Analyzing Storage Needs in Energy Systems with Variable Renewable Energy Integration

Lessons from Calliope for WITCH

by

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TU Delft

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Summary

This thesis explores the integration of flexibility measures in the European energy system. The thesis uses an integrated assessment model to simulate the integration of flexibility based on parameters from an energy system model with a high spatial and temporal scope.

The key objectives include evaluating different flexibility technologies' roles in enhancing future energy systems' reliability and resilience. The foundation of the thesis is identifying and evaluating the most promising storage technologies. Thereafter, the storage technologies are placed into the context of energy modeling, highlighting their strengths, weaknesses, and ability to be modeled.

The research uses the WITCH (World Induced Technical Change Hybrid) model. However, this research is based only on the region of Europe. The WITCH model can run simulations under different climate policy scenarios, including the business-as-usual (BAU) and carbon tax (ctax) pathways. Variables and parameters such as flexibility measures and associated costs are modeled to reflect future energy system configurations based on pre-run cost-optimal configurations from the Calliope framework.

The thesis results show that the main flexibility measures from the literature are storage, grid expansion, demand response, and sector coupling. These measures can enhance the energy system's integration of variable renewable energy sources. Climate policies, i.e., carbon taxes, enable higher levels of VRE and, therefore, flexibility measures, resulting in lower emissions and more efficient energy systems. Fundamentally, the results show a different approach to flexibility than that utilized in long-term models. Using aggregated parameters from energy systems models' pre-run configuration is a novel method of informing other models. This coupling method is effective when the variables of the two models can be harmonized. The thesis discussion raises areas for future research. The main discussion point is the effectiveness of using pre-run optimization results. The 2030 and 2050-based data provide the energy system's transitional nature. However, extracting insight for a purely transitional model like WITCH proved challenging. Furthermore, the impact of scaling the data from Calliope to match the WITCH data ranges needs further investigation. Lastly, the implications of the elasticity of substitution between the individual flexibility measures, e.g., between storage capacity expansion and transmission grid expansion.

Alignment with master thesis program

This thesis aligns with the objectives of the energy track Master Complex Systems Engineering and Management (CoSEM) at TU Delft. The research focuses on the flexibility requirements in future energy systems with high penetration of variable renewable energy. Finding solutions to integrate higher levels of VRE has been one of the main focus points of the master.

The Energy track of the CoSEM program provides a comprehensive education in energy markets and future energy systems, focusing on renewable energy, electricity, and gas infrastructures and how possible interventions for their improvement can be designed. This thesis mirrors these educational goals by examining the impact of increased VRE penetration on the energy system and the consequent need for advanced flexibility measures, including energy storage solutions.

The thesis's interdisciplinary nature, integrating technical analysis with policy implications, reflects the CoSEM program's emphasis on socio-technical system design.

This thesis's interdisciplinary and complex challenges align with the master's focus on socio-technical systems. Lastly, the thesis can inform policymakers about real-world applications of the strategies found.

Contents

Abbreviations, Tables and Figures

Abbreviations

Abbreviation	Definition
VRE	Variable Renewable Energy
DSM	Demand Side Management
PHS	Pumped Hydro Storage
BAU	Business as Usual
ctax	carbon tax
CAES	Compressed Air Energy Storage
CCGT	Combined Cycle Gas Turbine
O&M	Operations and maintenance
LCOE	Levelized Costs of Energy
LCOS	Levelized Costs of Storage
EV	Electric Vehicles
TPES	Total Primary Energy Supply
ESS	Electrical Storage Systems
STS	Short-Term Storage
LTS	Long-Term Storage
CHP	Combined Heat and Power
CSP	Concentrated Solar Power
CCS	Carbon Capture and Storage
GHG	Green House Gasses
kWh	Kilo Watt Hours
CAPEX	Capital Expenditures
OPEX	Operating expenses
AC	Alternating current
DC	Direct current

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1 Introduction

To realize the climate goals set out in the Paris Agreement, adopting and integrating renewable energy technologies within the energy system is crucial [47, 37, 54]. This integration has already begun transforming the energy landscape, as solar photovoltaics (PV) and onshore and offshore wind turbines have experienced significant cost reductions. However, integrating Variable Renewable Energy (VRE), such as solar and wind, introduces challenges associated with intermittent energy production [30]. Consequently, the design of the socio-technical aspects of future energy systems must address these challenges and implement solutions to ensure grid stability. This will ultimately enable a reliable and sustainable transition to renewable energy sources.

Historically, energy systems have been balanced using fast-reacting fossil fuel-based generators, which act as backup capacity [57]. VREs are, however, inherently site-specific, variable, and uncertain. Combined with the phase-out of fossil fuels, these characteristics necessitate a radical transformation of the energy system to become more flexible [52]. Increasing the grid capacity for transmission and local distribution of site-specific power supply are examples of increased flexibility. Additionally, the daily and seasonal mismatch of energy supply and demand entails storing the energy for later use [38].

Storage technologies can enable the match between variable energy generation and demand. By transforming the electricity into different energy carriers, the energy can be stored in over-generation and used in times of under-generation. The implementation of storage-enabling technologies is, however, not straightforward. The technology choice and the capacity needed to be implemented depends on socio-technical considerations [36].

Models are used to predict what technological, economic, political, and societal changes are needed to facilitate a future renewable-based energy system. Energy-economy-climate models are employed for ex-ante policy evaluation by generating scenarios of pathways towards a renewable future [21]. A popular energy-economy-climate model is the World Induced Technical Change Hybrid (WITCH) model, which will be the focus of this research.

Energy-economy-climate models often inhibit high levels of data aggregation due to computational constraints. A high level of aggregation could lead to a potential loss of crucial information, as it lacks spatiotemporal resolution. This limitation is significant as it may lead to an under- or overestimation of the electricity sector to balance Variable Renewable Energies (VREs) [34].

To address this, the integration of two scales of energy models is proposed: a short-term power system model to capture the precise interactions of technologies and a long-term integrated assessment model (IAM) to understand the interactions between the energy system, economy, and climate. Combining these scales allows the modeling of needed flexibility to be improved, enabling more informed policy decisions supporting the integration of VRE and flexibility. This approach incorporates a more realistic parameterization derived from different energy system configurations from Calliope. These configurations will be used as inputs to enhance the representation of flexibility in WITCH by identifying the key predictors and values that determine flexibility. This research aims to empower policymakers to make well-informed decisions regarding the required installed capacity and the appropriate technology types for flexibility to achieve policy goals.

This thesis is organized as follows: Chapter 1 identifies the academic research gap, outlines the research questions, and describes the approach to address them. Chapter 2 introduces the fundamental concepts and key ideas related to flexibility in energy systems. Chapter 3 details the modeling methods for flexibility used in this research. In Chapter 4, the model's results designed to predict flexibility are presented and analyzed. Chapter 5 examines the output of the WITCH model after incorporating the new interactions. Finally, Chapter 6 discusses the thesis findings and provides concluding insights.

1.1. Academic knowledge gap

This section will introduce and delineate the central concepts of the research. Starting with a general introduction to IAMs and WITCH in 1.1.1, moving further towards Calliope in 1.1.2 and the link between the two models. Furthermore, the literature on coupling long-term and short-term energy models will be discussed in 1.1.3.

1.1.1. Integrated Assessment Model: WITCH

Integrated assessment models (IAMs) evaluate global energy systems under various scenarios, often over timescales of several decades. These models assess the interactions between policies, such as emission mitigation, and their effects on the energy system and climate change. To capture these dynamics, IAMs typically model specific energy supply and demand sectors and constraints on land use, greenhouse gas emissions, and adaptation responses to climate impacts.

The WITCH model is an IAM that focuses on modeling the dynamics of climate change mitigation and adaptation. To enable detailed insights, the energy sector representation is hard linked with the rest of the economy. This linking enabels the optimization of energy investment and resources. The WITCH model combines a top-down aggregated optimal growth model with a detailed energy descriptive model structured around a Constant Elasticity of Substitution (CES) framework. Specifically, the electricity sector's CES structure comprises four supply elasticities values: zero, 2, 5, or infinity [11]. These parameters aim to model the substitutability between supply technologies. The value zero implies no substitutability, so the technologies can not replace each other. These technologies are summed independently of costs. The infinite elasticity suggests that the two technologies can replace each other completely; therefore, the choice of technology solely depends on the costs. The CES structure is the basis for the technology selection in the final energy mix in WITCH.

The impact of using different CES structures on VRE integration and final representation has been researched by Carrera and Marangoni (2017). Their findings showed that the initial values of the level of VRE matter significantly in the final technology selection in the modeled system [10]. Consequently, an accurate representation of storage and other flexibility measures in the earlier modeled years of Integrated Assessment Models (IAMs) and accurate technology diffusion representation is vital to capture real-world phenomena.

Challenges persist in achieving an adequate level of spatiotemporal detail when using IAMs. The WITCH model simulates the interactions between energy, economic, and climate systems to understand climate mitigation pathways. These global interactions are computationally intensive, this necessitates multi-year time steps to capture their complexities effectively. Therefore, the high level of aggregation required for global impacts leads to a loss of spatiotemporal detail.

This high level of aggregation is not necessarily a problem when modeling traditional power systems with high levels of fossil fuel-based generators. Operation in this system is more predictable because supply technologies are dispatchable [8]. However, the aggregation does cause a mismatch in the representation of the operations of VRE.

To solve these challenges, two types of strategies can generally be applied. One type is internal model improvements to represent VRE integration and operations, whereas the other type uses complementary, more specific models to parameterize the interaction or to benchmark outcomes [8]. Studies on the first type of improvements of IAMs have sought to find the right level of energy system representation within the IAM. Due to the computationally intensive interactions of the climate-energy-economy models, increasing temporal details to the level needed to represent the operations of VRE is often not feasible. Therefore, efforts in the representation of operations of technologies have been the primary goal to improve the internal interactions of the IAMs [46].

Furthermore, recent efforts to internally improve WITCH stem from modeling additional constraints to match the behavior of systems with high levels of VRE penetration. One of these efforts was the ADVANCE project, where multiple IAMs were improved by adding explicit constraints to describe VRE integration within energy systems better. For WITCH specifically, flexibility and capacity constraints were added [35], [44].

Using a complementary model is based on the understanding that different models have unique strengths and weaknesses. Therefore, specific interactions and operations can be modeled externally rather than attempting to achieve optimal detail within an IAM. This external model can enhance and provide valuable insights to the IAM. However, challenges emerge when developing suitable linking methods and frameworks to facilitate data flow between the models. In this thesis, the model that will provide insights into the flexibility needs in the European energy system is the Sector-coupled Calliope model. Sector coupling refers to integrating different energy sectors, such as the power, heating, industry, and transportation sectors. Transforming energy to other forms possibly allows energy to be utilized across these sectors. The Sector-coupled Calliope model is particularly well-suited for informing the IAM because sector coupling inherently requires high levels of flexibility, which allows for insights into optimal configurations of flexibility within an energy system. Additionally, the level of flexibility in Calliope allows for high VRE penetration levels. This could provide insights into what is needed to facilitate these penetration levels.

1.1.2. Calliope

Calliope is a framework for constructing energy system models with high spatial and temporal resolution. The framework allows for creating and analyzing energy system models on multiple scales, ranging from urban districts, to countries, to entire continents [41]. This thesis focuses on the continent-level scale.

Given that WITCH time steps (timeslices) are fixed at five years, adding temporal resolution is unfeasible. This limitation highlights the need for enhanced technological representation to improve storage and flexibility modeling within the system. This enhanced technical representation will be constructed using Calliope.

One promising development that Calliope has been used for is the generation of a range of possible configurations of future energy systems. This approach uses technically and economically feasible, spatially explicit, practically optimal results (SPORES). [43]. The SPORES represent viable configurations that enable a functioning energy system in 2050 within a certain percentage of the least-cost optimal configuration. Produced via a weight-based algorithm, these SPORES are computed to exhibit diversity in feasible configurations [43].

Through SPORES, insights can be obtained about the must-haves within an energy system, i.e., elements of a future renewable energy system that must be present for it to function. System configurations can, for example, rely on varying levels of electrification of heat and transport, Storage, Biofuels, Wind energy, PV, and intra-European transmission. The SPORES indicate that, due to sector coupling, the impact of renewable variability can be reduced. Consequently, there are SPORES where firm capacity becomes almost obsolete, and PV and wind can primarily supply the demand. Therefore, the firm flexibility constraint in WITCH contradicts the SPORES results. For example, in a configuration with a high level of solar capacity, summer overproduction and winter underproduction is often handled by electrolysis in summer and combined-cycle gas turbines in winter. However, other configurations are possible, allowing decision-makers to quantify their trade-offs.

The Calliope team have generated SPORES for both the 2030 and 2050 energy system. This collection of the model runs provides a glimpse into a future energy system where reliance on fossil-based generation is reduced or almost eliminated. As the SPORES aim to reach a configuration that is close to cost optimality, they can function as an aspirational target. This does not mean that the results are binding, as cost optimality is not the main focus of shifting towards a more renewable-based energy system.

1.1.3. Coupling Short-Term and Long-Term Energy Models

This section discusses existing linkages between IAMs and more detailed models. The aim is to find practical methodological frameworks for data transferability between the long-term planning and details models.

Gong et al. (2023) introduced a price-based bidirectional coupling method between the Regional Model of Investments and Development (REMIND) IAM, and the hourly power sector model Dispatch and Investment Evaluation Tool with Endogenous Renewables (DIETER). The short-term model produced hourly prices, which the long-term model can use to produce investment strategies. This allows the IAM to align its investments with more detailed operational consequences, thereby increasing the accuracy of the effects of the investments in the IAM [19].

Sejlom et al. (2020) created a bidirectional coupling method for a long-term energy system model and a short-term power market model in Norway. Hydropower makes up a large part of the electricity supply in Norway. The basis of the linkages was identifying the exogenous and endogenous variables that would be used for the link. The power system model provided the specific link between demand variables and hydropower to the IAM. The linkage iteratively communicated the demand from the IAM, and the hydropower capacity from the power model until the results converged. This allowed for an alignment in the most relevant features of the models, therefore allowing the transferability of results [50].

Other methods include using a multivariate regression model to link IAMs with a detailed hourly global electricity model. The regression model was used to downscale the IAM output to a timescale that could be used as input for the power system model. With these more stylized methods, it is crucial that the down-scaling is varied to ensure that the data represent the IAM interactions [8].

Other than using a power system model, dispatch models can be used for coupling. In the dispatch model, the maximum contributions of technologies to the total capacity can be defined. The capacities from the IAM are then used as input for the dispatch model to see if the demand can be met. Correction to levels of installed capacities is then communicated back to the IAM, thereby strengthening the assumptions in the IAM on system reliability [58].

Research has also been conducted on coupling models to enhance storage representation. Long-term energy planning and a power flow optimization model were coupled to create the coupling. The main focus was to find the impact of storage on system reliability and cost, which aligns with the goals of this thesis. The power flow model minimized the levelized cost within the system under different storage configurations. Thereby finding the optimal storage capacities for IAM-based energy systems [31].

In addition to the so-called hard-linking methods introduced above, soft-linking can be used to inform IAM with more detailed outputs from short-term models. This method transformed annual demand profiles to half-hour-based profiles. The power model added constraints on technologies' capabilities to supply energy. The results with and without using the short-term model can then be compared to assess the effectiveness of the soft coupling [12].

Overall, the studies demonstrate the use of both soft-linking and hard-linking models to integrate different modeling approaches. Hard-linking involves connecting two models and running them in parallel until they converge on a solution that satisfies the constraints of both models. In contrast, the soft-link approach uses the results from the IAM to inform the detailed model. In this thesis, the pre-computed SPORES will serve as the basis for linking, presenting unique methodological challenges compared to running the detailed model in real-time.

Building on lessons from previous coupling efforts, this research can benefit from strategies used to bridge long-term and short-term models. Variables employed to align these models provide valuable insights. Two main strategies emerge from the studies: Firstly, technology capacities from the long-term model can be used in short-term models to simulate feasibility and determine the additions needed to support these capacities. This approach helps evaluate whether the proposed capacities are achievable and what additional measures are necessary. Secondly, a cost-based coupling strategy involves the short-term model generating hourly price signals for specific costs, which can guide investment decisions in the long-term model. This method provides a dynamic feedback loop where short-term price signals influence long-term capacity investments. By incorporating the relevant strategies, this research aims to use the insights from the different scales of the models to allows for more informed policy decisions within the energy system.

1.2. Research approach

By combining the insights from the two model scales, the representation of flexibility in WITCH will be reevaluated. This process aims to refine or redefine the relationships between the energy systems configuration and the flexibility needed. The central research question that will be used in the research is constructed as follows:

- ***What is the influence of varying levels of variable renewable energy penetration on the storage requirements in a future energy system?***

The main research question will be answered by by dissecting the problem into multiple sub-questions.

1.2.1. Sub-questions and data requirement

1. ***What technologies or groups of technologies are available to manage flexibility in future energy systems?***

   A comprehensive literature review will be conducted to address the research question. This review will first identify various measures that can enhance flexibility and place them within the context of energy system modeling. It will then focus on storage technologies as a critical component of flexibility. This analysis will delineate their potential roles, effectiveness, and interplay in future energy systems. The review will assess their suitability for inclusion in energy system models by exploring leading technologies and the need for specific technology combinations. Finally, the findings will be compared with the flexibility measures currently incorporated in the Calliope framework to identify potential gaps and opportunities for improvement.

   Data Requirements: Literature on the modeling of flexibility in energy systems and their dynamics and effectiveness of dealing with VRE. Output data of the sector-coupled Euro-Calliope SPORES.

2. ***How do different renewable technology policy scenarios shape the demand for flexibility in future energy systems?***

   An analysis of the near-optimal runs of Calliope for 2030 and 2050 will be used to find the level of flexibility needed in energy systems with varying levels of VRE penetration. The trade-offs between the flexibility measures will be researched using detailed data visualization and analysis. The trade-offs are analyzed by comparing different configurations in the form of SPORES, which represent pathways toward climate-neutral energy systems. Examples of other configurations are the specific storage technologies and their discharge capacities. Additional steps are needed to ensure that the data from Calliope can be transferred to a model that simulates the energy system over time. Firstly, the features from Calliope that will be used to construct the storage needs must be modeled in WITCH. If some features are already present, fitting modeling strategies will be developed to restrain from double counting. When this mapping of variables between the models is finalized, we can construct the quantitative relationships between the variables. These relationships will be used to predict the level of flexibility needed in WITCH.

   Data Requirements: Euro-Calliope SPORES. The 2030 and 2050-based SPORES output will provide the data needed to construct the storage requirement per system configuration. Additionally, the features of WITCH are required to build the variable mapping.

3. ***How can integrating specific energy system dynamics improve the modeling of flexibility needs in long-term energy models?***

   The flexibility needs will be modeled via the interactions between VRE and flexibility, the costs of these flexibility measures, and the change of the interactions and the costs over time. The interactions between VRE and flexibility from the previous research question will be the basis of the WITCH module.

   Research indicates that the cost of flexibility can potentially make up 50% of the generation costs in future energy systems [24]. Therefore, accurate cost parameters for integrating VRE are crucial, particularly in energy modeling that aims to optimize for minimal costs [27]. This aspect of the research seeks to determine the optimal balance between when it is necessary to specify individual costs and when broader cost aggregation is appropriate.

   The cost parameters will be derived from projection of both installation and utilization costs. These projections will enable accurate simulation of social welfare optimization in the WITCH model for higher levels of VRE. This will provide policymakers with precise cost estimates and clear pathways toward a sustainable energy system. The utilized data is relatively static, meaning that the parameters are based on data points instead of data with a trajectory. Therefore, the data has to be translated into data over time. Modeling strategies will be developed to deal with this translation. These interactions will then be programmed into WITCH's mathematical formulation, using variables, parameters, constraints, and equations to model the energy system. The variable mapping constructed in earlier research phases will guide this data translation.

With the translated Calliope parameterization and dynamics, the WITCH model can be used to obtain the flexibility needed over time. The existing scenarios in the WITCH model will be used to assess how the dynamics from Calliope behave under different climate scenarios. This output of WITCH will show the results of the interactions between the installed capacity and the flexibility needed, which could impact the energy mix, the emissions, and the GDP loss in Europe. The data will be presented in the form of graphs. The graphs present the data over time, showing the results for a collection of variables for multiple years to highlight the trajectory of the values. These outcomes will be compared to the model runs in WITCH without the new module flexibility module. The insights from this comparative analysis should reveal whether the representation of flexibility in the European energy system has been improved.

Data Requirements: Previous sub-questions and the existing WITCH model. Additionally, the translation of static data to data over time will be based, where possible, on the literature. The output of WITCH will be utilized for the comparative analysis.

Data Requirements: Costs parameters from Calliope and literature. Methodologies for constructing costs over time from the literature.

After answering these sub-questions, the insights will be used to answer the main research question. The relationship between VRE penetration and flexibility needs will become quantified, and areas of future research can be identified based on the challenges that arise from the analysis.

2
Flexibility in Energy Systems

This chapter contextualizes storage requirements within the broader energy system configuration. Section 2.1 explores the importance of modeling for finding storage requirements in energy planning. Section 2.2 discusses the necessity of flexibility in future energy systems and examines various strategies to achieve it. Section 2.3 provides an in-depth analysis of different storage types and their respective use cases. Finally, section 2.4 and 2.5 relate the literature review findings to energy modeling.

2.1. Energy modeling

The expected increase in the penetration of VRE technologies in the energy system necessitates a strong strategy for successful integration. One key reason for this need is that the existing power system is neither designed nor optimized for VRE technologies [53], [17]. This strategy should focus on the technical and economic challenges associated with the unpredictable fluctuating nature of wind energy and solar PV [20].

Energy storage systems (ESS) are gaining traction in both literature and industry. ESS can balance supply and demand by storing excess energy for later use. This stored energy is released when there is a shortage, providing solutions for both short-term and long-term imbalances[4]. While the distinction is not always clearly defined, short-term storage (STS) generally manages daily fluctuations, whereas long-term storage (LTS) addresses seasonal variations (e.g., [33]). Centralized modeling of ESS in the energy sector can provide a benchmark for optimal system performance and highlight areas requiring policy intervention [15].

Aside from pumped hydro storage, energy storage is seldom used in current energy systems, with most technologies still at the experimental stage on a utility scale [39]. This raises questions about the current handling of flexibility in energy systems. Traditionally, flexibility has been needed to handle the variability, uncertainty, and forecast errors in load demand and manage generator maintenance and outages. To address these conventional needs, operational strategies, flexible generation, demand-side management (DSM), and transmission infrastructure have been essential [20].

However, with increasing VRE penetration, the nature of flexibility needs has evolved. New challenges include the variability and uncertainty inherent to VRE and their uncorrelated and spatially distributed characteristics [28]. These new needs increase the importance of having robust and adaptive flexibility measures within the power system.

Simulation results can serve as a benchmark to understand the impacts of VRE features on the energy system. For long-term planning, where market dynamics can vary significantly, these results can guide policy interventions and serve as a foundation for strategic planning. This helps identify and address the need for flexibility in systems with increasing levels of VRE [20].

The storage level needed in a power system is determined by the level of VRE penetration and the level of flexibility measures other than storage in the system. [5], [23]. The effects of the intermittency, unpredictability, and location dependency of VRE on flexibility needs increases with higher penetration.

