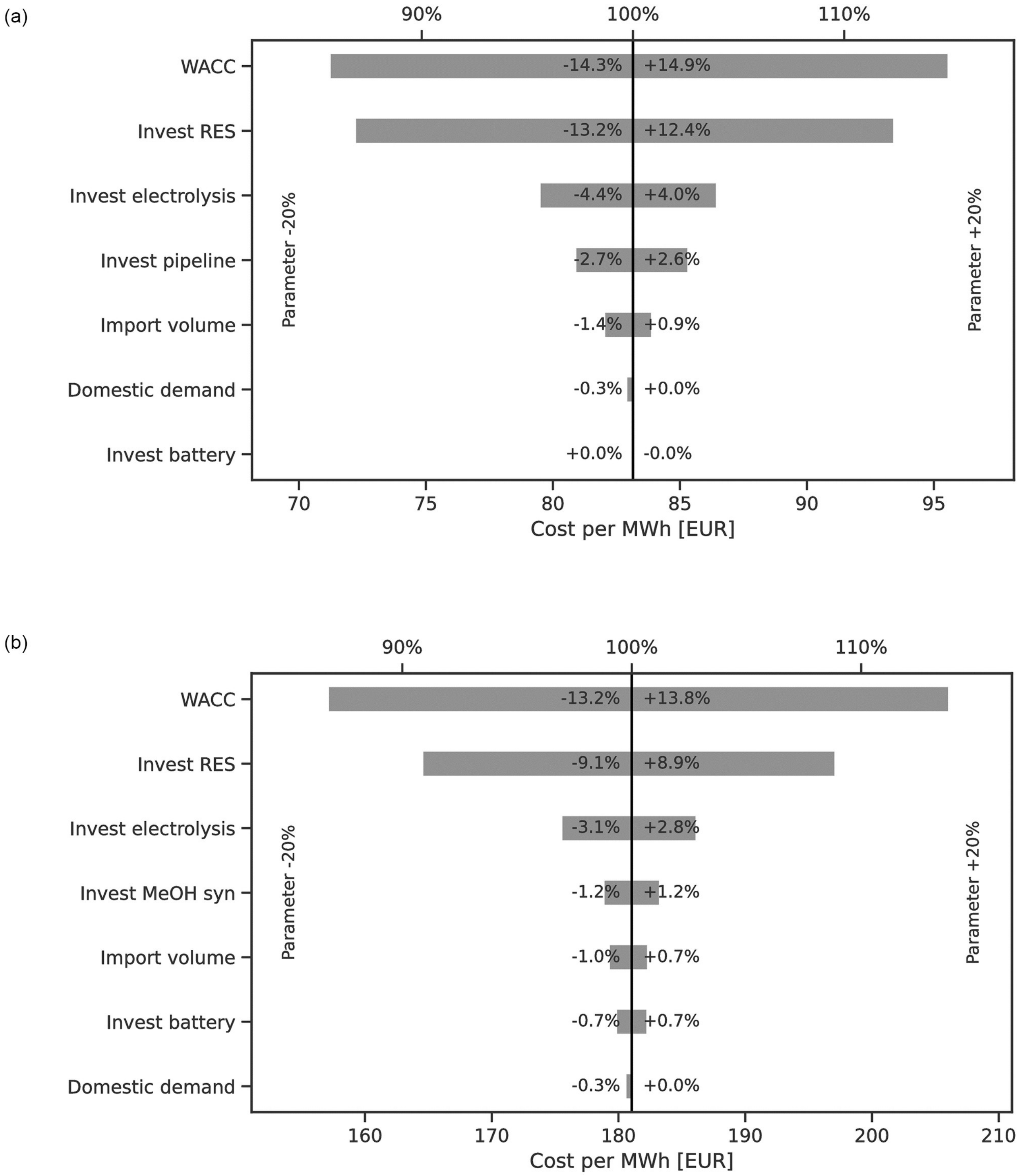

Fig 8. Sensitivities for two ESCs (left) H_2 (g) pipeline and (right) methanol by ship from ES to DE for 2030. Parameters listed on the left y-axis were varied by ±20%. The x-axis shows the resulting LCoE after variation and the relative change. The highest impact on the LCoE can be attributed to the choice of WACC followed by the cost of renewables and hydrogen electrolysis.

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on the LCoE. For both ESCs one additional major cost contributor based on the cost composition analysis was added, i.e. CAPEX for H_2 pipeline including compressors and methanol synthesis.

The results show the highest influence on LCoE to be from the choice of WACC, followed by variations to CAPEX of RES and then the CAPEX of electrolysis or the ESC specific contributor (investment in pipeline or MeOH synthesis).

Reduction of CAPEX for batteries has no effect for the pipeline-based ESC and only a small symmetric effect on the methanol ESC. Variations of domestic demand and import volume are negligible. This is to be expected because the relevant supply curve range does not show considerable changes to the LCoE in the relevant area around 500 TWh of electricity demand.

Lower WACC scenario

As indicated by the sensitivity analysis, the choice of WACC has the highest influence on the two ESCs analysed. Following this result we revisit the earlier analysis of LCoE and LCoH and rerun our model assuming 5% p.a. WACC (= −50%). Resulting LCoE are shown in Fig 9 and LCoH in Fig 10. The lower assumption is optimistic in comparison to other investigations like [48], but plausible and in line with recent reports like [52, 53] and in the face of similar or lower WACC reported for e.g. PV projects [49]. For large scale projects the assumption is also more reasonable as the projects include arguably high national interests and therefore support. The lower WACC leads to reductions of LCoE and LCoH each by around 35%. This exceeds most of the original scenario reductions seen between 2030 to 2050 due to technological learning. Under these more optimistic WACC assumptions one can find within each ESC one exporter and for each exporter one ESC with LCoE below 100 EUR/MWh_{LHV}. Similarly

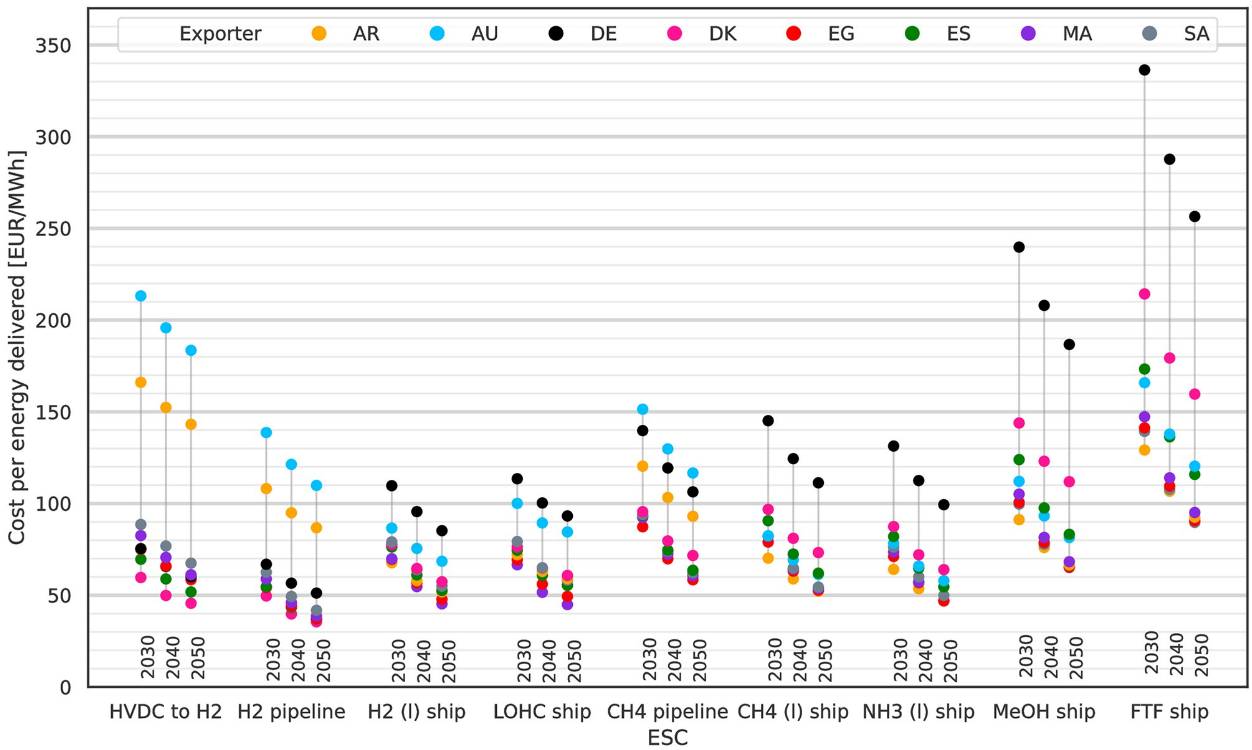

Fig 9. LCoE for 2030 to 2050 at a reduced WACC of 5% p.a.. Lowering the WACC reduces LCoE by around 35%.

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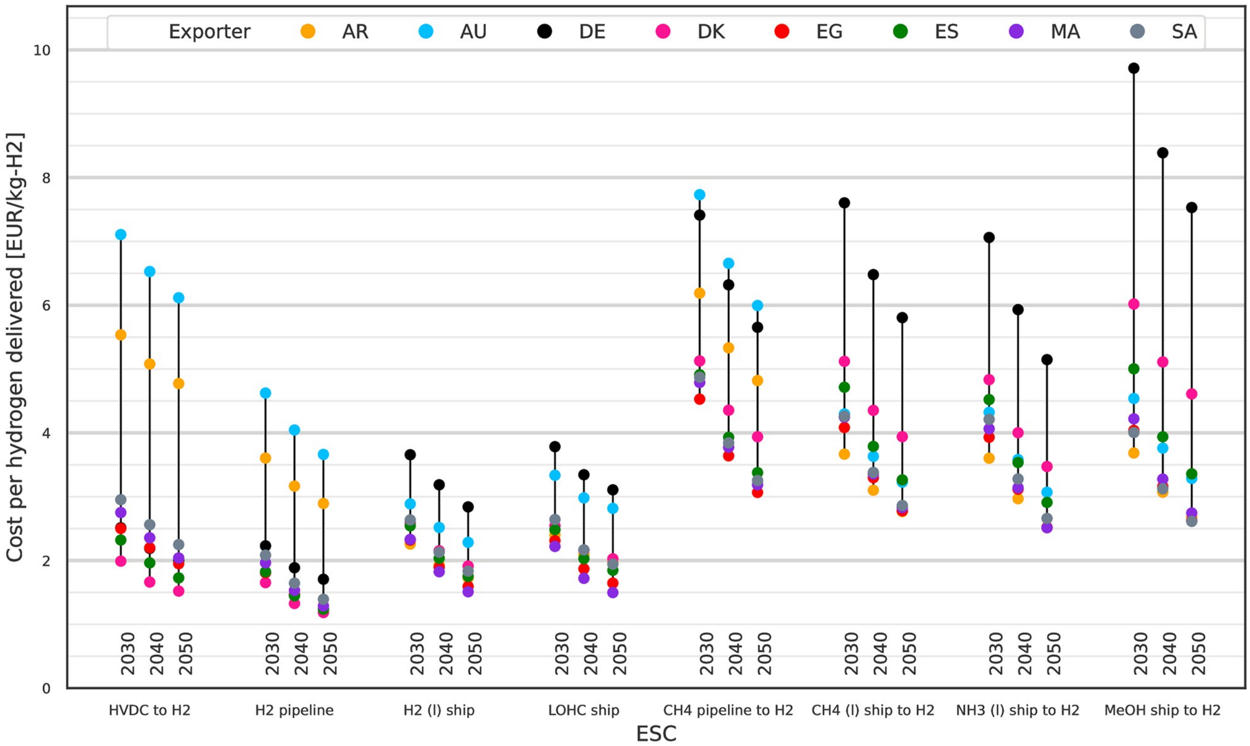

Fig 10. LCoH for 2030 to 2050 at a reduced WACC of 5% p.a.. Lowering the WACC reduces LCoH by around 35%.

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options for LCoH below 4 EUR/kg_{H2} are available for all ESCs and exporters. What is left unchanged is the order of preference for exporting countries within each ESC; given that the change to WACC affects all exporters the same way this result is not surprising.

Lowest LCoE are 50 EUR/MWh_{LHV} in 2030 to 36 EUR/MWh_{LHV} in 2050 by H_2 pipeline from DK which are also the lowest LCoH at 1.7 EUR/kg_{H2} in 2030 to 1.2 EUR/kg_{H2} in 2050. By 2050 more than 20 ESCs offer options for imports of hydrogen at 2 EUR/kg_{H2} (60 EUR/ MWh_{LHV}) or lower, most of them being by a static transport connection via H_2 pipeline or HVDC but also including some shipping options.

Comparison with today's commodity prices

We evaluate the competitiveness of our ESCs by comparing the future cost scenarios against today's market prices for the fossil-based counterpart commodities. The comparison between market prices and costs is not strictly valid because it ignores price formation in markets, but it can give a useful indication for the economic attractiveness of the ESCs. Fig 11 shows commodity prices relative to the average and median LCoE under 2050 technology assumptions with 5% p.a. and 10% p.a. WACC.

In our results methanol becomes available starting at 360 EUR/t from SA which is around 50% above 2020 market prices but within the range of market prices from 2021 and later. The current market prices are also within the range of the median methanol cost, indicating at least four exporter options for methanol within that cost range. Under less favourable financing conditions, cost differences exceed 100% and even the highest historical market prices are well below the 600 EUR/t median for methanol at 10% p.a. WACC. The constellation is similar for imports of FT fuel which hit break-even with the European average Diesel 2022 market price

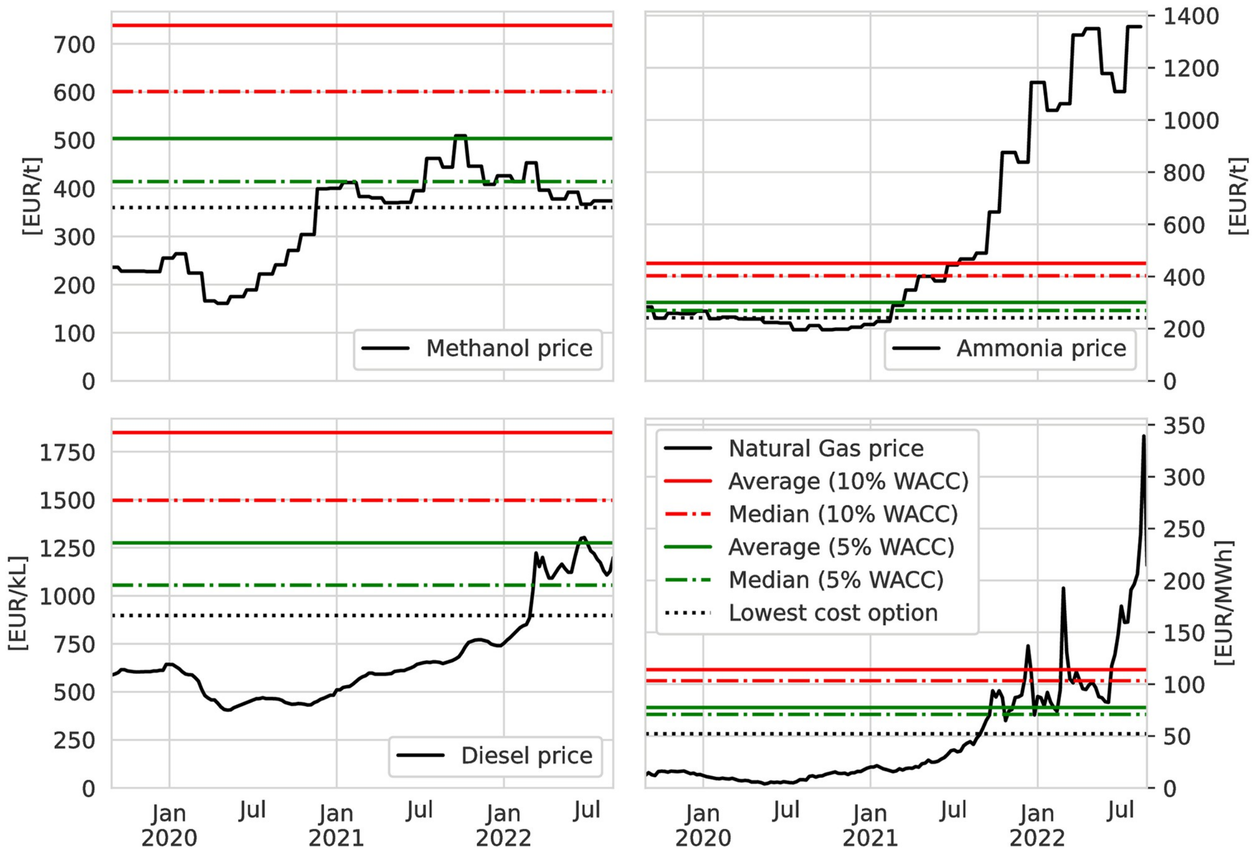

Fig 11. Comparison of market prices of current fossil-based commodities with modelled costs for synthetic ESC-based alternatives. Market prices are for Methanol based on MMSA Europe Spot FOB [31], Ammonia based on German export prices for ammonia [54], Natural gas based on Dutch TTF C1 future [55], FT fuel based on EU Diesel prices without taxes [56]. Statistics for natural gas are based on the costs for the CH_4 pipeline and shipping CH_4 (l) ESCs. The median value thus represents four exporter options for FT fuel, ammonia and methanol. For methane the median value represents eight exporter options.

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under favourable WACC assumptions but are not attractive compared to 2021 and earlier market prices or under higher WACC.

Market prices of ammonia and natural gas are strongly correlated with natural gas, it being the major cost-driving feedstock for today's ammonia production. Until the middle of 2021 prices for natural gas and ammonia were moderate and about 50% below the costs of the lowest cost option available from our ESCs. In the second half of 2021 market prices started to increase and reached up to ten-fold of previous levels during the energy crisis in Europe. In the long-term market prices in Europe for natural gas and therefore also for ammonia can be expected to stay well above pre-2021 levels as pipeline-based gas imports are substituted with LNG. At higher market prices our modelled import costs are within the cost range of being attractive. Even median import costs for the less favourable 10% p.a. WACC scenario are below currently seen market prices.

The differences between costs and market prices can also be bridged through CO_2 prices on the direct emissions of fossil-based energy carriers, which may also make higher LCoE with unfavourable financing conditions (10% p.a. WACC) more attractive. Bridging e.g. a cost difference of 500 EUR/kl for diesel/FT fuel would be equivalent to a CO_2 price of 187 EUR/t_{CO_2}. A difference of 100 EUR/t on methanol could be compensated by a CO_2 price of 73 EUR/t_{CO_2}.

For natural gas a CO_2 price of 126 EUR/t_{CO_2} could cover a difference of 25 EUR/MWh_{LHV} which is the difference seen between mid July 2021 spot market prices and median LCoE from our scenarios. Such CO_2 prices are realistic when compared to the estimated CO_2 emission prices for 2030 of 129 EUR/t_{CO_2} under stricter EU regulation [57] and are well within the range of the estimated social cost of carbon from CO_2 emissions in DE of 195 EUR/t_{CO_2} to 250 EUR/t_{CO_2} (2020 to 2050) [58].

This shows that under fast-track technology deployment that makes the 2050 cost projections appear earlier and under favourable financing conditions leading to low WACC, the differences in LCoE to the fossil chemical energy carrier alternatives could in some cases be overcome in the near future. It also shows the important role of enabling an environment of lower financing cost (WACC) to reduce the costs. Until the cost gap between synthetic RES-based and fossil energy carriers is closed, a purely cost-driven switch from fossil to synthetic fuels is improbable. Supporting policies, e.g. CO_2 prices and fuel quotas, or softer factors which incentivise change, e.g. adjusted customer preferences, exporter independence and diversification or business self-regulation following e.g. corporate social responsibility (CSR) or environmental social and corporate governance (ESG) criteria, will be required to drive the change.

Discussion

Limitations

The results we presented in this study are subject to a range of limitations. Some general limitations are due to the nature of the methods used while others arise from our model assumptions.

GIS-based analysis at low resolutions for determining RES potentials can over- or underestimate real potentials as it ignores local siting limitations below the resolution limit or not contained in the data input, e.g. terrain. The RES potentials and generation are likewise affected by using 2013 as representative weather year which disregards multi-year weather and climate change induced variations on RES generation and costs. By including exogenous technology development and learning for costs which use fixed projections for technology capacities being deployed in the future, we ignore the influence our ESCs capacities could have on world-wide learning and development. This limitation similarly extends to process efficiencies which are exogenously fixed and learning independent. For cost assumptions the validity and uncertainties cannot be assessed ex ante, a pitfall famously encountered by cost projections for RES technologies like PV which in hindsight were often too high [59]. Also some technologies might realise technological maturity faster or slower than others leading to earlier or later cost decreases in some ESC thus influencing the time-horizon of the results presented. There could also be path dependencies where existing infrastructure influences the choice of ESCs, such as existing LNG terminals leading to an advantage for SNG imports. Lastly assuming identical WACC for all countries and ESCs increases comparability but is not realistic; WACCs are generally country- and project-specific. More specific to our model we conducted investment optimisation for greenfield conditions in an islanded system. This assumption may not be appropriate where significant infrastructure for reuse or co-use already exists. Such cases are to be expected e.g. for electrical transmission lines and pipeline systems in the EU. Integrating energy exports with existing systems rather than deploying islanded systems can open opportunities e.g. for reuse of existing heat sources at lower costs than sourcing of the energy from inside an ESC. Reuse of existing infrastructure and integration both would lower the costs along an ESC. A similar effect should be expected from integration of technologies along the

ESCs, e.g. heat generated by electrolysis used for DAC, which was not considered either. Further we use simplified transport assumptions: Energy transport properties only scale by distance using representative average values which ignore e.g. topography, and we neglect shipping terminal costs. For forwarding electricity and chemicals between production locations and centralised facilities we assume copperplate-like transport without connection costs or losses on the exporter side and likewise for distribution systems on the importer side. On the demand side we presume an annual energy demand for domestic electricity as well as chemical energy carrier demand without specific demand pattern. This may cause unrealistically high amounts of low-cost, highly correlated electricity from PV to be used for domestic demand rather than some of its peak supply for the production of chemical energy carriers. The lack of demand pattern for the chemical energy carriers waives the need for short-term or long-term storage prior to end use where non-H_2 energy carriers may be better suited than any pure H_2 option. For the demand we further exclude differences in conversion efficiencies from energy carriers to energy services for better comparison. Potential competing demand by imports of other countries which may compete for the same ESCs is omitted as well as a to be expected increasing demand in DE exceeding 120 TWh. Aggregated demand may exceed available supply potential from some countries, e.g. DK, or regions, e.g. EU, cf. Fig 3. The decisions for transport, distribution and energy demand are expected to lead to an underestimation of LCoE. Another boost to LCoE can be expected as other nations start to import equally significant volumes of energy carriers, thus driving MCoEs in the supply curve and competition for best RES sites, unequally affecting LCoE from some exporters more, e.g. DK, than others, e.g. AU, AR. Attempting a generalisation for diverse distribution and end-use cases appears inadequate to us as it may lead to potentially misleading or easily misunderstood results. Instead we offer basic results on which further studies using sector or project specific parameters may be undertaken for which our results and model can act as a starting point.

In the broader picture we have considered imports to a single country, Germany, in our study. In reality there is to be expected a complex web of trade and competition between importing and exporting countries and individual actors. Our study is a first step into this direction.

Comparison with other studies

Opportunities to compare our modelling results with other studies are limited to the various different system boundaries common in literature. [3] investigated import of FTD and SNG from the Maghreb region. For 2030 they arrived at 85.3 EUR/MWh_{LHV} for FTD and for regasified SNG 98.8 EUR/MWh_{LHV} assuming 5% p.a. WACC without O_2 sale benefits. Compared to our results with 5% p.a. (and 10% p.a.) WACC for imports from Morocco (MA) in 2030, their costs are lower than ours reaching 147 EUR/MWh_{LHV} (213 EUR/MWh_{LHV}) for FT fuel and within a similar range for CH_4 (l) by ship at 82 EUR/MWh_{LHV} (120 EUR/MWh_{LHV}). Differences can be found in [3] assuming DAC CAPEX to be a third of what we assumed and use a lifetime of 30 years compared to 20 years. They also assumed 37% lower CAPEX for AE, low cost cavern hydrogen storage rather than steel tanks, higher AE efficiencies and made use of heat integration into their process. Fasihi et al. [60] estimated 2050 costs for local ammonia production to be 260 EUR/t_{NH3} to 300 EUR/t_{NH3} for the best sites including AR, AU and the WANA region. For 'most habitable regions of the world' they estimate costs of around 450 EUR/t_{NH3}. The costs we arrived at in our study covers a similar range with costs (exclusing DE) between 242 EUR/t_{NH3} to 330 EUR/t_{NH3} for the optimistic WACC case of 5% p.a. and 360 EUR/t_{NH3} to 492 EUR/t_{NH3} for the conservative WACC of 10% p.a.. The main differences between the studies are are the different assumptions on WACC with [60] assuming 7% p.a.

and their significantly lower CAPEX assumptions for hydrogen and battery storage. In terms of RES system compositions the authors saw a PV dominated system with complementary onshore wind deployed, while we see in our study quite different combinations of PV, offshore and onshore wind being deployed depending on the exporter and ESC.

Results from Niermann et al. [61] for hydrogen imports from Algeria by HVDC, ship with H_2 (l) and the LOHC DBT show significantly higher import costs at 6% p.a. WACC when compared with our results for MA in 2030 with 5% p.a. WACC: They report 11.5 EUR/kg_{H2} for LOHC shipping (we: 2.2 EUR/kg_{H2}), 13.2 EUR/kg_{H2} for H_2 (l) shipping (we: 2.3 EUR/kg_{H2}) and 15.6 EUR/kg_{H2} for HVDC imports (we: 2.8 EUR/kg_{H2}) The stark cost difference is driven by their assumptions of a different electrolysis technology (PEM) with different technological parameters, fixed electricity costs of 50 EUR/MWh_{el} and inclusion of seasonal storage as well as distribution costs, i.e. assumptions which are expected to drive costs for pure hydrogen storage (gaseous or liquid) and investment costs for the LOHC chemical substantially.

Lastly compared to [15] we see comparably flat supply curves for regions with large RES potentials. The lowest costs for H_2 (l) exports from Patagonia (AR) seen by Heuser et al. [15] are at 3.06 EUR/kg_{H2} excluding shipping cost. The authors further estimate the shipping costs to add another 0.53 EUR/kg_{H2}. These results are significantly higher than our results for 2050 with 2.5 EUR/kg_{H2} and 1.7 EUR/kg_{H2} at 10% p.a. and 5% p.a. WACC respectively. The difference in cost can be partially attributed to the inclusion of the collection infrastructure on the exporter side necessary for transporting the energy carrier from the distributed points of production to the coast for exports.