On the other hand, flexibility measures such as flexible generation, DSM, and expansion of the transmission infrastructure can mitigate some of this need. Therefore, the balance between the proportion of VRE and the robustness of other flexibility options collectively determines the optimal level of storage required to maintain grid stability and supply reliability. Therefore, there is no clear-cut relationship between storage and other variables. This nuanced need for storage makes modeling challenging. According to Haas et al., a range of further challenges arises in modeling storage for long-term planning [20]:

- Diversity of ESS: Differentiating between short-term and long-term storage and identifying the optimal mix of these technologies.
- Complex Lifetime and Efficiency Functions: Multiple variables, including usage cycles and operating conditions, influence the efficiency and lifetime of storage technologies, making the modeling non-linear.
- High Temporal and Spatial Resolution: Accurate modeling of ESS dynamics requires high temporal and spatial resolution to capture the interactions they operate on.
- Complete Valuation of ESS: Evaluating its full range of services, including potential competition with other flexibility sources like transmission, generation infrastructure, and demand-side management.
- Cross-Sectoral Integration: As energy sectors grow increasingly interconnected, cross-sectoral optimization is necessary

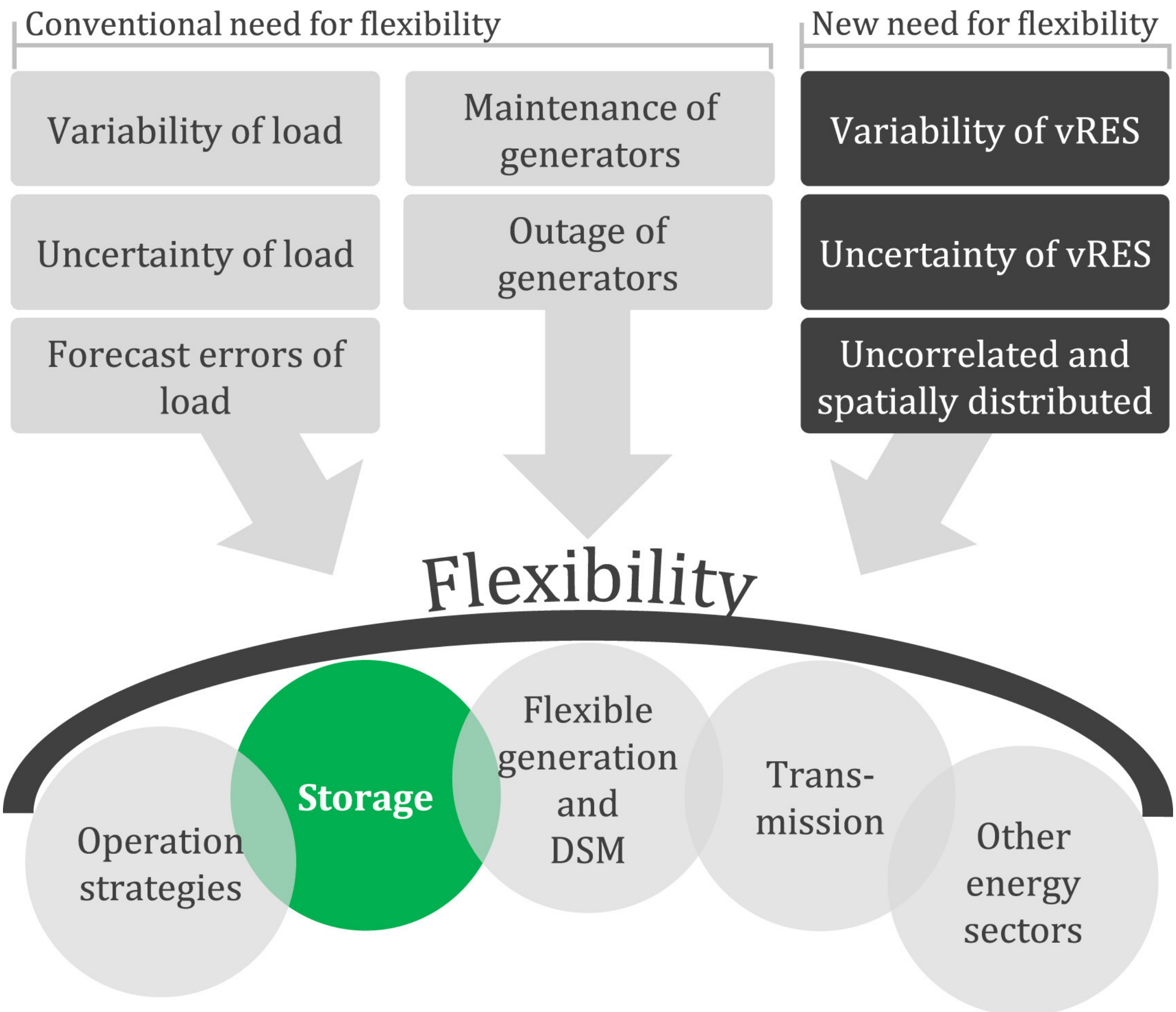


Figure 2.1: Traditional and new need for flexibility in energy systems [20]

2.2. Flexibility measures

Having established that increased VRE necessitates additional system flexibility, we will delineate various flexibility measures from the literature and connect them to storage and energy system modeling. However, before defining the technologies that can induce flexibility in an energy system, flexibility itself needs to be defined in the context of an energy system. No one definition defines the concept. In this work, the definition of flexibility is based on the work by Papaefthymiou and Dragoon (2016). They define flexibility as the capability of adjustable power system components to generate or consume power at varying rates, across different periods, and in response to diverse conditions within the power system [40].

2.2.1. Grid expansion

The first flexibility measure to be discussed is the expansion of the electricity grid. Expanding and interconnecting grids across regions and time zones plays a crucial role in balancing supply and demand more effectively. For instance, when one region faces high demand, another may have excess generation capacity, which can be shared through these interconnected grids. This geographical and temporal diversity helps smooth out the variability of VREs, reducing the overall reliance on storage.

Studies have also explored the role of energy storage in grid support and congestion management [38]. ESSs can alleviate grid congestion by absorbing excess energy, thereby reducing the need to transport power over long distances. This not only stabilizes the grid but also enhances its capacity to integrate higher levels of VREs like wind and solar power. By acting as a buffer, ESS can minimize the need for costly grid upgrades and improve overall grid reliability.

When combined, grid expansion and energy storage can significantly mitigate the mismatch between supply and demand, amplifying the benefits of each approach [38].

2.2.2. Demand-Side management

Demand-side management (DSM) involves incentivizing consumers to Demand-side management (DSM) involves incentivizing consumers to adjust their energy usage behavior. DSM can significantly balance supply and demand by shifting energy use from peak to off-peak periods. Time-of-use pricing and demand response programs encourage this shift, helping consumers align their usage with grid needs [20].

Research highlights the positive impact of DSM on integrating variable renewable energy (VRE). By aligning demand patterns with the supply patterns of VRE, DSM allows energy to be used directly as it is generated, reducing the need for storage or other intermediary steps [45].

A key benefit of DSM is that it allows for the direct use of VRE without the need for inefficient energy transformation or storage. By smoothing the demand curve, DSM shifts energy use to periods of high renewable generation or low overall demand, effectively reducing peaks and filling troughs. For instance, during high solar generation in the middle of the day, DSM can encourage activities like charging electric vehicles or running industrial processes. Conversely, it can reduce energy usage through automated processes during periods of low VRE supply.

2.2.3. Flexible generation Technologies

Flexible generation refers to power plants that can rapidly adjust their output up or down as needed [20]. This capability is useful for filling the gaps in supply caused by fluctuations in VRE output. Additionally, gas turbines can operate steadily at partial loads, which can help with grid stability. A range of fuels can be used for flexible generators, most prominently in gas form. This gas can be fossil, biomass-based, or synthetic methane. The technologies include more traditional thermal power plants and advanced technologies like combined cycle gas turbines (CCGT). CCGT offers high efficiencies and faster response time compared to traditional generation[25]. Furthermore, flexible gas turbines can use synthetic gas created via sector coupling, creating a new incentive to increase the installed capacity of this sector coupling.

Research indicates that a diverse mix of flexible generations can benefit system flexibility. A diverse mix gives many degrees of freedom to find a fitting mix of generations to fill the gaps left by VRE, adding to grid stability and reliability [16].

2.2.4. Sector coupling

Sector coupling involves integrating different energy sectors, such as electricity, heating, and transportation, to improve overall system efficiency and flexibility. A type of sector coupling that is already widely utilized is power-to-heat. The power sector is effectively coupled to the heating network via heat pumps and electric boilers. The heat can be stored or used directly for residential or industrial purposes[48].

Another concept that has been gaining traction is power-to-gas. The technologies that fall under the category of power-to-gas use excess renewable energy to synthesize gasses. Usually, hydrogen is created via electrolysis, which can be used as an energy carrier or fuel. With hydrogen, a range of hydrocarbons can be made using $\mathrm{CO_2}$. Gasses like methane can be stored in the existing gas infrastructure, possibly reducing the overall cost of the synthesis[6].

Both power-to-heat and power-to-gas can absorb excess electricity, decreasing storage needs. However, the two concepts are interlinked, with sector coupling and storage often utilizing hydrogen.

2.3. Storage

2.3.1. Integration of storage

This section will delineate the implications of the differences between short-term and long-term energy storage. Furthermore, technologies that can represent the two types of storage are identified.

Short-term storage (STS) technologies primarily operate on a daily scale. Therefore, they often store relatively small energy levels compared to long-term storage. The technologies usually have fast response times and can discharge the stored energy quickly. Managing daily fluctuations means these storage technologies must be discharged and charged multiple times daily, allowing them to benefit from high efficiencies [29].

Long-term storage technologies (LTS) are designed to address seasonal energy supply and demand variations. These technologies store energy over extended periods, ranging from weeks to several months, requiring larger installations to store high amounts of energy. The technologies used for LTS are often less efficient than those used for STS storage. This trend of having highly efficient but lower energy capacity technologies for STS and lower efficiency but higher energy capacity technologies for LTS emerges from the literature [26].

Finding the balance between integrating short-term and long-term storage technologies optimizes the energy system's resilience. As renewable energy penetration increases, the need for both types of storage becomes increasingly important.

2.3.2. Short-Term Storage Technologies

Batteries

Batteries have high efficiency, rapid response times, and are geographically independent[59]. The type of battery that has been labeled as having the most potential to be used on a utility scale is lithium-ion batteries. These batteries have round-trip efficiencies that can reach up to 90%, making them a good fit with the need for frequent cycling[45].

The cost of batteries is declining steadily. This decline can be attributed to the economies of scale in production and the experience of lithium-ion production as everyday batteries. However, uncertainties remain concerning the lifespan and degradation, which could impact the investment incentives [16].

Flywheels and Capacitors

Batteries are not the only technology that can be used for STS. Flywheels and capacitors, with their unique characteristics, have the potential to add to the system's flexibility. Flywheels can store rotational kinetic energy and have high power density. Due to the rotational energy, flywheels can deliver power almost instantaneously, which could help with frequency control in the grid. Limitations include the low energy capacity capacity and high self-discharge rates [1].

Capacitors store energy electrostatically and can charge and discharge fast. They offer high efficiency and relatively high power density. However, the low energy density makes them less suitable on a utility scale [45].

2.3.3. Long-Term Storage Technologies

Hydrogen Storage

Hydrogen storage has the advantage of large-scale capacity. This is reached by storing hydrogen in salt caverns or designated tanks, which are pressurized to increase energy density. Large installations entail that high amounts of overproduction energy can be stored via hydrogen. However, the efficiencies are low due to the many processes needed to create, store, and reverse the hydrogen back to electricity. New infrastructure development is also required, which adds to the overall cost[60].

Pumped Hydro Storage and Compressed Air Energy Storage

Pumped hydro storage (PHS) involves storing energy by pumping water from a lower reservoir to a higher one during periods of excess energy supply. When power is needed, the water is released, driving turbines of different sizes to generate electricity. Creating multiple-sized turbines allows PHS to output at different rated powers, adding flexibility. Additionally, PHS has a high efficiency. The disadvantage of PHS is that the technology is geographically dependent and can influence ecosystems on location. Therefore, the increase in hydro-based energy is questioned in the literature [2].

CAES operates on a similar principle but uses compressed air stored in underground caverns. The stored air is released to drive turbines when electricity is needed. CAES offers lower geographical constraints than PHS, although it typically has lower efficiency and higher operational costs [5].

Molten Salts and Other Seasonal Storage Options

Emerging long-term storage technologies, such as molten salts, are gaining attention for their ability to store thermal energy for extended periods. Molten salt storage, commonly used in concentrated solar power (CSP) plants, stores heat from solar energy in molten salts, which can later produce steam and generate electricity [7].

In summary, integrating short-term and long-term storage technologies is essential for managing the variability and uncertainty associated with high levels of VRE penetration. Each technology offers unique advantages and challenges, necessitating a strategic approach when selecting and implementing the optimal mix of storage solutions based on the specific needs of the energy system [51].

2.4. Technology selection in energy modeling

The debate about the cost competitiveness of VRE technologies is leading to a strategy of waiting for a 'unicorn technology' to appear. This waiting strategy can lead to cost increases of the transition of 61% [22]. Therefore, the modeling of future energy systems should rely as much as possible on proven technologies. This has been one of the starting points of the Sector Coupled Calliope model. Therefore, the choice was not to add new storage of flexibility measures identified in the literature not represented in Calliope.

2.5. Implications for energy modeling

The findings discussed in this chapter highlight the need for energy models to incorporate diverse flexibility measures and storage technologies to accurately reflect the demands of systems with high levels of VRE. As the integration of VREs continues to grow, energy models must evolve to account for the complex interplay between short-term and long-term storage solutions, grid expansion, demand-side management, flexible generation, and sector coupling. These elements are essential for capturing the total flexibility required to maintain grid stability and reliability. Furthermore, the ability to simulate various flexibility strategies and storage technologies within energy models will provide valuable insights into optimal configurations for future energy systems. This approach will enable more informed policy decisions and investment strategies, facilitating a smoother transition to renewable energy. By addressing the challenges of spatial and temporal resolution, lifetime and efficiency dynamics, and cross-sectoral integration, energy models can offer a more comprehensive framework for understanding and optimizing the role of flexibility in energy systems.

3

Methods and data

This chapter will describe the research methods and the utilized data. Section 3.1 delineates the data used. Section 3.2 shows the method of combining the data. After that, the method of comparing WITCH and Calliope will be described in 3.4. Section 3.6 shows the process of calculating flexibility costs in the system. Lastly, the method of constructing the WITCH module is described.

3.1. Data

In this section, we will describe the methods for utilizing the output of the Calliope framework. Although the generation of SPORES is not part of this thesis's research, we will first explain this process. Understanding how these spores are generated is essential for comprehending the subsequent discussions and analyses presented in this work.

3.1.1. Method of using the SPORES for this thesis

Calliope is a versatile, multi-scale energy system modeling framework for linear optimization. The framework can manage and optimize various energy technologies and systems, including renewable energy sources, storage technologies, and conventional power plants.

The model can run on different scales, making it a valuable tool for analyzing policy interventions or strategies under different scenarios[9]. The high spatial and temporal resolution allows for analyzing detailed technology characteristics and inter-technology dynamics. However, due to cost optimization, the output of the energy system model is often one configuration of the energy system. The probability that this exact energy system still aligns with the policy goals or other exogenous factors that are not modeled is slim. Therefore, the construction of the SPORES was developed. These SPORES results can offer configurations more aligned with political, social, and environmental topics [42]. This range of configurations allows us to find data points aligning with WITCH's assumptions. Additionally, the must-haves in the system can be found and translated into WITCH.

3.1.2. SPORE Generation Algorithm

The SPORES generation algorithm is based on an iterative process where the configurations are changed while meeting the constraints imposed on the optimizations. The algorithm systematically changes the parameters of the base model to find these alternative configurations. The parameter that are changed consists, amongst other, of generation capacity, storage options, and grid expansion. This creates a new optimization problem that is solved using Calliope's linear programming capabilities. The process starts with a base scenario representing the optimal energy system configuration. The algorithm then minimizes one or more parameters to create a new scenario. The optimization of the new scenario is compared to the base case scenario to check whether the costs are within the predefined percentage from the base case. The process is repeated iteratively, with each new scenario building on the results of previous iterations, until the configuration approaches a near-optimal solution [43]. The SPORES used in this work represent model runs that deviate by 10% from the cost-optimal scenario.

3.1.3. 2030 and 2050 runs

In this work, two clusters of SPORES will be used to parameterize flexibility needs. The first cluster focuses on the predicted energy system for 2030, where the modelers anticipated an increase in variable renewable energy (VRE) compared to the current European energy system. However, carbon neutrality is not expected to be achieved by this time. The 2030 dataset is based on a short-term projection of changes to the energy system, including expected demand growth rates, VRE growth rates, increased hydrogen utilization, and low levels of sector coupling. This dataset is useful for finding pathways in the early years of the transition to VRE in WITCH.

The second cluster represents the 2050 energy system, which is required to be carbon neutral. This carbon neutrality is attained by implementing high levels of VRE and phasing out most carbon-intensive generation sources. The 2050 dataset assumes carbon neutrality by 2050, necessitating a strong increase in VRE penetration to align with climate goals. Although it encompasses ambitious goals, efficiencies are scaled to expected values in both generation and utilization. Thus, the 2050 scenarios are designed to explore pathways to deep decarbonization and large-scale energy system transformation.

In both clusters, demand is calculated based on specific changes in electrification within certain sectors, while demand for other sectors is based on 2018 data. These two datasets differ significantly in their assumptions and configurations, providing insights into the relationship between VRE and flexibility across different timelines.

3.2. Combining the data

The difference in VRE penetration between the 2030 and 2050 model runs is crucial for quantifying the relationship between the VRE levels and the flexibility needed. The datasets will be systematically compared to find correlations between the level of VRE technologies in the system and the identified flexibility measures from Chapter 2. The two data frames are generally consistent in the types of flexibility technologies utilized.

3.3. Flexibility measures aggregation

The next step involved using the categories provided by the literature review in Chapter 2 to quantify the flexibility measures in the Sector Coupled Calliope SPORES. The storage categorization has already been made in Calliope. Transmission expansion was also explicitly modeled in the 2050 runs. However, in the 2030 runs, the transmission grid was kept at the same level. Demand response was modeled by using electric vehicles (EV). The bidirectional flow of EVs was used to enable dynamic charging and discharging of the cars. The choice was made to use the level of total capacity of the batteries of EVs as a measure of the flexibility provided by demand response. Calliope modeled both light transport and heavy-duty vehicles. The assumption was made that heavy-duty cars can not be used for dynamic charging and discharging as they have a more constant daily utilization rate. Flexible generation was represented by combined cycle gas turbines (CCGT) and combined heat and power (CHP) turbines. The capacity of these turbines was aggregated under the variable flexible generation. Hydropower was modeled as a constant in Calliope; no further expansion was assumed compared to the current level.

The Sector-coupled Calliope model allows for a multitude of mechanisms for sector coupling. Therefore, the choice was made not to represent sector coupling in one variable but to make the separation between heating and cooking sector coupling and transport sector coupling. The names of the types of sector coupling relate to the sector the energy carrier will be used in. Synthetic- and biofuel-based methane is the primary component of the heating and cooking variable, and biofuel- and synthetic liquids for the transport sector coupling.

The aggregation overview for the flexibility measures is visualized in Table 5.1.

Table 3.1: Categories and Technologies

Category	**Technologies**
Storage	Battery
	Pumped hydro
	Hydrogen storage
	Methane storage
Transmission	AC transmission
	DC transmission
EV Penetration	Light transport EV
Flexible Technologies	CCGT (electricity)
	CHP biofuel extraction (electricity)
	CHP methane extraction (electricity)
	CHP WTE back pressure (electricity)
Hydropower	Hydro run of river
	Hydro reservoir
Heating & Cooking Sector Coupling	Hydrogen to methane
	CHP biofuel extraction (heat)
	CHP methane extraction (heat)
	CHP WTE back pressure (heat)
	Biofuel to methane
Transport Sector Coupling	Biofuel to liquids (diesel)
	Biofuel to liquids (kerosene)
	Hydrogen to liquids (kerosene)
	Biofuel to diesel
	Hydrogen to liquids (diesel)

3.4. Comparing the models

The flexibility technologies identified in the literature are all present in the sector-coupled Euro-Calliope model. To couple the flexibility requirements between the Euro-Calliope and WITCH models, these technologies must also be represented in WITCH. The next step in this coupling process is mapping the flexibility variables between Calliope and WITCH. If any variables are missing, they will be modeled as dummy variables with associated costs. These dummy variables help refine the cost estimates related to flexibility. However, they do not capture the specific dynamics and interactions with other variables in the model when used in this way.

3.4.1. Scaling of the data

The technologies that comprise the flexibility measures are summed to get the total value of flexibility in the category. The resulting data frame is the primary input for constructing the model to predict flexibility. The aim of the model is to predict the absolute level of flexibility in the system based on the level of VRE in the European energy system. Due to different assumptions of the models on the ability to use and transform primary energy from wind and solar throughout all the demand sectors, the maximum level of VRE was significantly different. Therefore, the data had to be scaled. Scaling the data involved finding the maximum level of absolute VRE penetration in the two models. After that, the flexibility measures were scaled proportionally to the decrease in absolute VRE penetration. The maximum level of VRE capacity is 6 TW and 2.15 TW for Calliope and WITCH, respectively. Therefore, the data was scaled with a factor of 2.8. This allowed the use of the whole spectrum of SPORES instead of only using the runs of 2030, where the absolute penetration of VRE was comparable to the maximum level of VRE in

WITCH throughout all the years.

3.5. Constructing the regression

The scaled data on flexibility and the VRE technologies will provide the model input for predicting the flexibility level. The choice was made to create a linear regression model of the VRE and flexibility, which aims to predict the total level of flexibility. Therefore, the values of all the flexibility variables are summed to create a new variable: total flexibility (i.e. total installed capacity of flexibility in the European energy system). The expectation is that, with the increase in VRE, the total level of flexibility will also increase to deal with VRE's inherently site-specific, variable, and uncertain nature.

3.5.1. Filling in the regression

With the linear regression, we can predict the total flexibility. The specific distribution of the flexibility measures can be calculated from the total flexibility. The following steps can summarize this process.

1. **Linear Interpolation:** A linear interpolation of the existing data created a continuous range of values. This step ensures that the analysis covers the entire range of possible VRE penetration levels, even those not explicitly present in the initial dataset.
2. **Create Bins and Calculate Average Levels:** Nine equal-width bins were created for the predicted total flexibility. Each bin represents a specific range of predicted flexibility levels, allowing for grouping energy systems with similar flexibility requirements. The average level of each flexibility option within each bin was calculated. This aggregation provides insights into the typical composition of flexibility measures for different levels of VRE penetration.

This structure should provide a model where the VRE penetration from WITCH can be the input. After that, the bin associated with that specific level of VRE can be assigned. With the bin, the distribution of the flexibility measures within the total flexibility prediction can be allocated.

3.6. Constructing the levelized costs

When the prediction model of flexibility needed in the system is constructed, the next step is determining the costs of implementing flexibility. Where possible, these costs will be derived from the cost parameters provided by the Calliope output data. This section will outline the method for calculating the costs of various flexibility measures by aggregating cost parameters and transforming them into other units where needed. The cost calculation for flexibility measures includes three main components:

1. Capital Expenditure (CAPEX): The initial investment required to deploy the technology.
2. Operational Expenditure (OPEX): Annual costs associated with operating and maintaining the technology.
3. Efficiency: The technology's efficiency affects the total output and operational costs.