Concluding the comparison with existing literature yields consistent results where comparison is possible within a broader range. Differences to literature can be tracked and explained based on significantly different technology, cost and model assumptions.

Conclusion

In this paper we modelled large scale, islanded production and export of chemical energy carriers to Germany (DE) from Australia (AU), Argentina (AR), Denmark (DK), Egypt (EG), Spain (ES), Morocco (MA) and Saudi Arabia (SA). We compared these Energy Supply Chains (ESCs) with their equivalents for domestic production of chemical energy carriers in Germany. For the nine different ESCs we minimised greenfield investment costs to determine the Levelised Cost of Energy (LCoE) per MWh_{th} of the specific chemical energy carriers as well as Levelised Cost of Hydrogen (LCoH) per kg_{H2} after dehydrogenation of the energy carriers. We determined and used local Renewable Energy Source (RES) potentials via GIS-analysis, considered the influence of local electricity demand on exporters' supply curves and included the intermittency of RES sources via modelled hourly time-series.

In all investigated scenarios domestic sourcing of the individual chemical energy carriers in DE is among the most expensive options. Sourcing through ESCs from other countries is in almost all cases cheaper. Under conservative assumptions of 10% p.a. WACC we find the lowest LCoE (LCoH) for 2030 to be 75 EUR/MWh_{LHV} (2.5 EUR/kg_{H2}) from DK by H_2 (g) pipeline. Under optimistic assumptions of 5% p.a. WACC the costs reduce to 50 EUR/MWh_{LHV} (1.7 EUR/kg_{H2}). With technological development, costs further decrease by 2050 to 55 EUR/ MWh_{LHV} (10% p.a. WACC) and 36 EUR/MWh_{LHV} (5% p.a. WACC). Other than Denmark, imports from Spain and Western Asia and Northern Africa by hydrogen pipeline are also attractive, e.g. at between 37 EUR/MWh_{LHV} to 42 EUR/MWh_{LHV} (2050, 5% p.a. WACC). With optimistic 5% p.a. WACC assumptions, import options for any to all of the investigated chemical energy carriers and from all exporters become available at cost of 100 EUR/MWh_{LHV}

or lower. Importing FT fuels by ship is the most expensive ESC with the largest cost range we investigated, with the costs ranging 90 EUR/MWh_{LHV} to 256 EUR/MWh_{LHV} under best assumptions (2050, 5% p.a. WACC). The lowest cost options and exporters for importing energy are also the lowest cost options for imports of hydrogen. While better financing conditions and fast-track technology development lead to lower costs for imported energy and hydrogen, they do not lead to changes in in the order of preference regarding technology and exporter if they affect all exporters and ESC similarly.

As a rule of thumb LCoE increase with the complexity and energy intensity of an ESC. Costs for RES are the major cost driver usually contributing 39% to 55% to the total cost of an ESC. Electrolysis costs play only a minor role with on average 5% of the costs of an ESC. Costs for ESCs using ammonia, methane, methanol and FT fuels are additionally driven by the costs for synthesis and costs for hydrogen storage using above-ground steel tank, which is used to ensure feedstock availability for the inflexible synthesis processes.

Our findings support the notion that no best one-size-fits-all solution exists for chemical energy carrier imports. In fact no single exporter or ESC shows a unique techno-economic advantage over the others, leading to the conclusion that preference for one energy carrier, ESC and exporter should not be given solely based on small differences in LCoE and LCoH. This allows supply of energy carriers and feedstocks to be sourced from a diverse selection of countries, without affecting costs too strongly. For large volume imports of energy and pure hydrogen, imports by H_2 (g) pipeline or electricity by HVDC with domestic electrolysis are favourable. Alternatives incur only slightly higher costs. Our results support the notion that the choice of chemical energy carrier should be based on the requirements for end-use including short-term and long-term storage necessity, energy service conversion efficiency and distribution logistics rather than the cost alone. Accordingly future analysis of full ESCs could provide more insights by using specific demand assumptions and distinguishing between specific energy service or chemical needs. Such analysis could further include local production (captive) scenarios compared to our nation-level analysis. Finally, qualities of ESCs like reliability of supply, long-term cost predictability, local value chains and employment generation, which are generally not represented by the investment costs, need to be investigated and considered.

To overcome the limitations of this study and increase insight into energy imports, future research should focus on differentiating WACC based on exporter and technologies, include spatially resolved RES and collection infrastructure, include additional relevant energy carriers and ESC designs like CO_2-cycling and import of secondary, energy-intense products like refined-iron or other valuable hydrocarbons and investigate sensitivities of results also to technical aspects like process flexibilities and synthesis must-run conditions.

Supporting information

S1 Appendix. ESF, LCoE and curtailment.
(PDF)

S2 Appendix. Technical model structure.
(PDF)

S3 Appendix. Model equations.
(PDF)

S1 Fig. Energy Supply Chains visualisations.
(PDF)

S2 Fig. Electricity generation mix and supply curves.
(PDF)

S3 Fig. Cost composition for other years, lower WACC.
(PDF)

S4 Fig. RES eligible area masks.
(PDF)

S1 Table. Tabular results: Levelised Cost of Energy.
(PDF)

S2 Table. Tabular results: Levelised Cost of Hydrogen.
(PDF)

S3 Table. Technology assumptions.
(PDF)

S4 Table. Conversion efficiencies.
(PDF)

S5 Table. Shipping parameters.
(PDF)

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Supervision: Tom Brown.

Writing – original draft: Johannes Hampp.

Writing – review & editing: Michael Düren, Tom Brown.

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Flexing with lines or pipes: Techno-economic comparison of renewable electricity import options for European research facilities

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Abstract

Where local resources for renewable electricity are scarce or insufficient, long-distance electricity imports will be required in the future. Even across long distances, the variable availability of renewable energy sources needs to be managed for which dedicated storage options are usually considered. Other alternatives could be demand-side flexibility and concentrated solar power with integrated thermal energy storage. Here their influence on the cost of imported electricity is explored. Using a techno-economic linear capacity optimization, exports of renewable electricity from Morocco and Tunisia to CERN in Geneva, Switzerland in the context of large research facilities are modeled. Two different energy supply chains are considered, direct imports of electricity by HVDC transmission lines, and indirect imports using H2 pipelines subsequent electricity generation. The results show that direct electricity exports ranging from 58 EUR/MWh to 106 EUR/MWh are the more economical option compared to indirect H2-based exports ranging from 157 EUR/MWh to 201 EUR/MWh. Both demand-side flexibility and CSP with TES offer significant opportunities to reduce the costs of imports, with demand-side flexibility able to reduce costs for imported electricity by up to 45 %. Research institutions in Central Europe could initiate and strengthen electricity export-import partnerships with North Africa to take on a leading role in Europe's energy transition and to secure for themselves a long-term, sustainable electricity supply at plannable costs.

Introduction

Research facilities and communities are striving to become more sustainable, with a focus on reducing their carbon emission footprint. Among those working towards this goal are the High-Energy Physics (HEP) community and the research facilities at the European Organization for Nuclear Research (CERN) in Geneva, Switzerland [1]. A significant contribution to the carbon footprint of research institutions is made by electricity-related scope 2 emissions [2] from the use of fossil fuels in electricity generation. To some extent, these emissions can be lowered by increasing energy efficiency, but any remaining emissions have to be addressed by making the electricity supply carbon-neutral. This may be achieved by displacing fossil fuels in electricity generation with low-emission alternatives like Renewable Energy Sources (RES) from wind and solar technologies, primarily Photovoltaic (PV). However, expanding RES capacities becomes increasingly difficult with increasing shares of RES in the electricity mix due to their land requirements and weather-dependent availability needing to be managed. In Central Europe, both pose major challenges because of high population density, low land availability [3], and strong seasonality of RES.

One strategy to address the challenges is to deploy RES in areas with lower population density and more favorable climatic conditions, for example, solar-dependent RES closer to the equator, where diurnal and seasonal variations are reduced [4]. In several cases, Northern African countries including Morocco (MA) and Tunisia (TN) have been considered in the past as locations to produce electricity using RES and export it to European countries, see for example [5–8]. One initiative which became widely known in the 2000s was DESERTEC with plans to import electricity from Northern Africa to Europe [9]. A more recent example is the company Xlinks, which announced in 2021 its plans for the "Morocco-UK power project", a project to export electricity from MA to United Kingdom (UK) [10]. The project aims for building RES capacities in MA, a mix of wind and solar PV of a total of 10.5 GW capacity, combined with 20 GWh battery storage for managing their weather-dependent availability. The electricity is intended to be exported by subsea High-Voltage Direct Current (HVDC) transmission line with a capacity of 3.6 GW along the Western European continental coast to Devon, UK. Other underwater, long-distance HVDC transmission line projects are under construction or planned in Europe with its neighboring continents [5], like the EuroAsia interconnector [11], showcasing the technical and economic feasibility of such projects.

In the realization of large RES projects, reliable partnerships and off-take guarantees for the imported electricity are essential, as these reduce a project's risks and improve financing conditions through reduced cost of capital [12]. Through favorable financing conditions, RES-based projects can become economically feasible and attractive compared with fossil-based energy projects, as they are typically characterized by high upfront investment and low operational costs as opposed to fossil-based projects with low investment and high operational costs [13].

Herein lies an opportunity for synergies between research institutions and potential energy import projects to be explored. CERN has a high electricity demand, namely around 1250 GWh in 2018 during "Run 2" of the Large Hadron Collider (LHC) [14]. Like other large consumers of electricity, low and stable electricity prices are important for CERN and its current as well as future operations. At the moment CERN is supplied through the French electricity grid [14], which had a low carbon intensity $67\,\mathrm{g_{CO_2}/kWh}$ in 2018 compared to other European countries, due to France's high share of nuclear power [15] in its electricity supply. More recently the French nuclear power plant fleet has been experiencing a rising number of problems. And with the fleet's future unclear, maintaining current levels of carbon emissivity and electricity prices in the French grid will become impossible without the addition of significant RES capacities [16]. CERN, as an international research institution, could use the opportunity to pursue an import project for RES-based electricity from a neighbor country outside Europe, securing for itself and other interested research institutions a supply of electricity at long-term stable and plannable costs, thereby reducing the project risks and increasing the chances of the project being realized and adding to the French and European energy transition.

In assessing the viability of such a potential project, techno-economic modeling and analysis play a crucial role to understand associated limitations as well as technical and economic details. There exists a large body of literature on techno-economic analysis for projects exporting energy from Northern Africa to Europe with different foci. Electricity has been investigated with great interest in the past, e.g. [17–20] and recently Hydrogen (H_2) has become increasingly discussed for the same purpose, e.g. [21–23]. A very limited number of studies include both electricity and hydrogen exports in their analysis, like van der Zwaan et al. (2021) [8], and thereby allowing for comparative insight into these two alternatives.

While it is recognized that techno-economic modeling which includes RES needs to account for the variable availability of RES, e.g. through a sufficiently high temporal resolution [24], fewer analyses explore how this variability is managed. One common approach is the use of one or a combination of storage technologies [25]. The other is demand-side flexibility, which despite being a promising alternative [26], is often neglected [27]. With demand-side flexibility, the electricity demand is shifted in time based on the availability of RES-based electricity supply.

This study addresses these two common shortcomings – a comparison between hydrogen and electricity and demand-side flexibility as an alternative to storage – and compares the costs of imported electricity, RES shares, and storage requirements for large-scale electricity exports by HVDC and H_2 pipeline from MA and TN to Central Europe.

Method

General

The methodology for this paper is based on Hampp et al. (2023) [28] with some modifications. The investigated import projects, from now on referred to as Energy Supply Chains (ESCs), are modeled based on their techno-economic properties. For each ESC and exporter, an independent green-field capacity expansion model is built, where the model determines technical capacities to meet the requested electricity demand under optimal annualized system costs and perfect foresight in a linear program. Annualised costs c_i for each component i are calcualted using the Equivalent Annual Cost (EAC) method:

$$c_i = C_i \cdot (A_i + \mathrm{FOM}_i) \tag{1}$$

where C_i represent the components investment and FOM_i the Fixed Operation & Maintenance costs. A_i is the annuity factor for the component with lifetime t_i and cost of capital r:

$$A_i = \frac{(1+r)_i^t \cdot r}{(1+r)_i^t - 1} \tag{2}$$

To properly represent the variability of RES availability, a full year is modeled with an hourly time resolution. Python for Power System Analysis (PyPSA) [29] is used as an energy system modeling framework to implement the capacity expansion models. A major change to the original methodology from [28] is the substitution of the software package GlobalEnergyGIS (GEGIS) [30] with *atlite* [31]. While both packages can be used for modeling availability time series for RES from weather data and to determine land-availability potentials, *atlite* has a more modular and extensible approach which is utilized in this study.

As import destination Geneva is selected as a proxy for Central Europe. In Geneva and the surrounding regions, CERN and other large European research institutions are situated. The location also features a well-connected grid infrastructure through which potential synergies the European electricity grid could be created.

Renewable potentials and availability

As exporting countries MA and TN are chosen. Both countries are outside of but neighboring Europe in the Mediterranean and are thus in proximity to Geneva. As both countries are closer to the equator, they experience lower seasonality and a longer time of diurnal sunshine duration for higher availability of solar-based RES, PV, and Concentrated Solar Power (CSP). Due to lower population densities in MA and TN compared to Central Europe, their land availability for RES is also more favorable. For both countries, their southernmost administrative regions are excluded to reduce the spatial spread of potential RES sites. Eligible areas for each RES technology are identified using GEBCO [32] for slope and sea depth, WDPA [33] for protected areas, Corine Land Cover [34] for land cover types and proximity restrictions to populated areas and IMF data [35] on shipping sea routes. The resulting eligible areas are included in S4 Appendix. Using the eligible areas, RES potentials are determined by assuming technical potentials of $3\,\mathrm{MW/km^2}$ for offshore as well as onshore wind, and $17\,\mathrm{MW/km^2}$ for solar PV and CSP, based on [36]. Weather data for modeling RES hourly availability using *atlite* [31] is based on reanalysis data from ERA5 [37] for 2013. For the conversion from weather data to RES availability different models are implemented in *atlite* and used here, namely for onshore a *Vestas V112 3MW* and for offshore wind a *NREL offshore 5-MW baseline wind turbine* are used. Solar PV is modeled using the crystalline silicon model by Huld et al. (2010) [38]. For CSP the field of solar tower power station is represented with a solar-position dependent field and tower irradiation-to-heat efficiency which emulates detailed system simulations using *NREL SAM* [39] in combination with a fixed-efficiency power block. All RES locations are classified based on their annual capacity factor into 50 quality classes for each technology to construct country-specific electricity supply curves. For each technology and quality class, an hourly availability time series is generated which is made available to the capacity expansion model. Local electricity demand in the exporting regions MA and TN are considered by removing the estimated amount of annual electricity demand from the lowest-cost resources in the respective annual supply curves, see [28] for details. The annual electricity demands for MA (122 TWh) and TN (64 TWh) are synthetic demand estimates for 2030, generated using *GlobalEnergyGIS* [30] with 2013 as a reference weather year and GDP and population growth based on the SSP2 [40] scenario.

Technologies

As electricity generation technologies, (1) solar PV, (2) onshore wind and (3) offshore wind are included in all scenarios and ESCs. Furthermore in additional scenarios the influence of having (4) CSP with integrated Thermal Energy Storage (TES), as a special RES with an integrated storage option, as a fourth energy source available is analyzed.

Two types of ESCs are considered which both deliver electricity to the importer site in Geneva:

1. "HVDC" ESCs: Electricity is directly transported from the exporter to the importer by HVDC transmission line

2. "H_2 pipeline" ESCs: Electricity is first used to produce H_2 on the exporter side, and the H_2 is then transported by H_2 pipeline to the importer side where it is used for electricity generation using a Closed-Cycle Gas Turbine (CCGT).

The CCGT turbine for H_2-to-electricity conversion is chosen for its lower investment costs compared to large-capacity fuel cells. The ESCs and technologies are visualized in Fig 1. Technology costs and efficiencies are assumed for 2030 and listed in Table 1. Costs are assumed for large-scale facilities and scale linearly with capacity, no additional scaling exponent is applied. Efficiencies are assumed constant and load-independent. HVDC transmission lines and pipelines are transport modeled also with fixed, distance-dependent transport efficiencies. No standing losses for battery, hydrogen, and thermal energy storage are assumed. Technology costs and other currency values are

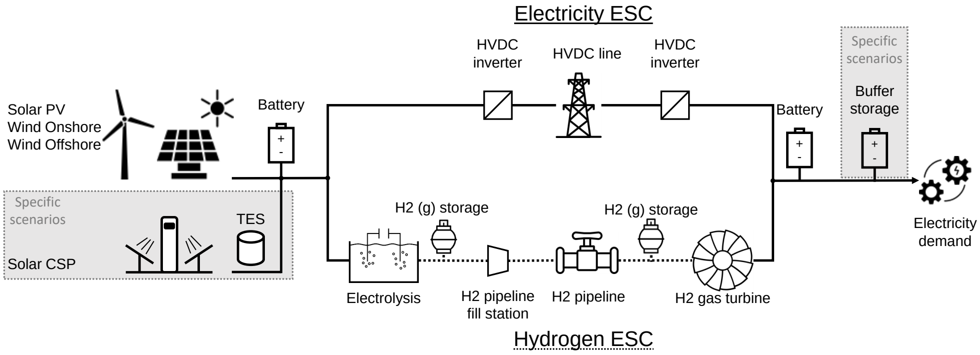

Fig 1. Technologies used for modeling the electricity imports ESCs and during specific scenarios.
(Top) ESC shows the technologies involved with direct electricity imports by HVDC, (Bottom) shows technologies for indirect imports by H_2 pipeline. Specific to certain scenarios is the inclusion of CSP with TES and the capacity of the electricity buffer storage for demand-side flexibility modeling. Icons are CC-BY-3.0 [41–47] and own creation.

reported in EUR_{2015}. Within the model technology costs are annualized using the equivalent annual cost method, considering technology investment and Fixed Operation & Maintenance (FOM) costs with 10 % Weighted Average Cost of Capital (WACC). The method for calculating annualized component costs and a discussion of the choice of WACC are discussed in greater detail in [28].

Table 1. Technology assumptions for the model for 2030.
Sources and a detailed description of the selected technologies are listed in S2 Appendix.

Technology	Investment [EUR_{2015}]		FOM [%/year]	Lifetime [year]	Efficiency [%]
Wind onshore	1035.56	EUR/kW_e	1.22	30	-
Wind offshore	1523.55	EUR/kW_e	2.32	30	-
Solar PV	347.58	EUR/kW_e	2.48	40	-
CSP field & receiver tower	98.15	EUR/kW_{th}	1.1	30	-
CSP TES	13.15	EUR/kWh_{th}	1.1	30	-
CSP power block	687.5	EUR/kW_e	1.1	30	41.2
Battery storage	142	EUR/kWh_e	0	25	-
Battery inverter	160	EUR/kW_e	0.34	10	98
Electrolysis (Alkaline)	450	EUR/kW_e	2	30	68
Hydrogen storage tank	12.23	EUR/kWh_{H2}	2	20	-
HVDC inverter pair	162.36	EUR/kW_e	2	40	98
HVDC line overhead on-land	432.97	EUR/(MW km)	2	40	97.7/1000 km
HVDC line underwater	471	EUR/(MW km)	0.35	40	97.7/1000 km
H_2 (g) pipeline fill station	4478	EUR/MW_{H2}	1.7	20	97.9
H_2 (g) pipeline on-land	226.47	EUR/(MW km)	3.17	50	97.9/1000 km
H_2 (g) pipeline underwater	329.37	EUR/(MW km)	3	30	97.9/1000 km
H_2 gas turbine (CCGT)	830	EUR/kW_e	3.35	25	58
Demand-side flexibility (Buffer storage)	0	EUR/MWh_e	-	-	-

Based on the assumptions made for conversion between electricity and H_2, a maximum round-trip efficiency for the H_2 ESCs of 39.44 % can be established. When considering transport efficiencies and losses, a lower efficiency for the full H_2 ESCs can be expected.

Import routes

The same routes are used for HVDC transmission lines and H_2 pipelines from both of the exporting countries. With the applied methodology the exact starting locations of the export routes do not impact the results, here Fez, MA, and Kairouan, TN, are chosen due to their central locations and access to pre-existing infrastructure in their respective country. From the starting points, the export routes head towards the coast and cross the Mediterranean to follow along the coastline of either Spain or Italy. From MA the path follows along the Spanish coast mostly underwater to Montpellier in France and then via Lyon to Geneva. For TN the path connects to Sicily by underwater line and from there follows the Italian coastline on-land to northern Italy and then Geneva. These routes are chosen to follow the shallow (less than 400 m) coastline of Spain with undersea HVDC lines to reduce public resistance and complicated permitting, the same reason as the Xlinks project chooses an underwater connection instead of a shorter on-land connection. The comparable underwater route for Italy along the coastline would for most parts be below a sea depth of 800 m. For such depths few projects exist, therefore the route is avoided as it would pose additional technological challenges. Instead, the route for Italy is chosen to follow existing High-Voltage Alternating Current (HVAC) lines from southern to northern Italy. The resulting routes as shown are comparable to those presented by Hess (2018) [48] and should not be considered definite. To account for potential deviations from these routes, the route lengths are scaled by a detour factor of 1.2 for HVDC [49] and 1.4 for pipeline [21]. This factor also helps to account for collection infrastructure on the exporting sides of MA and TN, which is not considered separately. The routes for MA and TN both have a total length of 1900 km. They are shown in detail in Fig 2 and the individual distances are given in Table 2.

Table 2. The distances considered for the different ESCs and exporters. Total distances for both exporters are the same with different shares of distance for the on-land and underwater paths.

Distances [km]	Total (underwater)	HVDC[a]	H_2 pipeline[b]
Morocco (MA)	1900 (1380)	2280 (1656)	2660 (1932)
Tunisia (TN)	1900 (150)	2280 (180)	2660 (210)

[a] Distances scaled by a detour factor of 1.2 based on [49].
[b] Distances scaled by a detour factor of 1.4 based on [21].

Export, technology and demand-sid flexibility scenarios

Imports from MA and TN to Geneva are compared between different scenarios:

- The two different ESCs, import by HVDC transmission line and H_2 pipeline
- With and without CSP & TES available as generation and storage technologies
- With different demand flexibilities for shifting the electricity demand pattern

The electricity demand in all scenarios is set to a constant baseload of 3.6 GW to keep comparability with the Xlinks project.

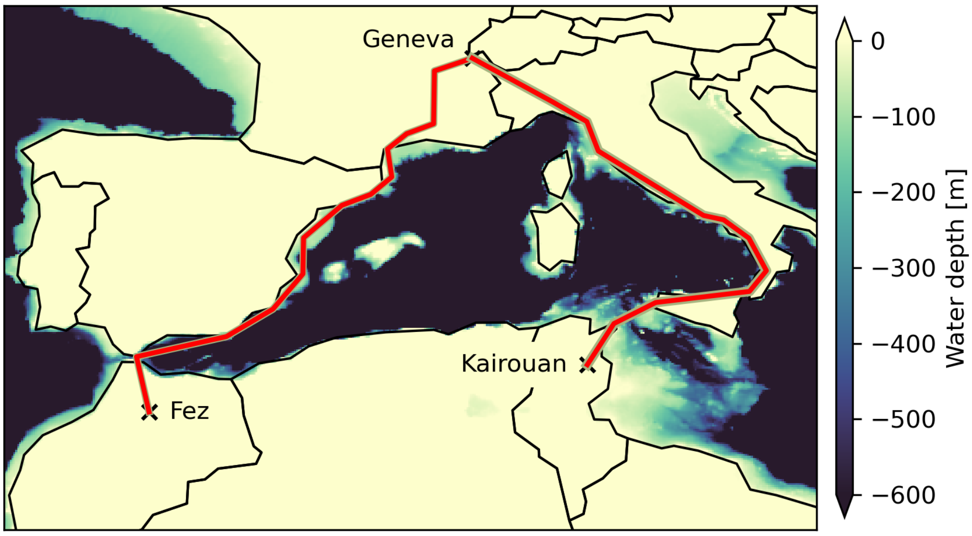

Fig 2. Import routes from MA and TN to Geneva, Central Europe, which are selected for this study.
The route from Fez, Morocco, follows the Spanish coastline underwater. The route from Kairouan, Tunisia, follows the Italian coastline on-land as the sea depth would make underwater development challenging. Country shapes made with Natural Earth [50] data, water depth based on [32].

Demand-side flexibility in the different scenarios refers to the ability to consume the requested amount of electricity at an earlier or later time. Increasing demand-side flexibility allows the model to meet electricity demand at an earlier or later time. This opens an additional option for the model to address the variable availability from the RES other than through storage capacities. The scenarios for demand-side flexibility range from "Baseload", i.e. the case where the electricity demand of 3.6 GW has to be continuously supplied, to "Annual" matching where there are no restrictions on when the electricity is supplied, only the total amount of $3.6\,\mathrm{GW} \cdot 8760\,\mathrm{h} = 31\,536\,\mathrm{GWh}$ needs to be supplied by the modeled ESCs. Scenarios with flexibility in shifting their demand, i.e. scenarios between "Baseload" and "Annual", allow the model to shift an electricity demand equivalent to the scenario name to an earlier or later time. The demand flexibility is implemented using an electricity buffer storage before the electricity consumer, which the model can use at no costs and with a maximum electricity storage capacity equivalent to the scenario name, e.g. for the "Daily" scenario with a capacity of $86.4\,\mathrm{GWh} = 3.6\,\mathrm{GW} \cdot 24\,\mathrm{h}$. Similarly, the remaining flexibility scenarios allow for demand shifting within "Weekly" for 168 h, "Biweekly" for 336 h, "Monthly" for 744 h and "Quarterly" for 2208 h. Technically the demand-side flexibility is implemented by extending the *PyPSA* models from [28] with a for-free *store*-component before the final electricity demand with its' maximum capacity limited to the amount of demand-side flexibility.

Results

Costs for importing electricity

The costs for importing electricity through the HVDC and H_2 pipeline ESCs are presented in Fig 3 for all scenarios modeled for this study, with both MA and TN as exporters and different levels of demand-side flexibilities. The figure shows the Levelised Cost of Electricity (LCoE), which is calculated as the total system costs divided by the annual total of electricity delivered. Tabular results are also included in S1 Appendix.

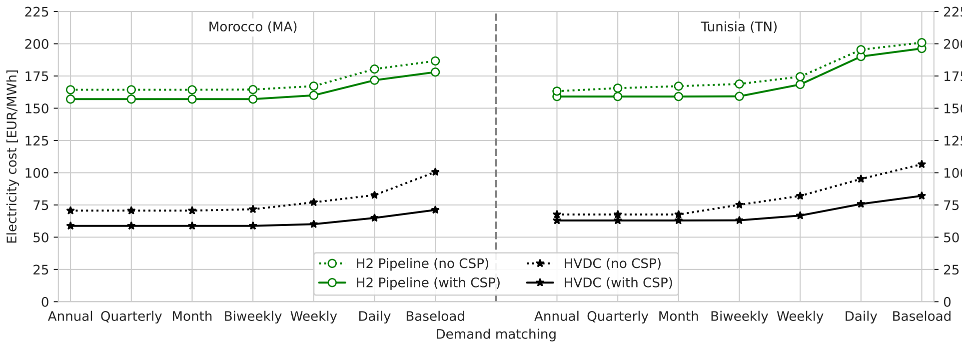

Fig 3. Cost of direct and indirect imports electricity from MA (left) and TN (right) in all scenarios.
The results are qualitatively and quantitatively similar for MA and TN. Direct imports by HVDC are 2 to 3 times cheaper than indirect imports and power generation from H_2. Electricity costs are highest when baseload electricity is required. Using a combination of CSP with TES as additional RES can offer additional cost benefits.

For both MA and TN exporters, the costs of importing electricity are similar. The costs of importing electricity directly through the HVDC ESC range from 58 EUR/MWh to 106 EUR/MWh. For indirect imports through the H_2 pipeline ESC, the costs are more than twice as high, starting from 157 EUR/MWh to 201 EUR/MWh. Scenarios with both CSP and TES for electricity generation and energy storage (referred to as “with CSP”) have lower costs compared to their scenario counterparts where both technologies are not available (referred to as “no CSP”). In the case of HVDC ESCs, the cost benefits of having CSP are higher, reaching up to a reduction of 25 EUR/MWh or 25 % in the “Baseload” scenario. On the other hand, the cost benefits of having CSP in H_2 ESCs are relatively low at the highest 10 EUR/MWh or 6 %. More systematic cost benefits for scenarios of both ESCs can be found with increasing demand-side flexibility. Here the costs of all imports can be reduced by 20 EUR/MWh to 40 EUR/MWh or 20 % when relaxing the requirement for “Baseload” to “Annual”-matched electricity supply. Since the costs and other results are very similar for MA and TN, for the remainder of this study the presentation will focus on the results for MA with and without CSP. Additionally, the focus will be on comparing “Baseload” and “Annual” scenarios, as they show the biggest differences and the results of the remaining flexibility scenarios are found to be these two scenarios. Figures showing the results for TN and all flexibility scenarios are included in S3 Appendix.

Electricity generation mix

Electricity for direct export and H_2 production is procured from a mix of wind and solar RES. A major difference between the scenarios is the availability of CSP and TES for electricity generation. Fig 4 and Fig 5 show the total electricity generation by technology for the HVDC and H_2 ESCs, comparing scenarios with and without CSP. RES capacities available for electricity generation but unutilized are shown as curtailed electricity. While the total amount of produced electricity is similar for all scenarios of the same ESC, the H_2 ESC requires more than double the amount of electricity compared to the HVDC ESC due to the round-trip conversion losses between electricity and H_2. Without transport energy demand and losses, the conversion of electricity to H_2 and back has a round-trip efficiency of 39.44 %. The electricity is provided from a mix of solar PV (or CSP if available in the scenario), combined with small amounts of wind. Solar-based RES are at an advantage in Northern Africa due to the low seasonality and the diurnal availability pattern. This availability pattern allows PV to be combined with battery storage and CSP with TES to provide baseload electricity relatively easily.

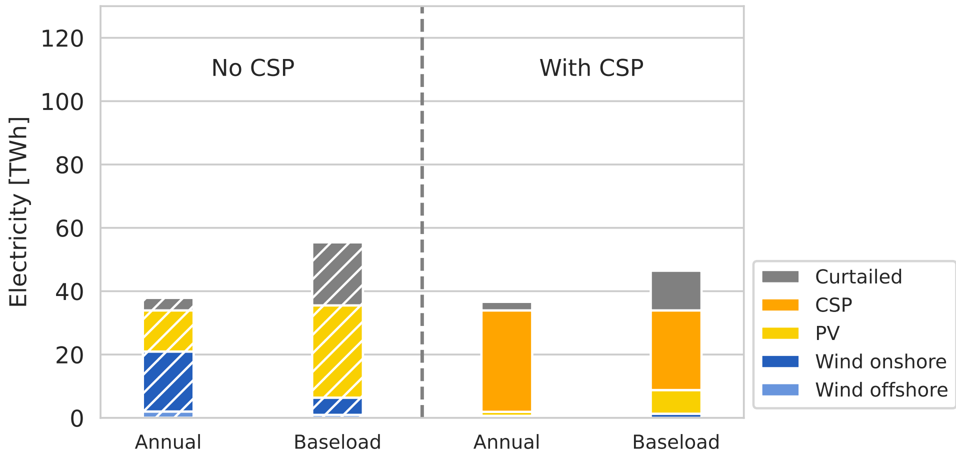

Fig 4. Electricity generation mix for direct imports by HVDC from MA. Scenarios without CSP and TES (left) compared to scenarios with both technologies available (right) for the two most contrasting scenarios for demand-side flexibility, “Baseload” and “Annual” matching, are compared. Without CSP and TES, electricity is generated from a mix of PV and onshore wind, where PV dominates in the “Baseload” scenario. In scenarios with CSP and TES, their combination leads CSP to be the dominant source of electricity, and the low-cost TES leads to lower levels of curtailed electricity.

Storage and transport capacities

The capacities for storage, transport, and H_2 conversion infrastructure from MA for scenarios including CSP are shown in figure Fig 6. The capacities are reported in electricity equivalents (GWh_e, GW_e) for better comparison. This means that the H_2 storage and pipeline capacities are multiplied by the CCGT efficiency and TES capacities are multiplied by the CSP power block efficiency (cf. Table 1).

The transport capacities for both HVDC and H_2 ESCs are similar across all scenarios, which indicates the limited surplus capacity and a high utilization rate for this infrastructure. The model has in principle the option to build storage capacities also after the transport infrastructure, that is downstream after the HVDC lines and H_2 pipeline on the exporting side. However, most storage is built on the exporting side in MA to maintain the high utilization rate of the transport infrastructure and to buffer the variable availability of RES there, rather than on the importing side.

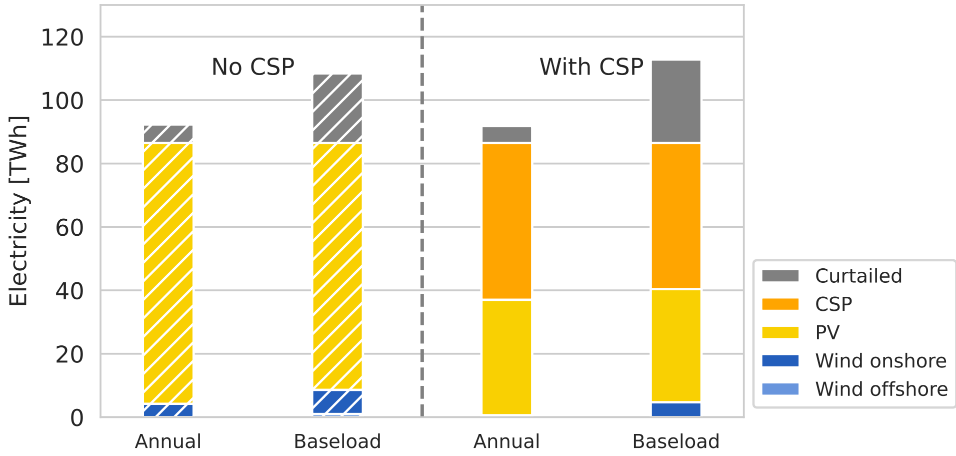

Fig 5. Electricity generation mix for indirect imports by H_2 from MA. Scenarios without CSP and TES (left) compared to scenarios with both technologies available (right) are compared. In contrast to Fig 4, PV generally provides a larger share of electricity in all scenarios and the total electricity generation is more than two times higher compared due to the round-trip-efficiency of converting between electricity and hydrogen.

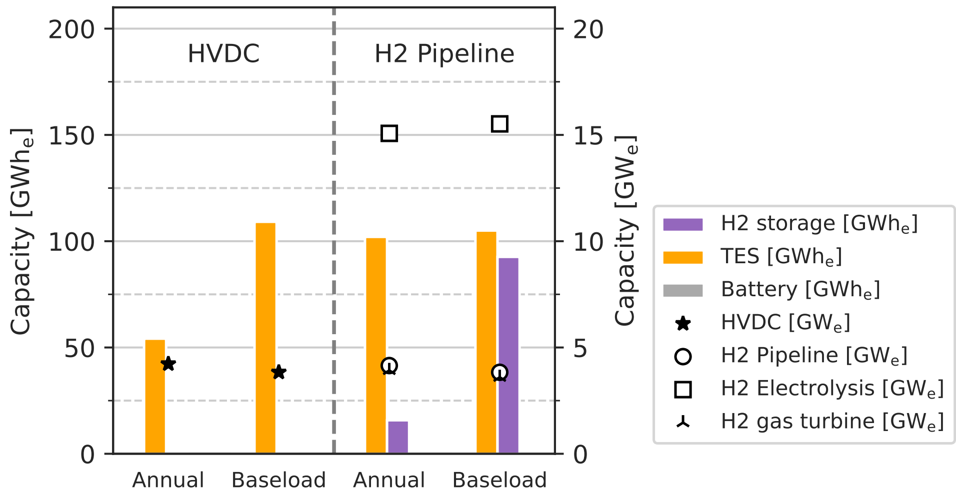

Fig 6. Capacities for storage, transport, and H_2 technologies for (left) direct and (right) indirect imports from MA in scenarios with CSP and TES. Storage capacities are in GWh$_e$ (bars, left y-axis), transport and H_2 technologies are in GW$_e$ (markers, right y-axis). All capacities are reported in electricity equivalents, see text for details. As demand becomes less flexible, storage capacities increase and are the highest in the scenarios for "Baseload" electricity supply.

The storage capacities of the H_2 ESC scenarios are about twice as high as those of the corresponding HVDC ESC scenarios. Between "Annual" and "Baseload" scenarios, the total storage capacities increase as the supply needs to meet demand on a stricter schedule. The overall storage capacities built range from 54 GWh_e to 110 GWh_e for direct imports via HVDC and 118 GWh_e to 198 GWh_e for indirect imports via H_2 pipeline. The storage capacities between the ESCs can also be compared based on how long they can provide the fixed demand of 3.6 GW. In the case of HVDC-based, the capacities last between 15 h to 31 h. For H_2 pipeline-based imports, the storage capacities last for a duration of 16 h to 37 h, the round-trip conversion to and from H_2 is accounted for the TES capacity, as the energy stored in the TES is exposed to conversion losses when being moved downstream along the H_2 ESC, cf. Fig 1.

As for the deployed technologies, battery storage is deployed in only some scenarios of the HVDC ESC and only when TES is not available, cf. ??. In the scenarios as shown in Fig 6, where TES is available it fully replaces battery storage due to its lower costs. In the case of the H_2 ESC, the increasing storage capacity requirements are met with the help of H_2 storage, due to its even better economics and integration of bulk H_2 storage compared to the alternatives TES and battery storage. At the same time TES plays a smaller role in the overall storage capacity while playing an important role in improving the economics of H_2 electrolysis by increasing the electrolysis' utilization factor. The necessary electrolysis capacities for the H_2 ESC with more than 15 GW at first glance seem high in comparison to the transport infrastructure capacity of below 4 GW_e. As for the TES, the round-trip efficiency of 39.44 % for H_2 conversion has to additionally be taken into account for the electrolysis capacities, leading to a minimum requirement of $^{3.6\,GW}/_{39.44\,\%} = 9.13\,GW_e$. This gives a utilization rate of around 60 % for the electrolysis in the shown scenarios. This utilization rate is well-above the possible utilization rate from a pure solar-based RES supply mix (cf. Fig 5) which is exposed to the day-night cycle. This points to the role of TES in the H_2 ESCs, as being to increase the utilization rate of electrolysis, rather than providing bulk energy storage capacities. This role is reserved for the H_2 storage.

Import cost compositions

The import costs can be broken down into individual cost components, which is shown in Fig 7. Approximately half of the total costs are for electricity generation from RES. Between "Annual" and "Baseload" scenarios, there are two components responsible for driving costs up. The first is the increasing RES costs linked to increasing RES capacities (cf. Fig 4, Fig 5), and the second the increasing storage costs linked to their increasing capacities, required to provide the baseload electricity supply.

Between the HVDC and H_2 ESCs, the cost difference is related to H_2 production and electricity generation from H_2. RES costs are nearly double for the H_2 pipeline compared to the HVDC-based imports, as conversion losses along the ESC accumulate and need to be compensated by higher electricity generation. The H_2 electrolysis and electricity generation from H_2 by gas turbine add another 25 % to the total costs and are additional cost components that are not required by the HVDC ESC. The comparison also shows that the transport-related costs, i.e. for HVDC transmission lines and H_2 pipeline including auxiliary equipment, are similar across all ESC and none of the alternatives has a unique advantage over the others. H_2 imports do not profit from lower transport costs.

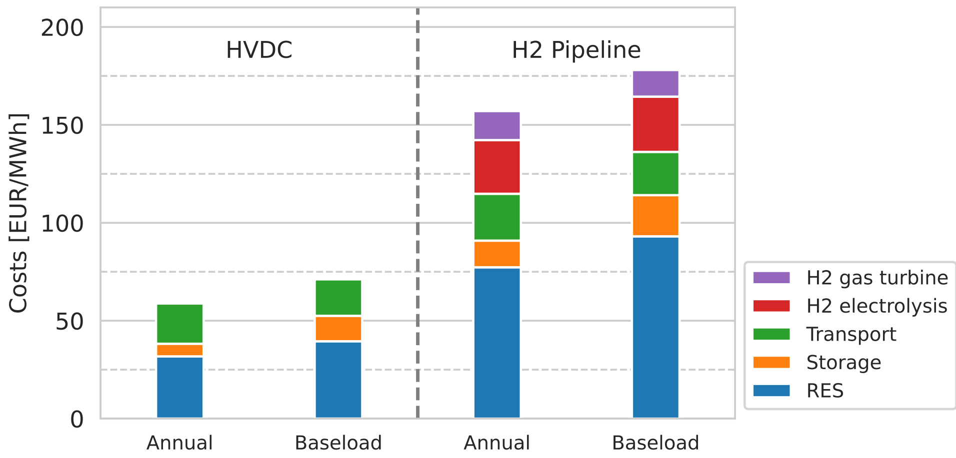

Fig 7. Composition of import costs for (left) direct and (right) indirect imports from MA in scenarios with CSP and TES.
The costs for transport are similar across scenarios and both ESC. The H_2 conversion steps add additional costs and electricity demand, leading to higher RES capacities required and RES-related costs. Between "Annual" and "Baseload" demand matching differences in costs are due to additional storage capacities and RES overcapacities, required for balancing weather-depended RES availability.

Discussion

The LCoE for importing electricity determined in this study are within the range of other studies. Compared to an earlier study by the author [28] where direct and indirect imports of H_2 by pipeline and HVDC were compared, in this study the advantages of directly importing electricity as the demanded energy carrier are again underlined. Hess (2013) [51] estimated around 120 EUR/MWh for HVDC-based electricity imports without demand-side flexibility. For imports of H_2 via blending in natural gas pipelines Timmerberg et al. (2019) [21] estimated in low and high cost scenarios to be between 59 EUR/MWh_{H2} to 123 EUR/MWh_{H2}, or 102 EUR/MWh to 212 EUR/MWh after taking into account the CCGT efficiency relevant in this study. The range found by Timmerberg et al. for low and high-cost scenarios is quantitatively similar to the range found here due owing to demand-side (in-)flexibility, indicating the importance of considering demand-side flexibility in such studies. The benefits of demand-side flexibility found here are also comparable to those found by Walter et al. (2023) [26] who determined possible reductions to costs for hydrogen of 30 EUR/MWh from full temporal demand-side flexibility.

Results based on the methodology and models used here are sensitive to made technology assumptions (cf. Table 1) and changes to these assumptions can have strong effects on the results, see [21, 28] for details. Since a transport modeling approach is used, not all physical aspects of the electricity transmission and H_2 pipeline infrastructure could be incorporated, notably the intrinsic ability of H_2 pipelines to buffer and store gas through linepack, although this effect is estimated small in comparison to natural gas pipelines [52]. The ESCs are modeled stand-alone and without consideration for existing infrastructure and potential options for reuse and synergies thereof. This especially includes potentially beneficial interactions with the European energy system are beyond the scope of this study and have been examined in detail by others, for example by Hess (2018) [48] and Wetzel et al. (2023) [53].

With the LCoE estimated to be below the average non-household consumer prices for electricity in France, which were at 120 EUR_{2022}/MWh in 2022 [54], the analysis provides grounds for considering the presented scenarios as potentially economically attractive projects. While today's electricity demand of CERN in particular, is sufficient to take off only a fraction of the electricity import volumes discussed here, future expansion and upgrades to the research facilities could lead to an increase of their electricity demand. Expansion and upgrades provide opportunities to evaluate and increase the demand-side flexibility with the potential economic benefits as outlined here. Demand-side flexibility in this study is characterized in a simplified way by assuming full demand-side flexibility capacity at zero associated costs. In reality, making available and using demand-side flexibility might be linked to costs along with the need for technical as well as organizational preparations to research equipment and usage patterns, which may dictate additional usage constraints beyond the flexibility capacity.

With the stated limitations it should become clear that this study does not constitute a feasibility study. With the focus on the techno-economic cost perspective, other aspects including societal and ecological are not explored. A more detailed investigation should incorporate an interdisciplinary approach to also evaluate to fill these gaps and investigate the social, ecological, and political consequences of detailed import projects and contain a site-specific analysis in MA or TN compared to the generalized, near country-wide analysis conducted here.

Conclusions

The presented study analyzed importing electricity from RES from Northern Africa to Central Europe directly by HVDC transmission line and indirectly by H_2 pipeline. From a cost perspective, direct imports of electricity are more attractive than indirect imports by H_2 pipeline. The costs for electricity imports by HVDC transmission lines are estimated to be between 58 EUR/MWh to 106 EUR/MWh. Imports by H_2 pipeline are estimated to cost more than twice as much, between 157 EUR/MWh to 201 EUR/MWh. Demand-side flexibility for electricity can reduce the costs of imported electricity by up to 45 %, as the demand can adapt to the weather-dependent availability of the RES supply. The less flexible the electricity demand is, the more surplus infrastructure and storage capacities are required. Using CSP with TES in addition to wind and PV for the electricity mix can reduce costs further, as it allows for the use and deployment of comparatively low-cost, integrated TES as alternative energy storage to battery and H_2 storage. This study does not evaluate the feasibility of the proposed projects and does not assess the demand-side flexibility of research institutions. It shows that electricity from RES can be imported cost-effectively and are a possible way for Central European research institutions to reduce their energy-related scope 2 carbon emissions. In times of rising and uncertain electricity prices, research institutions could step forward to become partners and guaranteed off-takers in a project importing electricity from Northern Africa, thereby reducing project risks and securing for themselves a supply of low-cost and sustainable electricity.

Supporting information

S1 Appendix. Tabular results of Levelised Cost of Electricity

S2 Appendix. Technology assumption details

S3 Appendix. Extended and additional figures

S4 Appendix. Regions and land availability analysis results

Acknowledgements

The author extends his special gratitude to the following persons for their helpful and dear-worthy comments and suggestions: Leon Schumm, Martina Hampp, Michael Düren and Tom Brown.

Abbreviations

H_2 Hydrogen

CCGT Closed-Cycle Gas Turbine

CERN European Organization for Nuclear Research

CSP Concentrated Solar Power

EAC Equivalent Annual Cost

ESC Energy Supply Chain

FOM Fixed Operation & Maintenance

GEGIS GlobalEnergyGIS

HEP High-Energy Physics

HVAC High-Voltage Alternating Current

HVDC High-Voltage Direct Current

LCoE Levelised Cost of Electricity

LHC Large Hadron Collider

MA Morocco

PV Photovoltaic

PyPSA Python for Power System Analysis

RES Renewable Energy Source

TES Thermal Energy Storage

TN Tunisia

UK United Kingdom

WACC Weighted Average Cost of Capital

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S1 Appendix. Tabular results of Levelised Cost of Electricity

Table A. Tabular results of LCoEs in EUR/MWh for all scenarios modeled for this study.
Values are visualized in Fig 3.

	CSP	with CSP				no CSP			
	ESC	HVDC		H_2 pipeline		HVDC		H_2 pipeline	
	Exporter	MA	TN	MA	TN	MA	TN	MA	TN
Flexibility									
Annual		59	63	157	159	71	68	164	163
Quarterly		59	63	157	159	71	68	164	166
Monthly		59	63	157	159	71	68	164	167
Biweekly		59	63	157	159	72	75	164	169
Weekly		60	67	160	168	77	82	167	174
Daily		65	76	172	190	83	95	180	195
Baseload		71	82	178	196	101	107	187	201

S2 Appendix. Technology assumption details

Table B. Details on the technology assumptions made in the model for 2030, as listed in Table 1.
The *currency year* indicates the monetary year of all costs taken from the specific publication. Where the *currency year* is not 2015, inflation adjustment is done assuming 2 % p.a. inflation rate.

Technology	Source	Currency year	Additional information
Wind onshore	[2]	2015	Technology “20 Onshore turbines”.
Wind offshore	[2]	2020	Technology “21 Offshore turbines” nominal investment minus grid connection costs.
Solar PV	[2]	2020	Technology “22 Utility-scale PV”.
CSP field & receiver tower	[1], [3]	2020	CAPEX based on [1] 2020 numbers, combined with CAPEX degression taken from ATB database “moderate” scenario; costs include solar field, solar tower, and EPC cost for the default installation size of 104 MW(e) plant. Total costs (223,708,924 USD) are divided by active area (heliostat reflective area, 1,269,054 m2) and multiplied by design point DNI (0.95 kW/m2) to obtain EUR per kW_{th} value. Exchange rate: 1.16 USD to 1 EUR. FOM calculated from the ratio between CAPEX and FOM of [3] for CSP in “Moderate” scenario. Lifetime taken from [3].
CSP TES	[1], [3]	2020	CAPEX based on [1] 2020 numbers, combined with CAPEX degression taken from ATB database “moderate” scenario; costs include the TES and EPC cost for the default installation size 104 MW(e) plant and 2791 MW(th) TES. Total costs (69390776.7 USD) are divided by TES size to obtain EUR per kW(th). Exchange rate: 1.16 USD to 1 EUR. FOM calculated from the ratio between CAPEX and FOM of [3] for CSP in “Moderate” scenario. Lifetime taken from [3].
CSP power block	[1], [3]	2020	CAPEX based on [1] 2020 numbers, combined with CAPEX degression taken from ATB database “moderate” scenario; costs include the power cycle incl. BOP and EPC cost for the default installation size (104 MWe plant). Total costs (135185685.5 USD) are divided by power block nameplate capacity size to obtain EUR per kW(el). Exchange rate: 1.16 USD to 1 EUR. FOM calculated from the ratio between CAPEX and FOM of [3] for CSP in “Moderate” scenario. Lifetime taken from [3].
Battery storage	[4]	2015	Technology “180 Lithium Ion Battery”, Energy storage expansion cost investment.
Battery inverter	[4]	2015	Technology “180 Lithium Ion Battery”, Output capacity expansion cost investment.
Electrolysis (Alkaline)	[5]	2015	Technology “86 AEC 100MW”.

Continue on the next page

Table B (cont.)

Technology	Source	Currency year	Additional information
Hydrogen storage tank	[6]	2020	Table SI.9, technology "GH2 (L)" with 450 EUR per kg of h2 converted to MWh using LHV with LHV to MWh. The currency year assumed 2020 for the initial publication of reference and observing note in SI.4.3 that in their reference no currency year is explicitly stated.
HVDC inverter pair	[7]	2011	Table A.2
HVDC line overhead on-land	[7]	2011	Table A.2
HVDC line underwater	[8]	2018	Estimated costs for a connector between Europe and North America (bidirectional, 4 GW, ca. 3000 km length and 3000m depth). Costs from publication are based on existing and currently under construction undersea cables.
H_2 (g) pipeline fill station	[9], [10]	2015	CAPEX from [9] from figure 14 of PDF, pg. 164, for staging 35 to 140 bar at a capacity of 6000 MW(HHV) single line pipeline and converting for LHV of H2. Lifetime from [9] figure 24 of PDF, pg. 168. FOM from [10] table 3 and table 5 with the pessimistic (highest) value chosen for a 48-inch pipeline with 13 GW_{LHV} at 100 bar pressure; the forecast year is not specified, assumed 2020 based on remarks in PDF.
H_2 (g) pipeline on-land	[11], [9]	2020	CAPEX Assumption for a 48-inch single line pipeline, incl. compressor investments, 16.9 GW peak capacity, 2750 EUR/m, 434 MWe/1000 km for compressor, 3.4 MEUR/MWe for compressor, from [11] table 35. FOM and lifetime from [9] Assumption for a 140 bar, $>$ 6000 MW HHV single line pipeline, incl. booster station investments. Considering LHV by scaling with LHV/HHV=0.8462623413.
H_2 (g) pipeline underwater	[12], [13]	2014	CAPEX oriented on to [12] for 36-inch CH4 submarine pipeline multiplied by 2.86 which is a common factor found for cost estimates between CH4 and H2 pipelines. FOM and lifetime from [13], assuming the same as for a CH4 pipeline.
H_2 gas turbine (CCGT)	[2]	2015	Technology "05 Gas turb. CC, steam extract.".
Demand-side flexibility	-	-	Guesstimate.