Levelized Cost of Energy and Levelized Cost of Storage: The LCOE and LCOS are the standard cost parameters to compare the costs of technologies over their lifetime [56]. It represents the per-unit cost (e.g., EUR/kWh) of building and operating a generating plant over its assumed lifetime. The formulas for calculating LCOE are:

$$\text{Annualized\_Capex} = \text{capex} \times \frac{\text{discount\_rate} \times (1 + \text{discount\_rate})^{\text{lifetime}}}{(1 + \text{discount\_rate})^{\text{lifetime}} - 1} \tag{3.1}$$

$$\begin{aligned} \text{Total\_Annual\_Costs} = {} & \text{Annualized\_Capex} + \text{om\_annual} \\ & + (\text{om\_prod} \times \text{efficiency} \times \text{hours\_per\_year}) \end{aligned} \tag{3.2}$$

$$\text{Total\_Energy\_Production} = \text{efficiency} \times \text{hours\_per\_year} \times \text{lifetime} \tag{3.3}$$

$$\text{LCOS} = \frac{\text{Total\_Annual\_Costs}}{\text{Total\_Energy\_Production}} \tag{3.4}$$

For storage technologies, we will define the CAPEX, OPEX, round-trip efficiency, and lifetime for battery storage, pumped hydro storage, hydrogen electricity storage, and hydrogen storage. Using the equations 3.1, 3.2, 3.3, and 3.4, the LCOS will be calculated.

The approach for calculating the cost of conversion technologies resembles that of storage costs, with some key differences. The LCOE for each conversion technology will be computed using one-way efficiency over the entire process chain rather than round-trip efficiency. Conversion costs are based on transforming electricity or raw biomass into fuels, considering only the efficiency of fuel creation, as these fuels are used directly without further conversion.

An analysis of Direct Air Capture (DAC) will also be conducted. The parameters for DAC will be defined, and the associated costs will be calculated in Euro per kilogram. Since various conversion technologies depend on DAC to varying degrees, the specific amount of carbon required to produce one kWh of fuel will be used to determine these costs.

Additional efficiencies and costs are associated with combined technologies, as they are not standalone processes. For example, creating synthetic methane involves hydrogen production and direct air capture of CO_2, with these costs added to the concept of synthetic hydrogen. Hydrogen storage is the only combined technology in the storage category, involving both synthesis and storage facility creation, increasing costs.

Transmission costs are calculated by the leveled cost of expansion and O&M costs. The alternating current (AC) and direct current (DC) costs are aggregated into one value using the formula:

$$\text{Levelized Transmission Cost} = \frac{\text{Total Investment Cost} + \text{Total O\&M Cost}}{\text{Total Energy Transmitted}}$$

Where:

$$\text{Total Energy Transmitted} = \text{Energy Cap Max} \times 8760 \times \text{Lifetime}$$

$$\begin{aligned}\text{Total O\&M Cost} = {} & \text{O\&M Annual Investment Fraction} \\ & \times \text{Total Energy Transmitted} \\ & \times \text{Levelized Cost per MWh}\end{aligned}$$

Finally, the levelized costs are calculated in EUR/kWh and then converted to T$/TWh to match the scale used in WITCH.

3.7. Weighted Average of the Costs

The decision was made not to model each new technology separately in WITCH. Instead, parameters from Calliope were incorporated into WITCH using dummy variables to represent additional flexibility costs. Costs were calculated for individual technologies, while flexibility levels were predicted for broader technology clusters, such as *storage* and *heating and cooking sector coupling*. Therefore, the choice was made to aggregate costs using a weighted average of the individual technologies within each flexibility measure.

3.7.1. Calculation of Weights

Weights for each technology were calculated by dividing its capacity by the total capacity of the relevant group. For example, the total capacity of heating and cooking technologies was computed, and the capacity of each technology within this group was divided by this total to obtain weights. These weights represent each technology's relative importance or contribution within its group.

3.7.2. Calculating Weighted Average costs

The weighted average cost for each group was calculated by multiplying the LCOS of each technology by its normalized weight and then summing these values. This method ensures that the calculated LCOS reflects the contributions of each technology proportionately.

3.8. Finding the pathway of flexibility integration

The WITCH model represents the interaction between the climate, energy, and economic systems. This is crucial for understanding and addressing the multifaceted challenges of climate change, especially concerning the large-scale integration of variable renewable energy (VRE) technologies [55].

Due to this transitional nature of the WITCH model, the data from Calliope will have to be translated into interactions over time. Calliope provides data from an optimization of one year in the future. We have data from 2030 and 2050, enabling us to see the temporal aspect of flexibility. This change over time, in combination with the parameterization of flexibility based on specific configurations of the energy system, enables us to translate the data to WITCH.

Therefore, the next step in the modeling phase will be to map the variables between the two models to understand the differences in their representations of the energy system. Variables represented in both models can be used to parameterize the system's flexibility needs. Variables from Calliope that are missing will have to be added to WITCH with their associated costs. Additionally, the variables used in both models will be compared to the units and their levels. When units are different, they will be corrected. When the value of flexibility variables in WITCH exceeds the levels in Calliope, they must be fixed to ensure compatibility between the findings in Calliope and the interactions in WITCH.

Once the variables of the models are synthesized, the interactions from Calliope can be programmed into a new module in WITCH. This module aims to use the energy system's configuration at each timestep to calculate the required level of flexibility while considering the present level of flexibility. Based on the cost calculations, this will result in additional costs while enabling the model to reach higher shares of VRE.

The cost parameters obtained from Calliope are based on 2050 predictions. These costs are not expected to remain constant over time [49]. Therefore, a cost reduction function must be included in the data.

3.9. Integration of the flexibility dynamics into WITCH

In this section, the interactions of flexibility and VRE will be integrated mathematically to incorporate them into WITCH. The units in WITCH and Calliope are consistent, so there is no need to transform the data to other units. The parameters from Calliope are loaded into WITCH, and the interactions with the endogenous variables were constructed via equations. The equations aim to calculate the total flexibility needed in the system at every timestep (t) and for every region (n).

The first step is to calculate the absolute VRE penetration by summing the installed capacity of the wind and solar technologies. This equation is visualized in 3.5.

$$\begin{aligned}\text{VRE\_PENETRATION}(t,n) = &\ K\_EN.l(\text{'elpv'}, t, n) + K\_EN.l(\text{'elwindon'}, t, n) \\ &+ K\_EN.l(\text{'elwindoff'}, t, n)\end{aligned} \tag{3.5}$$

Where:

$$\begin{aligned}
\text{VRE_PENETRATION}(t,n) &= \text{The total penetration of Variable Renewable Energy (VRE) at time } t \\
&\quad \text{and region } n. \\
K_EN.l(\text{'elpv'},t,n) &= \text{The installed capacity of photovoltaic solar energy (PV) at time } t \\
&\quad \text{and region } n. \\
K_EN.l(\text{'elwindon'},t,n) &= \text{The installed capacity of onshore wind energy at time } t \\
&\quad \text{and region } n. \\
K_EN.l(\text{'elwindoff'},t,n) &= \text{The installed capacity of offshore wind energy at time } t \\
&\quad \text{and region } n.
\end{aligned}$$

With the VRE penetration, we can predict the level of flexibility needed in the system at every t and n. This equation is given in 3.6

$$\text{K\_EN\_FLEX}(t,n) = 0.70 + 1.44 * \text{VRE\_PENETRATION}(t,n) \tag{3.6}$$

Where:

$$\begin{aligned}
\text{K_EN_FLEX}(t,n) &= \text{The estimated flexibility requirement at time } t \text{ and region } n. \\
\text{VRE_PENETRATION}(t,n) &= \text{The total penetration of Variable Renewable Energy (VRE) at time } t \\
&\quad \text{and region } n. \\
0.70 &= \text{A constant term representing the baseline flexibility requirement.} \\
1.44 &= \text{A coefficient that scales the flexibility requirement based on the level of} \\
&\quad \text{VRE penetration.}
\end{aligned}$$

The K_EN_FLEX variable represents the total flexibility needed in the system relative to demand. This flexibility is modeled as a variable rather than a parameter, allowing the WITCH solver to optimize it. This approach models the trade-offs between increasing VRE penetration, which requires additional flexibility, and opting for a higher carbon capture and storage (CCS) to achieve carbon neutrality. The solver balances the costs of adding flexibility with the costs and benefits of CCS, enabling a more efficient path to carbon neutrality.

The K_EN_FLEX variable holds the predicted level of flexibility. The next step is to find the flexibility bin that is associated with the level of K_EN_FLEX at that timestep and in that region. This process is modeled by iteratively checking if the value is lower than the outer value of the flexibility bins. Starting from the lowest bin up towards the highest bin. After that, the flexibility variables can be given a value based on the bin. This process is modeled via the following loop:

$$\begin{gathered}
\text{For each } v \in \text{FlexVars}: \\
\text{For each } (t,n): \\
\text{For each } b \in \text{FlexBin}: \\
\text{If } K_{\text{EN_FLEX}}(t,n) \leq \text{OuterValue}(b), \\
\text{then } k_{\text{en_flex_dist}}(v,t,n) = \text{Allocation}(v,b),
\end{gathered}$$

Where:

$$\begin{aligned} v &: \text{Flexibility variable being looped over.} \\ (t, n) &: \text{The time } t \text{ and region } n \text{ being evaluated.} \\ b &: \text{The current flexibility bin.} \\ K_{\text{EN\_FLEX}}(t, n) &: \text{The estimated flexibility requirement at time } t \text{ and region } n. \\ \text{OuterValue}(b) &: \text{The upper bound of the flexibility bin } b. \\ k_{\text{en\_flex\_dist}}(v, t, n) &: \text{The distribution of the flexibility variable } v \text{ at time } t \text{ and region } n. \\ \text{Allocation}(v, b) &: \text{The allocation of flexibility variable } v \text{ based on the flexibility bin } b. \end{aligned}$$

Within the k_en_flex_dist parameter, the predicted levels of flexibility at t and n are held. The difference between the values of the level of the existing flexibility variables in WITCH and the values found in the new module can then be calculated via the equations given in 3.7, 3.8, 3.9.

$$\Delta\text{K\_EN\_FG}(t, n) = \text{k\_en\_flex\_dist}(\text{'flexible\_techs'}, t, n) - \sum_{\text{jel\_firm}} \text{K\_EN.l}(\text{jel\_firm}, t, n) \tag{3.7}$$

Where:

$$\begin{aligned} k\_en\_flex\_dist(\text{'flexible\_techs'}, t, n) &= \text{Total predicted flexible generation capacity needed} \\ K_{\text{EN.l}}(\text{jel\_firm}, t, n) &= \text{Sum of the flexible generators' capacity endogenous to WITCH} \end{aligned}$$

$$\begin{aligned} \Delta\text{Q\_EN\_FEV}(t, n) = \text{Scalar} \times (&\text{k\_en\_flex\_dist}(\text{'ev\_pen'}, t, n) \\ &- (\text{Q\_EN.l}(\text{'edv'}, t, n) + \text{Q\_EN.l}(\text{'plg\_hybrid'}, t, n))) \end{aligned} \tag{3.8}$$

Where:

$$\begin{aligned} \text{Scalar} &= 1000 \\ \text{k\_en\_flex\_dist}(\text{'ev\_pen'}, t, n) &= \text{Total predicted EV battery capacity needed} \\ \text{Q\_EN.l}(\text{'edv'}, t, n) &= \text{Current capacity of electric vehicles} \\ \text{Q\_EN.l}(\text{'plg\_hybrid'}, t, n) &= \text{Current capacity of plug-in hybrid vehicles} \end{aligned}$$

$$\begin{aligned} \Delta\text{K\_EN\_GRID}(t, n) = &(\text{k\_en\_flex\_dist}(\text{'transmission'}, t, n) - \text{k\_en\_flex\_dist}(\text{'transmission'}, t-1, n)) \\ &- (\text{K\_EN\_GRID.l}(t, n) - \text{K\_EN\_GRID.l}(t-1, n)) \end{aligned} \tag{3.9}$$

Where:

$$\begin{aligned} \text{k\_en\_flex\_dist}(\text{'transmission'}, t, n) &= \text{Total predicted transmission capacity needed} \\ \text{K\_EN\_GRID.l}(t, n) &= \text{Current transmission capacity} \end{aligned}$$

The last step in the module was calculating the final costs based on the needed flexibility. To translate the weighted average levelized costs in 2050 to those that can be used as input for the flexibility costs at each t, a function must be fitted to represent a cost reduction. The choice was made to fit a polynomial function to the cost data. The function was fit to have a cost increase three times the level in 2020 compared to 2050 [49]. An overview of the cost reduction can be found in A. The construction of the polynomial is presented in 3.10.

$$\text{cost}(t) = \text{cost}_{2050} \times \left(a + b \times (t - 2050) + c \times (t - 2050)^2\right) \tag{3.10}$$

Where:

$$\begin{aligned}
a &= 1 \\
b &= -0.02 \\
c &= 0.0002 \\
\text{cost}_{2050} &= \text{Cost in the year 2050} \\
t &= \text{Years}
\end{aligned}$$

The final connection is between the predicted installed capacity and the annual energy output of the flexibility measures. When specific utilization data was unavailable, we assumed that the flexibility measures operated at rated power for 2,000 hours per year. For technologies with available utilization data, the power-to-energy ratio was determined based on that data. Using these assumptions and data, the additional flexibility costs were calculated over time using the following equation:

$$\begin{aligned}
&\text{COSTS_FLEX}(t,n) = \\
&\quad \sum_{i \in \mathcal{SC}} \left[k_en_flex_dist(i,t,n) \times \text{p2e_ratio}(i) \times \text{costs}(i,t,n) \right] \\
&\qquad + \sum_{j \in \mathcal{S}} \left[k_en_flex_dist(\text{storage},t,n) \times \text{stor_ratio}(j) \times \text{p2e_ratio}(j) \times \text{costs}(j,t,n) \right] \\
&\qquad + \Delta K_{\text{FG}}(t,n) \times \text{p2e_ratio}(\text{flexible_techs}) \times \text{costs}(\text{flexible_techs},t,n) \\
&\qquad + \Delta Q_{\text{FEV}}(t,n) \times \text{p2e_ratio}(\text{ev_pen}) \times \text{costs}(\text{ev_pen},t,n) \\
&\qquad + \Delta K_{\text{GRID}}(t,n) \times \text{p2e_ratio}(\text{transmission}) \times \text{costs}(\text{transmission},t,n)
\end{aligned} \tag{3.11}$$

Where:

$$\begin{aligned}
\mathcal{SC} &= \text{The set of all sector coupling types.} \\
\mathcal{S} &= \text{The set of all storage types (e.g., batteries, pumped hydro).} \\
k_en_flex_dist(i,t,n) &= \text{The distribution of flexibility variable } i \text{ at time } t \text{ and region } n. \\
\text{p2e_ratio}(i) &= \text{The power-to-energy ratio for flexibility variable } i. \\
\text{costs}(i,t,n) &= \text{The historical costs associated with flexibility variable } i \text{ at time } t \text{ and region } n. \\
\Delta K_{\text{FG}}(t,n) &= \text{The change in capacity of flexible generators at time } t \text{ and region } n. \\
\Delta Q_{\text{FEV}}(t,n) &= \text{The change in capacity of EV batteries at time } t \text{ and region } n. \\
\Delta K_{\text{GRID}}(t,n) &= \text{The change in capacity of grid expansion at time } t \text{ and region } n.
\end{aligned}$$

The process of constructing the final WITCH model from the Calliope data is summarized in figure 3.1.

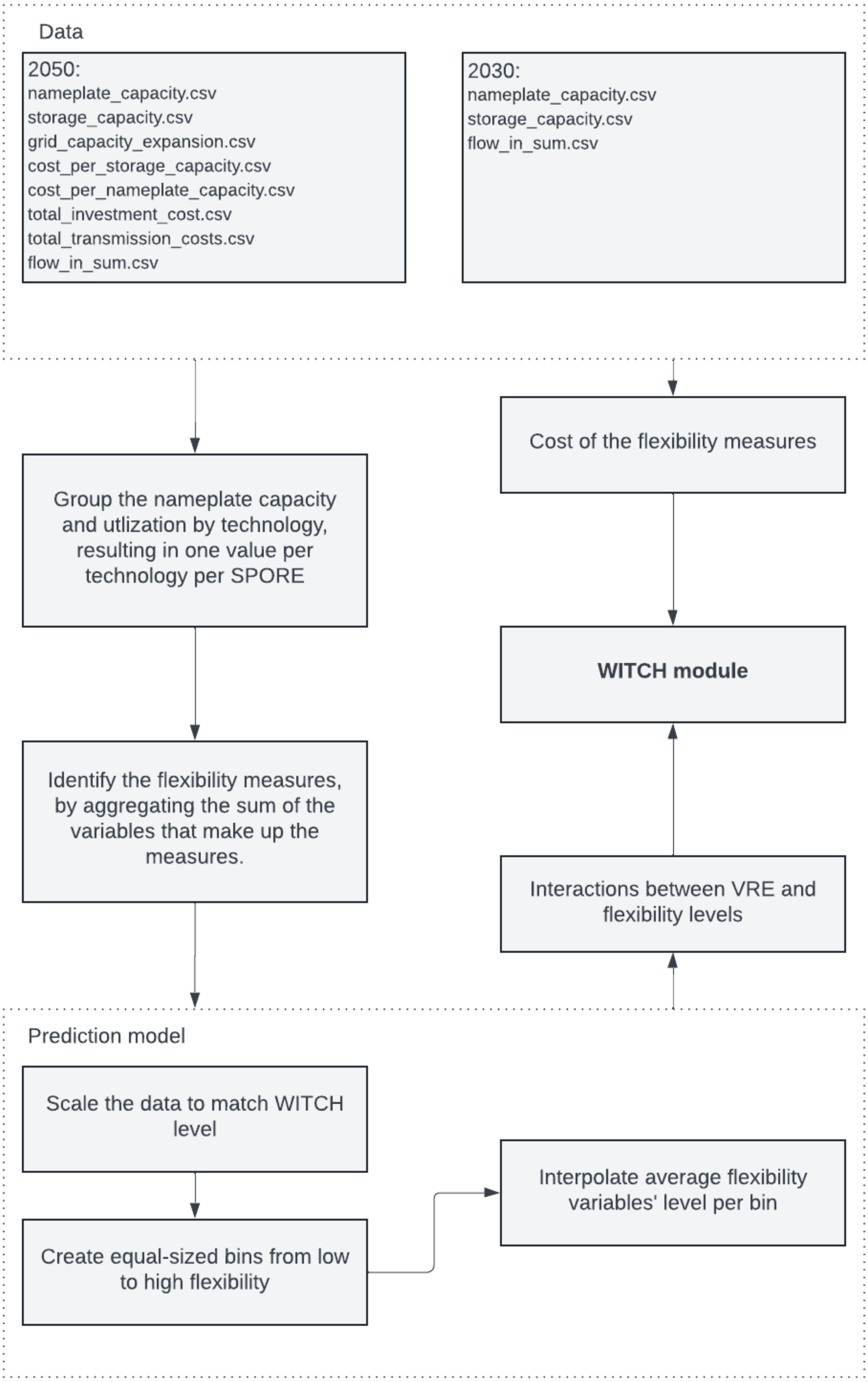


Figure 3.1: Process of mapping Calliope results to WITCH

3.10. Analysis method

The simulations can be run to generate data, with the interactions formalized into equations for WITCH. The WITCH output data will be categorized into economic, environmental, and energy-based results. The analysis will focus on how the new module affects these three categories. Specifically, we will compare the model's output with and without the new interactions. This comparison will highlight the impacts of the enhanced interactions and assess whether the proposed method of linking models provides a more accurate representation of flexibility than the current approach. The analysis will cover the capacity mix for electricity generation to see if the increased level of flexibility influences the total capacity needed and the level of specific capacities of technologies. The generation of electricity will be visualized and compared to the installed capacity. With the inclusion of the new flexibility module, the expectation is that less installed capacity will be needed for the same generation level. The increased level of flexibility could allow for higher levels of generation utilization. This will be tested by plotting the curtailment of the different technologies. Additionally, the differences in primary energy supply in Europe will be analyzed.

These energy system features will be visualized and analyzed under different energy policy scenarios. The WITCH model can simulate various policy scenarios, and this work will focus on two: Business As Usual (BAU) and Carbon Tax (ctax). By running the model under these scenarios, we can test the sensitivity of the new flexibility module to different policies. The model is expected to require higher levels of flexibility under the ctax scenario since the increased use of VRE, driven by the carbon tax, is a primary predictor of flexibility needs.

The code used to plot the variables is available in Appendix B. To ensure readability, some level of aggregation was applied to certain technologies in the visualizations, which slightly reduces the granularity of the WITCH model output.

A sensitivity analysis will also examine how WITCH's current constraints affect the adoption of flexibility measures. This will be done by relaxing the constraints on VRE implementation based on Calliope assumptions. This approach will help identify which constraints limit VRE integration level, which could explain why VRE penetration is lower in WITCH than Calliope.

4 Flexibility modeling results

This chapter presents the results of developing the model to predict the level of flexibility needed in the energy system. Section 4.1 explores the influence of Variable Renewable Energy (VRE) penetration on the system. It discusses how VRE configuration affects the required level of flexibility, focusing on the correlation between VRE penetration and the system's flexibility needs. Section 4.2 presents the results of a comparative analysis between the Calliope and WITCH models. The section includes a detailed examination of the differences in storage capacity, VRE penetration, flexible generation, and EV battery capacity between the models. Section 4.3 presents the regression analysis results used to predict the total level of flexibility needed in the system. The linear relationship between VRE penetration and total flexibility and the regression model's effectiveness in capturing this relationship are discussed. In Section 4.4, the final section analyzes the costs associated with different flexibility measures. The section provides a breakdown of the levelized costs of various technologies and groups, highlighting their significant cost differences.

4.1. Influence of VRE in the system

To construct a more detailed parameterization of flexibility needs in the energy system, the relationship between VRE configuration and the needed level of flexibility needs to be examined. The correlation matrix between the variables in Calliope is provided in A. It can be seen that VRE penetration is a significant contributor to the system's need for flexibility. Moreover, the specific capacity mix of PV and wind installations appear to influence the flexibility, which is consistent with findings in the literature (e.g., [13]; [14]; [3]). However, the 2030 data had a higher average PV level because PV currently makes up a large share of the energy level in Europe. Therefore, when used as a predictor, systems with higher levels of PV tend to predict lower levels of flexibility on average. Consequently, the choice was made to leave it out. Therefore, only VRE penetration was chosen to predict the system's flexibility.

4.1.1. Flexibility distribution in the system

After combining the 2030 and 2050 data, the flexibility measures could be constructed for each SPORE. The results of the levels of the flexibility measures for each SPORE are visualized in 4.1. Visualizing the data in a parallel coordinates plot was chosen to gain insights into the trade-offs between the different flexibility measures. However, as seen in the plot, no clear patterns appear in the data showing when a system needs specific types of flexibility. For example, high levels of PV could result in higher levels of summer over-generation, which could be handled by producing high levels of synthetic fuels. The lack of these clear patterns shows that a robust mix of different types of flexibility generally provides enough total flexibility to allow high VRE penetration. The data clearly distinguishes between the total level of flexibility needed in the system for low and high VRE penetration. The 2030 data points generally show a lower need for flexibility overall than the 2050 data points. The 2050 data points start around the 0.5 normalized VRE penetration in the plot.

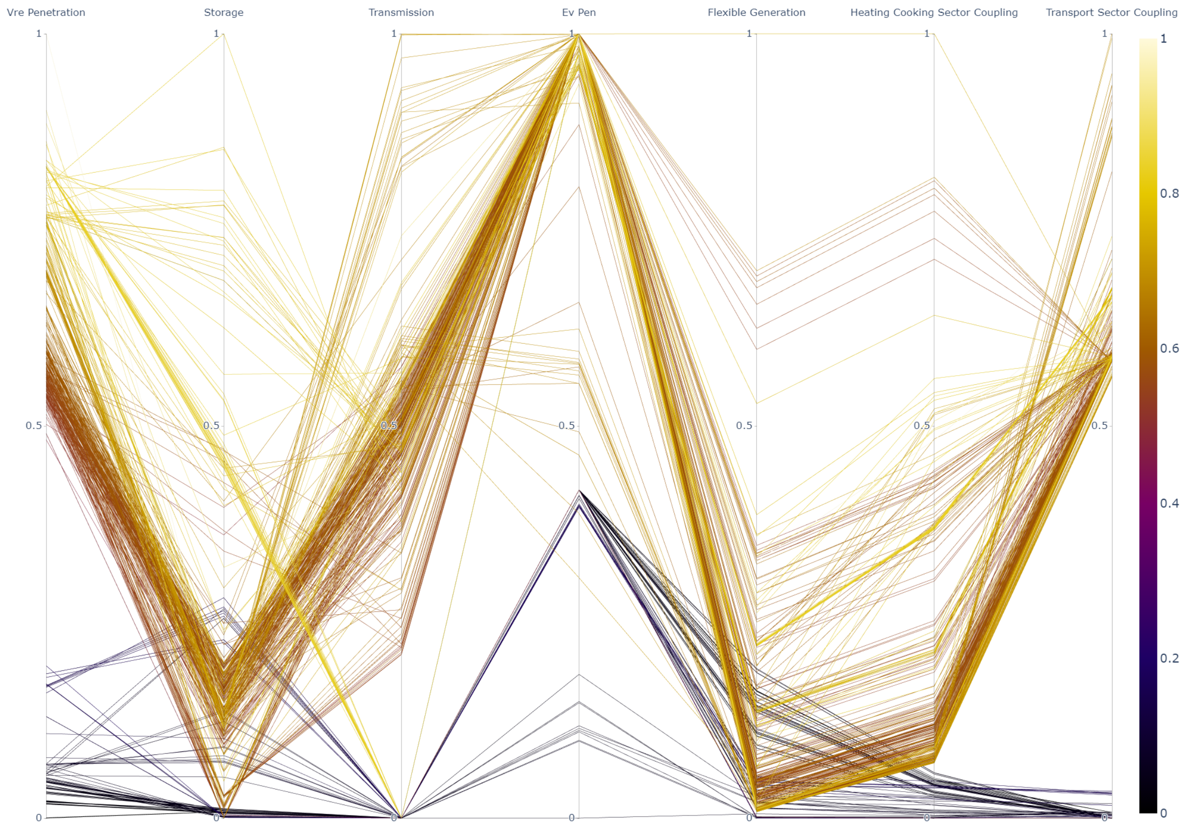


Figure 4.1: Parallel coordinates plot of flexibility variables and the level of VRE penetration

4.2. Comparison of Calliope and WITCH

We conducted a comparative analysis by examining boxplots of various critical variables in the year 2050, which helped us identify significant differences between the models. The Calliope data is based on the 2050 SPORES, and for WITCH, the database is constructed via various pre-run outputs of WITCH under various policy scenarios. The scenarios used for this mapping and the outcomes of the variable mapping can be found in the Appendix B. When a variable's value is higher in WITCH than in Calliope, it may lead to predictions that fall outside the data distribution provided by Calliope. In such cases, the variable is fixed to ensure the results remain robust and can be effectively integrated into the WITCH model.

Firstly, the level of storage capacity is analyzed in Figure 4.2. The value of the storage variable in the WITCH model is substantially lower than in Calliope. These differences can be attributed to the higher spatial and temporal detail incorporated in Calliope. The detailed modeling of the dynamics of the technologies exposes the mismatch between supply and demand, both in time and geographically. This high resolution allows Calliope to capture the variability and intermittency of renewable energy sources accurately. For instance, solar and wind power generation can fluctuate significantly within a day and across seasons, necessitating substantial storage solutions to balance supply and demand consistently.

In contrast, being a more aggregate model, WITCH does not capture these dynamics to the same extent. WITCH focuses on a broader temporal and spatial scope, which does not capture temporal and geographical mismatch to the same extent.

The boxplot comparison of VRE penetration between WITCH and Calliope in Figure 4.2 demonstrates substantial differences in the modeled outcomes, which can be attributed mainly to Calliope's advanced sector coupling capabilities. With its high-resolution modeling and detailed sector coupling, Calliope captures the intricate interactions between various energy sectors: power, heating, transportation, and industry. This integrated approach allows Calliope to optimize the utilization of VRE across these sectors, thereby achieving higher levels of VRE penetration. The model's ability to coordinate the supply and demand across different sectors means that excess renewable energy in one industry can be effectively utilized in another, enhancing overall system flexibility and efficiency. WITCH does not have these capabilities and relies more on gas and oil as primary energy supply for the transport, industry, and residential sectors.

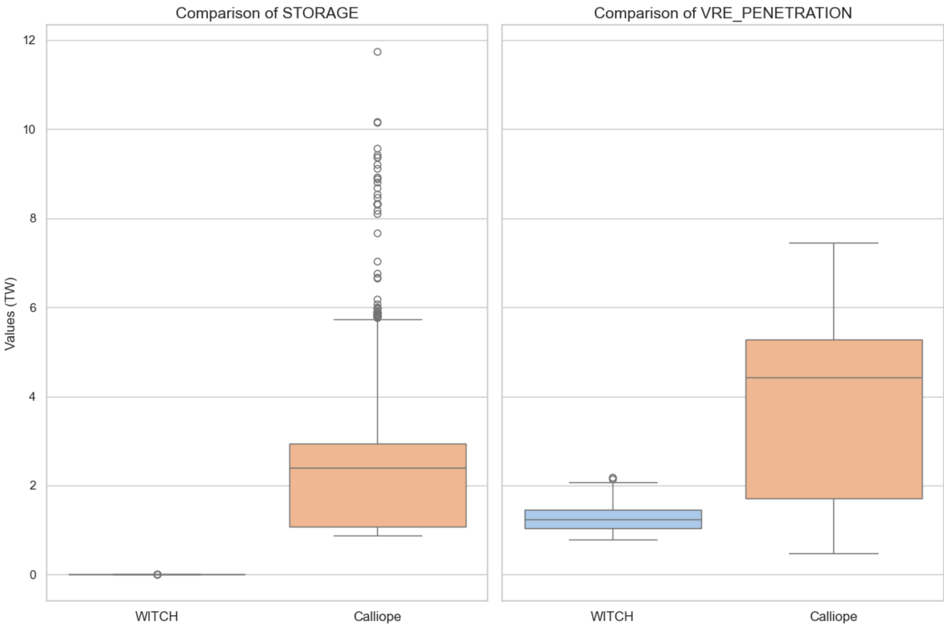
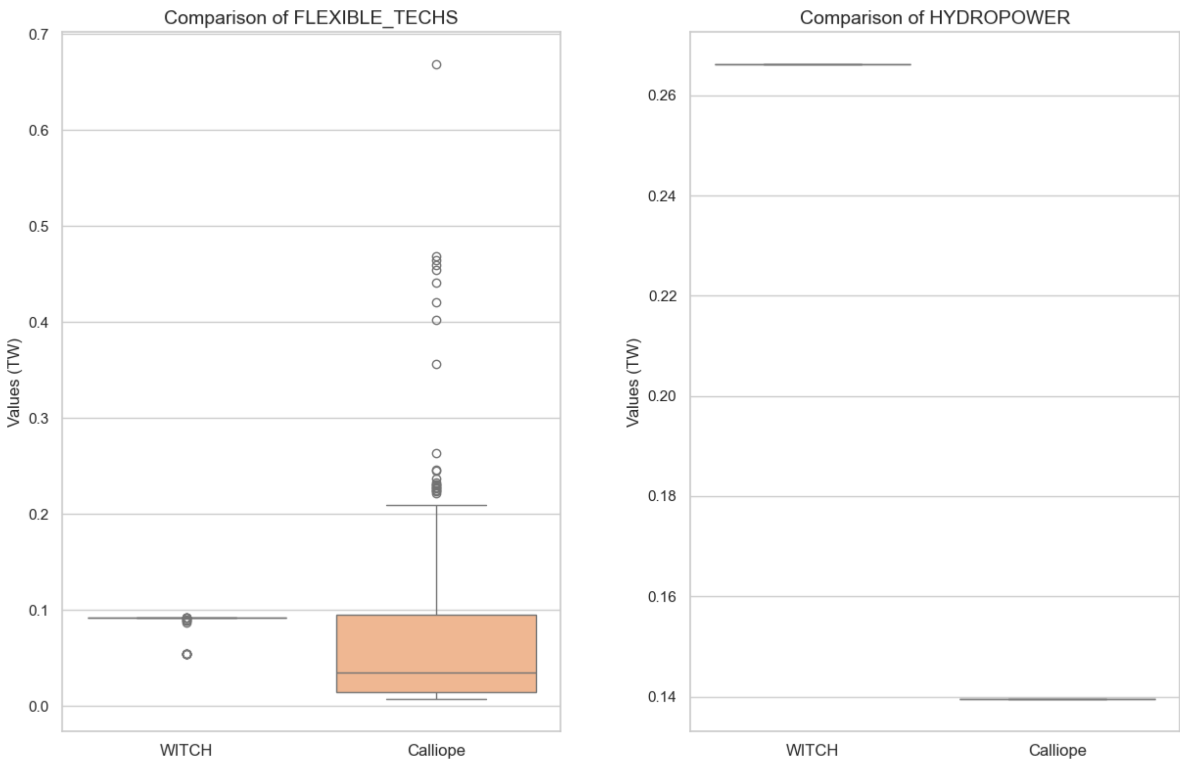


Figure 4.2: VRE penetration and Storage penetration levels in WITCH and Calliope.

Figure 4.3 compares the penetration levels of flexible generation technologies in WITCH and Calliope. The plot shows a more comprehensive range of values in Calliope, indicating greater variability or a broader implementation spectrum of these technologies. In contrast, WITCH displays a more concentrated range of values. However, the mean values in WITCH are higher. Therefore, there will be instances in the model where the level of flexible generation is higher in WITCH than is needed from the Calliope parameterization.

Additionally, Figure 4.3 compares the penetration levels of hydropower in WITCH and Calliope. Both models show a relatively narrow range of values, indicating less variability in hydropower penetration. Hydropower values in WITCH are consistently higher than those assumed in Calliope. Therefore, no additional constraint will be needed to regulate the hydropower capacity in WITCH.



(a) Flexible generation penetration levels in WITCH and Calliope.

(b) Hydropower penetration levels in WITCH and Calliope.

Figure 4.3: Comparison of penetration levels in WITCH and Calliope.

Figure 4.4 compares the total level of EV battery capacity for WITCH and Calliope. Transmission expansion is not compared because the yearly expansion in WITCH cannot be directly compared to the total expansion projected for 2050 in Calliope.

The WITCH model shows lower EV penetration levels with a moderate range of variability. In contrast, Calliope displays a similar level on the lower end of the range but reaches significantly higher values. This indicates that higher EV penetration may be necessary in the system to achieve the required level of flexibility in WITCH.

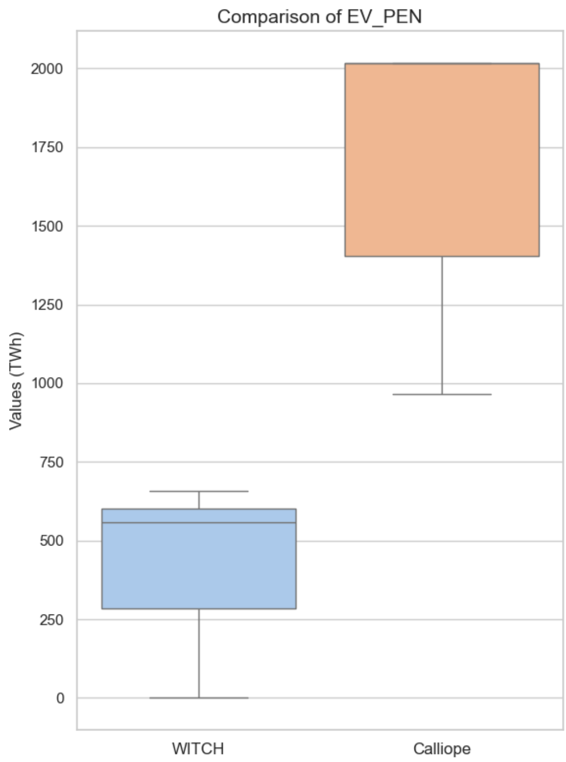


Figure 4.4: EV levels in WITCH and Calliope.

4.3. Regression results

In this section, the results of the model to predict the level of flexibility needed in the system are presented. The data exploration did not clear up the relationship between the configuration of the energy system and flexibility measures. Therefore, the choice was made to examine the flexibility in the system as a whole and deconstruct it afterward. Using the VRE penetration scaled to the WITCH level, we analyzed the system's total necessary level of flexibility. This relationship is illustrated in Figure 4.5, where we plot the total flexibility against this predictor.

The positive linear relationship between VRE penetration and total flexibility becomes evident from the plot. We applied a linear regression model to quantify this relationship. This model is designed to predict the total level of flexibility required in the system based on varying levels of VRE penetration.

The equation governing the relation between total flexibility and VRE penetration is presented below.

$$\text{Predicted Total Flexibility} = \alpha + \beta_1 \times \text{VRE Penetration}$$

Where:
- α is the intercept, which represents the lowest average level of flexibility found in the SPORES
- β_1 is the coefficient for VRE Penetration,

Figure 4.5 shows a noticeable gap in the data due to only using the datasets from 2030 and 2050, leaving 20 years without data. This gap may hide the true nature of the relationship between total flexibility and VRE penetration. Despite this, the data generally suggests a positive correlation, indicating that as VRE penetration increases, so does the need for flexibility. This trend is represented by the red line, which models the expected increase in flexibility. The scatter of data points around this line also highlights the variability in responses to increased VRE penetration, suggesting that flexibility needs may vary widely across different scenarios.

The linear model in Figure 4.5 shows a strong relationship between total flexibility and VRE penetration, with an R^2 value of around 0.7. This means that changes in VRE penetration can explain 70% of total flexibility changes. This result highlights the model's ability to capture the connection between these

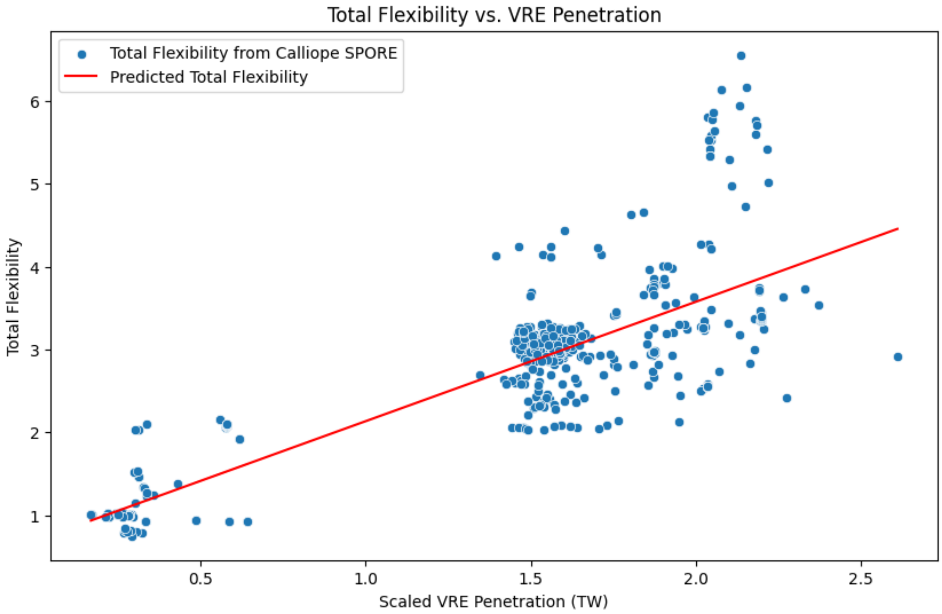


Figure 4.5: Actual and predicted values of total level of flexibility as a function of VRE penetration.

variables, which emphasizes the importance of VRE penetration in predicting flexibility needs. The metrics of the regression can be found in Appendix B.

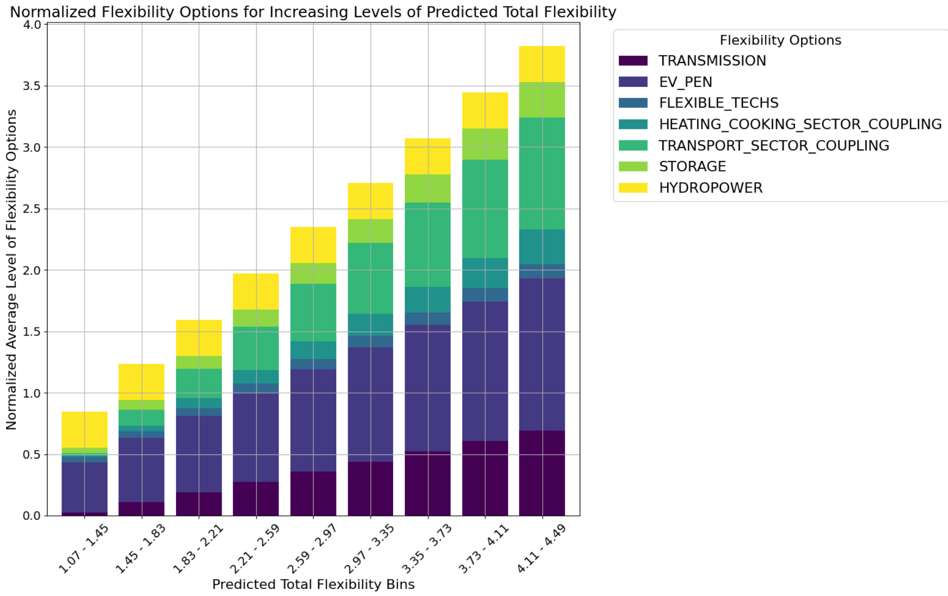


Figure 4.6: Normalized total flexibility bins with the flexibility measures distribution.

The flexibility bins in Figure 4.6 illustrate the increase in total flexibility, indicated by the positive linear relationship observed in the regression. The y-axis shows the normalized level of total flexibility; the x-axis shows the range of the predicted level of flexibility for each box. The value of the predicted level of flexibility is a function of the penetration of VRE. Each bin encapsulates a different distribution of flexibility variables, with hydropower held constant. With this model, we can parameterize the total level of flexibility needed and the specific level for each flexibility measure in WITCH. The values below the bins indicate each bin's total predicted flexibility range. The complete model code can be found in B.

Figure 4.6 shows that the flexibility measures increase relatively proportional to the total flexibility, except for hydropower. The first box indicates a relatively high utilization of hydropower and EV for flexibility. The other measures play a minimal role. The transport sector's coupling and transmission increased strongly in the subsequent bins. These values are normalized. Therefore, this distribution does not represent the actual distribution of flexibility.

Table 4.1: Flex Bin Data with Metrics in TW (EV in TWh)

Flex Bin	Trans- -mission (TW)	EV_PEN (TWh)	Flexible Techs (TW)	Heating/ Cooking Sector (TW)	Transport Sector Coupling (TW)	Storage (TW)	Hydro- -power (TW)
1	0.055	560.002	0.015	0.002	0.002	0.525	0.056
2	0.249	607.513	0.018	0.013	0.015	0.674	0.056
3	0.435	651.065	0.020	0.023	0.027	0.810	0.056
4	0.621	694.617	0.022	0.034	0.040	0.946	0.056
5	0.798	736.190	0.025	0.044	0.052	1.075	0.056
6	0.976	777.763	0.027	0.054	0.064	1.205	0.056
7	1.162	821.315	0.029	0.065	0.076	1.341	0.056
8	1.348	864.867	0.032	0.075	0.089	1.477	0.056
9	1.534	908.419	0.034	0.086	0.101	1.613	0.056

Table 4.1 shows the actual values of the flexibility measures within each bin. The units for each metric are specified as follows: EV Penetration is measured in TWh, while all other metrics are measured in TW. As the bins progress from 1 to 9, most flexibility measures show an increasing trend. This reflects the growing demand for flexibility as VRE penetration increases. Notably, the Hydropower measure remains constant across all bins, indicating a stable contribution from hydropower regardless of the flexibility bin. Additionally, it can be seen that some flexibility measures grow exponentially, like transmission and both the sector coupling categories. Others start with relatively high starting values and increase only marginally compared to their starting values, like storage and EV penetration.

4.4. Cost analysis results

In this section, the cost results will be visualized and analyzed. First, the costs of the individual technologies will be presented. Then, the costs of the groups will be analyzed.

Table 4.2 shows the costs of each technology considered in this work. The categories are the flexibility measures, and the technology column represents the technologies that form the flexibility measures together. The levelized cost of each technology is given. EV penetration and transmission are the only flexibility measures not aggregated from technologies with different costs. Therefore, the calculation of the costs for transmission and EV was based on one value. The additional kWh of EV battery capacity cost was set at 0.25 EURkWh [32]. The costs of transmission expansion were based on Calliope parameters. The cost of methane storage is not parameterized in Calliope, as the current gas infrastructure in Europe is used. However, in this thesis, the assumption was made that additional costs were needed for the knowledge development of the use of synthetic methane. Therefore, the costs are set at the same level as those for hydrogen storage. The costs for storage are not aggregated, as one of the main points of the thesis was the more precise depiction of storage in WITCH.

Table 4.2: Levelized Cost (EUR/kWh) for Various Technologies, Categorized by Group

Category	Technology	Levelized Cost (EUR/kWh)
Transport Sector Coupling		
	Biofuel to Liquids	7.97
	Hydrogen to Liquids	17.71
	Biofuel to Diesel	0.97
	Biofuel to Methanol	4.05
Heating/Cooking Sector Coupling		
	Hydrogen to Methanol	17.32
	Biofuel to Methane	1.68
	Hydrogen to Methane	16.55
	CHP Biofuel Extraction Heat	0.25
	CHP Methane Extraction Heat	0.25
	CHP WTE Back Pressure Heat	0.25
Storage		
	Battery	0.19
	Pumped Hydro	0.03
	Combined Hydrogen Storage	3.22
	Methane Storage	3.22
EV Penetration		
	EV	0.25
Transmission		
	Transmission	5.08

There are significant differences in costs among the technologies. For example, the short-term storage technologies (e.g., batteries and pumped hydro) have lower costs than the rest. The additional heat costs from combined heat and power plants are relatively low. The most striking result is the high cost of hydrogen-based fuels. The hydrogen-to-methanol, hydrogen-to-methanol, and hydrogen-to-liquids have levelized costs within the 17 EUR/kWh range, around two times as high as the biofuel-based fuel. This can be explained by the costs of the conversion technology, the hydrogen synthesis, and the carbon capture. The breakdown of the cost of these hydrogen-based fuels is visualized in Figure 4.7

This analysis shows the importance of considering costs throughout the technology process. DAC's expenses can significantly influence the energy system's costs when this system relies heavily on synthetic fuels from hydrogen.

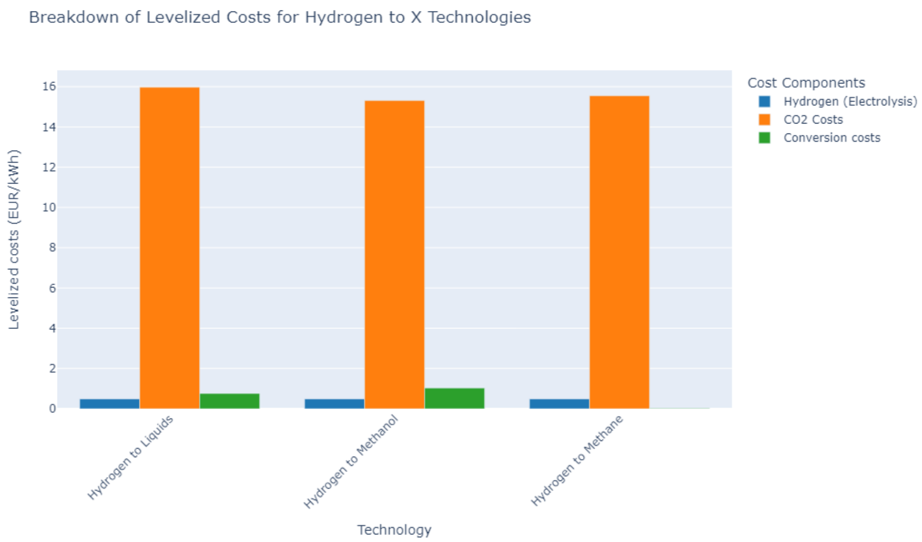


Figure 4.7: Breakdown of the synthetic fuel cost.