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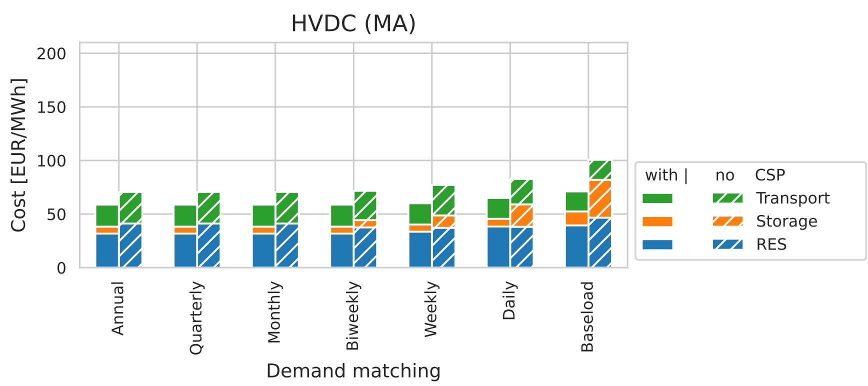
S3 Appendix. Extended and additional figures

S3A Appendix. Import cost compositions

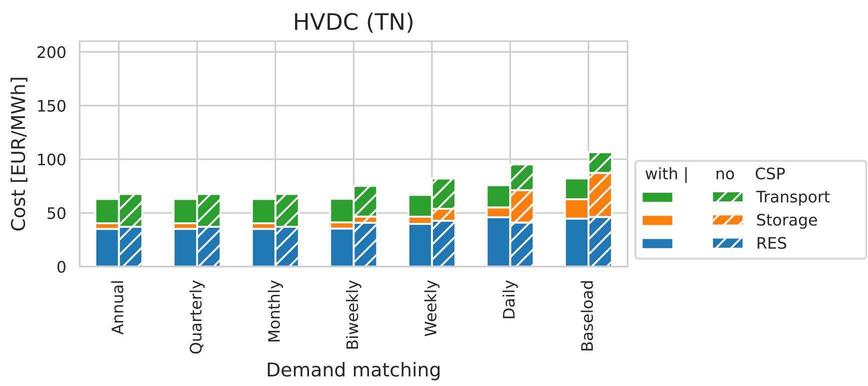
In Fig 7 the cost compositions for ESCs from MA with CSP are shown. An extended version of this figure is shown below in Fig A for all flexibility scenarios, scenarios without CSP, and all scenarios from TN.

The categories used in Fig 7 and the figures below are the following:

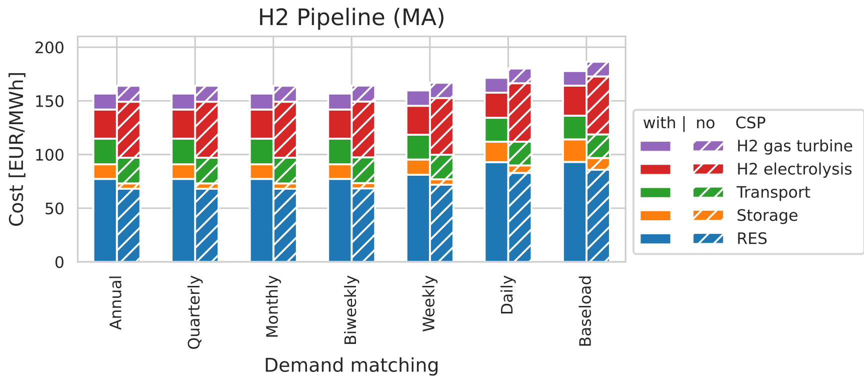
- RES: Electricity generation from offshore wind, onshore wind, PV and CSP; excluding TES
- Storage: Battery storage, TES, H_2 storage
- Transport: All HVDC and H_2 pipeline components, incl. inverter and compressor stations
- H2 electrolysis: H_2 electrolysis for converting water and electricity to H_2
- H2 gas turbine: CCGT cost for converting H_2 back to electricity



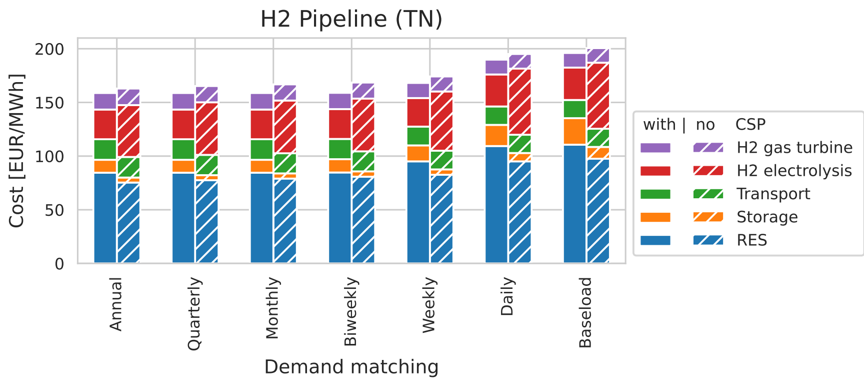
(a) HVDC from MA.



(b) HVDC from TN.



(c) H_2 Pipeline from MA.

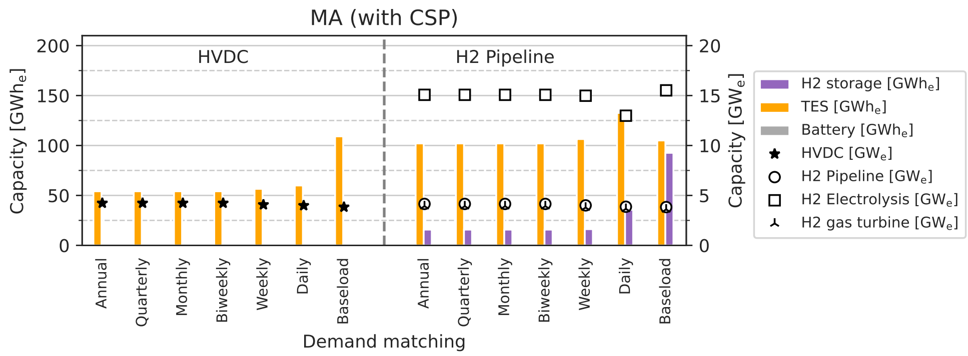


(d) H_2 Pipeline from TN.

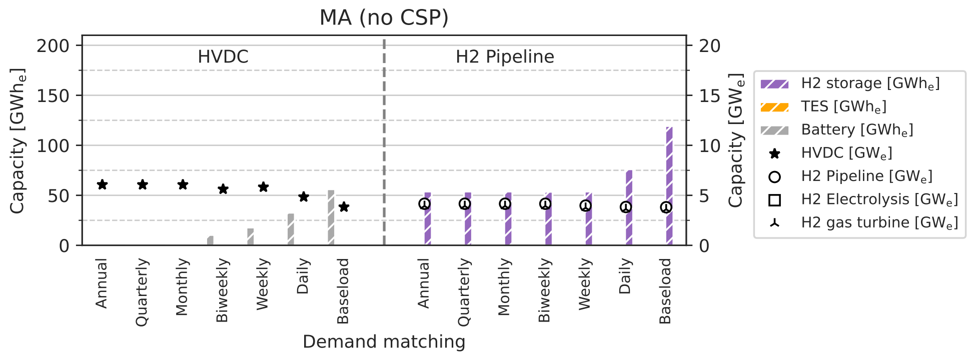
Fig A. Cost compositions in EUR/MWh for all scenarios calculated in this study with and without CSP.
(a) HVDC from MA, (b) HVDC from TN, (c) H_2 pipeline from MA, (d) H_2 pipeline from TN. Extended and additional versions of Fig 7. Hatched bars indicate scenarios without CSP and TES, solid bars with both technologies.

S3B Appendix. Capacities for storage, transport and Hydrogen technologies

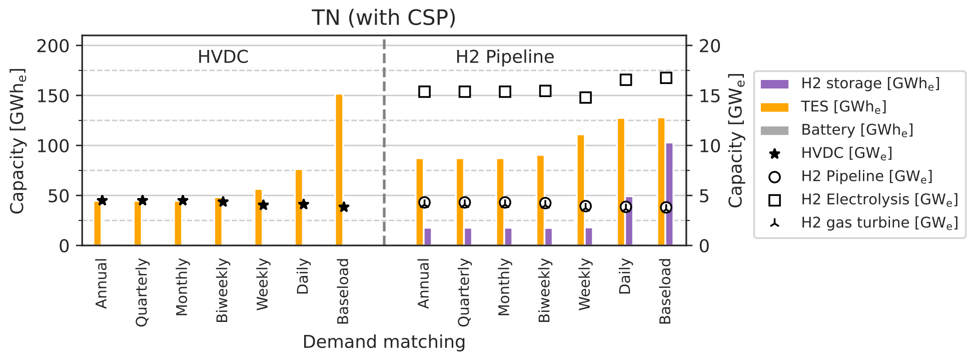
In Fig 6 the capacities for storage, transport, and H_2 technologies for ESCs from MA with CSP are shown. An extended version of this figure is shown below in Fig B for all flexibility scenarios, scenarios without CSP, and all scenarios from TN.



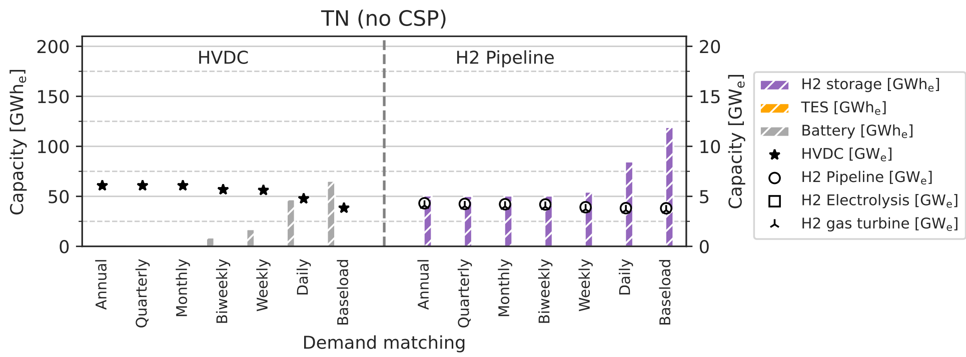
(a) ESCs from MA with CSP and TES.



(b) ESCs from MA without CSP and TES.



(c) ESCs from TN with CSP and TES.

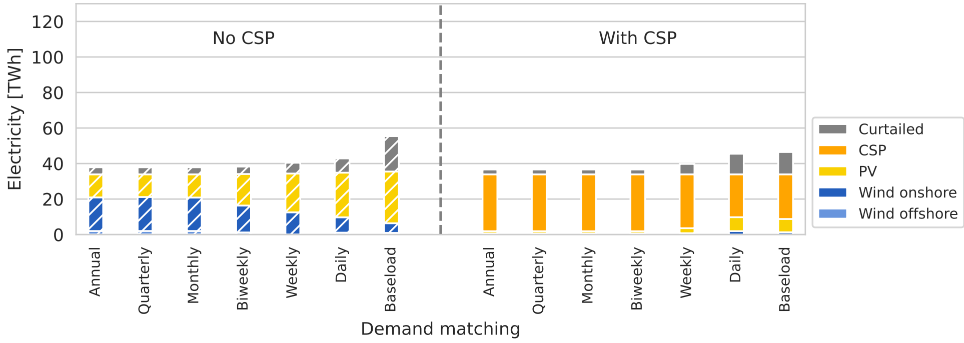


(d) ESCs from TN without CSP and TES.

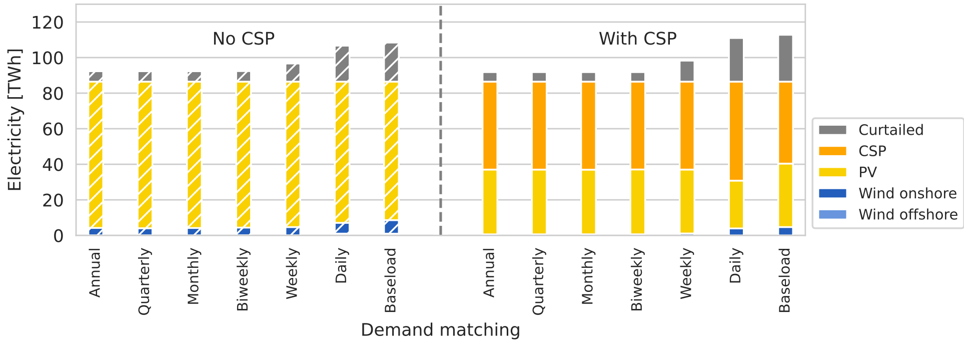
Fig B. Capacities for storage, transport, and H_2 technologies.
(a) from MA with CSP, (b) from MA without CSP, (c) from TN with CSP, (d) from TN without CSP. Extended and additional versions of Fig 6. All capacities are reported in electricity equivalents, see text for details. Hatched bars indicate scenarios without CSP and TES, solid bars with both technologies.

S3C Appendix. Electricity mix

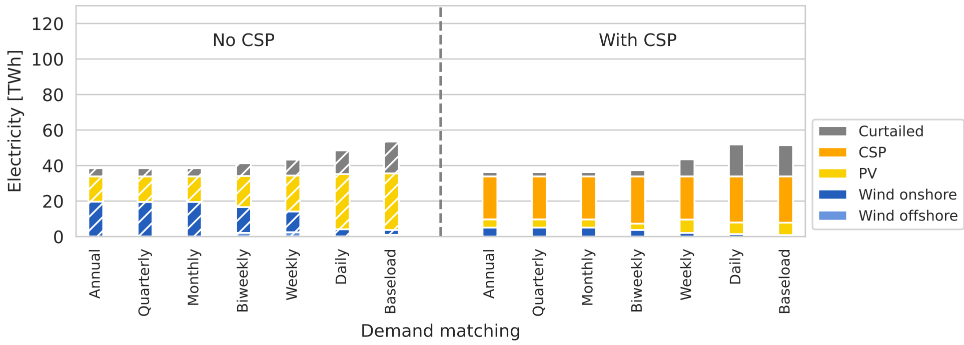
In Fig 4 and Fig 5 the capacities for storage, transport, and H_2 technologies for ESCs from MA with and without CSP are shown. An extended version of this figure is included below for all flexibility scenarios, scenarios without CSP, and all scenarios from TN.



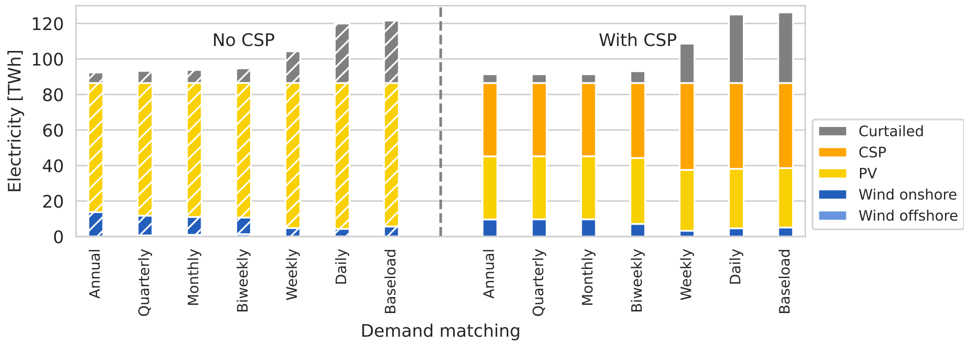
(a) HVDC from MA.



(b) H_2 pipeline from MA.



(c) HVDC from TN.



(d) H_2 pipeline from TN.

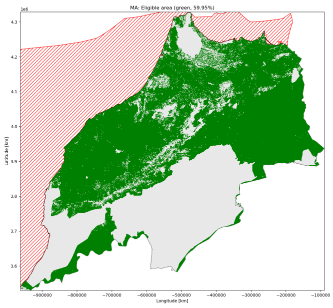
Fig C. Electricity generation mix for ESCs without and with CSP and TES technologies available to the model.
(a) for HVDC from MA, (b) for H_2 pipeline from MA, (c) for HVDC from TN, (d) for H_2 pipeline from TN. Extended and additional versions of Fig 4 and Fig 5. Hatched bars indicate scenarios without CSP and TES, solid bars with both technologies.

S4 Appendix. Regions and land availability analysis results

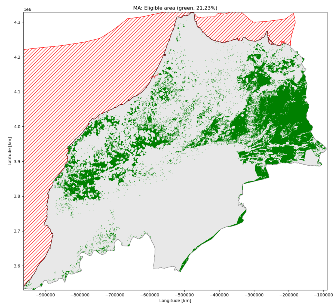
S4A Appendix. Morocco

The following administrative regions based on Database of Global Administrative Areas (GADM) [1] were included in the analysis for MA: Tanger - Tétouan, Gharb - Chrarda - Béni Hssen, Taza - Al Hoceima - Taounate, Rabat - Salé - Zemmour - Zaer, Grand Casablanca, Fès - Boulemane, Oriental, Chaouia - Ouardigha, Doukkala - Abda, Tadla - Azilal, Meknès - Tafilalet, Marrakech - Tensift - Al Haouz, Souss - Massa - Draâ.

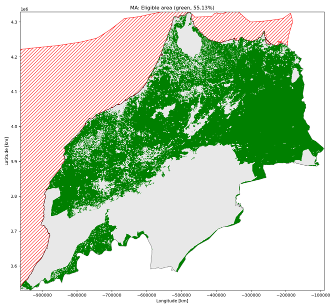
Eligible land for individual technologies after land availability analysis is shown below in Fig D.



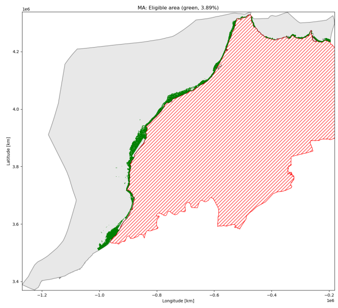
(a) Solar PV.



(b) Solar CSP.



(c) Wind onshore.

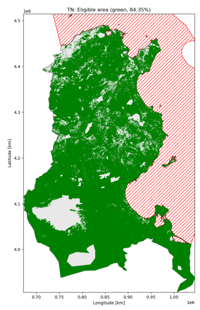


(d) Wind offshore.

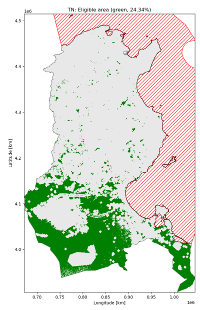
Fig D. Areas in Tunisia considered eligible and considered for RES. (a) for solar PV, (b) for solar CSP, (c) for wind onshore, (d) for wind offshore.

S4B Appendix. Tunisia The following administrative regions based on GADM [1] were included in the analysis for TN: Bizerte, Ariana, Tunis, Manubah, Béja, Nabeul, Ben Arous (Tunis Sud), Jendouba, Zaghouan, Siliana, Le Kef, Sousse, Kairouan, Monastir, Mahdia, Kassérine, Sidi Bou Zid, Sfax, Gafsa, Tozeur, Gabès, Kebili, Médenine.

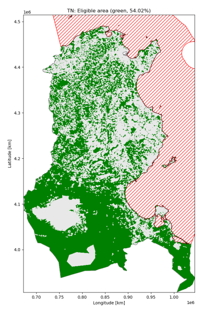
Eligible land for individual technologies after land availability analysis is shown below in Fig E.



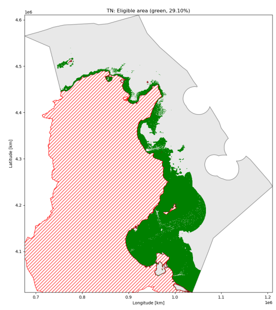
(a) Solar PV.



(b) Solar CSP.



(c) Wind onshore.



(d) Wind offshore.

Fig E. Areas in Tunisia considered eligible and considered for RES. (a) for solar PV, (b) for solar CSP, (c) for wind onshore, (d) for wind offshore.

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D PUBLICATION 4

This chapter has been published as

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J.H. Data Curation, Investigation, Methodology, Software, Writing – Review and Editing

CellPress

Future Energy

Ultra-long-duration energy storage anywhere: Methanol with carbon cycling

Tom Brown[1,*] and Johannes Hampp[2]

Tom Brown leads a group of energy system modelers at the Technische Universität Berlin, where he holds the professorship for digital transformation in energy systems. His group researches future pathways for the energy system, with a particular focus on revealing the trade-offs between energy resources, network expansion, flexibility, and public acceptance of new infrastructure. He is a strong supporter of openness and transparency in research and is one of the lead developers of the widely used open-source software Python for Power System Analysis (PyPSA).

Johannes Hampp is a researcher at the Potsdam Institute for Climate Impact Research and is finishing a doctorate at the University of Gieβen in energy system modeling. His research focuses on the production of hydrogen and hydrogen derivatives and on the effects of regional differences in renewable endowments around the world on energy and feedstock supply chains.

Ultra-long-duration storage for variable renewable energy

Wind and solar generation are rapidly expanding around the globe as their costs come down and societal pressure to reduce greenhouse gas emissions rises. To supply a high fraction of electricity demand with variable sources, different types of storage are needed to balance daily, weekly, seasonal, and interannual weather fluctuations. Battery storage can bridge several hours of low solar and wind feed-in. However, if wind and solar penetration rises to cover all demand in the absence of other generation technologies, longer duration energy storage becomes necessary to supply multiple days or weeks of dark wind lulls and seasonal variations in supply and demand, as well as to bridge years of low renewable production. While the term long-duration energy storage (LDES) is often used for storage technologies with a power-to-energy ratio between 10 and 100 h,[1] we introduce the term ultra-long-duration energy storage (ULDES) for storage that can cover durations longer than 100 h (4 days) and thus act like a firm resource. Battery storage with current energy capacity investment costs of 100–200 €/kWh would be too costly for these long periods. Simulations show that for renewable systems to be competitive with dispatchable low-carbon technologies, ULDES would need to cost at most around 10 €/kWh.[2] (Note that all costs are given in 2020 euros, while all fuel energy units and efficiencies refer to the lower heating value.)

Underground hydrogen storage for ULDES

Hydrogen storage is a promising candidate for ULDES, whereby hydrogen is produced by electrolysis of water, stored and then used to generated electricity in a gas turbine or fuel cell.[3–5] While aboveground pressure vessels can cost 10–40 €/kWh, depending on their rated pressure, storing hydrogen underground in solution-mined salt caverns has much lower costs in the range 0.1–0.5

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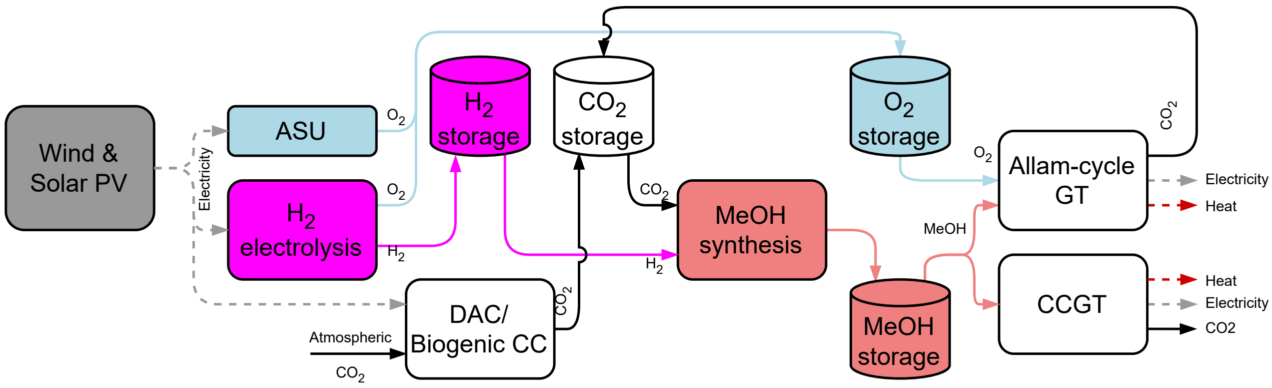

Figure 1. Schematic of methanol storage with carbon cycling

The Allam turbine combusts methanol in pure oxygen and returns the carbon dioxide to join the electrolytic hydrogen for synthesis to methanol. Methanol is stored as a liquid at ambient temperature and pressure, oxygen is stored as a liquid at −183° C, and carbon dioxide is stored as a liquid at 7 bar and −50° C; only hydrogen is stored as a gas (at 250 bar) while it is buffered before going into the methanol synthesis. Figure inspired by Baak et al.[8]

€/kWh. Several salt caverns with sizes up to 274 GWh are already used for storing hydrogen at petrochemical facilities in the United Kingdom and in Texas in the United States. Despite the attractive cost, hydrogen salt caverns face several challenges. Many regions do not have salt deposits, such as large parts of Africa, southeast Europe and southeast Asia.[3] In those countries that do have suitable salt deposits for caverns, they are often highly localized: in the northeast of the island of Ireland, centrally in Great Britain, and in the north of the Netherlands and Germany, to name a few examples.[3] The distance of cavern sites from hydrogen supply and demand presents a transportation challenge: bringing electricity to electrolyzers at storage sites would mean a significant expansion of power transmission lines, while placing electrolyzers close to renewables sites and transporting the hydrogen would require a hydrogen pipeline network.[6] Small-diameter hydrogen pipelines have been in service for decades, and existing fossil gas pipelines could be repurposed for hydrogen, but open challenges remain such as the embrittlement of pipeline steel and the global warming potential of hydrogen leaks.[7] There may be delays when building new transmission lines or hydrogen networks or problems during the simultaneous scale up of hydrogen supply, transport, and storage. Proposals for new salt cavern storage have encountered public opposition, with concerns that range from ground shifting above caverns and the impacts of saline discharge from solution mining on marine wildlife to general concerns about hydrogen safety. On the generation side, the high combustion temperature of hydrogen leads to high nitrogen oxide emissions from gas turbines, which must be managed with strategies such as water injection.

Methanol for ULDES

Methanol as ULDES could offer an alternative to hydrogen storage. A concept for methanol storage with carbon cycling from Baak et al.[8] is sketched in Figure 1 with all inputs and outputs. Methanol can be synthesized from electrolytic hydrogen and carbon oxides (so called "e-methanol"). E-methanol is already produced today at a scale of thousands of tons per year in Iceland, and a similar process is used for methanol at megaton scale using gasified coal in China, where the methanol is used in the chemical industry.[9] Methanol is liquid at ambient temperature and pressure, and can thus be stored in large aboveground tanks, just as oil products are today, at costs of around 0.01–0.05 €/kWh. A single 200,000 m^3 cylindrical tank with diameter 80 m and height 40 m can store 880 GWh of methanol. When combusted with pure oxygen in a transcritical Allam cycle turbine using carbon dioxide as the working fluid, up to 98% of the carbon dioxide from combustion can be captured with minimal effort, producing power at efficiencies of up to 66%.[10] The oxygen for the turbine can be taken from the water electrolysis and stored cryogenically as a liquid in aboveground steel tanks or separated from the air. A 50 MW_{th} plant using the Allam cycle is already operating in Texas[11] and several commercial plants are planned in the United States and Europe in the 300 MW range. The captured carbon dioxide can then be stored as a liquid in aboveground pressure vessels to be used again for methanol synthesis, thus closing the carbon cycle. The Allam cycle is chosen for its high efficiency and high capture rates, which avoids having to source carbon dioxide from elsewhere. By combusting in pure oxygen rather than air, the system avoids both nitrogen oxide emissions and the thermodynamic cost of separating the carbon dioxide from the exhaust gases. Any carbon dioxide that leaks can be topped up either from biogenic sources or captured directly from the air.

Existing literature on methanol

Ideas for a methanol economy, by which methanol could be used in transport, chemicals, power, and heat, go back at least to the 1980s, when Friedrich Asinger suggested using methanol as an alternative to imported hydrocarbons, first from coal gasification and later based on electrolysis using nuclear power.[12] More recently, methanol has been discussed using renewable power as the primary energy source.[9,13,14] While many studies see a role for methanol in industry as a precursor chemical for producing olefins and aromatics, for long-distance shipping, or as an intermediate for kerosene production for long-distance aviation, its potential role in long-duration storage is less explored. It has been favorably compared to methane for storage in terms of round-trip efficiency but without carbon cycling or economic analysis.[15] Cycling of carbon, oxygen, and hydrogen-derivatives has been suggested in the concept of "thermal hydrogen"[16] but not in the context of very high penetrations of renewable energy and inter-annual storage. Carbon cycling with Allam turbines has been considered for methanol storage recently,[8] but the focus was on the levelized cost of storage (LCOS) based on static assumptions about capacity factors, rather than a dynamic analysis in interaction with variable renewables and other storage options like batteries. What has been missing is a dynamic analysis for high levels of wind and solar in a more realistic power system setting over many weather years, which we provide in this commentary.

Importance of flexibility for methanol synthesis

In production facilities using fossil fuels, methanol synthesis is run with high-capacity factors. Maintaining these high load levels with fluctuating hydrogen supply from variable electricity would require large-scale hydrogen storage to buffer the hydrogen, which may not be available as discussed above. While hydrogen can be buffered in pressure vessels for several hours, multi-day periods of low wind and solar generation would present a challenge for inflexible synthesis operation. Although there is little published experience from large facilities, recent research literature as well as initial indications from demonstration plants suggest it should be possible to run methanol synthesis flexibly enough to avoid large hydrogen storage. This can be done by reducing synthesis minimum part-load levels to 10%–20%,[17–19] temporarily shutting down synthesis,[17,20] flexibly ramping within minutes,[17] and flexibilizing the distillation.[18,21] We will assume that the synthesis unit can be turned on and off as long as ramping limits of 10% of capacity per hour are respected. Simulations done for green methanol synthesis show that flexibility in the form of unlimited ramping and 10% minimum part-load can reduce the levelized cost of methanol by 21%–34% compared to inflexible operation.[22] We explore the sensitivity to the flexibility assumptions in supplemental information section S4.1.

Optimization methodology for Europe

To compare methanol with hydrogen storage, we optimized the supply of a stylized constant electricity demand with wind, solar, and storage in the United Kingdom, Germany, and Spain using a single continuous time series of historical hourly weather data for the years 1950–2020.[23] The capacities of wind, solar, battery storage, and either hydrogen or methanol ULDES were optimized to supply the demand in every hour of the 71 years of data. Such a long time span was taken in order to include both seasonal as well as inter-annual variability, since wind in particular is known to go through decadal cycles of variation. No discounting over the 71 years was applied, since the large number of years is used in the spirit of robust optimization across different weather conditions. The years are linked by the storage states of charge and asset capacities.

We consider four scenarios for ULDES:

1. H_2 pressure vessel: hydrogen storage in aboveground steel pressure vessels, combined cycle gas turbine (CCGT) for electricity generation
2. H_2 salt cavern: hydrogen storage in underground salt caverns, CCGT for electricity generation
3. MeOH Allam CCU: methanol storage, all storage in aboveground steel tanks or pressure vessels, no must-run requirement for methanol synthesis, synthesis ramping limited to 10%/h, Allam cycle turbine, majority carbon dioxide cycled from Allam turbine, direct air capture (DAC) or biogenic CO_2 for topping up
4. MeOH CCGT DAC/bio: methanol storage, all storage in aboveground steel tanks or pressure vessels, no must-run for methanol synthesis, synthesis ramping limited to 10%/h, CCGT without CO_2 capture instead of Allam, all CO_2 for methanol synthesis from DAC (or biogenic sources)

Cost projections assuming utility-scale facilities were taken for the year 2030 and are listed in Table S1. A weighted average cost of capital of 5% is used. It is assumed that up to 98% of carbon dioxide can be captured from the Allam turbine and that lost carbon dioxide is compensated with DAC powered by electricity and heat from a heat pump. Since no fossil fuels are available, the scenarios have no net carbon dioxide emissions. Methanol is synthesized directly from carbon dioxide and hydrogen. All code and data are openly available, as detailed in supplemental information section S2. Sensitivities to the major input assumptions are analyzed in supplemental information section S4.

Simulation results for Europe

The system cost breakdowns for providing electricity are shown in Figure 2;

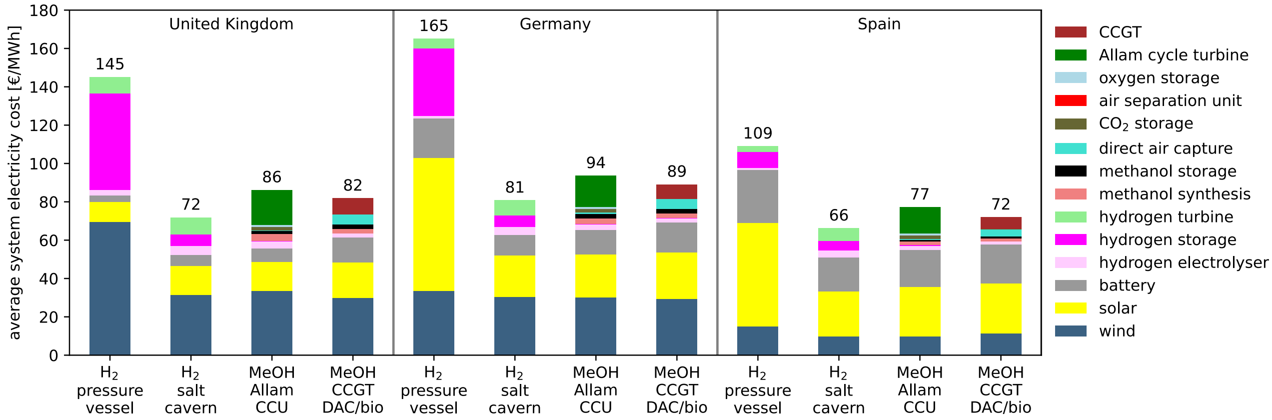

Figure 2. Average electricity costs for systems based on wind and solar

The first two scenarios use hydrogen (H_2) storage; the second two have methanol (MeOH) storage, the first with carbon cycled from an Allam turbine, while in the second, carbon dioxide is taken from direct air capture (DAC).

further results on costs, capacities, energy, and prices can be found in Table S2. Choosing underground salt caverns over pressure vessels for hydrogen storage reduces total costs by 39%–51%. Expensive steel pressure vessels reduce the optimal storage capacity and force the system to build excessive wind and solar capacity, which is then curtailed. While the United Kingdom with its good wind resources builds excess wind, excess solar is favored in less windy and sunnier Germany and Spain, whose predominantly daily variations need less multi-day storage in pressure vessels than wind in the United Kingdom. Using methanol storage with aboveground tanks for all stored substances is 16%–20% more expensive than underground hydrogen storage. Since using the methanol system is still 29%–43% lower in cost than using aboveground pressure vessels for hydrogen, it presents the most cost-effective solution of those studied here where salt deposits are not accessible. The round-trip efficiency for hydrogen storage at 38% is higher than for methanol storage with carbon cycling at 35%.

Focusing on the results for Germany, the Allam cycle covers just 9.2% of electricity demand. The rest is covered either directly by wind and solar or by batteries (see Sankey-style diagrams in Figure S1). 89% of the carbon dioxide used for the methanol synthesis is captured from the Allam turbine and stored, while the remaining 11% comes from DAC. There is a trade-off between storing all of the CO_2 from the Allam turbine with a very large CO_2 storage versus venting some CO_2 and using DAC at times when electricity is cheap. Similarly for the oxygen supply for the Allam turbine, 91% of the oxygen is stored from the electrolysis, while 9% comes from the air separation unit.

Significant cost contributions for methanol storage come from the Allam cycle turbines. Following Mitchell et al.,[10] we have assumed that the Allam cycle turbines cost twice as much as a CCGT; if the cost dropped to parity, the methanol storage system would be just 6%–7% more expensive than cavern hydrogen storage (see supplemental information section S4.4). Combusting the methanol in a CCGT without carbon capture, forcing the system to rely on DAC to source the carbon dioxide, is lower cost than the closed carbon cycle variant of methanol storage and 9%–14% more than underground hydrogen storage. In particular, costs are saved on the turbine itself as well as the storage of oxygen and carbon dioxide. However, this solution relies on scaling up DAC, which has not yet been demonstrated at large scale. The marginal cost of carbon dioxide with DAC is around 200 €/t CO_2 in the model; if biogenic CO_2 is available, it could reduce the cost further, although carbon dioxide is only a small part of the overall system cost. A sensitivity to doubling the DAC cost is performed in supplemental information section S4.5 and shows a low impact. Since the carbon is no longer cycled in this scenario, the methanol could also be imported from renewables-rich regions at lower cost.[24] Because of the energy demand of the DAC, the round-trip efficiency in this scenario is reduced to 29.5%.

Methanol for inter-annual storage

The energy filling level of the ULDES in the underground hydrogen and flexible methanol scenarios is plotted for Germany in Figure 3. With underground hydrogen storage, the storage is built to cover 50 days of electricity demand and follows a predominantly seasonal charging pattern, charging in the summer and then discharging in winter. Some hydrogen is shifted between years, while the rest of the inter-annual variability is managed by building wind and solar large enough for low-wind years and curtailing them in high-wind years. For methanol on the other hand, the storage is low enough cost to be used both for inter-annual as well as seasonal storage. It is built to cover 94 days of electricity demand.

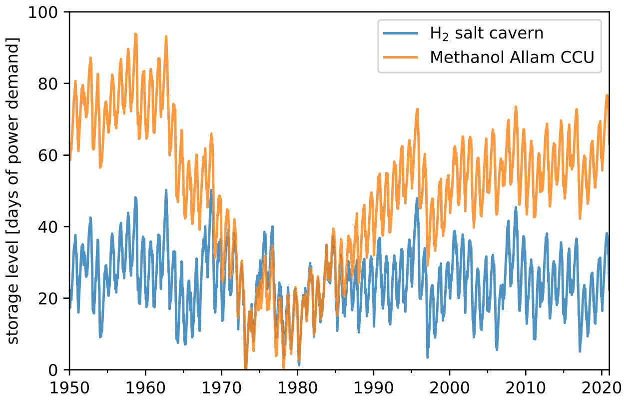

Figure 3. Filling levels for storage in Germany

Shown are the H2 salt cavern and Methanol Allam CCU scenarios over 71 historical years, measured in days of electricity demand that can be covered (i.e., energy content of the fuel multiplied by the efficiency of electricity generation)

Comparison with other studies

A study on methanol storage with carbon cycling that only considered a static calculation (without time series) found a round-trip efficiency of 30.1% and a LCOS of 240 €/ MWh_{el}.[8] Our round-trip efficiency is higher at 35% because we assume a higher efficiency for the Allam turbine (66% versus 60%) and for the methanol synthesis (83% versus 79%). However, our LCOS is higher, in the range 309–366 €/ MWh_{el}, because we include the cost of electricity for charging the storage and our Allam cycle has a lower capacity factor of 11%–14% compared to the fixed capacity factor of 50% assumed in Baak et al.[8] Our levelized cost of methanol in the MeOH Allam CCU scenario ranges from 103 to 118 €/MWh. If there is no carbon cycling and DAC is exclusively used, this cost rises to 113–127 €/MWh. The combined price range translates to 571–704 €/t MeOH, which is higher than pre-2022 fossil methanol prices of 200–400 €/MWh but in line with literature values for green methanol in 2030.[24] For underground hydrogen storage, the total amount of storage is more than double that found in a recent study looking at 35 weather years,[25] with the difference being caused by the higher cavern costs of 2 €/kWh in that study, which shift the balance toward less storage and more curtailment.

Simulation sensitivities

To assess the sensitivity of the results to the most influential model assumptions, further model runs are provided in supplemental information section S4 with the following changes: less flexible methanol synthesis, combining methanol and underground hydrogen storage, including fossil methane with carbon capture and storage, higher costs for DAC, lower costs for the Allam cycle, three additional countries, a strongly seasonal demand that simulates the electrification of space heating, and the removal of wind generation.

Simulation limitations

The simulations consider countries as a single location, which leads to some beneficial smoothing of wind and solar and neglects grid costs. Given that transporting hydrogen is more costly in money and energy than methanol, a more detailed spatial analysis would favor methanol. There is uncertainty around costs for 2030, particularly for technologies like the Allam cycle and DAC that are just in the process of scaling up. Our model assumes perfect foresight and ignores land constraints. Including more generation technologies, such as hydroelectricity or offshore wind, and storage technologies, such as redox flow batteries or compressed air energy storage, could lead to system cost reductions, depending on the assumptions used.

Strategic methanol reserve for resilience

The simulations above are robust to low wind and solar events that have occurred in the last 71 years. To insure the system against other extreme events, it would be inexpensive to over-dimension the methanol storage with, for example, a minimum filling level of 60 days of demand. This would provide resilience against the unpredictable effects of climate change, volcano eruptions that disrupt solar generation for several days,[26] geopolitical interruptions to imported energy carriers, and sabotage of energy interconnectors. Providing a strategic methanol reserve would be similar to the way that reserves for oil products and gas are maintained today.

Modularity and scalability

An attractive feature of methanol storage is that it can be scaled down without impacting costs too strongly. Most of the economies of scale are already realized from a size of 200 MW (referring to the electrolysis capacity),[8] and methanol synthesis units are on the market at sizes down to 10 MW.[27] This could make methanol interesting for smaller islands, off-grid systems, and other autonomous regions. In contrast, hydrogen pipelines and underground storage are large discrete infrastructure that first make sense from GW scale.

Business models in the short-term

Methanol ULDES or parts of the storage system may have business models before the full electricity system eliminates emissions. In locations where grid connection capacity is limited, renewable generators can be combined with ULDES to maximize their use of the connection point. While not carbon neutral, Allam turbines could be used in the short-term with fossil gas and the captured carbon dioxide could be used to produce methanol with green hydrogen, which could then be used in shipping or the chemicals industry.

Alternatives to Allam cycle

Although most of its components are widely produced, the Allam cycle itself has only been demonstrated in a 50 MW_{th} demonstration plant. Further commercial plants at 300 MW scale are planned. While this is further along the commercialization route than hydrogen turbines, there may still be problems that arise with the larger turbines or scaling up production fast enough. In this case, alternatives include fitting carbon capture to standard CCGTs, which have already been run with methanol,[9] or running the CCGT without capture and sourcing CO_2 from the air or biomass like the scenario MeOH CCGT DAC/bio. Fuel cells for methanol, either using methanol directly or with a reformer to hydrogen, are also possible, although a turbine may be more attractive given its inherent rotating inertia. The inertia from a turbine can also be used when it is not generating active power by disconnecting the generator from the turbine so that the generator operates as a synchronous condenser.

Alternative chemical energy carriers

We now compare storage with the energy carrier methanol to methane, ammonia, liquid hydrogen, and other liquid organic hydrogen carriers (LOHCs). The methane route is similar to methanol in that carbon must be cycled in the system, both can reuse existing fossil fuel infrastructure for storage and transport, the round-trip efficiencies are alike, and the costs of methanation and methanol synthesis are similar. On the downside, the costs of building new methane storage are higher than methanol, underground storage requires specific geology (but is more flexible than hydrogen), methane needs to be compressed for transport and storage, and gas pipelines require GW size for economies of scale. Using methane may also prolong existing business models for fossil gas. Leaks of methane must be carefully monitored and mitigated since it is a powerful greenhouse gas. Ammonia can be stored cryogenically or under pressure as a liquid and does not require carbon management since nitrogen can be separated from the air. On the downside, ammonia is highly toxic, its transport and storage is highly regulated, pure ammonia turbines have a low technological readiness, and, when ammonia is combusted in a turbine, it leads to nitrogen oxide emissions that need to be mitigated. Liquid hydrogen requires significant and continuous cooling power, which makes it unattractive for ULDES. LOHCs such as dibenzyltoluene have similar properties to methanol storage but have lower technological readiness, and the costs of the carrier compounds make it more expensive.

Future research needs

In order to understand methanol better as a long-duration energy storage option, there are several urgent research needs. The effects of flexible methanol synthesis on catalyst behavior, efficiency, and wear-and-tear should be demonstrated. More experience is needed on methanol synthesis with carbon dioxide rather than carbon monoxide. It would also be helpful if there were more operational information on the Allam cycle in the public domain. The trade-offs for storage of carbon dioxide and oxygen versus air capture should be explored. The possibility to separate the methanol synthesis from its usage geographically could be explored. For example, methanol and carbon dioxide could be transported to and from the facility by road, rail, pipeline, or ship. Ships could be built to transfer methanol outbound and carbon dioxide inbound given that their volumetric densities are similar.

Conclusions

While storing hydrogen underground in salt caverns is an attractive proposition for long duration storage, methanol storage can offer several advantages, including geographical flexibility, scalability, and easier handling. Its usage is complicated by the need to cycle carbon in order to ensure carbon neutrality, but we argue that this can be elegantly solved using Allam cycle turbines. New insights on methanol synthesis flexibility and promising demonstration facilities for the Allam cycle have given new impetus to this concept. Further research should firm up the prospects for ultra-long-duration methanol storage.

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at https://doi.org/10.1016/j.joule.2023.10.001.

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DECLARATION OF INTERESTS

The authors declare no competing interests.

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PyPSA-Earth. A new global open energy system optimization model demonstrated in Africa

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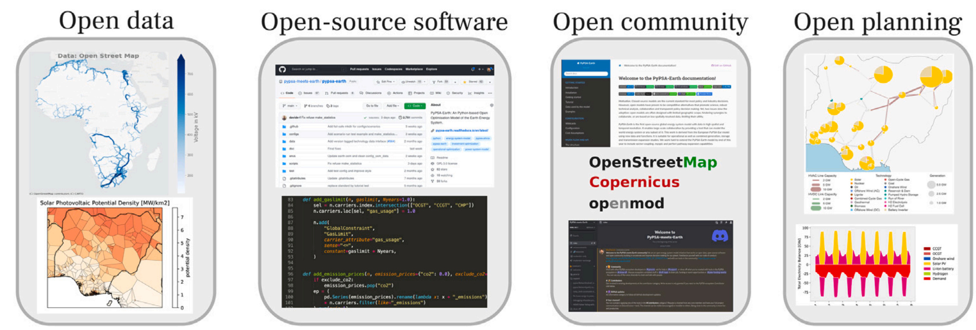
GRAPHICAL ABSTRACT



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ABSTRACT

Macro-energy system modelling is used by decision-makers to steer the global energy transition towards an affordable, sustainable and reliable future. Closed-source models are the current standard for most policy and industry decisions. However, open models have proven to be competitive alternatives that promote science, robust technical analysis, collaboration and transparent policy decision-making. Yet, two issues slow the adoption: open models are often designed with particular geographic scope in mind, thus hindering synergies from collaborating, or are based on low spatially resolved data, limiting their use. Here we introduce PyPSA-Earth, an open-source global energy system model with data in high spatial and temporal resolution. It enables large-scale collaboration by providing a tool that can model the world's energy system or any subset of it. The model is suitable for operational as well as combined generation, storage and transmission expansion studies. In this study, the novel power system capabilities of PyPSA-Earth are highlighted and demonstrated. The model provides two main features: (1) customizable data extraction and preparation with global coverage and (2) a PyPSA energy modelling framework integration. The data includes electricity demand, generation

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and medium to high-voltage networks from open sources, yet additional data can be further integrated. A broad range of clustering and grid meshing strategies help adapt the model to computational and practical needs. Data validation for the entire African continent is performed and the optimization features are tested with a 2060 net-zero planning study for Nigeria. The demonstration shows that the presented developments can build a highly detailed power system model for energy planning studies to support policy and technical decision-making. We anticipate that PyPSA-Earth can represent an open reference model for system planning, and we welcome joining forces to address the challenges of the energy transition together.

1. Introduction

1.1. Motivation

Energy system planning models are broadly adopted around the world. They are used as instruments to inform policy and investment decision-making, such as operational, supply diversification, and long-term infrastructure planning studies. Inscrutable 'black-box' models, despite being criticized in academia [1], are still the standard for high-impact modelling such as the African Continental Power System Plan [2]. This prevents transparent decision-making while having other major drawbacks, as described in [1]. Open-source models evolved to overcome these typical black-box model problems and can perform equivalent or even more tasks, but at no charge, while additionally supporting transparent and robust analyses [3]. In many examples, the European Commission applies open tools and requests their use in funded projects, proving its belief in the benefits of openness and transparency [4]. Now with the encouraging rise of more than 31 models in 2019 [5], simultaneously, concerns of failed collaboration and duplication are arising that cost taxpayer money [6]. As a result, it becomes increasingly important to avoid duplication and provide modelling solutions that allow global united efforts. For these reasons, in this study, we propose an open-source community-backed flexible energy system model able to represent any arbitrarily large region of the world power system in high spatial and temporal resolution that leverages other existing open-source projects to serve industry, policymakers, and researchers.

1.2. Literature analysis

In general, models are idealized representations of real physical systems. To ease building idealized systems, 'frameworks' have been developed to provide pre-compiled equations, algorithms, solver interfaces and/or input/output features. A framework becomes a 'model' only when data is added that describes real physical systems [7]. In this view, PyPSA is a framework and PyPSA-Eur and PyPSA-Earth are models for the European and Earth energy system, respectively. Nowadays, the open-source community is rich in energy system modelling frameworks that can provide similar functionalities. Table 1 compares some available functionalities across selected widely-adopted modelling frameworks [3,8,9]. Undoubtedly, each developer team might be capable of filling in missing features, but the functionality of the frameworks is only one important part of models, the other one, often even more relevant, is the integration of data.

Existing models are often designed to implement data with limited geographical coverage, such as a specific province, country or continent [22]. Continental models with implemented high-resolution data have proven to be the most maintained and active, possibly by covering many regions of interest and giving the user options for the aggregation level [23,24]. In contrast, there are several examples where single-country models have soon become outdated, poorly documented or inactive [25–27]. While global energy system models exist, they currently need to improve. The pioneering global energy system models that impacted policy and research discussions are closed source; for instance, LOADMATCH from Jacobson et al. [28] and LUT model from Breyer et al. [14]. GlobalEnergyGIS [29], an open-source tool which can create energy system model data for any arbitrary region, is used in the Supergrid model [30], but misses network data or a workflow management system that are important for flexible and reproducible data processing [31]. Similarly, the GENeSYS-MOD model is a global open-source model; however, it is written in GAMS, preventing free use and offers no data processing workflows [32]. Another promising candidate is the recently released OSeMOSYS Global model, which includes a workflow management system but misses network topology data as well as unit-commitment and power flow constraints that have been shown to strongly affect model results [9,33].

Similarly, existing PyPSA models are geographically limited. While PyPSA as a framework is adopted worldwide by many companies, non-profit organizations and universities (see example studies in [34]), no global model solution is available. Providing a global energy system model ecosystem solution has the potential to unlock collaboration potentials that accelerate and improve the energy transition planning.

1.3. Contributions

This paper presents PyPSA-Earth, an open-source global energy system model with data in high spatial and temporal resolution. We classify PyPSA-Earth as an energy system model even though the manuscript focuses on the electricity sector. We do this for three reasons: first, the underlying model framework allows sector-coupling, meaning modelling not only electricity, but also other sector such as heating and transport; second, the model can already build hydrogen networks and supply hydrogen demands which is not demonstrated in this study but visible in the source code; and finally, existing work is ongoing to implement the data for the other sectors. Across the manuscript high spatial resolution implies the ability to represent a regional (e.g. country) energy system with a flexible number of sub-regions, each of them describing an arbitrary large (e.g. counties) or small (e.g. provinces) proportion of the region under consideration. Similarly, high temporal resolution means that the time series used in dispatch analyses can be hourly, sub-hourly or larger than an hour, in agreement with the requirements of the energy model. Details on the data and methods are explained in Section 3.

Users can flexibly model the world or any subset of it. Using an automated workflow procedure, they can (a) generate energy system model relevant data and (b) perform planning studies. The novel contributions of PyPSA-Earth are detailed as follows:

1. New model creates arbitrary high spatial and temporal resolution representation of power systems around the world
2. Automated workflow generates national, regional, continental or global model-ready data for planning studies based on open or optionally closed data
3. Integration and linking of multiple data sources and open-source tools to process raw data, e.g. OpenStreetMap
4. Provision of new spatial clustering strategies to simplify the high-resolution model
5. Data and model validation for the African continent and Nigeria
6. Development of 2060 net-zero energy planning study for Nigeria

PyPSA-Earth includes several novel modelling features that make this manuscript unique. While the model leverages previous open-source tools, such as PyPSA-Eur [23], the aim of modelling the globe with flexible spatial and time resolution, the filtering methodology,

Table 1
Comparison of selected features for energy system modelling frameworks that are applied in Africa.

Software	Version	Citation	Language	Free and open	Power flow	Transport model	LOPF[d]	SCLOPF[e]	Unit commitment	Sector-coupling	Pathway optimization[f]
Calliope	v0.6.8	[10]	Python	✓		✓			✓	✓	
Dispa-SET	v2.4	[11]	GAMS	✓		✓			✓		
GridPath	v0.14.1	[12]	Python	✓		✓	✓		✓		✓
LEAP	2020.1.63	[13]	NA[a]							✓	
LUT	2021	[14]	GNU[b]			✓	✓			✓	✓
NEMO	v1.7	[15]	Julia	✓	✓	✓	✓		✓		
OSeMOSYS	2022	[16]	GNU[c]	✓		✓				✓	✓
PLEXOS	9	[17]	NA[a]			✓	✓	✓	✓	✓	✓
PYPOWER	5.15.5	[18]	Python	✓	✓	✓	✓		✓		
PyPSA	v0.20.0	[3]	Python	✓	✓	✓	✓	✓	✓	✓	✓
SPLAT-MESSAGE	2022	[19]	GAMS			✓			✓	✓	
TIMES[g]	2022	[20]	GAMS			✓	✓		✓	✓	✓

[a]NA = no information available.
[b]Mix of GNU-Mathprog and Matlab.
[c]Available in GNU Mathprog, Python and GAMS.
[d]Linearized optimal power flow [3].
[e]Security constrained linearized optimal power flow [3].
[f]Includes myopic and perfect foresight optimizations over multiple years [21].
[g]Times is open source but not free as licensing for GAMS is required to operate the model.

the automatic data fetching by OpenStreetMap, and the data workflow procedures here detailed are a novelty. Accordingly, PyPSA-Earth is not an extension of any previous models but a novel approach and tool that is first presented in this manuscript with a focus on the African continent. In the following, PyPSA-Earth is presented and quantitatively validated for the African continent and Nigeria; its optimization features are finally tested for a 2060 net-zero energy planning study for Nigeria's electricity sector.