4.4.1. Costs of flexibility groups

The costs of the flexibility groups are calculated as the weighted average of their components. However, not all groups have components that cost different amounts. The sector coupling and storage groups do have varying component costs. The storage group is broken down further to maintain a high level of detail of storage representation in WITCH. As a result, only the sector coupling group's costs are calculated using the weighted average. The breakdown of the influence of the components of sector coupling on the costs is visualized in Figure 4.8.

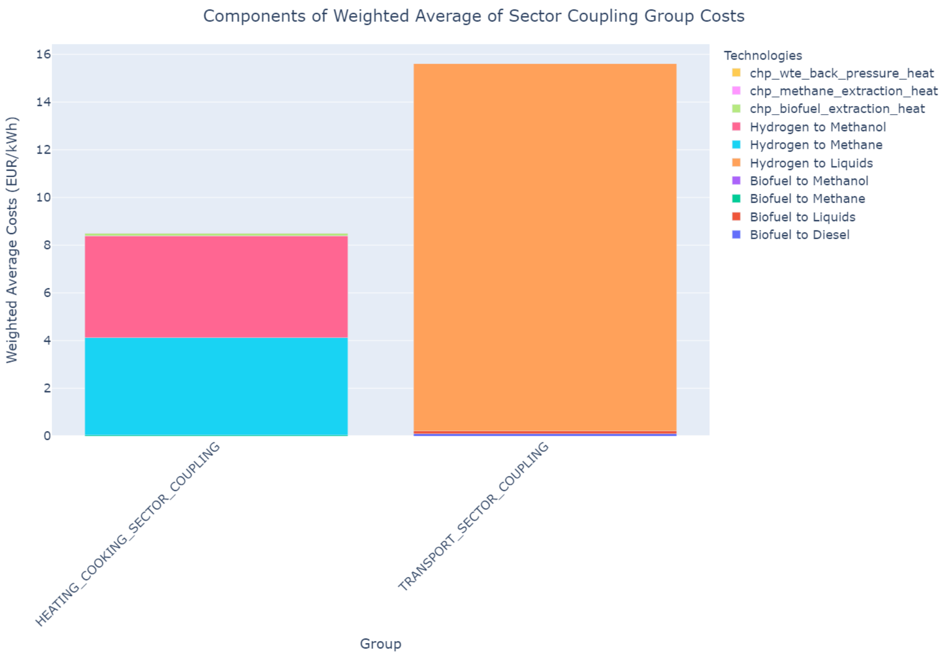


Figure 4.8: Weighted components of sector coupling categories.

Figure 4.8 shows the influence of the high costs of hydrogen-based fuels on the cost of sector coupling as a whole. The transport sector coupling is almost entirely made up of the costs of hydrogen-to-liquids. The heating and cooking sector coupling cost is primarily covered by hydrogen to methane and methanol. This leaves us with the final cost parameters to be included in the WITCH module. The costs are shown in Table 4.3.

Group	Weighted Average Levelized Cost (EUR/kWh)
EV PEN	0.2540
Heating Cooking Sector Coupling	8.5166
Transmission	5.0750
Transport Sector Coupling	15.6065
Storage (Battery)	0.1908
Storage (Pumped Hydro)	0.0301
Storage (Hydrogen)	3.2232
Storage (Methane)	3.2232

Table 4.3: Weighted Average Levelized Cost of Flexibility measures

5

Results of flexibility modeling in long-term energy model

In this chapter, the results of the final analysis will be presented. First, the policy scenarios are introduced in 5.1, delineating the existing structures governing flexibility and VRE penetration. After that, the new interactions under different policy scenarios are compared in section 5.2, 5.3, 5.4, and 5.5. Lastly, the sensitivity of the model's parameters that influence the integration of flexibility in the system is studied in 5.6.

The model's outcomes are not intended to forecast future energy systems' transformations precisely. Instead, they stem from an optimization process aiming for welfare-maximizing. Thus, the results should be viewed as an economically optimal scenario to guide policymakers on resource allocation and promote low-carbon energy technologies to meet emission targets.

5.1. Policy analysis

The policy analysis will be based on two distinct policy scenarios:

1. Business as usual (BAU): no additional carbon mitigation based climate policy
2. Carbon Tax (ctax): The WITCH model allows for different ctax scenarios. The ctax that was utilized for this work is the default ctax. This entails a carbon price of 30 \$(2005) per $\mathrm{tCO_2}$equivalent. This price will increase over the years using the average Ramsey consumption discount rate. The ctax is initialized in the year 2020.

5.2. Generation mix

Figure 5.1 illustrates the energy production mix for the BAU and ctax scenarios. Using the tax policy scenario, renewable energy-based and carbon-capture-based technologies become more economically viable. This leads to a higher penetration of these technologies compared to fossil-fuel-based generation. This difference between the BAU and the ctax is evident from the electricity generation figure. The penetration of Variable Renewable Energy (VRE) increases significantly in the ctax scenario. The high levels of VRE necessitate higher biomass levels with carbon capture and storage (CCS) plants due to the flexibility constraint that requires a counterpart to the higher level of VRE with increased firm capacity.

There are also similarities between the two models. In general, the generation increases until 2050 and then stabilizes. Additionally, the role of nuclear energy decreases steadily in both scenarios, aligning with the shift to VRE and flexible generation.

In the ctax scenario, there is a substantial reduction in the use of coal between 2010 and 2030. This reflects the influence of the carbon tax, which should target coal, as it has high emissions. The use of biomass without CCS is high in the BAU in 2030 compared to the ctax. In the ctax, biomass utilization with CCS will become more pronounced in 2040. The biomass with CCS seems to replace the biomass without CCS in the ctax steadily. The contribution of hydropower remains consistent across all scenarios, which shows the established role in the energy mix as a reliable renewable source.

Both wind and solar energy grow significantly in the ctax scenario. Solar power, in particular, shows a substantial increase, while wind stays relatively constant over time. This results in a substantially higher PV-to-wind ratio than in the Calliope scenarios. The energy production mix stabilizes after 2050 in all scenarios. This suggests that most technological shifts and capacity additions will occur primarily within the next three decades in Europe.

The model runs with _old represent the WITCH model output without the flexibility module, the _new represent the model runs with the flexibility module. A few differences arise when comparing the new module with the old interactions within the BAU scenario. Solar energy penetration is slightly lower when the new module is included. Additionally, the old model has lower biomass generation in the later years. This indicates a need for more firm capacity in the latest model. The early years of the model show only slight differences between the old and the new BAU.

Comparing the new module within the ctax scenario. The model shows results comparable to those of the BAU scenario. Lower levels of generation are needed because of the higher levels of efficiency from the flexibility measures. Solar PV energy generation remains constant mainly, while wind energy production is significantly lower.

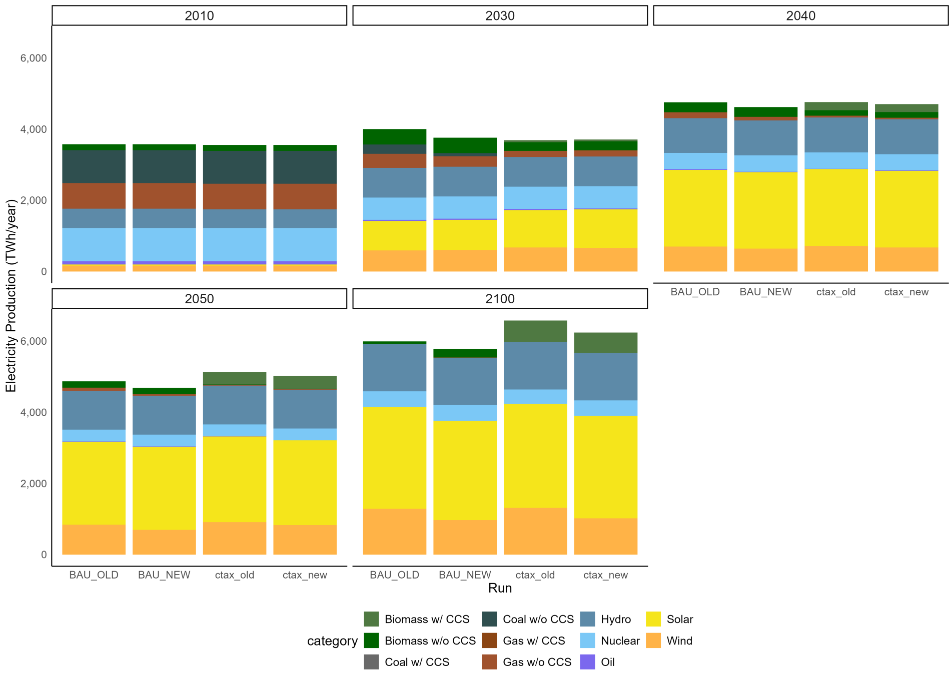


Figure 5.1: Comparison of the Electricity generation under the BAU and ctax policy scenario in Europe

5.2.1. TPES

The chart Figure 5.2 compares the Total Primary Energy Supply (TPES) mix for old and new BAU and ctax scenarios across various years (2010, 2030, 2040, 2050, and 2100). In comparing the old BAU to the new BAU, biomass contribution is slightly higher in the new BAU in 2050 and 2100.

The new module will significantly lower coal demand in 2030. The gas contribution is similar between the old and new across all years, with a slight increase in the new BAU scenario in 2100. Solar and wind energy contributions are higher in the old BAU, with a visible increase in solar power in the later years (2040, 2050, and 2100). Hydro and oil remain consistent between the old and new BAU.

Comparing the ctax with and without the new module, the most prominent difference is the utilization of biomass, which is higher with the flexibility module in the later modeled years. Gas use is significantly lower in the later years, indicating that the lower levels of gas with the new module are partly covered by biomass. The summed TPES is higher without the new module, which shows the efficiency gains from introducing the flexibility. The contribution of solar is slightly lower with the latest module in the early years. After that, the wind energy supply will decrease strongly in 2100.

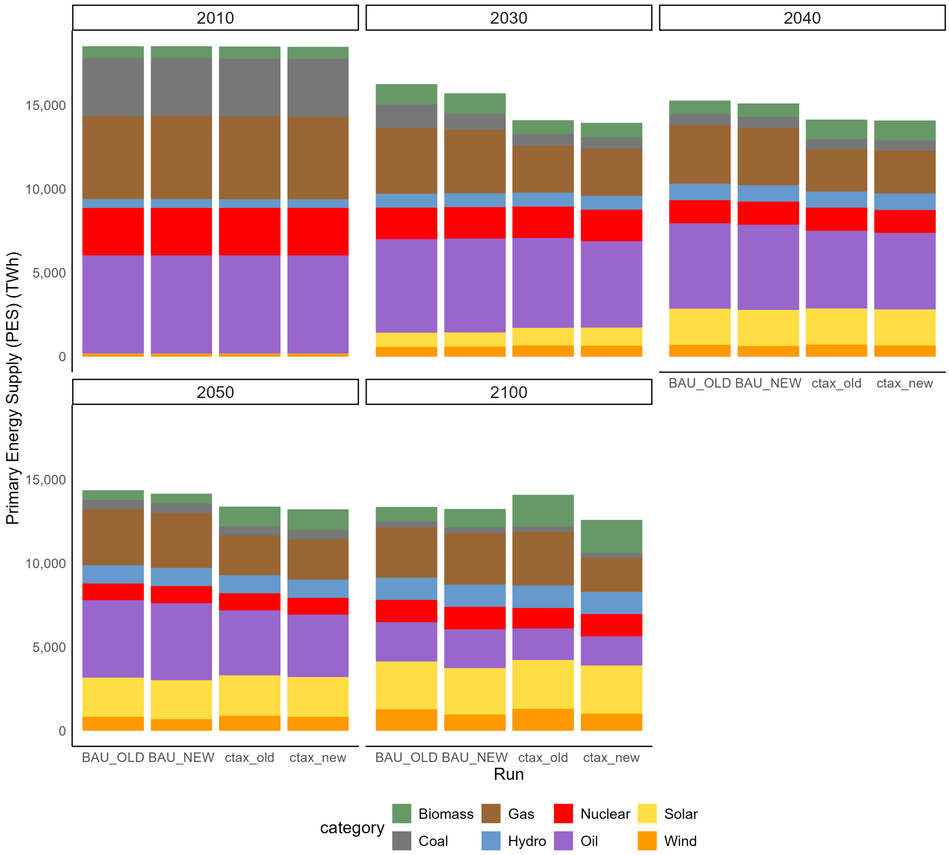


Figure 5.2: Comparison of the TPES under the BAU and ctax policy scenarios in Europe

5.2.2. Installed capacity

Graph 5.3 shows the installed capacity in Europe for the different policy scenarios. The intermittent nature of wind and solar power can be evaluated by comparing the generation and installed capacity share. The installed capacity of wind and solar energy is significantly higher than that of biomass and nuclear energy, which shows that the capacity factor of these technologies is lower. The technologies' distribution is relatively similar with and without the new flexibility module. The main difference between the old and the new is the installed capacity of wind. The capacity of wind is significantly lower when the new module is included. Showing that wind energy can be utilized more effectively.

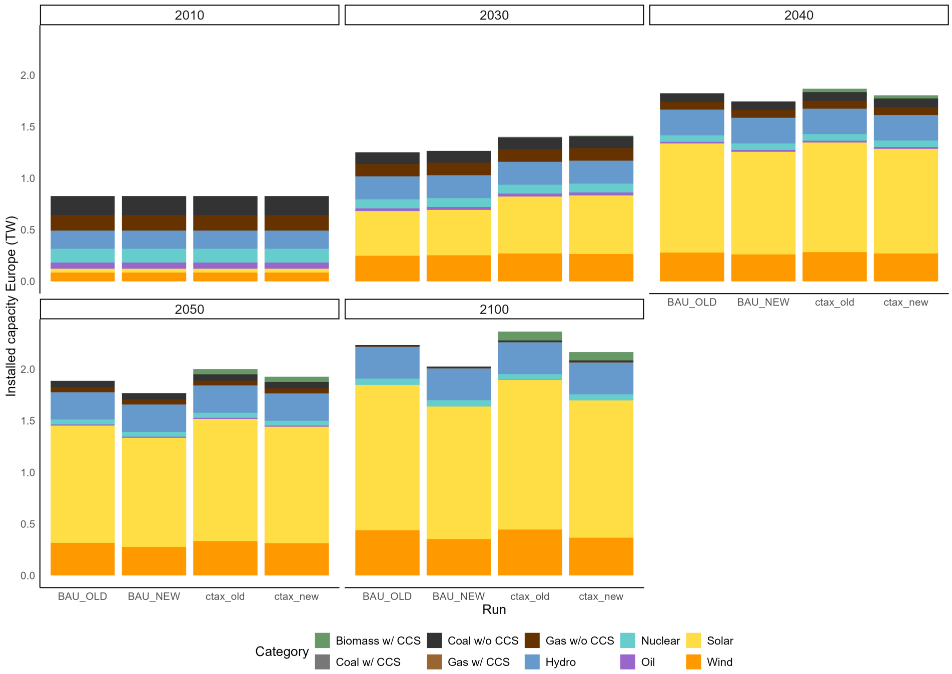


Figure 5.3: Comparison of the installed capacity of electricity generation under the BAU and ctax policy scenario in Europe

One way to test the efficiency gained by introducing the new module is to look at the curtailed energy. Figure 5.4 shows the curtailment over the years for the model with and without the new module under the two scenarios. Under the BAU scenario, the curtailment decreases with the new module around 2040. This remains lower until 2075 when there is a small drop in curtailment for the model with the old interactions. After 2075, the curtailment in the module with the old interaction rises strongly.

The output under the ctax scenario shows similar results. With the new interactions, the curtailment is overall lower than with the old interactions. Overall, the results are consistent with the installed capacity differences, where we see more significant differences in the later modeled years.

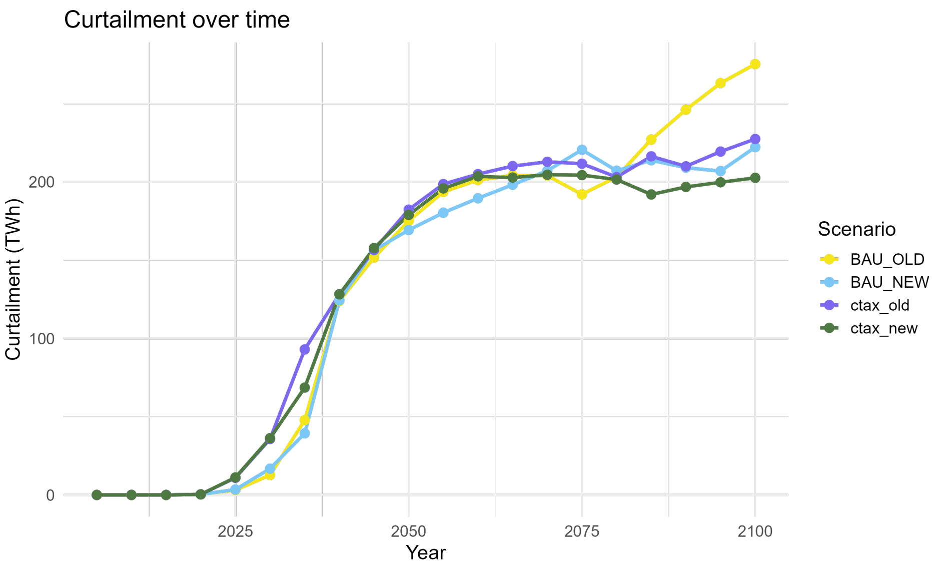


Figure 5.4: Comparison of the curtailment under the BAU and ctax policy scenarios in Europe

5.3. Flexibility under different policy scenarios

With the level of VRE penetration, the total level of flexibility in the system can be predicted. Figure 5.5 presents the expected level for each scenario. The flexibility bins are plotted to show which bin the prediction falls in for each timestep. The flexibility needs increase rapidly in both the ctax and the BAU in the earlier years. This rapid increase stops around 2040, when both scenarios undergo a relatively stable progression until 2100. The progression, therefore, inhibits the qualities of a logarithmic-like curve. The ctax predicted total flexibility is consistently higher than the BAU. Thus, the ctax reaches the fourth bin around 2040. Thirty years later, the BAU reaches the fourth bin in 2070. In 2100, the two scenarios end up at around the same predicted level of flexibility in the system. This can be explained by the similar levels of VRE installed capacity at that time.

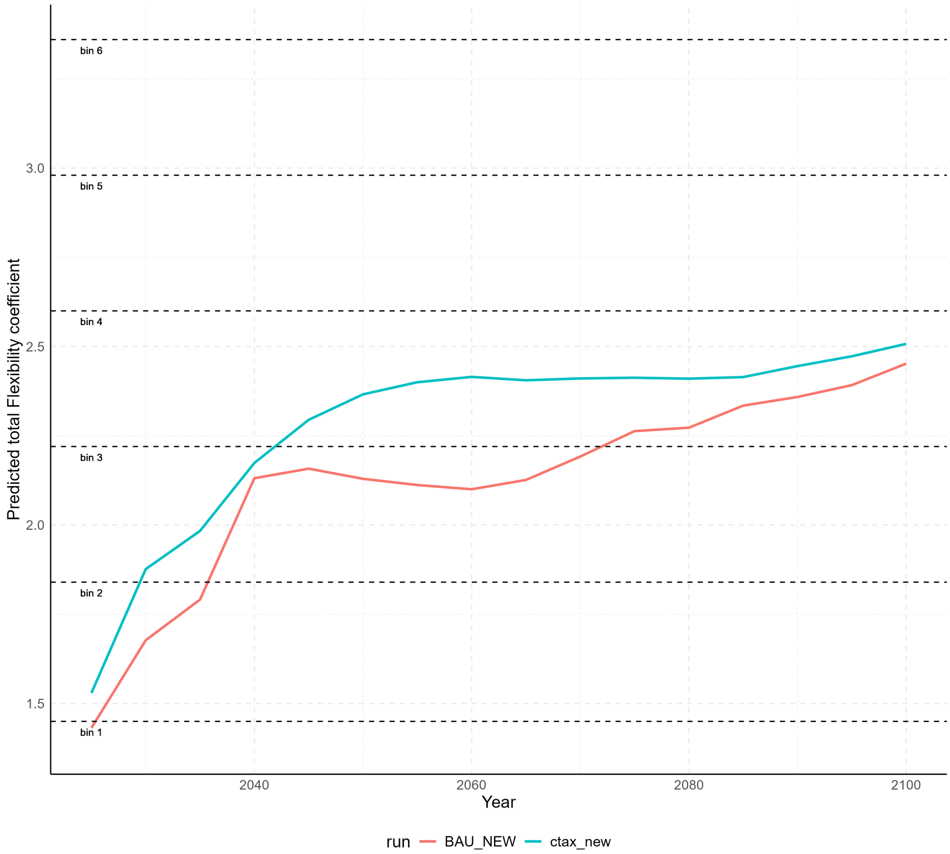


Figure 5.5: Comparison of the flexibility under the BAU and ctax policy scenario in Europe, and the level of the relevant bins

This behavior of the predicted total flexibility results in the allocation of the flexibility variables shown in Figure 5.6. The transparent bars before 2020 represent that the equation is initialized after 2020. The allocation of the flexibility variables from the total flexibility are parameters. Therefore, the distribution of flexibility is constant within each flexibility bin. The results show that three different flexibility bins are utilized over the model time in Europe. Notably, the initial jump in flexibility required by 2025 is substantial compared to current levels, with subsequent increases being less intense. This suggests a need for an aggressive introduction of flexibility in the earlier years based on the data.

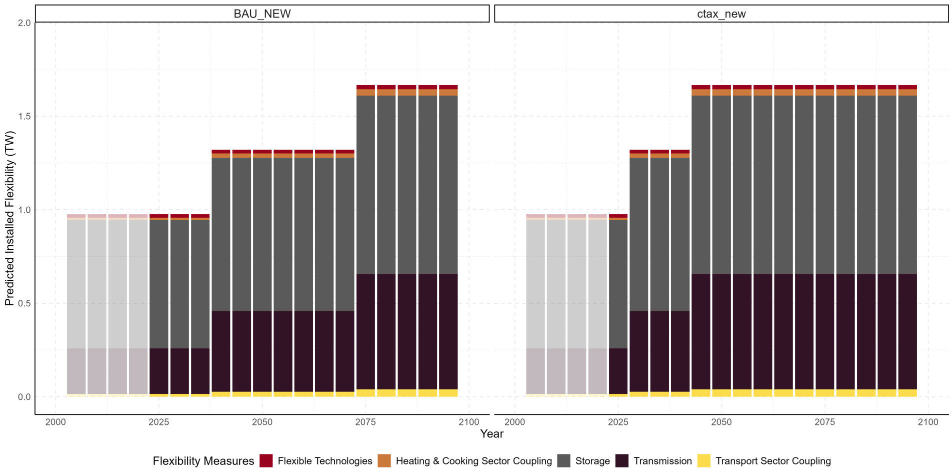


Figure 5.6: Comparison of the flexibility measures under the BAU and ctax policy scenario in Europe

Figure 5.7 illustrates the system's storage discharge capacity for specific technologies. The disaggregation was implemented to represent the storage capacity for each technology with more accuracy. The decision was made to maintain a constant storage distribution within each bin. Consequently, the storage levels remain relatively constant across the grouped years. However, when the model transitions to a different bin, the storage levels adjust accordingly.