All code and validation scripts are shared open-source under GPL 3.0 license. The data, often extracted by python script activation, is available under multiple open licenses. For a detailed license listing, see [35].

1.4. Organization of the paper

The rest of the paper is organized as follows. Section 2 introduces the novel PyPSA-Earth model that can perform large-scale modelling studies. The data processing novelties are detailed in Section 3. Data validation for the African continent is performed in Section 4, and a quantitative case study on Nigeria is discussed in Section 5. Finally, the limitations of the model are discussed, and the conclusions are drawn.

2. PyPSA-Earth model

This section describes the scope of the PyPSA-Earth model, its features as well as the role of the initiative that is facilitating the model developments.

2.1. Scope

The PyPSA-Earth model is a novel open-source data management and optimization tool that aims to provide policymakers, companies and researchers with a shared platform for a wide range of macro-energy system analyses needed to achieve the energy transition together. The option to create a tailored country, continental or global model under a unique code repository maximizes synergies and wider user benefits. For instance, one user in Africa can implement new features and data, improve the documentation or implement bug fixes that immediately benefit all other users worldwide.

By leveraging on existing methodologies and PyPSA-based tools [34], PyPSA-Earth has been developed to enable, among others, the following studies in any country or region on the planet:

1. energy system transition studies
2. power system studies
3. technology evaluation studies (e.g. energy storage, synthetic fuels and hydrogen pipelines)
4. technology phase-out plans (e.g. coal and nuclear)
5. supply diversification studies
6. electricity market simulations.

In this manuscript, we focus on the power system modelling features of PyPSA-Earth.

2.2. Features

The following features are implemented in PyPSA-Earth:

1. flexible model scope: from Earth to any subregion
2. high temporal and spatial resolution
3. model-ready data creation
4. co-optimization of investment and operation
5. single or multi-year optimization
6. flexible addition of arbitrary optimization constraints, e.g. socio-economic, technical, or economic.

Moreover, the PyPSA-Earth model has been developed with the following non-functional requirements:

1. easy to use and learn
2. highly customizable and flexible
3. modular to include new features and data
4. fully reproducible.

The proposed features of PyPSA-Earth are a novelty compared to the literature in Section 1. Furthermore, new features can be created in or adopted from other PyPSA-based models that share a similar backbone. Examples are the work on endogenous learning with pathway optimization and multiple investment periods [36], dynamic line rating constraints based on spatially differing environmental conditions [37], the implementation of generic constraint settings that enable equity constraints such as applied in [38] and uncertainty analyses by input parameter sweeps or by exploring the near-optimal solution space [39].

The data and methods Section 3 presents more details on the presented features.

2.3. PyPSA meets Earth initiative

The PyPSA meets Earth initiative is an independent research initiative that aims to improve energy system planning with open solutions. It supports, builds and maintains the PyPSA-Earth model and is therefore briefly introduced. The initiative's vision is to support transparent

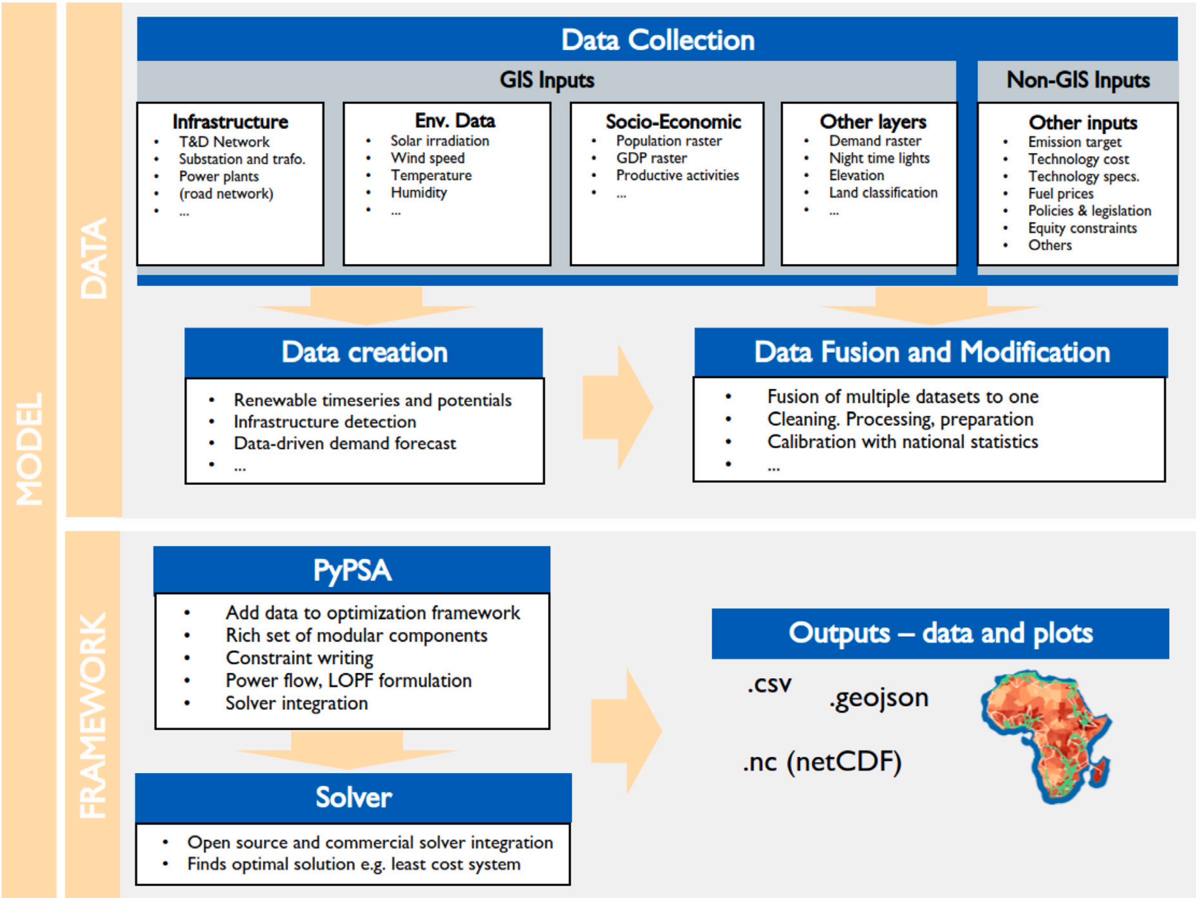


Fig. 1. PyPSA-Earth model design. After providing the configuration parameters and countries of interest, data is collected and processed to be then fed into the PyPSA model framework which enables to perform the desired optimization studies such as least-cost system transition scenarios.

and debatable decision-making on the energy matter that cannot be achieved with the status quo ruled by commercial inscrutable closed-source "black-box" tools. Current research activities in the initiative can be categorized into three distinct groups:

- open data
- open energy system model
- open-source solver.

First, the open data activities focus on open data creation, collection, fusion, modification, prediction and validation for energy system models. These data activities are not limited to aggregated country information but prioritize work on high spatial and temporal resolution data, which is fundamental for scalable and accurate mini-grid and macro-energy system model solutions. Second, the open energy system modelling activities focus on implementing new functions and data streams into the model, such as building a sector-coupled model with multi-horizon optimization that is useful across the globe. Third, open-source solver-related activities deal with benchmarks and efficient interfaces that help to adopt and develop open-source solvers. For instance, we created a benchmark that became a successful public funding proposal and attracted sufficient funding for the open-source solver HiGHS [40]. This activity pushes breakthroughs in large-scale optimization performance required for energy system models, which were until now reserved only for people that can afford commercial proprietary solvers.

In order to assure a continuous inflow of people that maintain, improve and use the software, as needed by open-source software [41], the initiative supports a free and open community where anyone can contribute. The initiative adopts:

- *GitHub* to publicly record issues, requests, solutions or source code-based discussions;
- *Discord* as a voice channel and messaging social platform for regular public meetings and exchanges;
- *Google Drive* to publicly store files and meeting notes.

Together, these tools provide the backbone of the open community supporting the initiative goals and activities (data, model, solver).

3. Data and methods

In this section, the novelties of PyPSA-Earth methodology are highlighted and described in detail. As depicted in Fig. 1, first, we introduce the workflow management tool that supports the model user experience. Then, data creation and processing approaches are discussed considering the main data blocks used by the PyPSA-Earth model: power grid topology and spatial shapes, electricity demand, renewable potential and power plant locations. Further, we describe some advanced pre-processing techniques, such as clustering and line augmentation, used to introduce data into the model in a robust and efficient way. Finally, we describe the energy system modelling and optimization framework with its solver interfaces.

3.1. Workflow management tool

First of all, similarly to PyPSA-Eur [23], PyPSA-Earth relies on the 'Snakemake' workflow management [42] that decomposes a large software process into a set of subtasks, or 'rules', that are automatically chained to obtain the desired output. Accordingly, 'Snakemake' helps sustainable software design that enables reproducible, adaptable and transparent science, as described in [43]. The whole PyPSA-Earth workflow was implemented as a new set of 'Snakemake' rules. For more details, Figure B.13 in Appendix B represents a workflow of PyPSA-Earth automatically created by 'Snakemake' for which the user can execute any part of the workflow with a single line of code. That is expected to improve the user and developer experience, as complex tasks are decomposed into multiple modular smaller problems that are easier to handle and maintain.

3.2. Network topology and model

The electricity network topology is one of the main inputs needed to build an energy system model which accounts for realistic power flow approximations across regions. The most comprehensive and accurate data on power grids are curated by the transmission system operator. In practice, the availability of open power grid data is still relatively low for many parts of the world, with the situation in Africa being extremely sparse.

A natural way to address the lack of power grid data is to utilize open geospatial datasets. Currently, a few open-source packages have been published to extract and build networks from such datasets (e.g. Gridkit [44], Transnet [45], SciGrid [44]). However, each package focuses on applications for a particular world region rather than on the global coverage and there still needs to be a ready-to-use solution which could be implemented into a global model. To fill this gap, we have developed an original approach which reconstructs the network topology by relying solely on open globally-available data. The developed approach is based on the OpenStreetMap (OSM) datasets that are a crowd-sourced collection of geographic information, which is daily updated and includes geolocation Refs. [46].

The electricity network topology is created in three novel steps: (i) downloading, (ii) filtering and cleaning the data, and (iii) building a meshed network dataset with transformer, substation, converter and high voltage alternating current (HVAC) as well as high voltage direct current (HVDC) components. Figure B.14 shows sample raw and cleaned networks along with the options for clustering and line augmentation that are introduced in Sections 3.7 and 3.8, respectively.

For the download step, the *esy-osm* tool is used to allow fast retrieval of OSM data through multi-threaded processing [47]. Appropriate OSM features are used to extract all necessary network components, including substations, transformers and power lines. Their geospatial description was cleaned in this process, and the data structure aligned with the PyPSA framework requirements.

Beyond that, to build the network, an approach has been developed to improve the quality of the OSM-extracted grid topology by accounting for a reasonable tolerance of OSM-derived coordinates.

3.3. Fundamental shapes

Fundamental shapes represent the smallest defined regions that gather various data types to characterize the energy system, such as in Fig. 2 or Figure B.15 in Appendix B. Before being ready for the model-framework execution, data is often provided in many different ways, e.g. geo-referenced point locations and raster data. To properly execute the modelling, such information is gathered and aggregated at the level of the fundamental shapes. These shapes can represent either administrative zones or spatial zones generated from the grid structure as shown in Figure B.15 in Appendix B, which is in the following discussed in more detail for onshore and offshore shapes.

For onshore regions, the model provides two ways to build fundamental data shapes. The first retrieves the so-called Global Administrative Areas (GADM) that represent administrative zones at various levels of detail (e.g. national, regional, province, municipality) [48]. The second one uses the substation GIS location to create Voronoi partitioned areas for each substation, which boundary is defined as equidistant to the centroid of the nearest sites [49]. The latter approach is beneficial to replicating the network accurately, while the former helps communicate results.

For offshore regions, the model uses only Voronoi partitioned areas to create fundamental shapes. These Voronoi areas are built from high voltage onshore nodes and are limited to the offshore extent by the Maritime Boundaries and Exclusive Economic Zones (EEZ) data for each country [50].

3.4. Electricity consumption and prediction

The model currently provides globally hourly demand predictions considering 'Shared Socioeconomic Pathways' [51] scenarios for 2030, 2040, 2050 and 2100 and weather years of 2011, 2013 and 2018. The demand time series is created using the new contributed *synde* package [52], which implements a workflow management system to extract the demand data created with the open-source Global-Energy GIS (GEGIS) package [29].

In principle, GEGIS produces hourly demand time series by applying machine learning methods [29] using as predictors temperature, population, GDP, industrial structure, heating, cooling technologies, among others, similarly to [53]. The observed absolute error of GEGIS in the validation test is considered acceptable for energy studies as it is 8% across 44 countries, yet with generally worse performance in low-income countries [29].

The coverage of the *synde* package is currently limited. Figure B.16 in Appendix B shows no data outputs for especially low-demand countries. A heuristic creates data for the countries with missing data by scaling the Nigerian demand time series proportionally to population and GDP. We validate this approach in Section 4.2.

3.5. Renewable energy sources

Renewable energy sources such as solar, wind and hydro time series are modelled with the open-source package *Atlite* [54]. *Atlite* (i) creates cutouts that define spatio-temporal boundaries, (ii) prepares cutouts, which means that environmental and weather data is added to geospatial boundaries by matching various datasets (ERA5 reanalysis data [55], SARAH-2 satellite data [56], and GEBCO bathymetry [57]), and finally, (iii) applies conversion functions to produce technology-specific spatially resolved time series and potentials [54]. Currently, the *PyPSA-Earth* model framework implements solar photovoltaic, on- and offshore wind turbines, hydro-runoff, reservoir and dam power resources. In the case of hydro, the runoff time series are obtained by *Atlite* for each powerplant location, as described in Section 3.6. As our new contribution, the hydro power output is thereby proportionally rescaled to match the total energy production of existing power plants by country [58]. At the time of writing, available in *Atlite* but not yet implemented in PyPSA-Earth are potentials and time series for concentrated solar power, solar thermal collectors, heat demand and dynamic line rating with a wide range of technology options. For details on the model implementation for each technology, we refer the reader to the *PyPSA-Eur* publication which the presented model mostly builds-upon [23]. A brief concept demonstration of *Atlite* is provided in Fig. 3.

3.6. Generators

Given the limitation of reliable datasets for power plants for the African region, the existing powerplantmatching tool [59] has been extended to include additional datasets, such as OpenStreetMap, to fine-tune the African model and validate the results with the final goal of maximizing accuracy and quality of the result.

Powerplantmatching has been successfully proposed to estimate the location and capacity of power plants in Europe. The validation performed with respect to the commercial World Electric Power Plants Database (WEPP) by Platts and the dataset by the Association of European Transmission System Operators (ENTSO-E) reaches an accuracy

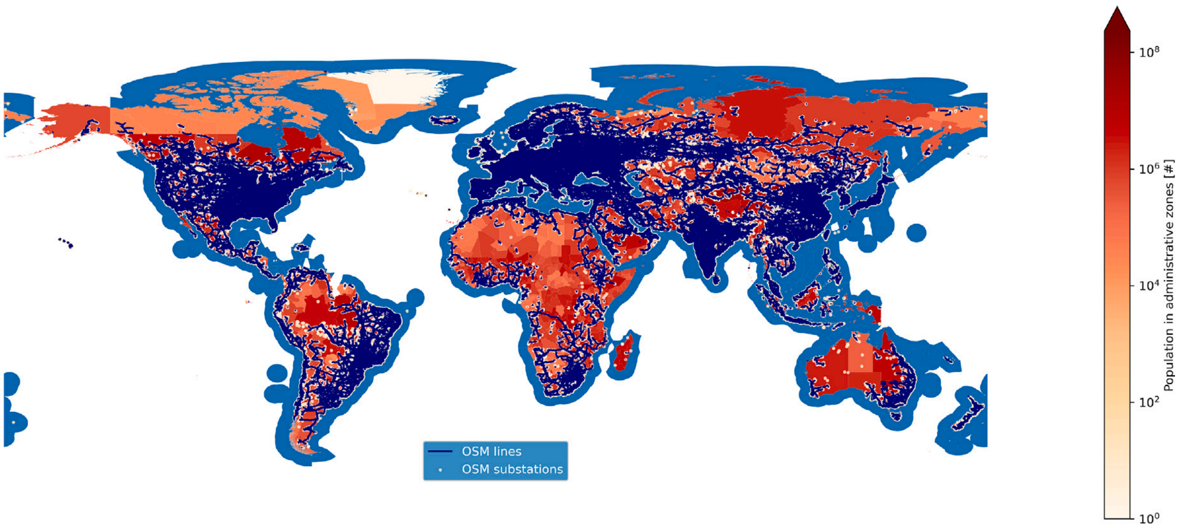


Fig. 2. Representation of transmission networks by Open Street Map (OSM) and shapes produced by PyPSA-Earth.

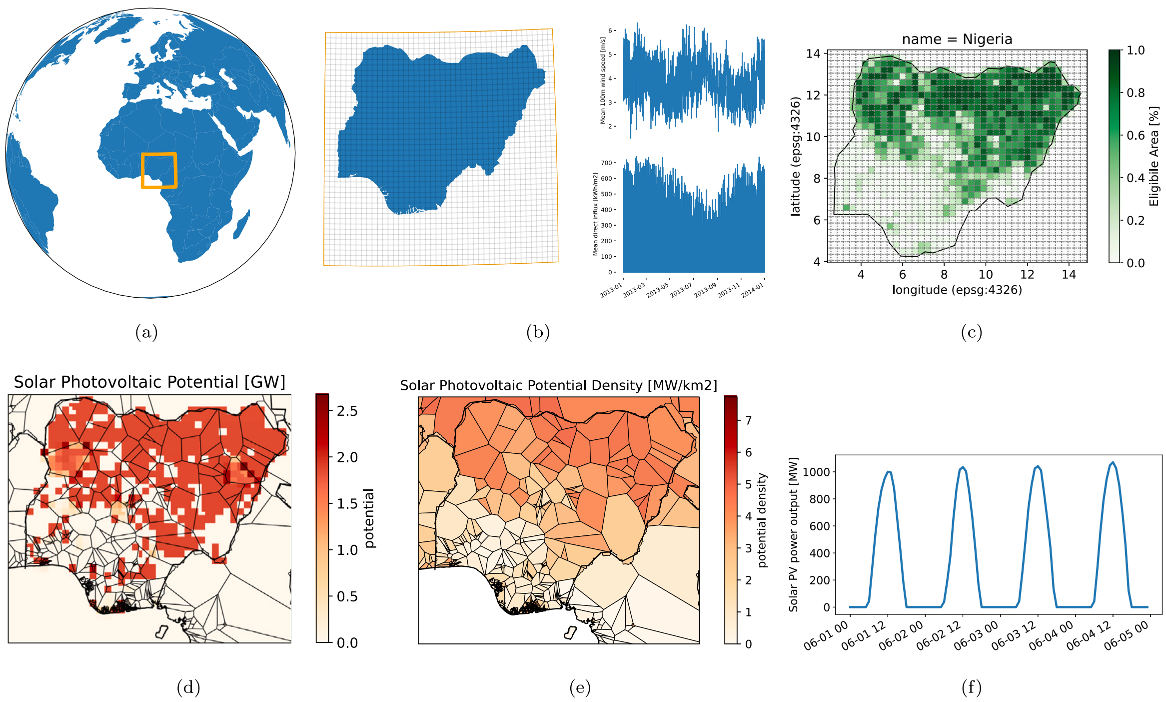


Fig. 3. A concept demonstration of Atlite for Nigeria. (a) Shows that environmental and weather data is extracted in a *cutout* for the region of interest. (b) The cutout is split in a raster of $(0.25°)^2$ or roughly $(27.5\ \mathrm{km})^2$ (length varies along latitude), whereby each cell contains static or hourly time series data. The example wind speed and direct irradiation influx time series are shown for one cutout cell that contains an *ERA5* extract of the Copernicus Data Store [55]. (c) Shows the eligible area raster, which is built by excluding protected and reserved areas recorded in *protectedplanet.net* and excluding specific land-cover types from *Copernicus Global Land Service* whose eligibility can vary depending on the technology. (d) Illustrates the maximal installable power raster, which is calculated by the eligible area and the socio-technical power density of a technology e.g. $4.6\ \mathrm{MW/km^2}$ for solar photovoltaic. (e) The raster is then downsampled to the region of interest or fundamental shape by averaging the proportion of the overlapping areas. (f) Finally, by applying a PV technology model to (b) and combining it with (e) we can define per region the upper expansion limit and the maximal hourly availability constraint for a given technology.

of around 90% using only open data [59]. By default, various open data sources are included, such as [60], ENTSO-E [61], GEO [62], and renewable statistics by IRENA [63] among others. The approach applied for *powerplantmatching* is based on the procedure depicted in Fig. 4 available in Appendix B, where the raw datasets are first downloaded, then filtered to remove missing or damaged data, and aggregated. Once the refined data are obtained, the datasets are pairwise compared to identify duplicated entries. Finally, non-duplicated data are merged into a unique dataset and used as a source for PyPSA-Earth. Only a few of these datasets have global scope (GEO, GPD and IRENA) and have been validated for Africa. In particular for Africa, where data is lacking, including all available open data can be critical to maximizing the accuracy of the results. Therefore, inspired by future work suggested in [64], we have extended the *powerplantmatching* tool to optionally

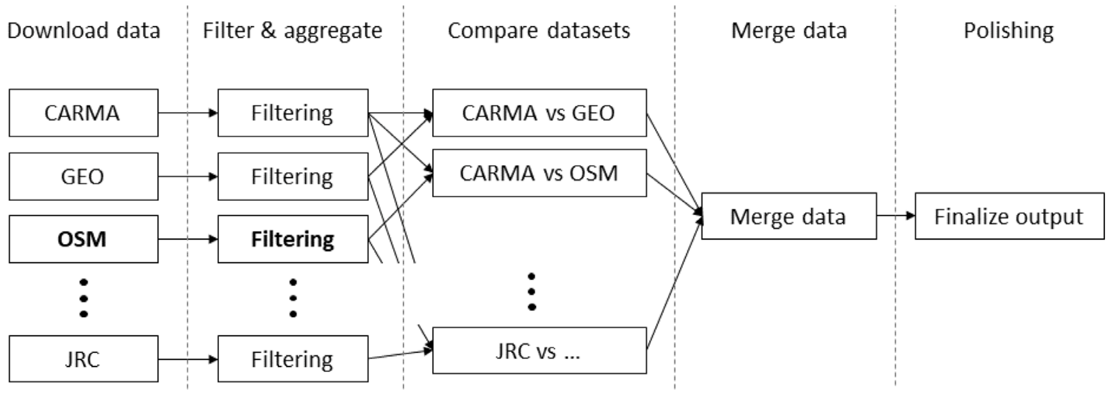


Fig. 4. Flowchart of the *powerplantmatching* procedure, including the novel OSM input (in bold) which was developed for PyPSA-Earth.

include and process OpenStreetMap data to improve the quality of outputs.

3.7. Spatial clustering approach

In order to tackle the computational complexity of solving a co-optimization problem of transmission and generation capacity expansion, the model offers state-of-the-art spatial clustering methods adapted from the PyPSA package and PyPSA-Eur model [3,65]. Spatial clustering allows aggregating nodes of the system to reduce the complexity of the model, which is essential for reducing the computational needs.

The available clustering methods provide a focus on (i) conserving the representation of renewable potentials as well as the topology of the transmission grid, (ii) accurately representing the electrical parameters to improve estimates of electrical power flows in an aggregated model, (iii) aggregating spatially close nodes disregarding other a-priori information of the network, or (iv) according to their location with regards to the country's subdivisions facilitating results interpretation for policy recommendations. An analysis of suitable clustering methods that depend on the modelling application is provided in [66].

In summary, (i) the clustering approach that focuses on a better representation of variable sources or sinks of the model is inspired by [67]. It includes variable potentials, i.e. capacity factors or full load hours for solar and wind, or the variable electricity demand as a distance metric between nodes. This is combined with a hierarchical clustering approach, similar to the suggestions provided in [68]. However, we only allow nodes to be aggregated when a physical transmission line connects them instead of assuming a synthesized grid in contrast with [68]. (ii) The clustering method that focuses on a better representation of the transmission grid was initially suggested by [69] to be applied to the case of electricity system modelling. It is a density-based hierarchical clustering operating on the line impedance. (iii) The network can also be reduced using a weighted k-means algorithm on the locations of the network nodes as explained in detail in [49]. (iv) Finally, using the GADM shapes allows aggregating all nodes in the same shape.

Any of these methods can be applied in single or two distinct iterations, as displayed in Fig. 5 for Nigeria. In each of these two iterations, a different method can be applied, choosing from (i)-(iv). In the first iteration, all nodes are clustered to a desired number of representative nodes, aggregating generators, flexibility options (electricity storage and transmission lines) and electrical demand. The second iteration is optional and allows the remaining nodes to be clustered again. However, now only the transmission network is effectively reduced such that the representation of renewable resources is fixed to the resolution of the previous iteration (compare the first row and second row of Fig. 5). The spatial resolution of the transmission network must always be larger or equal to the resource resolution, i.e. the clustering of the first iteration sets an upper bound.

3.8. Augmented line connection

The African network is often not well interconnected. This is due to isolated national planning data or the presence of isolated mini-grids that are popular electrification measures [70]. Therefore, we propose an algorithm to mesh a given network and assess different grades of connectivity. To investigate the benefits of meshed networks, PyPSA-Earth can perform a k-edge augmentation algorithm that guarantees every node has a modifiable number of connections to other nodes. Only if nodes do not already fulfil the connectivity condition, the algorithm will create new lines to the nearest neighbour by a minimum spanning tree. The new 'augmented' lines can be set to an insignificant size (e.g. 1 MW) to create new options for line expansion in the investment optimization. For example, Figure B.14 in Appendix B compares between the standard clustered network with 420 nodes and its augmented version. Only the model that includes augmented line connections can explore an interconnected continent.

3.9. Model framework and solver interface

The PyPSA-Earth model integrates the PyPSA model framework with its solver interfaces to perform planning studies; details on the mathematical modelling are provided in Appendix A for the sake of brevity. Using PyPSA has several benefits compared to other tools that are briefly introduced in the following. First, PyPSA enables large-scale optimization in Python. Python is well known for being user-friendly, but when analysing the memory consumption and speed for building optimization problems, it was considered non-competitive compared to tools based on the programming language Julia or C++ [71] – a bottleneck which also hinders large-scale optimization required for PyPSA-Earth. As a reaction, developers in the PyPSA ecosystem built *nomopyomo* overcoming the bottlenecks [5]. More recently, the same group has been working on a general package called *Linopy* that promises a 4–6 runtime speed up and a 50% improvement in memory consumption compared to the optimization problem formulator Pyomo, possibly making it also more memory efficient than the Julia alternative *JuMP* as indicated in [71]. Another point making the PyPSA dependency attractive is that it is one of the most popular tools, as suggested by GitHub stars in the GPST benchmark [72], possibly due to its standard component objects and the continuously maintained documentation [34]. Finally, the framework offers several solver interfaces (HiGHS, Cbc, GLPK, Gurobi, among others), providing flexibility in solving various optimization problems with open-source and proprietary solutions.

4. Validation

The data validation section aims to assess the data quality with publicly available data: at a continental level in Africa and a country level in Nigeria.

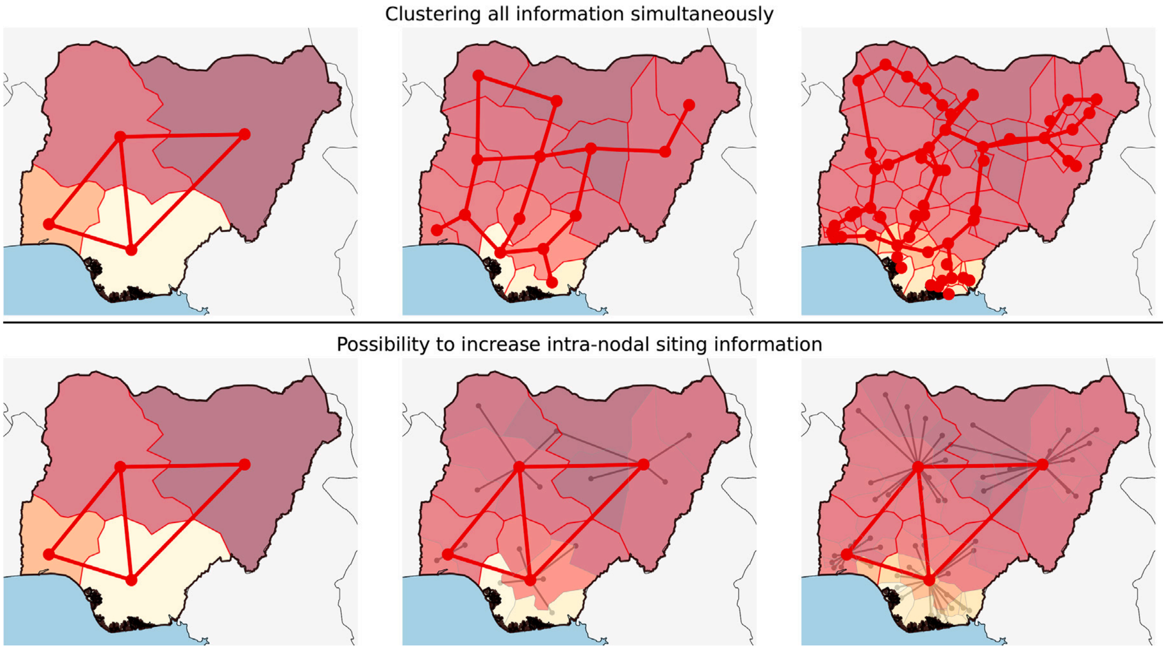


Fig. 5. Illustration of the clustering methodology applied for the transmission network (red nodes and edges) and resource resolution (grey nodes and edges). In the first row, we show how nodal data (i.e. generators, storage units, electrical loads etc.) is aggregated in tandem with the resolution of the transmission network. Three exemplary resolutions of the network for Nigeria are displayed here: 4, 14 and 54 nodes from left to right. The second row shows how the clustering also allows modelling the transmission grid at a different resolution than the resources. In this example, the transmission network contains 4 nodes connected by 4 lines (all in red) at every resolution, while 4, 14 and 54 generation sites become available (left to right). The background colour represents exemplary capacity factors in shades of red, for an arbitrary technology. The darker the colour, the higher the capacity factor.

4.1. Network topology and length

Validating the African power grid is challenging. Different from Europe, where ENTSO-E [73] provides reliable open data with continental scope, such a transparent data source is lacking in Africa, and only a few utilities release open data. The self-proclaimed most complete and up-to-date open map of Africa's electricity network is offered by the World Bank Group, which implements Open Street Map data, as well as indicative maps data from multiple sources [74]. However, the World Bank data should not be used as a single validation set because it may report outdated data, given that it has yet to be updated after 2020, and is partially based on indicative maps rather than on geo-referenced data, making the post-validation time-consuming. Conversely, PyPSA-Earth builds its grid topology directly from daily updated Open Street Map data. Finally, the World Bank data also provides less detailed information than Open Street Map; for instance, it does not give any information on the frequency, circuit or cable number, limiting the information that can be used for validation. The following compares grid statistics and topology on a Nigerian and African scale, including nationally reported data from the Nigerian energy commission.

First, the transmission lines are validated by comparing the total circuit lengths at different alternate current (AC) voltage levels. Transmission lines can carry one or more 3-phase circuits, each with at least three cables. Instead of looking only at the line length, which is the distance between high voltage towers, it is common to report the total circuit length, which multiplies each line length, e.g. distance from tower to tower, with the number of circuits [23]. Table 2 indicates that the Nigerian network length reported at the World Bank aligns approximately with the official transmission company statistics [75], suggesting that the World Bank data is either accurate in Nigeria or used as a reference by the transmission system operator. This officially reported total circuit length is approximately 35% longer than the original Open Street Map data or the modified and cleaned PyPSA-Earth derivative. Conversely, on a continental scale, Open Street Map provides approximately a 117% longer total circuit length than the reported World Bank data. To summarize, while Open Street Map data is qualitatively less available in Nigeria by looking at the statistics, it offers significantly more data on a continental scale.

To further compare and validate the data, Fig. 6 highlights good agreement between the network topology in Nigeria and Africa of Open Street Map and World Bank sources. However, in central and south Nigeria, the World Bank covers more power lines. On the African scale, the opposite is observed. Open Street Map covers more network structures in East and North Africa.

4.2. Electricity consumption

This subsection validates the demand prediction on the example year 2030 for every African country by comparing the individual country consumption for 2020 and 2030 with official continental annual electricity consumption used in PyPSA-Earth. Fig. 7 shows 2020 reported electricity consumption data per country, published from *Our World in Data* that is additionally refined by data from the global energy think-tank Ember and BP's statistical review of world energy [76]. The used electricity demand data in PyPSA-Earth roughly doubled from 2020 to 2030, indicating demand growth. While national demand predictions are often unavailable, the demand prediction is further validated by comparing it to other more common continental demand predictions. In Africa, *Our World in Data* reported an electricity consumption in 2020 of 782 TWh/a. For 2030, [77] predicted 1924TWh/a, [78] 1877 TWh/a and the PyPSA-Earth model data 1866 TWh/a, predicting more than a doubling of Africa's electricity consumption by 2030. In summary, looking at the total African electricity consumption suggests that the data used in the global PyPSA model is in the range of others.

4.3. Solar and wind power potentials

The validation of solar and wind potential is performed by comparing statistics by international organizations, such as IRENA, with

Table 2
HVAC and HVDC circuit line lengths of Nigeria and Africa from different sources.

Circuit lengths in 1000 km	Nigeria			Africa			Ref
	110–220 kV	220–380 kV	>380 kV	110–220 kV	220–380 kV	>380 kV	
World Bank Group[a]	9.3	12.1	0.0	59.4	63.5	41.0	[74]
Open Street Map (OSM)	6.3	9.1	0.0	87.9	180.7	76.7	[46]
Transmission Company of Nigeria	More than 20			–	–	–	[75]
PyPSA-Earth (cleaned OSM)	6.7	9.1	0.0	88.3	183.7	82.9	

[a]Information about circuits is missing.

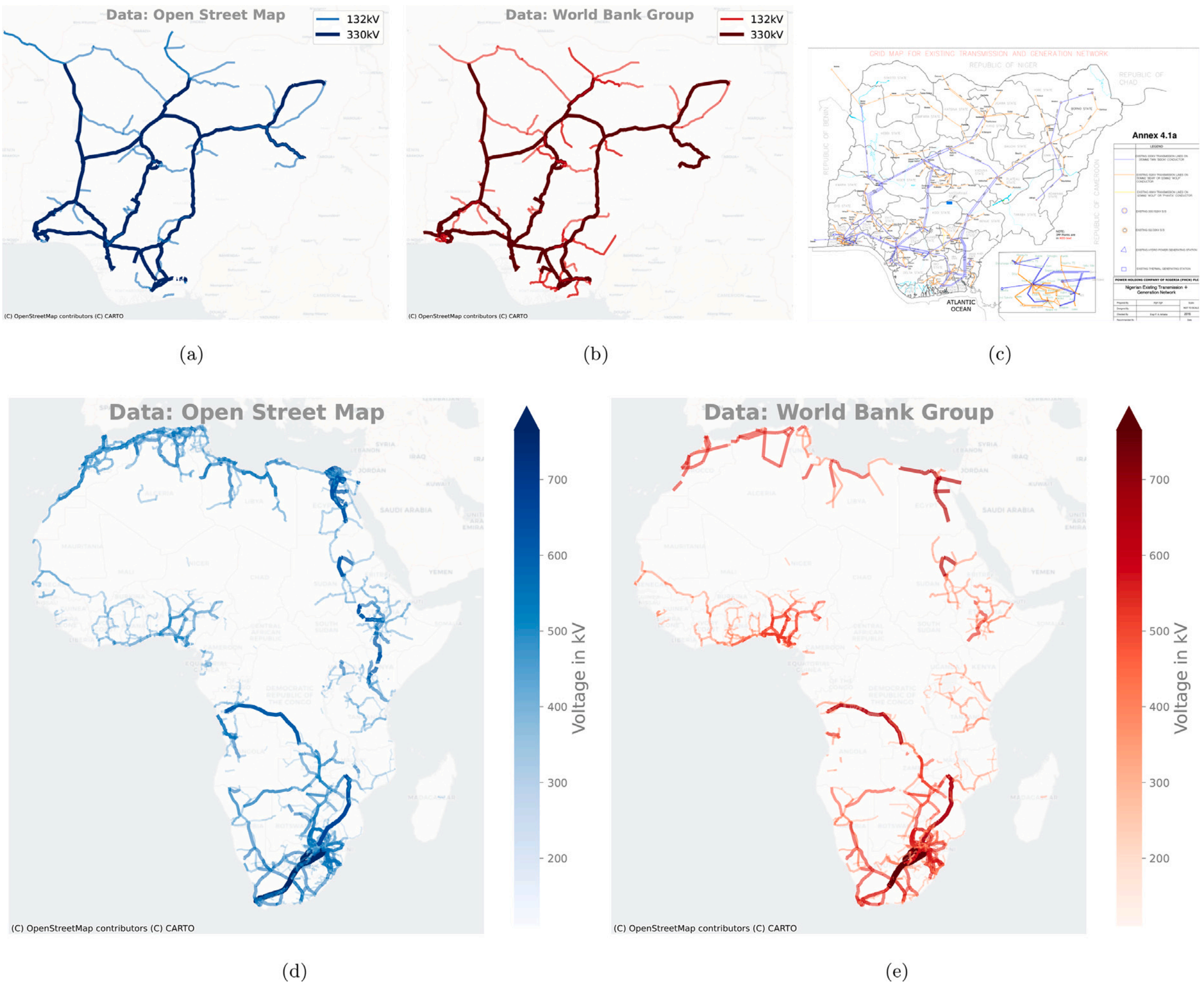


Fig. 6. Network topology of open available transmission network data (above 110 kV) from (a) & (d) Open Street Map, (b) & (e) World Bank Group and (c) the Nigerian Transmission Company. On the African scale, the voltage ranges from 110–765 kV in both data sets. The line format varies with the voltage level and includes transparency, thickness and colour.

the outputs of the PyPSA-Earth model, both including total generation capabilities and the specific power densities per unit of available land.

Solar and wind potentials are well-reported across the African continent. In 2021, the Global Wind Energy Council estimated for Africa a technical potential for wind generation of 180.000 TWh (PyPSA-Earth: 108.700 TWh), sufficient to electrify the continent 250 times relative to the 2019 demand [79]. Similarly, the International Renewable Energy Agency estimated in 2014 that the technical potential in Africa is 660.000 TWh (PyPSA-Earth: 122.200 TWh), which is sufficient to electrify the continent 916 times [80]. The discrepancy between the technical potentials observed in the PyPSA-Earth model and the institutional reports is due to the underlying assumptions. How many renewables can be installed in a region depends on two main assumptions: the excluded areas [km^2] and the power density per technology [MW/km^2], both discussed in the following.

While we define the available areas in a data-driven way similar to [23,80] (see details in Section 3.5), the remaining eligible area quantifies the technical potential per technology through the technical power density factor. However, this density applies only to land specifically and uniquely allocated to renewable production, yet this cannot easily be generalized to all non-protected land areas at the country level. Land areas are also necessary for non-technical activities such as economic activities, industries, farming, well-being, and housing. Accordingly, in PyPSA-Earth we considered a more conservative power density coefficient to account for such socio-economic considerations.

Focusing on solar photovoltaic power plants, we assessed the power density of the 41 largest installations in the world [81,82]: the average power density is 46.4 MW/km^2, the minimum 10.41 MW/km^2, and the maximum 150.0 MW/km^2. The type of solar module and the design of the solar photovoltaic plant drive this extensive range of values. For instance, the Cestas Solar Park in France uses high-performing solar

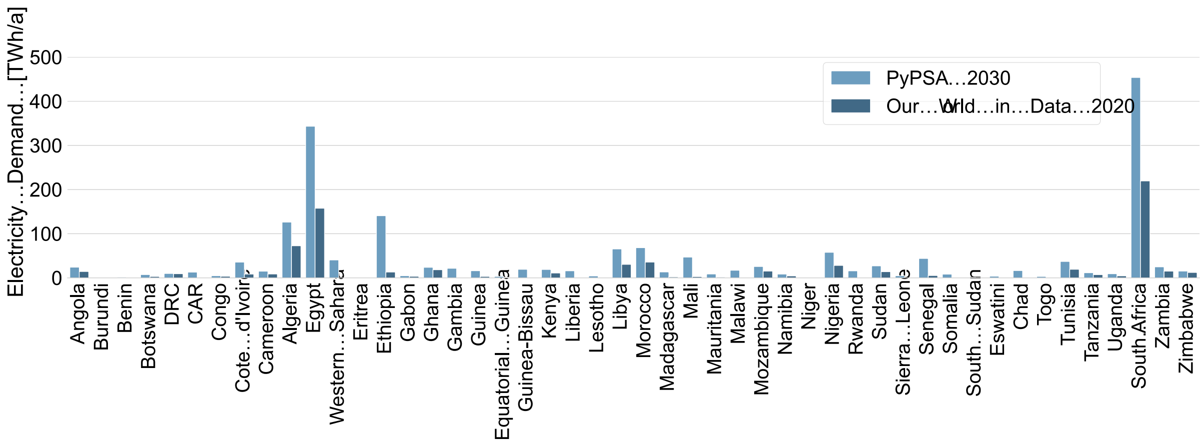


Fig. 7. Comparison of reported [76] and predicted annual electricity consumption data across African countries indicate in every country demand growth. For 2030, the African total electricity consumption of PyPSA aligns with other predictions from [77,78].

modules and additionally contains a compact east–west orientation solar field design leading to the 150.0 MW/km^2 extreme. Similarly to [23], we reduced the technical power density to 10% of the average power plant density to represent the socio-technical limit: 4.6 MW/km^2 for solar photovoltaic.

For onshore and offshore wind farm technologies, we verify power density assumptions by analysing seven existing utility-scale wind farms. The observed average technically feasible power density for onshore wind farms is 6.2 MW/km^2, and for offshore wind farms, 4 MW/km^2 [83]. Using the same approach as [23], we reduced these values from 6.2 to 3 MW/km^2 and from 4 to 2 MW/km^2 for onshore and offshore wind farms, respectively, to represent socio-technical power densities and give wind farms space to lower generation reducing wake-effects.

Currently, we apply the same socio-technical power density irrespective of the land cover type. However, roughly about 43% of the continent is characterized as extreme deserts [84], allowing these regions to be less conservative about the social-technical power density.

4.4. Power plant database

This section compares the site-specific power plant database used in PyPSA-Earth to national statistics.

Data on existing power plants is critical for accurate energy simulations as they affect long-term investments, dispatch, and stability of the energy systems. For validation purposes, relevant country statistics are provided by IRENA [85] and USAID [86]. While the PyPSA-Earth data is geo-referenced, including each power plant's location, type and nominal capacities of each power plant, the other sources only provide country statistics. Therefore, data used in PyPSA-Earth is of higher quality, especially for energy system modelling in high spatial resolution that would be impossible to perform only with the IRENA and USAID sources.

Fig. 8(b) shows that the PyPSA-Earth model matches the largest fraction of the installed capacity of existing databases, with 165 GW out of the 229 GW reported by IRENA. Most technologies are matched with adequate accuracy (2%–15% error), yet larger differences occur, especially for coal and gas power plants, partially due to the recent installation of power plants over the last 3–4 years, whose data has not been updated by the sources described in Section 3.6. In future work, adding more recent data sources may improve the data situation [87]. Furthermore, we note that, although the current PyPSA-Earth procedure does not include geothermal and CSP technologies, their capacity can be relevant for certain countries (e.g. Kenya, Morrocco and South Africa), but at an African scope, these technologies still represent a small fraction of the installed capacity. Therefore, the proposed validation is considered of good accuracy, supporting the appropriateness of the PyPSA-Earth model.

5. Demonstration of optimization capabilities in Nigeria

At COP26, Nigeria's president Buhari committed to net zero emissions by 2060 [88]. To demonstrate that the presented model can be useful for Nigeria's energy planning activities, we showcase the optimization capabilities of PyPSA-Earth. In particular, this section covers two least-cost power system optimizations, one for 2020 to reproduce the historical system behaviour and one representing a decarbonized 2060 scenario (see Figs. 10 and 11).

5.1. Nigeria 2020 - Dispatch validation

The 2020 scenario applies a dispatch optimization with linear optimal power flow constraints to simulate and validate the optimization results for Nigeria. Accordingly, only the operation of existing infrastructure is optimized for the lowest system cost, excluding any infrastructure expansion e.g. generation or transmission line expansion (see Fig. 10).

Starting with the scenario design. The power grid retrieved from OpenStreetMap is clustered into 54 nodes, representing the aggregation zones for the demand and supply. Since the existing network is more meshed than the OpenStreetMap based PyPSA-Earth network (see Fig. 6), a few augmented line connections with a negligible minimal capacity of 1 MW are added such that every node has at least two line connections, see (b) in Fig. 10, to overcome missing network data. A total demand of 29.5 TWh is considered for 2020 using the national demand profiles provided in PyPSA-Earth. The magnitude aligns with reports from *Our World in Data* (28.2 TWh) [76]. The demand profiles are distributed across all nodes proportional to GDP and population. With the available hourly electricity demand time series and the existing 2020 power plant fleet (validated in Section 4.4), the model calculates the optimal generator dispatch considering power flow constraints.

The dispatch validation shown in Table 3 compares the generation shares of the PyPSA-Earth results to those reported at *Our World in Data* [76]. The comparison highlights that PyPSA-Earth adequately represents the total electricity production shares by source in Nigeria with acceptable accuracy. Model results for the solar generation have a 100% accuracy compared to data provided by *Our World in Data*, gas generation is 2 TWh (10%) higher than the benchmark, while hydro generation is 0.3 TWh (5%) lower. These deviations could be explained by the 1.3 TWh (4%) higher assumption of total electricity demand and differences in the specific marginal costs of resources. Using the cost assumptions from [24], we derive an average marginal price for electricity of 59 €/MWh, which aligns with reported production costs in the range of 45 – 70 €/MWh [89].

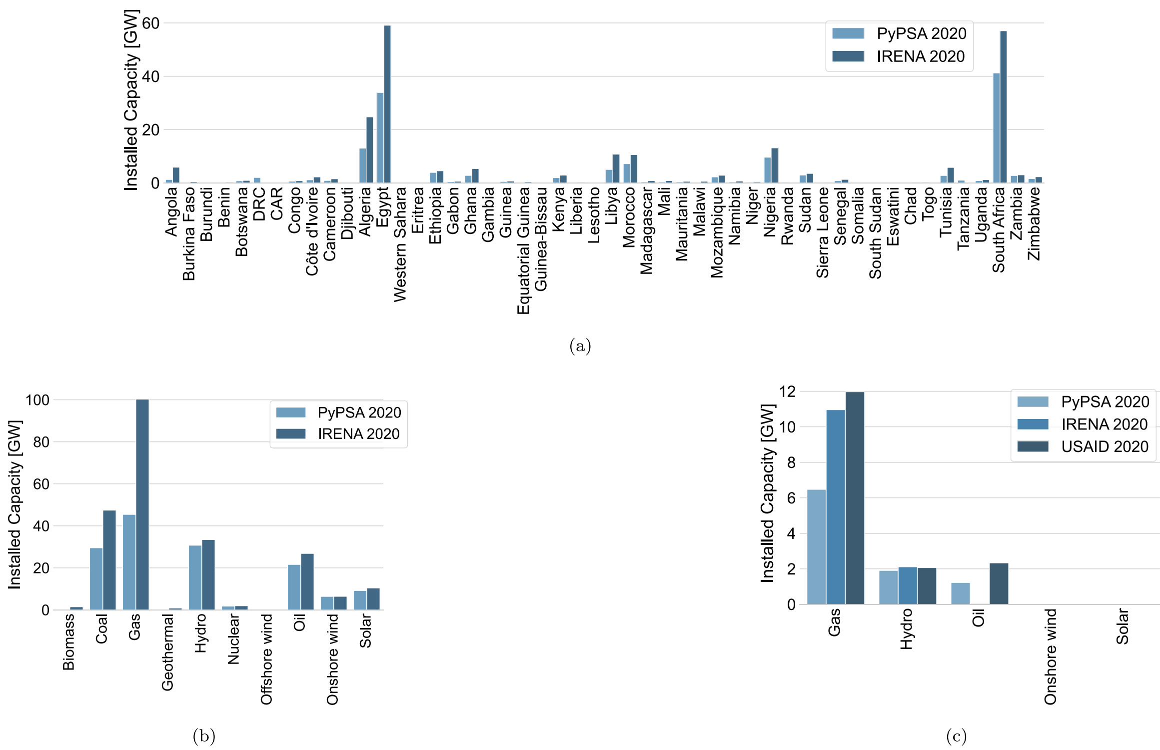


Fig. 8. Total installed generation capacity in Africa by (a) country and (b) technology, including a focus on (c) the installed capacities in Nigeria.

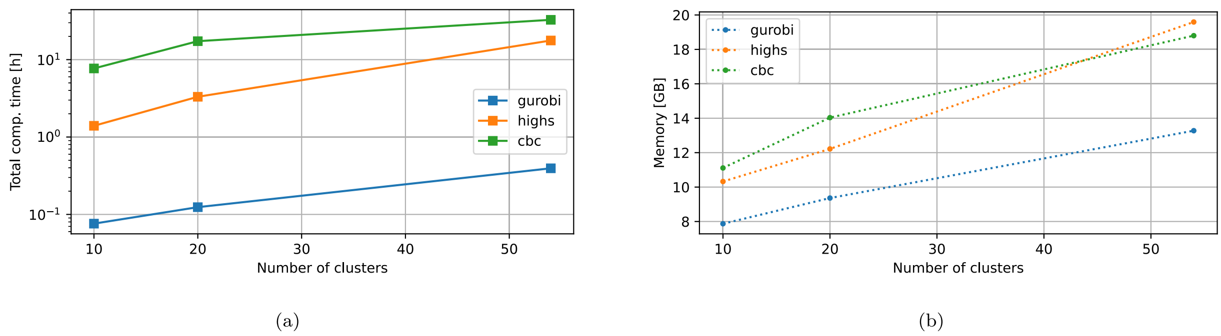


Fig. 9. Solution time (a) and memory requirements (b) for the 2020 Nigeria dispatch optimization for Gurobi 9.5.1, HiGHS 1.2.1 and CBC 2.10.8 solvers at different spatial resolution; solution time is weighted by threads.

Table 3
Nigeria 2020 dispatch comparison.

	Total	Hydro	Coal	Gas	Wind	Solar
PyPSA-Earth [TWh]	29.5	5.8	–	23.6	0	0.04
Our World in Data [TWh]	28.2	6.1	0.6	21.4	0	0.04

The computational needs for this scenario in terms of total solving time (computational time times the average load of the processors) and memory are shown in Fig. 9. We used four threads with Gurobi 9.5.1 solver while only a single-core with HiGHS 1.2.1 and CBC 2.10.8, since their parallel solving capabilities are currently limited. While the commercial Gurobi solver is very efficient, the results in Fig. 9 confirm that the open-source HiGHS solver can also optimize the network below one day with memory requirements that are available for laptops. Given the expected improvements for open-source solvers, the computational requirements are likely to decrease significantly [40].