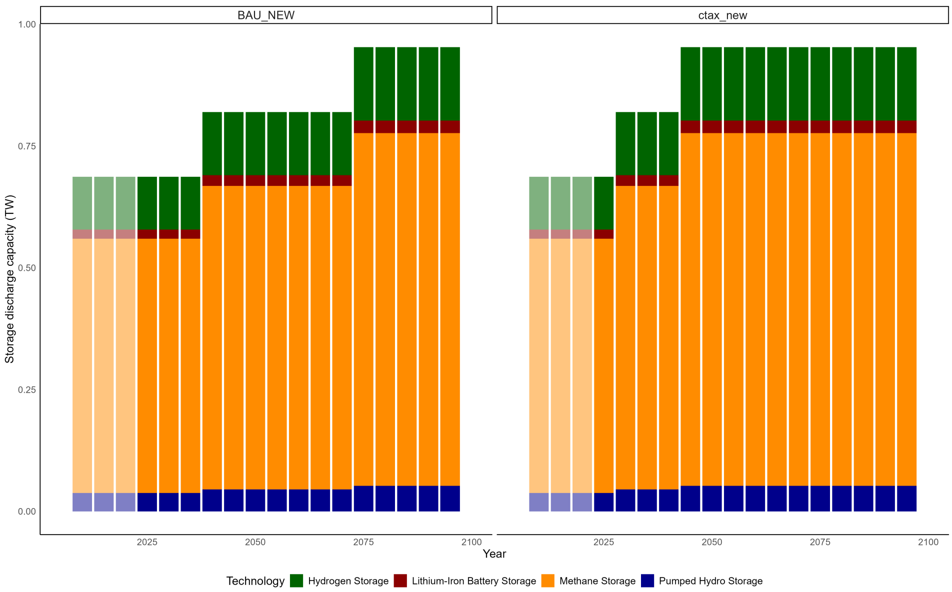


Figure 5.7: Comparison of the storage levels under the BAU and ctax policy scenario in Europe

5.4. Existing flexibility in the system

The next step for the model was to find the system's existing flexibility level. These existing levels of flexibility are subtracted from the predicted values to obtain the net flexibility needed.

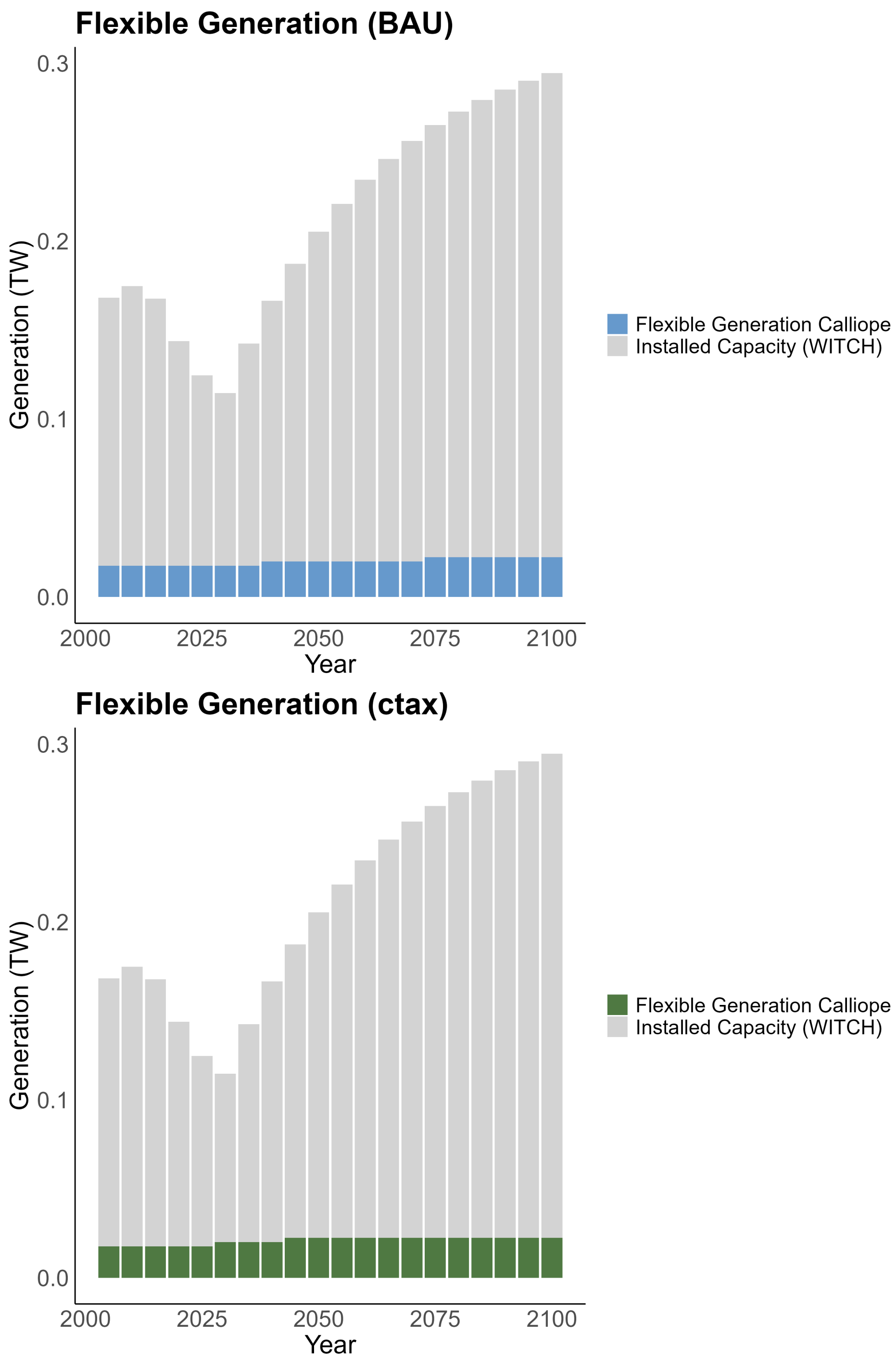


Figure 5.8: Comparison of the additional flexible generators needed under the BAU and ctax policy scenario in Europe

The existing level and possibly the additional level of flexible generators like gas and biomass are plotted in Figure 5.8. The grey bars show the existing level of flexible generators in WITCH over the years. The colored bars represent the level found in the flexibility model from Calliope. The flexible generation from Calliope is consistently and significantly lower than the level from WITCH. This can be explained by the broader representation of flexible supply in WITCH, where a multitude of different generators are modeled. Meanwhile, in Calliope, synthetic and bio-based fuels were used only in CCGT generators. The increases can be seen in the steps from one flexibility bin to the next in the colored bars. The data shows that Calliope relies less on flexible generation for flexibility compared to WITCH. Therefore, no additional flexible generation is needed.

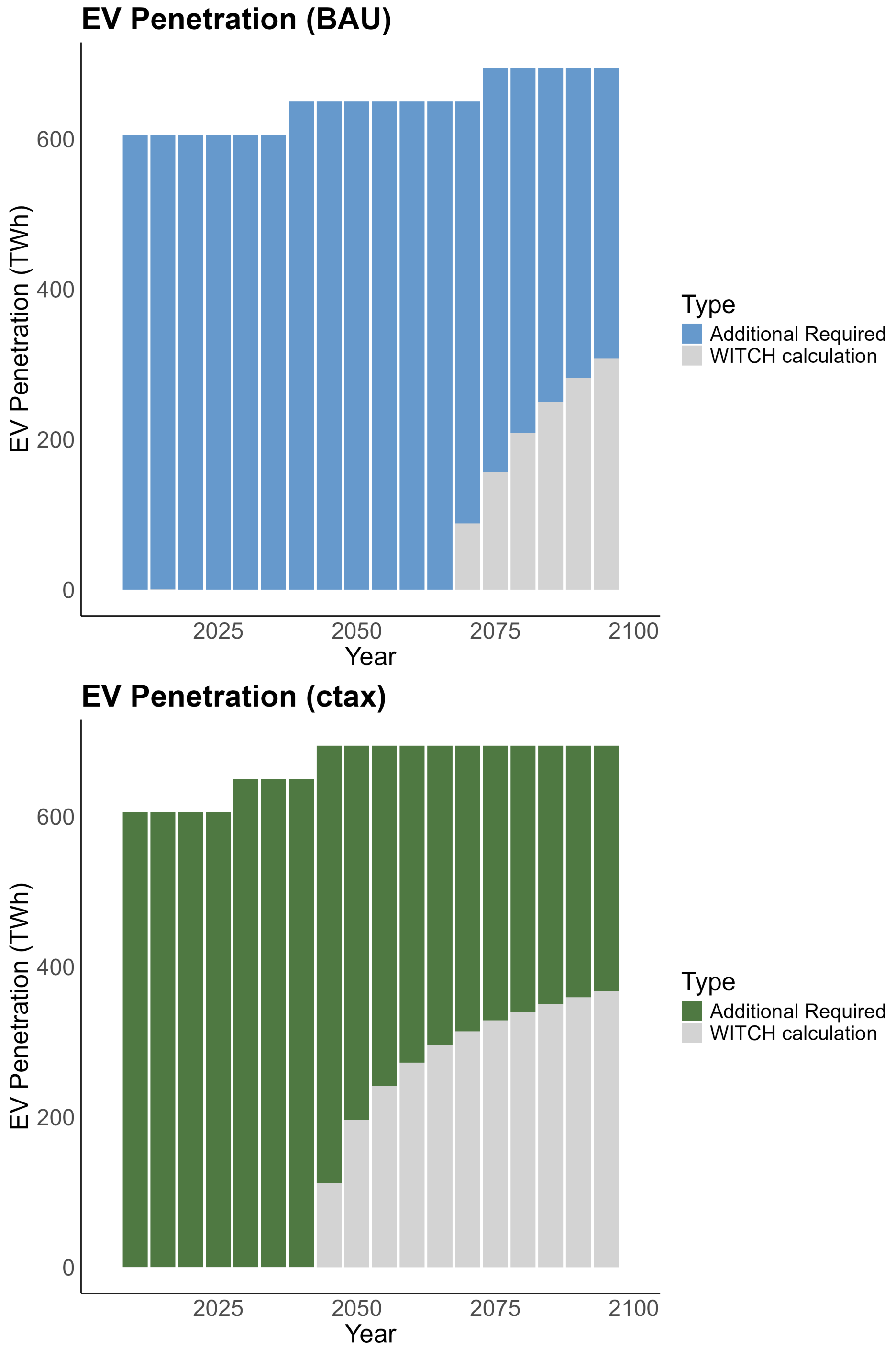


Figure 5.9: Comparison of the additional EV battery capacity needed under the BAU and ctax policy scenario in Europe

The additional and existing level of battery capacity from EVs is shown in Figure 5.9. The existing level of EV battery capacity in the BAU remains zero up until 2070. This late adoption entails a high level of additional EV needed to match Calliope's flexibility. The EV battery capacity when the WITCH model does decide to adopt EV is also significantly lower than the level calculated by Calliope.

In the ctax, the model adopts EV faster. This results in a substantial increase in EV battery capacity around 2045. However, this level is also lower than the calculated values from Calliope. Therefore, additional capacity is also needed in the ctax scenario.

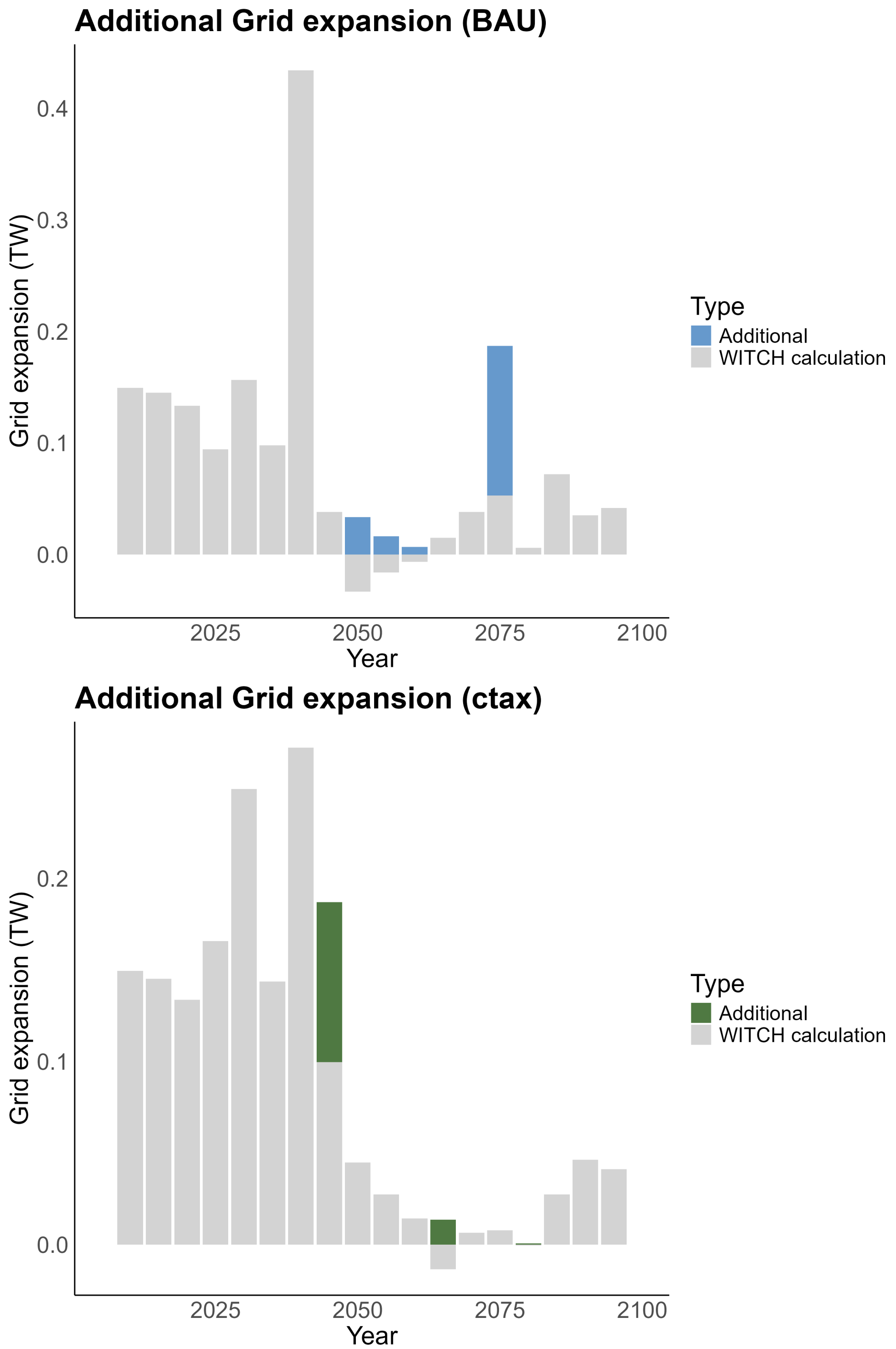


Figure 5.10: Comparison of the grid expansion needed under the BAU and ctax policy scenario in Europe

Figure 5.10 illustrates the grid expansion requirements for both the BAU and ctax scenarios. The WITCH model generally predicts a greater need for grid expansion than Calliope. This indicates that the more stylized modeling approach of interactions in WITCH results in lower interaction levels, as observed in the storage variables, and a higher anticipated grid capacity expansion. The results suggest that the new module compensates for reducing grid capacity by maintaining it at a baseline level.

Notably, the instances where additional grid expansion is required coincide with transitions to a new bin.

5.4.1. GDP loss

The economic impacts of flexibility on Europe are not the main focus of this thesis. However, we identified that cost parameters strongly influence the penetration of flexibility in the system. Therefore, the discounted GDP loss in Europe is shown in Figure 5.11. Comparing the new BAU to the BAU baseline represented by the dotted line at y = 0, there is an initial increase in GDP, which is not expected as additional costs are associated with the new module. The increase in GDP is probably an effect of the higher utilization of generated electricity, in combination with a low rise of VRE in the beginning stages of the model. The new BAU, ctax_old, and ctax_new all inhibit similar trajectories. Substantial decreases in GDP from 2025 until stabilizing around 2035, after rising again in the later years of the model. The total GDP loss of the new flexibility module remain within a close range of around 0.1 % compared to the old model in both scenarios.

Figure 5.11: Comparison of the economic variables under the BAU and ctax policy scenario in Europe

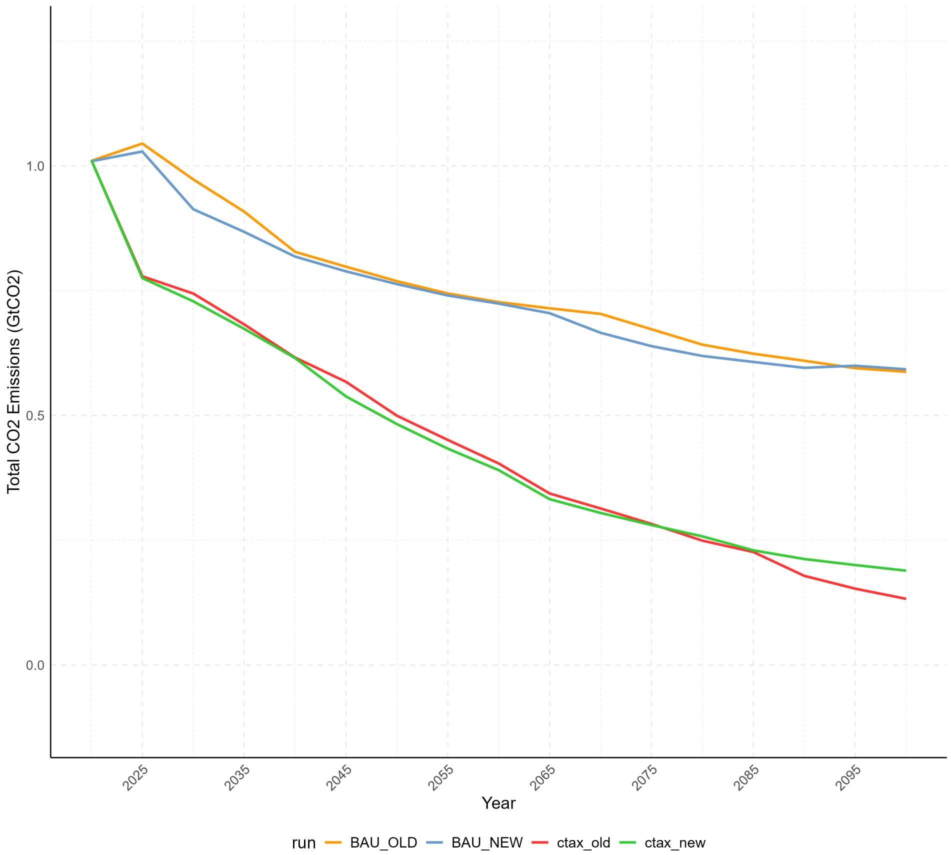


Figure 5.12: Comparison of the CO_2emissions under the BAU and ctax policy scenario in Europe

5.5. Emissions

Figure 5.12 shows the emissions trajectory for the old and the improved model under the two scenarios. It is important to note that the WITCH model utilizes both CCS and DAC to reduce these emissions. As a result, the actual net emissions are lower than what is depicted in the plot.

The model with the flexibility module with the BAU scenario shows a trajectory comparable to the old model. This alignment is consistent with the energy generation and TPES comparisons, where there were only slight differences between the old and the new models.

In the ctax scenario, the emissions reduce more rapidly than in the BAU. This reduction is driven by the carbon tax, which incentivizes using carbon-neutral generation. The new module shows a slight decrease in emissions compared to the old ctax model (ctax_old). This results from the higher utilization of energy from VRE, which decreases the need for other forms of generation.

Overall, the plot illustrates that the updated models follow similar trends to their older counterparts but with slight improvements in emission reductions. This indicates that the refinements in the new models contribute to more efficient and effective emission reduction strategies.

5.6. Sensitivity analysis

Sensitivity VRE utilization

The higher temporal and spatial resolution of the analysis of Calliope has revealed that with an increased level of VRE, the system faces binding additional costs that were not fully accounted for in the current version of WITCH. However, the extra flexibility introduced also brings advantages to the energy system. The sensitivity analysis aims to understand which constraint binds the system to lower VRE levels than the Calliope levels. Then, the constraints can be relaxed based on the higher utilization of VRE from the induced flexibility. This approach allows us to explore the potential for optimizing the balance between flexibility and cost, ensuring that the system can effectively accommodate higher levels of VRE without incurring high costs.

5.6.1. Capacity constraint

The effect of high levels of flexibility can be further researched by expanding the utilization level in the existing constraints on VRE integration. In WITCH, the utilization of power generated by VRE is represented by the capacity value. Although this capacity value was not directly researched in the thesis, a sensitivity analysis will be conducted to determine its influence on the need for flexibility. Currently, the capacity value is an exponentially decreasing function of VRE integration under the assumption that VRE utilization decreases as the VRE share increases. Flexibility options can mitigate the reduction in VRE utilization by supporting higher levels of VRE. Therefore, to test the sensitivity of the module, one additional capacity value will be tested for the *capacity value*. The new value is presented in Table 5.1.

Original value	**Tested value**
$0.9 \cdot \exp(\text{cv\_exp} \cdot \frac{Q\_EN(\text{'elwind'},t,n)}{Q\_EN.l(\text{'el'},t,n)})$	0.9

Table 5.1: Comparison of Old and Tested Capacity Values

The higher utilization of wind and solar energy should result in lower costs for solar and wind energy supply per generated energy, which could cause the model to select more VRE than the original capacity value level.

The capacity value is used in the capacity constraint, which is shown in equation A.1. The capacity constraint ensures sufficient supply to cover sudden increases in demand. This constraint mandates that the firm capacity be 1.5 to 2 times (depending on the region) the level of the yearly average load. Firm capacity is the *guaranteed capacity* in the model. For non-VRE technologies, the firm capacity equals the installed capacity. For VRE technologies, the capacity is multiplied by the capacity value and the capacity factor. The capacity factor represents the actual output over a period of time of the technology divided by its theoretical potential over that period. The capacity value quantifies the relationship between the increasing VRE level and the decreasing utilization level over time. As the proportion of VRE in the energy mix grows, the practical capacity value gets lower, reducing the utilization of each additional unit of VRE. This is where the introduction of the new module makes a difference. Flexibility measures ensure a high level of VRE utilization. Therefore, in the sensitivity analysis, the impact of the capacity value will be analyzed by comparing it with the outcomes from Calliope.

Sensitivity to technology cost

This sensitivity analysis section aims to find the impacts of the chosen coefficients of the cost reduction function. The coefficients were selected to represent a threefold cost increase in 2020 compared to the 2050 cost for the base-runs. This cost reduction function can effectively be seen as a scenario without subsidies. Now, we want to see if lowering this cost reduction curve impacts the integration of VRE into the system. This is achieved by decreasing the coefficients to model a lower value of costs in the earlier modeled years. By doing so, insight can be obtained on whether subsidies on flexibility would effectively obtain higher shares of VRE in the system.

Figure 5.13 shows the predicted total flexibility in the system under the ctax scenario. Additionally, the relaxed cost and relaxed capacity value runs are added. The relaxed cost results are identical to the initial tax run, showing that the cost reduction is not a driving factor in the VRE penetration directly.

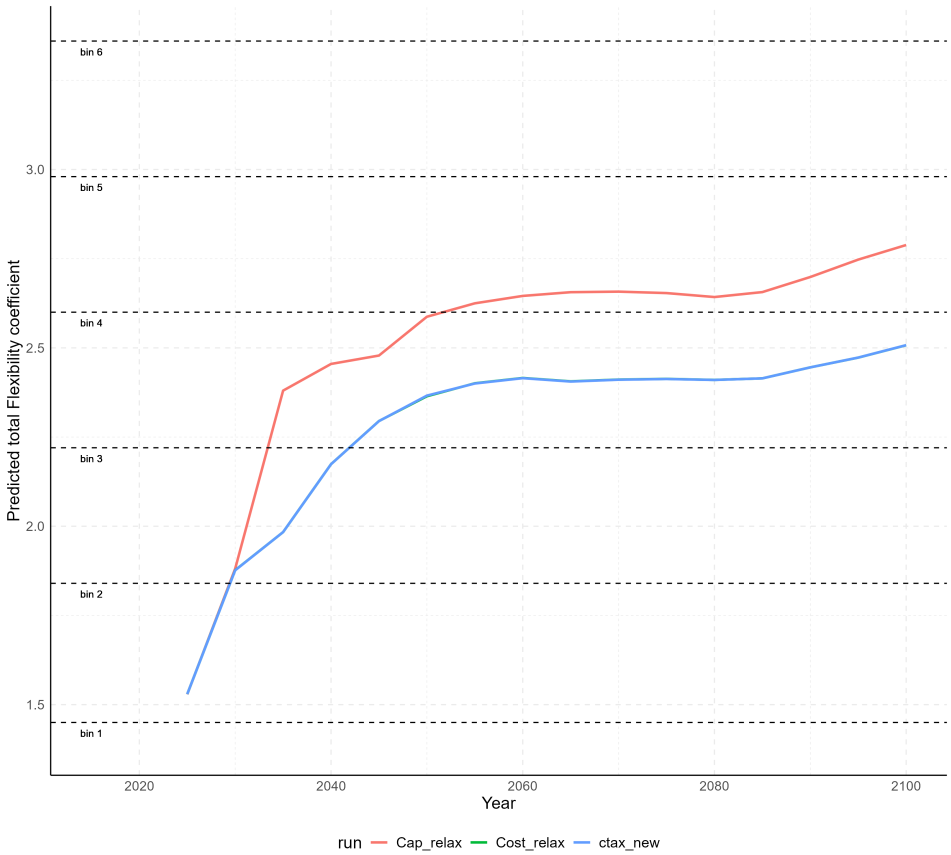


Figure 5.13: Sensitivity of the model to relaxing the capacity constraint and the cost reduction rate

The relaxed capacity value shows increased VRE penetration and thus, an increases in the needed flexibility.

This result is interesting because the higher capacity value ensures that more energy can be used from VRE, which leads to a lower installed capacity for the same level of VRE output. However, the higher capacity-to-energy ratio makes VRE a more feasible investment in WITCH. Therefore, the model chooses to have more VRE in the system. This shows the need for additional research on the exact interactions between the level of VRE, flexibility used, and VRE output in the system.

6
Discussion

6.1. Discussion

This thesis investigates the role of flexibility measures within the European energy system to accommodate increasing levels of variable renewable energy (VRE). Through simulation using the WITCH model and insights from the Calliope framework, it evaluates what levels of storage, grid expansion, demand response, and sector coupling are needed to ensure system resilience and reliability under varying climate policy scenarios. The work aimed to integrate the strengths of two different scales of energy modeling to make better policy decisions. The resulting methods suggest a novel approach to incorporating flexibility, refining, and adding to traditional methods used in long-term energy models.

6.1.1. Interpretation of research

In this section, the work's results are interpreted. In doing so, it can be evaluated whether the novel method of coupling Calliope and WITCH actually improves the modeling of flexibility.

Relating the method of coupling this work to earlier work, we can see some apparent differences. This thesis uses an unconventional method using pre-run Euro-Calliope SPORES instead of running Calliope directly with WITCH inputs. This required scaling the data to match the assumptions of both models. In contrast, the bidirectional model of Sejlom et al. scaled the data based on demand from the IAM, adjusting the short-term model's demand [50]. In the work by Sejlom et al., harmonizing the demand between models removed any uncertainty about the impact of scaling, which is a problem we do have in this work. Additionally, the choice was made to model flexibility as a parameter of increasing levels of VRE. This causes the WITCH model to make a trade-off between installing more VRE with the associated flexibility requirements or opting for a different form of energy generation. This is a different approach than coupling models to find the impacts of flexibility on the system, which was demonstrated by lai et al. (2021) [31].

This demonstrates that using external flexibility interactions to inform an Integrated Assessment Model (IAM) is complex. Coupling can be based on various variables, and differences in key assumptions between models create specific challenges that need resolution. The choice of coupling variables depends on the particular aspect of energy system modeling that requires enhancement. This work focused on the installed capacity for flexibility, so the model was coupled based on VRE penetration. However, coupling short-term and long-term models does not have to be exclusively based on VRE penetration. There is no one-size-fits-all approach; careful consideration and analysis are necessary to identify which variables govern the interactions the modeler seeks to improve.

The model's output provided insights into the trajectory of flexibility in the WITCH model under different policy scenarios. The capacities and implementation rates can be compared to existing literature and projections of flexibility in Europe's future energy system. It's important to remember that no model aims to predict the future precisely; instead, models offer insights into trade-offs and patterns that can help policymakers make informed decisions. Differences will inevitably occur between models due to variations in model formulation and heterogeneous data inputs. Therefore, comparing the absolute outputs of different models does not necessarily create insights on their relative effectiveness or accuracy. Instead, the focus should be on understanding the underlying assumptions and methodologies that drive these differences and how they inform potential policy pathways and strategies. This is shown, for example, by Gils et al. (2022), who compared the flexibility modeling in power sector models. The author acknowledged that comparing flexibility outcomes from different models is only relevant when necessary inputs are harmonized [18]. Therefore, to gain insights into whether the level of flexibility is within the ranges of other models, the inputs must first be harmonized.

6.1.2. Implications for research and policy

A significant advancement in IAM and power model coupling research is using pre-run SPORES, or other forms of a range of pre-run simulation results, to address the computational limitations of running two models simultaneously. The use of a regression model to couple models is not novel. Still, the use of the range of possible near-cost optimal to generate an average level of flexibility needed has not been performed. This method can also be used to refine different parameters in long-term models. For instance, the installed capacity and the resulting yearly energy generation needed for specific technologies to meet a demand profile from an IAM can be predicted.

Furthermore, the differences in WITCH's output when incorporating a more precise depiction of flexibility demonstrate that flexibility significantly influences the energy system. This shows policymakers need to consider flexibility measures integral to energy planning and policy development.

6.1.3. Limitations and future research

Utilized data

Conducting more runs of the Calliope model from earlier years is essential to obtain a more detailed understanding of the flexibility required at the start of the energy transition trajectories. The higher number of runs concentrated around 2050, compared to the lower number of runs around 2030, may result in a skewed representation of the average levels of the flexibility variables within the bins.

A more balanced distribution of runs across different years is necessary to accurately capture the initial stages of flexibility requirements. This is crucial because the early years of the transition set the foundation for how the energy system evolves and adapts to increasing shares of variable renewable energy (VRE). By only utilizing 2030 and 2050 runs, we could miss specific patterns of the integration of flexibility in the years between 2030 and 2050 and after 2050.

To address this, additional runs of Calliope, starting from earlier years up until 2100, could be conducted. These runs will provide a more granular view of how flexibility requirements evolve from the very beginning of the transition. They could also help identify critical periods where policy interventions and technological developments can have the most significant impact.

This is also important because the distribution within the flexibility runs in the bins. Average values are currently used; however, due to the interpolation, some assumptions have been made over the years with no data. Additional model runs could provide the data to diminish the need for interpolation.

Feedback sector-coupling and demand

The data utilized in this analysis is derived from the Sector-Coupled Calliope model, in which wind and solar energy supply most of the primary energy. The system's high level of modeled flexibility, especially from sector coupling, achieves this. The synthesis of synthetic and bio-based fuels reduces the demand for traditional fossil fuels. However, this nuanced process of synthetic and bio-based fuel production and its subsequent impact on traditional fuel demand has not been modeled in WITCH within this thesis.

As sector coupling increases, the overall demand for traditional gas and oil will decline, and more VRE is needed. Therefore, this interaction will cause a higher prediction of the required flexibility. This is the reason why the model predicts moderate amounts of flexibility.

Future research should incorporate sector coupling feedback into the fuel demand module. This should accurately represent the interplay between renewable, synthetic, and traditional energy sources. By doing so, it will be possible to understand better the full scope of flexibility requirements in a highly integrated and renewable-dominated energy system.

Elasticity of Substitution Between Flexibility Variables

Because the flexibility technologies are modeled as dummy variables and not incorporated into the CES structure of the WITCH model, the interactions between the flexibility measures are not precise. This limitation means that the model does not easily account for how increased storage capacity might influence the need for other flexibility measures, such as demand-side management or grid expansion. Research should explore the interactions between different flexibility options and develop models that can better represent these dynamics.

Real-time coupling

The method used in this thesis could be the basis for real-time coupling. A model like Calliope can validate the energy system configuration using real-time coupling. This removes the need for bins to 'match worlds' between the models. An actual level of flexibility can be obtained by running the model instead of using the SPORES. Variables identified in this study can then be used as input for Calliope. The results of the Calliope run can then be integrated into WITCH. This also ensures that variables not in a corresponding range, like the demand, can be corrected.

Cross-Regional Validation

Results that can be transferred to other regions require a thorough understanding of the specific dynamics of the energy system in those regions. The starting levels of VRE and flexibility can range significantly between regions, which impacts the trajectory of these variables. Furthermore, the regions could already have high levels of a certain flexibility measure, reducing the need for other flexibility measures. This highlights the need for a method to map flexibility needs with different starting values between models or regions. For example, the demand profiles and renewable energy potential vary significantly across the defined regions, affecting storage needs and flexibility requirements. Further research should focus on developing standard metrics and normalization techniques that can accurately represent these differences, enabling more reliable transfers of insights and results between models.

Role of costs in WITCH

The chosen polynomial function to model the decreasing cost as a function of cumulative utilization influences the costs of the entire system. Future research could assess the sensitivity of model results to different cost reduction functions in more detail, exploring coefficients or other functions that might better represent cost reductions based on empirical data where possible.

Additionally, the costs parameters in this thesis does not assume any subsidies for the new technologies introduced into the model. Subsidies could lower the initial costs and make implementing higher levels of VRE more economically feasible. Additional research on the influence of subsidies on flexibility in long-term models is needed. This is especially important for the newly introduced technologies, as there is no real-life data on their costs on a utility scale. Lastly, the interactions of the lifetime of the technologies with their costs are not modeled in this thesis. There is no real-life data on the exact lifetime of specific installations for sector coupling on this scale, making predicting the costs harder.

6.2. Conclusion

In this section, the sub-questions will be answered by summarizing the main findings of the work. Then, these conclusions are used to answer the main research question.

What technologies or groups of technologies are available to manage flexibility in future energy systems?

The literature review and subsequent analysis identify several key flexibility measures most promising for managing flexibility in future energy systems: storage technologies, transmission expansion, demand response management, and sector coupling.

The findings indicate that an integrated approach combining these technologies is essential to address both spatial and temporal mismatches between supply and demand. Specifically, storage technologies, such as batteries and hydrogen storage, play a crucial role in balancing short-term fluctuations, while transmission expansion helps mitigate regional disparities in energy availability. Demand response further enhances system flexibility by aligning energy consumption with availability, thus reducing the overall strain on the grid. Sector coupling can flatten the electricity demand curve and reduce fossil fuel demand in future energy systems.

Moreover, the research reveals that the required storage capacity is not solely determined by the direct mismatch between supply and demand; the deployment of other flexibility measures significantly influences it. For instance, effective demand response can reduce the need for extensive storage solutions.

How do different renewable technology policy scenarios shape the demand for storage in future renewable energy systems?

The analysis of various technology policy scenarios using the Sector-Coupled Euro-Calliope framework shows that achieving high VRE penetration with a cost increase of no more than 10% requires a strategic mix of flexibility measures. While the study didn't establish a direct link between specific system configurations and individual flexibility measures, it did identify a broader connection between overall flexibility demand and VRE penetration.

This relationship was quantified through a regression model, predicting total flexibility levels across different VRE penetration scenarios, categorized into specific bins. Although individual SPORES (Spatially explicit, Practically Optimal Results) didn't reveal strong dependencies between particular flexibility measures and system configurations, aggregating data allowed for estimating the required flexibility at various VRE penetration levels. The results suggest that total flexibility demand increases with VRE, and the distribution of flexibility measures shifts as VRE levels rise.

How can integrating specific energy system dynamics improve the modeling of flexibility needs in long-term energy models?

Integrating specific energy system dynamics into an IAM (Integrated Assessment Model) to better model flexibility needs has proven to be a complex challenge. The core objective was to develop a method to exchange data between two models by matching the worlds based on the VRE penetration variable. This alignment allowed us to determine the capacity required for each identified flexibility measure and the associated costs.

One key advantage of this approach is that it allows for a more precise definition of interactions and associated costs between different flexibility measures, which were previously modeled in a more aggregated or simplified manner. By incorporating detailed pre-run model results, the improved framework enhances the accuracy of cost estimations and the understanding of how various flexibility measures interact within the broader energy system.

However, this approach also introduces new complexities. The interactions with existing flexibility variables within the IAM remain relatively basic, potentially oversimplifying the dynamics within the IAM. These interactions may not fully capture the feedback loops and dependencies inherent in real-world energy systems, limiting the model's ability to predict long-term flexibility needs accurately. Additionally, aggregating data to match WITCH's structural assumptions while retaining sufficient detail proved particularly challenging. This trade-off raises concerns about the potential for oversimplification or misalignment between the modeled scenarios and actual system behaviors.

In favor of this integration, the explicit modeling of interactions and costs provides a more transparent and potentially more reliable framework for decision-making. Additionally, even with the higher associated modeled cost that comes with VRE, the model still implemented high levels of VRE. However, the current approach may still struggle to capture the nuanced interplay between the levels of the existing flexibility measures and the introduction of new ones.

6.2.1. Main research question

With the conclusion of the sub-questions, the main research question will now be answered.

What is the influence of varying levels of variable renewable energy (VRE) penetration on the storage requirements in a future energy system?

This research showed that VRE penetration significantly influences storage requirements in future energy systems. In the earlier years, as VRE penetration increased, there was a surge in storage capacity needs. This immediate rise reflects the critical role that storage plays in facilitating the integration of VRE, given the inherent variability and intermittency of renewable energy sources like wind and solar. Substantial storage infrastructure is required immediately to manage the initial influx of VRE effectively.

However, as VRE levels continue to increase, the growth rate in storage requirements begins to taper off. This trend suggests that beyond a certain point, other flexibility measures, particularly grid expansion and sector coupling, will become more prominent in managing the integration of VRE. This can be seen by the exponential increase in sector coupling and transmission expansion from the constructed model in this work.

By introducing these flexibility measures, the system can more effectively manage higher levels of VRE, thereby reducing the strain on storage resources over time. The assessment of flexibility measures found that their interactions not only influence the system's capacity to adopt high levels of VRE but also contribute to more efficient energy generation and a potential reduction in fossil fuel demand, particularly in the transport sector under the Carbon Tax scenario.

The analysis of policy scenarios (Business as Usual and Carbon Tax) using the WITCH model highlighted how flexibility measures and storage requirements evolve under varying conditions. In the Carbon Tax scenario, higher levels of VRE were economically viable due to the additional cost of fossil-based technologies. This scenario also saw a greater reliance on biomass with carbon capture and storage (CCS), which provided the necessary firm capacity to complement the variability of renewables.

In conclusion, VRE penetration significantly impacts storage requirements, but this can be managed effectively by deploying a strategic mix of flexibility measures. Policymakers play a crucial role in this transition. They must create supportive frameworks, encourage innovation, and focus on developing emerging technologies. A holistic approach to energy system design, grounded in existing technical configurations and energy models, is essential for modeling future trajectories. By taking these steps, policymakers can help ensure that future energy systems are sustainable, resilient, and capable of integrating high levels of renewable energy while remaining relatively cost-effective.

References

[1] Mustafa E Amiryar and Keith R Pullen. “A review of flywheel energy storage system technologies and their applications”. In: *Applied Sciences* 7.3 (2017), p. 286.

[2] Guido Ardizzon, Giovanna Cavazzini, and Giorgio Pavesi. “A new generation of small hydro and pumped-hydro power plants: Advances and future challenges”. In: *Renewable and Sustainable Energy Reviews* 31 (2014), pp. 746–761.

[3] Angel A Bayod-Rujula, Marta E Haro-Larrodé, and Amaya Martínez-Gracia. “Sizing criteria of hybrid photovoltaic–wind systems with battery storage and self-consumption considering interaction with the grid”. In: *Solar Energy* 98 (2013), pp. 582–591.

[4] Marc Beaudin et al. “Energy storage for mitigating the variability of renewable electricity sources: An updated review”. In: *Energy for sustainable development* 14.4 (2010), pp. 302–314.

[5] John Bistline et al. “Energy storage in long-term system models: a review of considerations, best practices, and research needs”. In: *Progress in Energy* 2.3 (2020), p. 032001.

[6] Herib Blanco and André Faaij. “A review at the role of storage in energy systems with a focus on Power to Gas and long-term storage”. In: *Renewable and Sustainable Energy Reviews* 81 (2018), pp. 1049–1086.

[7] Alexander Bonk et al. “Advanced heat transfer fluids for direct molten salt line-focusing CSP plants”. In: *Progress in Energy and Combustion Science* 67 (2018), pp. 69–87.

[8] Maarten Brinkerink. “Assessing 1.5-2° C scenarios of integrated assessment models from a power system perspective-Linkage with a detailed hourly global electricity model”. In: *IIASA YSSP* (2020).

[9] *Calliope — github.com*. `https://github.com/calliope-project`. [Accessed 18-07-2024].

[10] Samuel Carrara and Giacomo Marangoni. “Including system integration of variable renewable energies in a constant elasticity of substitution framework: the case of the WITCH model”. In: *Energy Economics* 64 (2017), pp. 612–626.

[11] Enrica De Cian et al. “The 2008 WITCH model: new model features and baseline”. In: (2009).

[12] JP Deane et al. “Soft-linking of a power systems model to an energy systems model”. In: *Energy* 42.1 (2012), pp. 303–312.

[13] Jérôme Dujardin et al. “Interplay between photovoltaic, wind energy and storage hydropower in a fully renewable Switzerland”. In: *Energy* 135 (2017), pp. 513–525.

[14] Orhan Ekren and Banu Yetkin Ekren. “Size optimization of a PV/wind hybrid energy conversion system with battery storage using response surface methodology”. In: *Applied energy* 85.11 (2008), pp. 1086–1101.

[15] SA Farghal and MR Abdel Aziz. “Generation expansion planning including the renewable energy sources”. In: *IEEE Transactions on Power Systems* 3.3 (1988), pp. 816–822.

[16] Paolo Gabrielli et al. “Optimal design of multi-energy systems with seasonal storage”. In: *Applied Energy* 219 (2018), pp. 408–424.

[17] Hans Christian Gils et al. “Integrated modelling of variable renewable energy-based power supply in Europe”. In: *Energy* 123 (2017), pp. 173–188.

[18] Hans Christian Gils et al. “Modeling flexibility in energy systems—comparison of power sector models based on simplified test cases”. In: *Renewable and Sustainable Energy Reviews* 158 (2022), p. 111995.

[19] Chen Chris Gong et al. “Bidirectional coupling of the long-term integrated assessment model REgional Model of INvestments and Development (REMIND) v3. 0.0 with the hourly power sector model Dispatch and Investment Evaluation Tool with Endogenous Renewables (DIETER) v1. 0.2”. In: *Geoscientific Model Development* 16.17 (2023), pp. 4977–5033.

[20] Jannik Haas et al. “Challenges and trends of energy storage expansion planning for flexibility provision in low-carbon power systems–a review”. In: *Renewable and Sustainable Energy Reviews* 80 (2017), pp. 603–619.

[21] Mathijs Harmsen et al. “Integrated assessment model diagnostics: key indicators and model evolution”. In: *Environmental Research Letters* 16.5 (2021), p. 054046.

[22] Clara F Heuberger et al. “Impact of myopic decision-making and disruptive events in power systems planning”. In: *Nature Energy* 3.8 (2018), pp. 634–640.

[23] Kai Heussen et al. “Unified system-level modeling of intermittent renewable energy sources and energy storage for power system operation”. In: *IEEE Systems Journal* 6.1 (2011), pp. 140–151.

[24] Lion Hirth, Falko Ueckerdt, and Ottmar Edenhofer. “Integration costs revisited–An economic framework for wind and solar variability”. In: *Renewable Energy* 74 (2015), pp. 925–939.

[25] Chad A Hunter et al. “Techno-economic analysis of long-duration energy storage and flexible power generation technologies to support high-variable renewable energy grids”. In: *Joule* 5.8 (2021), pp. 2077–2101.

[26] Hussein Ibrahim, Adrian Ilinca, and Jean Perron. “Energy storage systems—Characteristics and comparisons”. In: *Renewable and sustainable energy reviews* 12.5 (2008), pp. 1221–1250.

[27] Nils Johnson et al. “A reduced-form approach for representing the impacts of wind and solar PV deployment on the structure and operation of the electricity system”. In: *Energy Economics* 64 (2017), pp. 651–664.

[28] Jakub Jurasz et al. “A review on the complementarity of renewable energy sources: Concept, metrics, application and future research directions”. In: *Solar Energy* 195 (2020), pp. 703–724.

[29] Seama Koohi-Fayegh and Marc A Rosen. “A review of energy storage types, applications and recent developments”. In: *Journal of Energy Storage* 27 (2020), p. 101047.

[30] Chun Sing Lai et al. “A comprehensive review on large-scale photovoltaic system with applications of electrical energy storage”. In: *Renewable and Sustainable Energy Reviews* 78 (2017), pp. 439–451.

[31] Chun Sing Lai et al. “A review on long-term electrical power system modeling with energy storage”. In: *Journal of Cleaner Production* 280 (2021), p. 124298.

[32] Lukas Lanz et al. “Comparing the levelized cost of electric vehicle charging options in Europe”. In: *Nature Communications* 13.1 (2022), p. 5277.

[33] Tianye Liu, Zhen Yang, and Yuanyuan Duan. “Short-and long-duration cooperative energy storage system: Optimizing sizing and comparing rule-based strategies”. In: *Energy* 281 (2023), p. 128273.

[34] Francesco Lombardi, Matteo Vincenzo Rocco, and Emanuela Colombo. “A multi-layer energy modelling methodology to assess the impact of heat-electricity integration strategies: The case of the residential cooking sector in Italy”. In: *Energy* 170 (2019), pp. 1249–1260.

[35] Gunnar Luderer et al. “Assessment of wind and solar power in global low-carbon energy scenarios: an introduction”. In: *Energy Economics* 64 (2017), pp. 542–551.

[36] Xing Luo et al. “Overview of current development in electrical energy storage technologies and the application potential in power system operation”. In: *Applied energy* 137 (2015), pp. 511–536.

[37] Patrick Moriarty and Damon Honnery. “Can renewable energy power the future?” In: *Energy policy* 93 (2016), pp. 3–7.

[38] FM Mulder. “Implications of diurnal and seasonal variations in renewable energy generation for large scale energy storage”. In: *Journal of Renewable and Sustainable Energy* 6.3 (2014).

[39] Furquan Nadeem et al. “Comparative review of energy storage systems, their roles, and impacts on future power systems”. In: *IEEE access* 7 (2018), pp. 4555–4585.

[40] Georgios Papaefthymiou and Ken Dragoon. “Towards 100% renewable energy systems: Uncapping power system flexibility”. In: *Energy Policy* 92 (2016), pp. 69–82.

[41] Stefan Pfenninger and Bryn Pickering. “Calliope: a multi-scale energy systems modelling framework”. In: *Journal of Open Source Software* 3.29 (2018), p. 825.