5.2. Nigeria 2060 - Net-zero study

In the 2060 net-zero scenario, we perform a brownfield capacity expansion optimization. This means new renewable energy and transmission capacity can be built on top of existing infrastructure. Simultaneously, a dispatch optimization is performed subject to linear optimal power flow constraints. To explore new transmission grid structures, the meshing strategy is modified such that each node connects HVAC lines to at least three nearest neighbouring nodes and that a random selection of far distance nodes above 600 km connects HVDC lines, see (b) in Fig. 11. Using a random selection for long-distance HVDC can help identify valuable line connections before applying any heuristic that might not find these. In addition to the net-zero emission constraint, the 2060 total demand has been calibrated in agreement to [90] to about 250 TWh by linear interpolating the stated energy policies of IEA for Nigeria [63]. Observing the optimized infrastructure in Fig. 10, the overall optimal least-cost power system can be mostly supplied with solar energy and a mix of battery energy storage. Hydrogen energy storage with steel tanks is included as an expansion

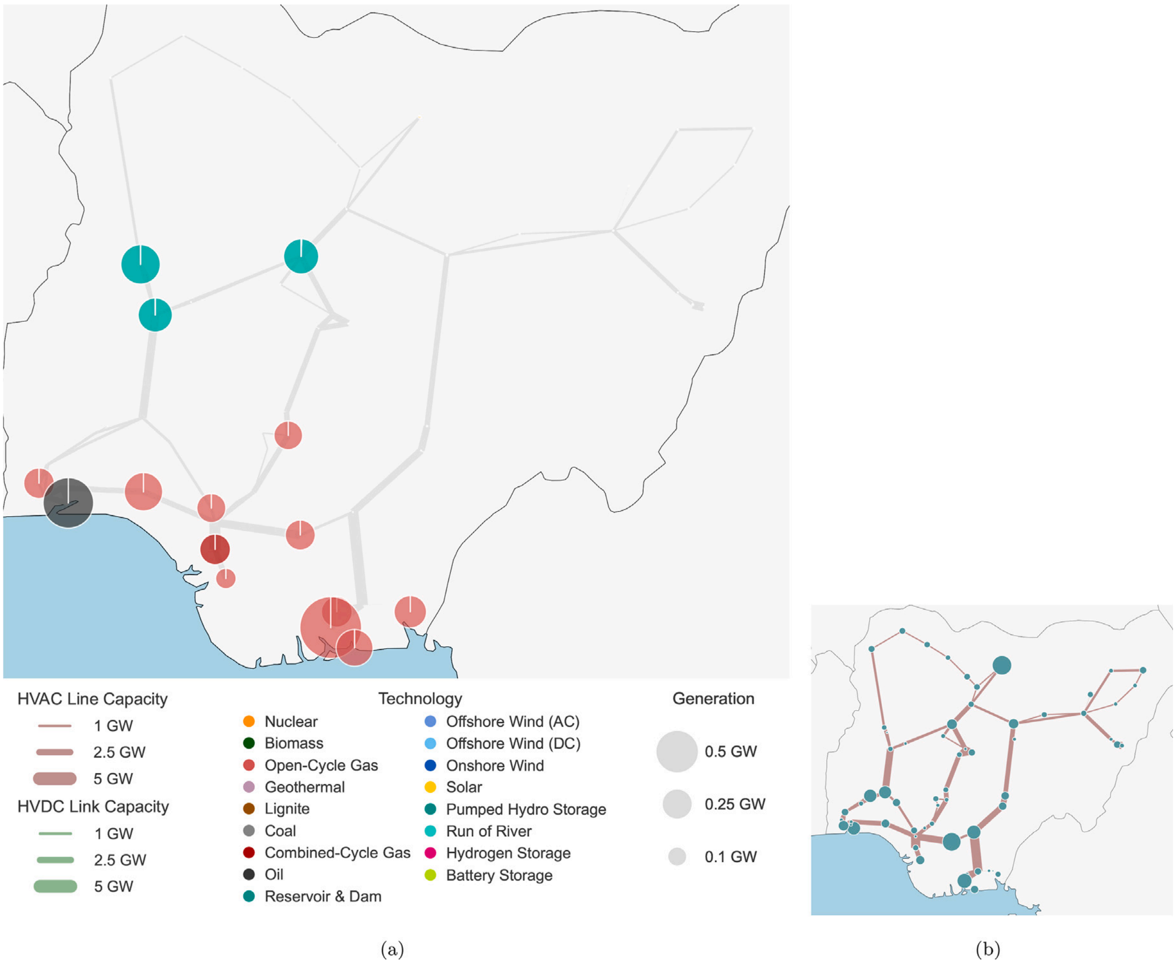


Fig. 10. Optimization results of Nigeria's (a) 2020 power system. The coloured points represent installed capacities. (b) Shows all network options on a different scale as (a) with the total electricity consumption per node.

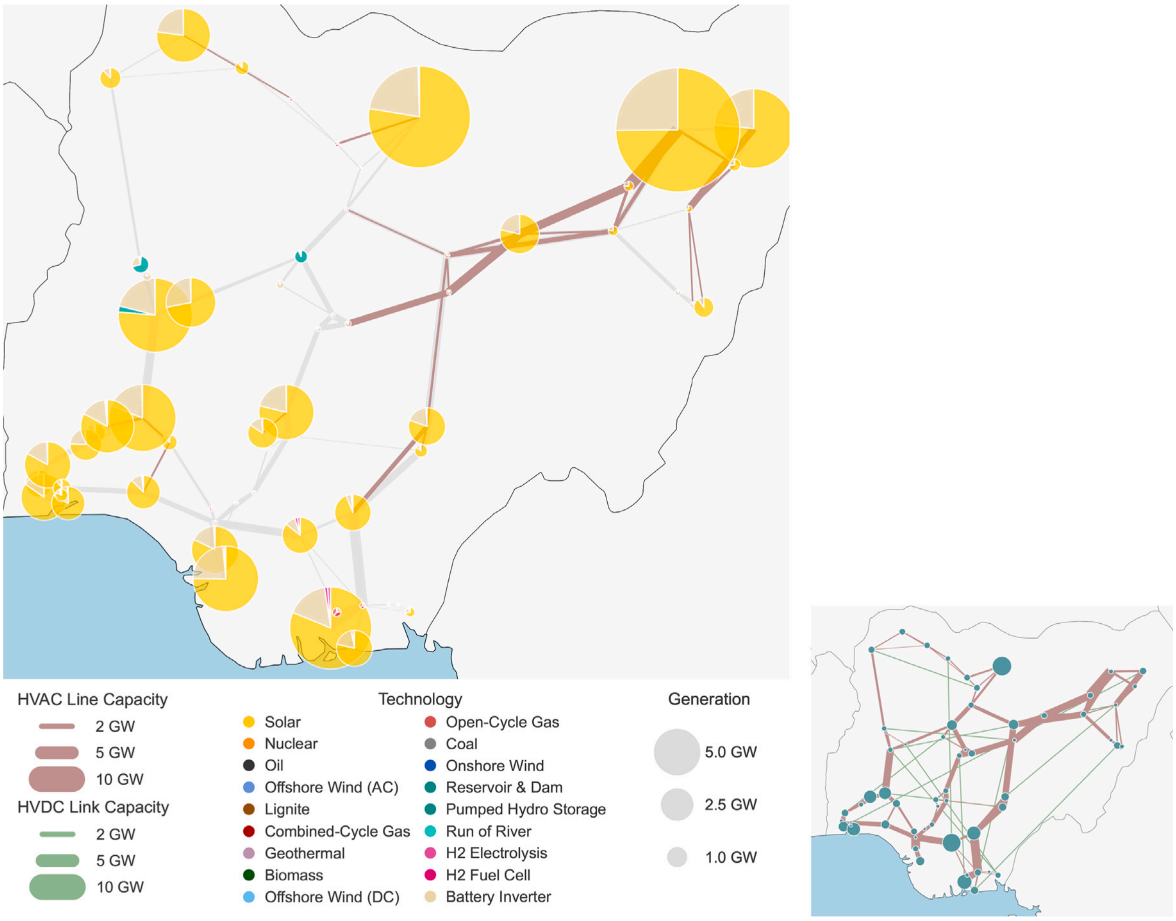
option. However, it is not significantly optimized, probably because we ignore fuel trade with other countries and the unique geo-location of the country. Nigeria lies close to the equator, where solar irradiation is homogeneous across the year, requiring less seasonal energy storage. The battery storage consists of an inverter component [€/MW] and a Li-Ion battery stack [€/MWh] that can be independently scaled by the model such as applied in [91]. The energy-to-power ratio (EP) indicating the sizing between these storage components is optimized in the range 4.5 h – 15.0 h with an average of 6.75 h. The total optimized Li-Ion battery storage discharging capacity and energy capacity is 67.9 GW and 459.7 GWh, respectively. The optimal solar capacity distribution is spatially uneven. Most solar is expanded in the country's north, where the solar potential is significantly higher [92]. It is also cost-optimal to build new transmission routes in the north and east of Nigeria, enabling the spatial distribution of electricity. The total optimized solar PV capacity is 256.9 GW, whereas about 20% of the solar energy is curtailed on an annual average. The HVDC options are not used significantly, indicating it is not cost-optimal in the scenario. Fig. 12 shows the dispatch profiles outputs of the optimization, which illustrates that most batteries charge during the day and discharge at night. Notably, to be conservative, with cost assumptions for 2050 [93], the average marginal prices reach only 51 €/MWh, compared to 59 €/MWh in the 2020 scenario. While we do not address in this demonstration uncertainty that could strengthen the results, future work can add modelling to generate alternatives and structured parameter sweeps [39] as well as robust optimization techniques [94]. Nevertheless, the results of the demonstration indicate that the optimized renewable electricity future for Nigeria could be cheaper than today.

6. Limitations and future opportunities

6.1. Missing network topology data

Modelling can only be as good as underlying data – the same applies to PyPSA-Earth. By relying on open sources to model energy systems, their data quality is a concern that we also acknowledge for the present paper. Yet, we also describe possible image recognition procedures to improve the data situation in PyPSA-Earth and potentially all energy models. This effort may complement the traditional effort by public institutions that disclose data of public relevance, such as installed network infrastructure, as performed by ENTSO-E [61].

Compared to Europe or North America, institutions that provide infrastructure data with geolocation for modelling have no analogues in Africa. The missing network data situation is limiting the use of energy system models. However, other types of data from which energy system components can be inferred exist on a much larger scale. Satellite imagery is one such data type. As part of the PyPSA meets Earth initiative, we are exploring opportunities to use neural network-based object detection applied to satellite imagery to enrich the existing datasets on energy infrastructure. In the past, such efforts have either been hard to apply on larger scales due to high requirements on manual input [95] or are coarse approximations to the true grid structure [96]. Under the umbrella of this initiative, we aim to develop precise and scalable methods and base our efforts on recent advances in the field.



(a) (b)

Fig. 11. Optimization result represent Nigeria's (a) 2060 power system. The coloured points represent installed capacities. Light grey and dark grey lines are existing and newly optimized transmission lines, respectively. (b) Shows all network options on a different scale as (a) with the total electricity consumption per node.

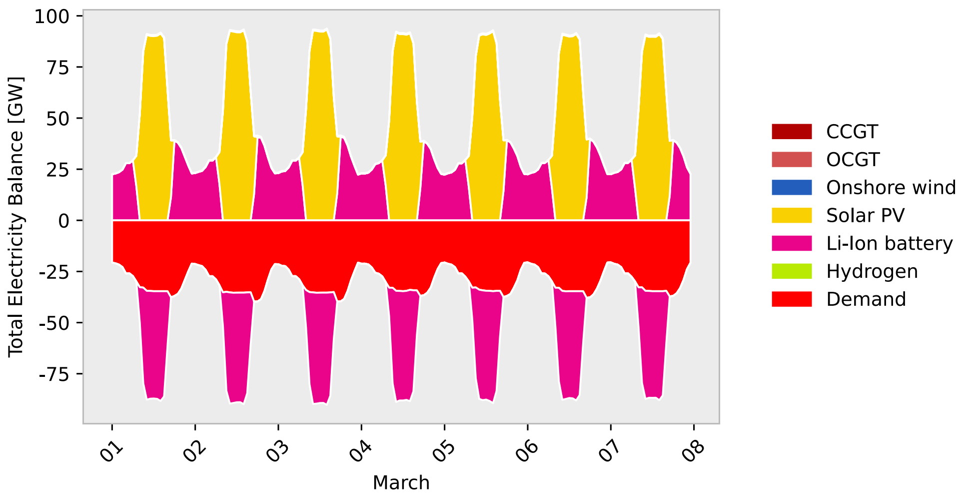


Fig. 12. Total electricity balance for the 2060 scenario. The time-series is hourly sampled for selected days in March including electricity supply (above zero) and consumption (below zero). CCGT and OCGT stands for closed and open cycle gas turbines, respectively.

6.2. Missing demand time series and prediction biases

Demand is a significant uncertainty factor in Africa due to the growth in magnitudes over the following decades that has implications on results created by PyPSA-Earth. Therefore, improving demand predictions is essential. We acknowledge this limitation in the data fed into our model and highlight research opportunities to address this challenge. PyPSA-Earth demand data is limited, as indicated in Section 3.4, by poor prediction performance for low-income countries due to input data biases and by missing machine learning output data for some low-demand countries due to software bugs. Additionally, while the open-source *synde* package [52] used in PyPSA-Earth extended the original GEGIS package for demand prediction by a workflow, there are opportunities to create a package focusing only on demand prediction substituting the GEGIS design that provides all energy model data in one package [29].

Developing a package focusing on sector-coupled energy demand forecast for macro-energy system modelling worldwide is an opportunity to improve the status quo of existing tools, not limited to the power sector. Further, instead of validating the demand with annual means, one should validate with hourly officially reported time series since the data quality is better indicated by the latter.

6.3. Imprecise global data

PyPSA-Earth relies on open data with global scope. This means that sometimes data is used that approximate country-specific details needed for national energy planning studies. While improving the global open data situation is one opportunity [97], another is to enable the integration of national and regional more precise data that can also be used as a source for validation. Therefore, PyPSA-Earth does not only use global data as default but will allow the integration of national or regional more precise data with specialized functions, here named "linkers".

6.4. Additional technologies

PyPSA-Earth includes the major transmission, generation and storage technologies. However, some system components are not yet included. Examples of not implemented generation technologies are Concentrating Solar Power (CSP), location-based geothermal, and other secondary technologies such as wave/tidal energy harvesting. While at a global scale these technologies represent a minor fraction, for country-specific analyses, they may have substantial implications, such as in the case of Kenya for geothermal or Morocco for CSP. Moreover, while currently only lithium-ion batteries and hydrogen energy storage are considered, other technologies may be considered and tested, such as the well-known Redox Flow batteries, Compressed-Air Energy Storage (CAES), Liquified-Air Energy Storage (LAES), that can have a large market in the future. Moreover, the dynamic calculation of the transmission capacity as a function of weather conditions [23], also known as Dynamic Line Rating (DLR) [98], still needs to be included.

These limitations, at the time of writing, represent future opportunities to improve the model and capture relevant technologies to perform detailed energy studies for all countries.

7. Conclusions

This paper presents the PyPSA-Earth model, which is an open-source global energy system model in high spatial and temporal resolution. It is making high-resolution modelling accessible to countries which so far had not detailed energy planning scenarios developed. Using a novel comprehensive workflow procedure PyPSA-Earth automatically downloads open data, provides model-ready data and integrates optimization features to address large-scale energy system planning. In agreement with the open-source spirit, the model is not built from scratch but derived from the European-focused PyPSA-Eur model adding global data as well as several new features.

The methodology is confirmed to be flexible and accommodate a high temporal and spatial resolution power model for national and regional energy planning with global scope. The validation performed for the African continent highlighted that PyPSA-Earth successfully provides power network and installed generation data that match trustworthy third-party national data with adequate accuracy, hence suggesting PyPSA-Earth to be a reliable model for energy planning. The 2020 and 2060 planning studies for Nigeria have further confirmed that net-zero emission scenarios for the electricity sector can be performed using PyPSA-Earth, leading to realistic results comparable with similar studies but in higher spatial detail. That further stresses the robustness of the approach and the flexibility of the methodology to be used in practical projects.

Given the need for reliable tools to foster the energy transition and the efficient use of resources, PyPSA-Earth can successfully support policymakers, utilities, and scholars in providing reliable, transparent, and efficient decision-making on energy studies. While several open-source projects are developed but discontinued, the authors of this paper and other PyPSA-Earth developers aim to foster collaborative energy system modelling on the same code-base to provide a well-maintained and robust tool rather than disperse resources across multiple models that get quickly outdated. Given the flexibility of the approach, additional improvements can be integrated, and scholars interested in contributing are invited to contact the model initiative team to join forces. Accordingly, this paper and the proposed tool can serve as a backbone, enabling further research and business activities to built on top to meet various energy transition planning needs that must be cheap and fast to develop for every nation and community on Earth.

Further studies may address the sector-coupled version of PyPSA-Earth. In addition to power and hydrogen data, sector-coupling requires various electric as well as non-electric demand and supply side data from other sectors, including heat, industry and/or transport. Other future work may interface energy modelling with economics modelling, add robust-optimization capabilities, improve demand forecasts in alignment with climate change scenarios, adapt imprecise global network data using object detection on satellite images or validate the model in other regions.

CRediT authorship contribution statement

Maximilian Parzen: Conceptualization, Project administration, Software development, Validation, Figure production, Writing and revising the manuscript. **Hazem Abdel-Khalek:** Software development, Validation, Figure production, Writing and revising the manuscript. **Ekaterina Fedotova:** Software development, Validation, Figure production, Writing and revising the manuscript. **Matin Mahmood:** Software development, Validation, Figure production, Writing and revising the manuscript. **Martha Maria Frysztacki:** Software development, Validation, Figure production, Writing and revising the manuscript. **Johannes Hampp:** Software development, Validation, Figure production, Writing and revising the manuscript. **Lukas Franken:** Writing and revising the manuscript. **Leon Schumm:** Software development, Validation, Figure production, Writing and revising the manuscript. **Fabian Neumann:** Conceptualization, Writing and revising the manuscript. **Davide Poli:** Writing and revising the manuscript. **Aristides Kiprakis:** Funding acquisition, Writing and revising the manuscript. **Davide Fioriti:** Conceptualization, Project administration, Software development, Validation, Figure production, Writing and revising the manuscript.

Declaration of competing interest

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

Data availability

Code and data to reproduce results and illustrations are available by using PyPSA-Earth v0.1 [34]. Further, instruction and configurations to reproduce the scenarios and plots are provided here: https://github.com/pz-max/pypsa-earth-paper.

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Appendix A. The mathematical modelling

The following paragraphs are an extract of [91], which formulates PyPSA-Earth based on [3,23,99,100].

The objective of PyPSA-Earth is to minimize the total Annualized Costs (AC) of the system shown in (A.1), comprised of the annualized capital and operational expenditures. Capital expenditures include capacity-related, long-term investment costs c at location i for generator $G_{i,r}$ of technology r, storage energy capacity $H^{store}_{i,s}$, charging capacity $H^{+}_{i,s}$ and discharging capacity $H^{-}_{i,s}$ of technology s and transmission line F_l. Operational expenditures include energy-related variable cost o for generation $g_{i,r,t}$ and storage charging $h^{+}_{i,r,t}$ and discharging $h^{-}_{i,r,t}$, as well as energy-level related storage cost $e_{i,s,t}$. Thereby, the operation depends on the time steps t that are weighted by duration w_t that sums up to one year $\sum_{t=1}^{T} w_t = 365 day * 24 \frac{h}{day} = 8760$ h.

$$\begin{aligned}\underset{G,H,F,g,h,e}{\text{minimize}}\ AC = \Bigg[& \sum_{i,r}(c_{i,r}\cdot G_{i,r}) + \sum_{l}(c_l \cdot F_l) \\ & + \sum_{i,s}(c^{store}_{i,s}\cdot H^{store}_{i,s} + c^{-}_{i,s}\cdot H^{-}_{i,s} + c^{+}_{i,s}\cdot H^{+}_{i,s}) \\ & + \sum_{i,r,t}(o_{i,r}\cdot g_{i,r,t}\cdot w_t) + \sum_{i,s,t}\left((o^{+}_{i,s}\cdot h^{+}_{i,s,t} + o^{-}_{i,s}\cdot h^{-}_{i,s,t})\cdot w_t\right) \\ & + \sum_{i,s,t}(o^{store}_{i,s}\cdot e_{i,s,t}\cdot w_t) \Bigg]\end{aligned} \tag{A.1}$$

The objective function is subject to multiple linear constraints to make scenarios more realistic, leading to a convex linear program with continuous variables. The constraints explained in the following in more detail consist of (i) demand equals supply constraint, (ii) geophysical and operational constraint for generators, storage units as well as power lines, (iii) Kirchhoff's current and voltage law constraints that represent the physics of electric energy flows in the power network, (iv) a recovering cyclic energy storage constraint and finally, (v) greenhouse gas emissions reduction constraint. Such linear problems have in general one unique objective value with sometimes multiple non-unique operational solutions [100], making complex problems solvable in reasonable amount of time (sometimes multiple days).

Firstly, the PyPSA-Earth model guarantees the energy balance by the linearized power flow in Eqs. (A.2) and (A.3) to guarantee the energy balance of the power network, which is very distinctive feature compared to most other planning models [3]. This is done by including Kirchhoff's Current Law and Kirchhoff's Voltage Law constraints. The equivalent formulation of Kirchhoff's Current Law in (A.2) guarantees that the net energy balance for each substation i match, accounting for local generation, storage, transmission system and inelastic electricity demand $d_{i,t}$. The variable $f_{l,t}$ identifies the power flow in the line l having networks' incident matrix $K_{i,l}$.

$$\sum_r g_{i,r,t} - \sum_s h^{+}_{i,s,t} + \sum_s h^{-}_{i,s,t} + \sum_l K_{i,l}\cdot f_{l,t} = d_{i,t} \quad \forall i,t \tag{A.2}$$

While Kirchhoff's Current Law accounts for both, AC and controllable DC lines, the Kirchhoff's Voltage Law only additionally constraints AC power lines. In PyPSA-Earth the voltage angle difference around every closed cycle in the network must add up to zero. PyPSA-Earth formulates this constraint using linearized load flow assumptions, in particular, cycle basis $C_{l,c}$ of the network graph where the independent cycles c are expressed as directed linear combinations of lines [101]. This leads to the constraints (A.3), where x_l is the series inductive reactance of line l [99]. As might be noted, the linearized power flow assumptions completely disregard the resistance. These assumptions introduce negligible errors when (i) the reactance is much larger than the resistance, such as for high voltage lines, and (ii) the voltage angle differences are small i.e. $sin(\delta) = \delta$ [101].

$$\sum_l C_{l,c}\cdot x_l \cdot f_{l,t} = 0 \quad \forall c,t \tag{A.3}$$

Secondly, since generator and storage units as well as transmission lines can experience geographical restriction, PyPSA-Earth can constrain the installed capacities and gives the options for lower as well as upper limits. Equations from (A.4) to (A.6) specify the power capacities for generators, storages and lines, respectively.

$$\underline{G}_{i,r} \le G_{i,r} \le \overline{G}_{i,r} \quad \forall i,r \tag{A.4}$$

$$\underline{H}_{i,s} \le H_{i,s} \le \overline{H}_{i,s} \quad \forall i,s \tag{A.5}$$

$$\underline{F}_{l} \le F_{l} \le \overline{F}_{l} \quad \forall l \tag{A.6}$$

Thirdly, while the previous constraint only limits the installations, some components require time-varying operational limits. Examples for such technologies are renewable generators, described by the subset RG, and power lines with dynamic line-rating (DLR) [102], whose operation highly depend on the weather signals. With roughly 20x20 km globally rasterized era5 weather data that are available for more than 30 years, calculated using Atlite, PyPSA-Earth can limit the rated power of generators $G_{i,r}$ and lines F_l by a location and time dependent variable, i.e. temperature, wind speed, humidity and solar irradiation, as mathematically described in (A.7) and (A.8).

$$0 \le g_{i,r,t} \le \overline{g}_{i,r,t}\cdot G_{i,r} \quad \forall i, r \in RG, t \tag{A.7}$$

$$0 \le f_{l,t} \le \overline{f}_{l,t}\cdot F_l \quad \forall l,t \tag{A.8}$$

Fourth, describing storage constraints. Storage charging $h^{+}_{i,s,t}$ and discharging $h^{-}_{i,s,t}$ are both positive variables and limited by the installed capacity $H^{+}_{i,s,t}$ and $H^{-}_{i,s,t}$ in (A.9) and (A.10).

$$0 \le h^{+}_{i,s,t} \le H^{+}_{i,s} \quad \forall i,s,t \tag{A.9}$$

$$0 \le h^{-}_{i,s,t} \le H^{-}_{i,s} \quad \forall i,s,t \tag{A.10}$$

This formulation keeps the feasible solution space convex, though does not prevent simultaneous charging and discharging, which is often an unrealistic effect that can heavily distort modelling results in net-zero scenarios. Setting adequate variable cost parameter solves this modelling artefact while keeping the problem formulation linear [100].

The storage energy level $e_{i,s,t}$ is the result of a balance between energy inflow, outflow and self-consumption described in (A.11). Additional to directed charging and discharging with its respective efficiencies $\eta_{i,s,+}$ and $\eta_{i,s,-}$, natural inflow $h^{inflow}_{i,s,t}$, spillage $h^{spillage}_{i,s,t}$ as well as standing storage losses that reduces the storage energy content of the previous time step by a factor of $\eta_{i,s,+}$ are considered.

$$\begin{aligned} e_{i,s,t} &= \eta_{i,s,+}\cdot e_{i,s,t-1} + \eta_{i,s,+}\cdot w_t \cdot h^{+}_{i,s,t} - \eta^{-1}_{i,s,-}\cdot w_t\cdot h^{-}_{i,s,t} \\ &\quad + w_t \cdot h^{inflow}_{i,s,t} - w_t\cdot h^{spillage}_{i,s,t} \quad \forall i,s,t \end{aligned} \tag{A.11}$$

The amount of energy that can be stored is limited by the energy capacity of the installed store unit $H^{store}_{i,s}$ [MWh], which allows independent storage component scaling shown in (A.12).

$$0 \le e_{i,s,t} \le H^{store}_{i,s} \quad \forall i,s,t \tag{A.12}$$

To fix the storage technology design, in (A.13) a technology-specific energy to discharging power ratio $\overline{T}_s$ is multiplied with the capacity of the discharging unit $H^-_{i,s}$ to define the upper energy limit per installed storage.

$$0 \leq e_{i,s,t} \leq \overline{T}_s \cdot H^-_{i,s} \quad \forall i, s, t \tag{A.13}$$

Further, Eq. (A.14) guarantees that the energy storage units are operated cyclically: the state of charge at the first and last period of the optimization period T (i.e. 1 year) must be equal.

$$e_{i,s,0} = e_{i,s,T} \quad \forall i, s \tag{A.14}$$

This cyclic definition is not mandatory but helps with the comparability of model results. It further avoids the free use of storage energy endowment, meaning that the model could prefer to start with a higher and end with a lower storage level to save costs.

Finally, PyPSA-Earth can constrain the total emissions. These emissions are tracked by a variable at each generator unit r and marginal emission intensity γ_r to constrain the total emission by a limiting parameter $\overline{GHG}$ as in (A.15).

$$g_{i,r,t} \cdot \gamma_r \leq \overline{GHG} \quad \forall i, r, t \tag{A.15}$$

Appendix B. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.apenergy.2023.121096.

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DECLARATION

I declare that I have completed this dissertation single-handedly without the unauthorized help of a second party and only with the assistance acknowledged therein. I have appropriately acknowledged and cited all text passages that are derived verbatim from or are based on the content of published work of others, and all information relating to verbal communications. I consent to the use of an anti-plagiarism software to check my thesis. I have abided by the principles of good scientific conduct laid down in the charter of the Justus Liebig University Giessen 'Satzung der Justus-Liebig-Universität Gießen zur Sicherung guter wissenschaftlicher Praxis' in carrying out the investigations described in the dissertation.

Tübingen, 30th December 2023

Johannes Hampp

COLOPHON

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