[42] Bryn Pickering, Francesco Lombardi, and Stefan Pfenninger. “Decision support for renewables deployment through spatially explicit energy system alternatives”. In: *EGU General Assembly Conference Abstracts*. 2021, EGU21–16205.

[43] Bryn Pickering, Francesco Lombardi, and Stefan Pfenninger. “Diversity of options to eliminate fossil fuels and reach carbon neutrality across the entire European energy system”. In: *Joule* 6.6 (2022), pp. 1253–1276.

[44] Robert C Pietzcker et al. “System integration of wind and solar power in integrated assessment models: a cross-model evaluation of new approaches”. In: *Energy Economics* 64 (2017), pp. 583–599.

[45] André Pina, Carlos A Silva, and Paulo Ferrão. “High-resolution modeling framework for planning electricity systems with high penetration of renewables”. In: *Applied Energy* 112 (2013), pp. 215–223.

[46] Kris Poncelet et al. “Impact of the level of temporal and operational detail in energy-system planning models”. In: *Applied Energy* 162 (2016), pp. 631–643.

[47] Joeri Rogelj et al. “Paris Agreement climate proposals need a boost to keep warming well below 2 C”. In: *Nature* 534.7609 (2016), pp. 631–639.

[48] Katrin Schaber. “Integration of Variable Renewable Energies in the European power system: a model-based analysis of transmission grid extensions and energy sector coupling”. PhD thesis. Technische Universität München, 2014.

[49] Oliver Schmidt et al. “Projecting the future levelized cost of electricity storage technologies”. In: *Joule* 3.1 (2019), pp. 81–100.

[50] Pernille Seljom et al. “Bidirectional linkage between a long-term energy system and a short-term power market model”. In: *Energy* 198 (2020), p. 117311.

[51] Rui Shan et al. “Evaluating emerging long-duration energy storage technologies”. In: *Renewable and Sustainable Energy Reviews* 159 (2022), p. 112240.

[52] Wei Shen et al. “A comprehensive review of variable renewable energy levelized cost of electricity”. In: *Renewable and Sustainable Energy Reviews* 133 (2020), p. 110301.

[53] Simon R Sinsel, Rhea L Riemke, and Volker H Hoffmann. “Challenges and solution technologies for the integration of variable renewable energy sources—a review”. In: *renewable energy* 145 (2020), pp. 2271–2285.

[54] Florian Steinke, Philipp Wolfrum, and Clemens Hoffmann. “Grid vs. storage in a 100% renewable Europe”. In: *Renewable energy* 50 (2013), pp. 826–832.

[55] *The WITCH model — witchmodel.org*. `https://www.witchmodel.org/`. [Accessed 19-07-2024].

[56] Thomas TD Tran and Amanda D Smith. “Incorporating performance-based global sensitivity and uncertainty analysis into LCOE calculations for emerging renewable energy technologies”. In: *Applied energy* 216 (2018), pp. 157–171.

[57] Elena Verdolini, Francesco Vona, and David Popp. “Bridging the gap: Do fast-reacting fossil technologies facilitate renewable energy diffusion?” In: *Energy Policy* 116 (2018), pp. 242–256.

[58] Artur Wyrwa et al. “A new approach for coupling the short-and long-term planning models to design a pathway to carbon neutrality in a coal-based power system”. In: *Energy* 239 (2022), p. 122438.

[59] Yuqing Yang et al. “Battery energy storage system size determination in renewable energy systems: A review”. In: *Renewable and Sustainable Energy Reviews* 91 (2018), pp. 109–125.

[60] Zhi Zhang et al. “Equalizing multi-temporal scale adequacy for low carbon power systems by co-planning short-term and seasonal energy storage”. In: *Journal of Energy Storage* 84 (2024), p. 111518.

A

Figures and equations

A.1. Correlation matrix

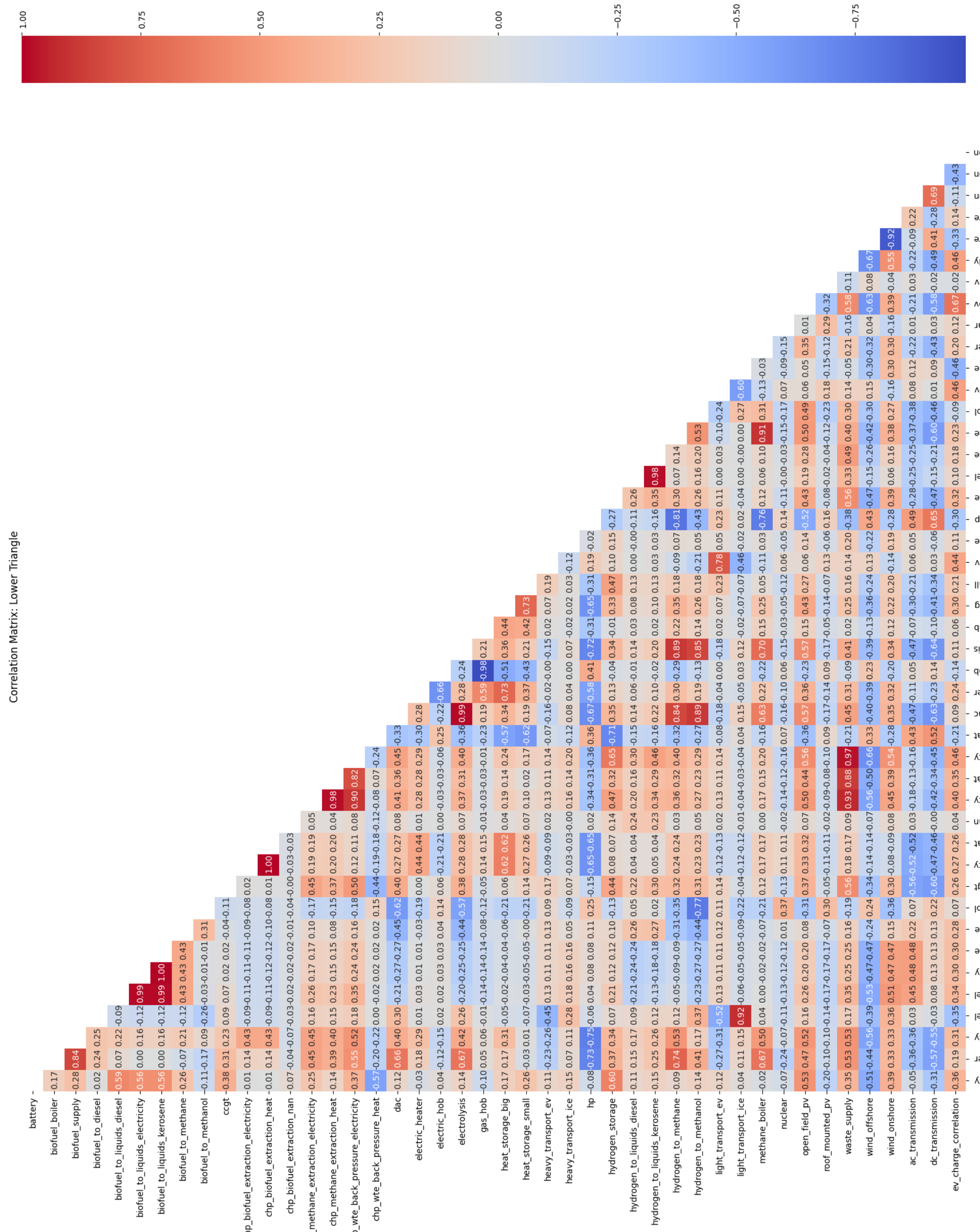


Figure A.1: Correlation matrix of the variables in Calliope

A.2. Cost reduction

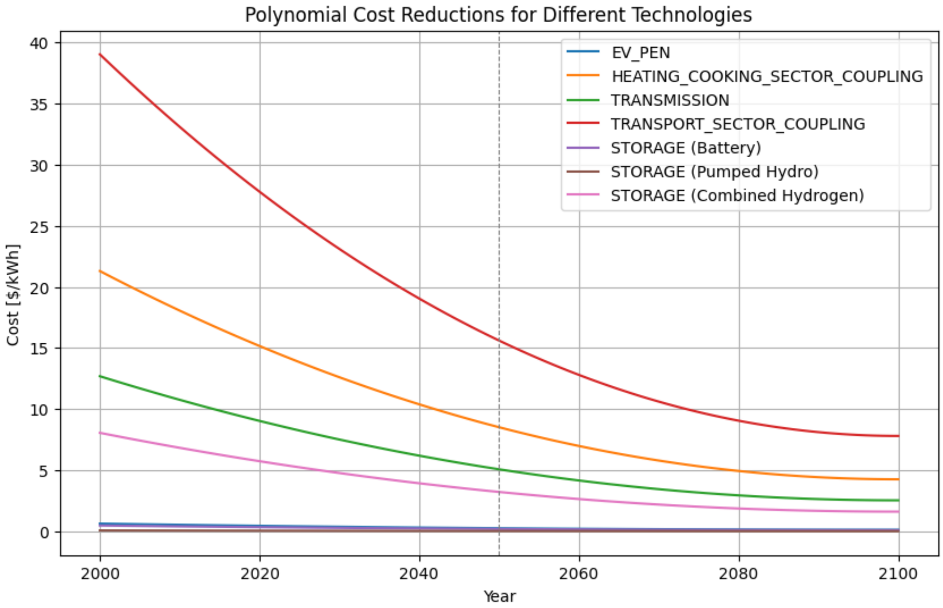


Figure A.2: Cost reduction flexibility measures

A.3. WITCH

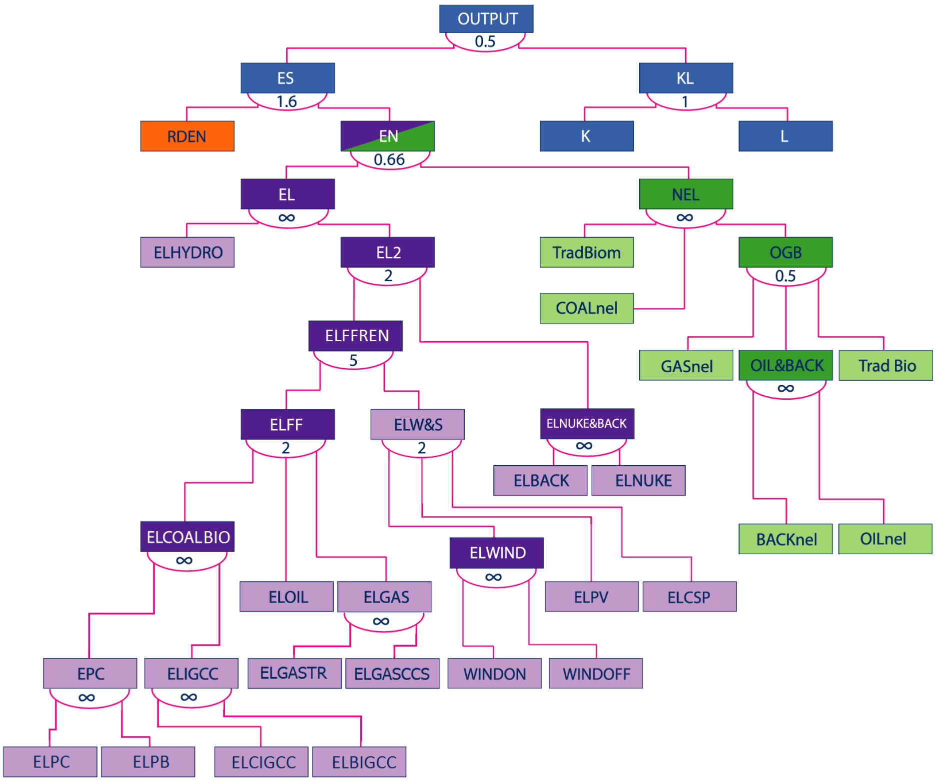


Figure A.3: Production function in WITCH

A.4. Equations

eqfirm_capacity_%clt%(t,n) $\quad \forall(t,n) \in$ mapn('%clt%') $\quad$ and $\quad$ year$(t) > 2005$

$$
\begin{aligned}
&\sum_{jel\_firm} K\_EN(jel\_firm,t,n) + \sum_{jreal\_stor} K\_EN(jreal\_stor,t,n) \cdot \text{cap\_coeff\_stor}(jreal\_stor) \\
&\quad + \Bigg(\sum_{(wind\_dist,wind\_class)} K\_EN\_WINDON(wind\_dist,wind\_class,t,n) \cdot \text{cap\_factor}(wind\_class) \\
&\quad + \sum_{(wind\_dist,wind\_depth,wind\_class)} K\_EN\_WINDOFF(wind\_dist,wind\_depth,wind\_class,t,n) \\
&\quad \cdot \text{cap\_factor}(wind\_class) \\
&\quad \cdot \text{cv\_coeff} \cdot \exp\left(\text{cv\_exp} \cdot \frac{Q\_EN('elwind',t,n)}{Q\_EN.l('el',t,n)}\right) \\
&\quad + \sum_{(solar\_dist,solar\_class)} \frac{K\_EN\_PV(solar\_dist,solar\_class,t,n) \cdot \text{solar\_mu}(solar\_class,'elpv')}{\text{yearly\_hours}} \\
&\quad \cdot \text{cv\_coeff} \cdot \exp\left(\text{cv\_exp} \cdot \frac{Q\_EN('elpv',t,n)}{Q\_EN.l('el',t,n)}\right) \\
&\geq \text{firm\_coeff}(n) \cdot \Bigg(Q\_EN('el',t,n) - \sum_{ices\_el} QEL\_OUT('edv',ices\_el,t,n) \\
&\quad - \sum_{ices\_el} QEL\_OUT('edvfr',ices\_el,t,n)/\text{yearly\_hours}
\end{aligned}
\tag{A.1}
$$

B

Source code

The entire code and all the data utilized in this thesis can be found on the GitHub repository: `https://github.com/Jessedehaan123/witch`.

B.1. Variable Mapping

B.1.1. WITCH Scenarios utilized to create the variable mapping

Scenario	Scenario	Scenario
NAV_Dem-15C-act_d	NAV_Dem-20C-act_d	SUP_1p5C_Elec
NAV_Dem-15C-act_u	NAV_Dem-20C-act_u	SUP_1p5C_Elec_HighVRE
NAV_Dem-15C-all_d	NAV_Dem-20C-all_d	SUP_1p5C_Elec_LimCCS
NAV_Dem-15C-all_u	NAV_Dem-20C-all_u	SUP_1p5C_Elec_LimNuc
NAV_Dem-15C-ele_d	NAV_Dem-20C-ele_d	SUP_1p5C_Regional
NAV_Dem-15C-ele_u	NAV_Dem-20C-ele_u	SUP_2C_Comb
NAV_Dem-15C-ref	NAV_Dem-20C-ref	SUP_2C_Comb_HighVRE
NAV_Dem-15C-tec_d	NAV_Dem-20C-tec_d	SUP_2C_Comb_LimCCS
NAV_Dem-15C-tec_u	NAV_Dem-20C-tec_u	SUP_2C_Comb_LimNuc
NAV_Dem-NPi-act	NAV_Dem-NPi-ele	SUP_2C_Default
NAV_Dem-NPi-all	NAV_Dem-NPi-ref	SUP_2C_Elec
NAV_Dem-NPi-tec	PEP-2C-AdvPE	SUP_2C_Elec_HighVRE
PEP-2C-AllEn	SUP_1p5C_Comb	SUP_2C_Elec_LimCCS
PEP-2C-Default	SUP_1p5C_Comb_HighVRE	SUP_2C_Elec_LimNuc
PEP-2C-LowCE	SUP_1p5C_Comb_LimCCS	SUP_2C_Regional
PEP-NPi	SUP_1p5C_Comb_LimNuc	SUP_NPi_Default
ssp2_bau		

Table B.1: List of Scenarios

B.2. Model to predict flexibility

```
# Scale the data to match WITCH data
data['VRE_PENETRATION'] = data['VRE_PENETRATION'] * 0.35
data['STORAGE'] = data['STORAGE'] * 0.40 # scalar for model
data['TRANSMISSION'] = data['TRANSMISSION'] * 0.40
data['EV_PEN'] = data['EV_PEN'] * 0.40 * 0.001  # scalar for model
data['FLEXIBLE_TECHS'] = data['FLEXIBLE_TECHS'] * 0.40
data['HYDROPOWER'] = data['HYDROPOWER'] * 0.40
data['HEATING_COOKING_SECTOR_COUPLING'] = data['HEATING_COOKING_SECTOR_COUPLING'] * 0.30 # scalar for model
data['TRANSPORT_SECTOR_COUPLING'] = data['TRANSPORT_SECTOR_COUPLING'] * 0.30 # scalar for model

```

```python
# Define flexibility variables excluding hydropower for total flexibility prediction
flexibility_variables = [
    'TRANSMISSION',
    'EV_PEN',
    'FLEXIBLE_TECHS',
    'HEATING_COOKING_SECTOR_COUPLING',
    'TRANSPORT_SECTOR_COUPLING',
    'STORAGE'
]

# Sum the flexibility variables to get total flexibility
data['Total_Flexibility'] = data[flexibility_variables].sum(axis=1)

# Define predictors for total flexibility
X_flex = data[['VRE_PENETRATION']]
X_flex = sm.add_constant(X_flex)  # Add a constant term for the intercept
y_flex = data['Total_Flexibility']

# Perform regression analysis to predict total flexibility
model_flex = sm.OLS(y_flex, X_flex).fit()
data['Predicted_Total_Flexibility'] = model_flex.predict(X_flex)

# Display the summary of the regression model for total flexibility
summary_model_flex = model_flex.summary()
print("Summary of Regression Model for Total Flexibility:\n", summary_model_flex)

# Retrieve coefficients
alpha = model_flex.params['const']
beta1 = model_flex.params['VRE_PENETRATION']

# Print the equation in GAMS form
equation_gams = f"* Equation to predict total flexibility\n" \
                f"eq_flexibility_prediction(t, n)..\n" \
                f"    Predicted_Total_Flexibility(t, n) =e= {alpha:.6f} + {beta1:.6f} * VRE_PENETRATION(t, n);"
print(equation_gams)

# Plot Total Flexibility vs. Predictors
plt.figure(figsize=(10, 6))
sns.scatterplot(x=data['VRE_PENETRATION'], y=data['Total_Flexibility'], label='Total Flexibility from Calliope SPORE')
sns.lineplot(x=data['VRE_PENETRATION'], y=data['Predicted_Total_Flexibility'], label='Predicted Total Flexibility', color='red')
plt.xlabel('Scaled VRE Penetration (TW)')
plt.ylabel('Total Flexibility')
plt.legend()
plt.title('Total Flexibility vs. VRE Penetration')
plt.show()

# Perform linear interpolation and extrapolation for missing VRE penetration values
# Generate intermediate VRE penetration values
vre_range = np.linspace(data['VRE_PENETRATION'].min(), data['VRE_PENETRATION'].max(), 100)

# Linear interpolation for each flexibility variable excluding hydropower based on VRE penetration
interpolated_data = pd.DataFrame({'VRE_PENETRATION': vre_range})
for var in flexibility_variables:
    interp_func = np.poly1d(np.polyfit(data['VRE_PENETRATION'], data[var], 1))  # Fit a linear model
    interpolated_data[var] = interp_func(vre_range)  # Generate interpolated values
    # Ensure no negative values
    interpolated_data[var] = interpolated_data[var].clip(lower=0)

# Keep hydropower constant
interpolated_data['HYDROPOWER'] = data['HYDROPOWER'].mean()

# Sum the interpolated flexibility variables to get total flexibility
interpolated_data['Total_Flexibility'] = interpolated_data[flexibility_variables].sum(axis=1) + interpolated_data['HYDROPOWER']

```

```python
# Normalize each flexibility variable using min-max scaling and store the min and max values for later
scaler = MinMaxScaler()
scaler.fit(data[flexibility_variables + ['HYDROPOWER']])
interpolated_data[flexibility_variables + ['HYDROPOWER']] = scaler.transform(interpolated_data[flexibility_variables + ['HYDROPOWER']])

# Create equal-width bins for Predicted Total Flexibility
flex_bins = np.linspace(interpolated_data['Total_Flexibility'].min(), interpolated_data['Total_Flexibility'].max(), 10)
interpolated_data['Flex_Bin'] = pd.cut(interpolated_data['Total_Flexibility'], bins=flex_bins, labels=False, include_lowest=True)

# Add the bin assignment back to the original data for GAMS
data['Flex_Bin'] = pd.cut(data['Predicted_Total_Flexibility'], bins=flex_bins, labels=False, include_lowest=True)

# Calculate the average level of each flexibility option within each bin
avg_flexibility_options = interpolated_data.groupby('Flex_Bin')[flexibility_variables + ['HYDROPOWER']].mean()

# Reverse the normalization to get back to actual values
avg_flexibility_options_actual = pd.DataFrame(scaler.inverse_transform(avg_flexibility_options), columns=flexibility_variables + ['HYDROPOWER'])

plt.rcParams.update({'font.size': 14})

plt.figure(figsize=(16, 10))
ax = avg_flexibility_options.plot(kind='bar', stacked=True, colormap='viridis', width=0.8, figsize=(16, 10))

plt.title('Normalized Flexibility Options for Increasing Levels of Predicted Total Flexibility', fontsize=18)
plt.xlabel('Predicted Total Flexibility Bins', fontsize=16)
plt.ylabel('Normalized Average Level of Flexibility Options', fontsize=16)
plt.xticks(ticks=np.arange(len(flex_bins)-1), labels=[f'{flex_bins[i]:.2f} - {flex_bins[i+1]:.2f}' for i in range(len(flex_bins)-1)], rotation=45, fontsize=14)
plt.yticks(fontsize=14)
plt.legend(title='Flexibility Options', bbox_to_anchor=(1.05, 1), loc='upper left', fontsize='large', title_fontsize='16')
plt.grid(True)
plt.tight_layout()
plt.show()

# Display the actual values of the needed flexibility variables for each box
print("\nActual values of the needed flexibility variables for each box per EJ demand:\n", avg_flexibility_options_actual)

# Save the data with bin assignments to a CSV file for GAMS import
print(data[['VRE_PENETRATION', 'Predicted_Total_Flexibility', 'Flex_Bin']])
```

Table B.2: Summary of Regression Model for Total Flexibility

Statistic	Value	
Dependent Variable	Total Flexibility	
R-squared	0.685	
Model	OLS	
Adjusted R-squared	0.685	
Method	Least Squares	
F-statistic	1324	
Date	Wed, 14 Aug 2024	
Prob (F-statistic)	8.75e-155	
Time	12:09:15	
Log-Likelihood	-566.84	
No. Observations	610	
AIC	1138	
Df Residuals	608	
BIC	1146	
Df Model	1	
Covariance Type	Nonrobust	
Variable	**Coefficient**	**Standard Error**
const	0.6926	0.060
VRE_PENETRATION	1.4416	0.040
Additional Statistics	**Value**	
Omnibus	123.847	
Durbin-Watson	1.179	
Prob(Omnibus)	0.000	
Jarque-Bera (JB)	313.401	
Skew	1.032	
Prob(JB)	8.83e-69	
Kurtosis	5.841	
Cond. No.	5.01	

B.3. LCOE and LCOS calculation

```python
# Constants
discount_rate = 0.05
hours_per_year = 8000

def annualize_capex(capex, lifetime, discount_rate):
    return capex * (discount_rate * (1 + discount_rate) ** lifetime) / ((1 + discount_rate)
        ** lifetime - 1)

def calculate_lcoe(capex, om_annual, om_prod, efficiency, lifetime, discount_rate,
    hours_per_year):
    annualized_capex = annualize_capex(capex, lifetime, discount_rate)
    total_annual_costs = annualized_capex + om_annual + (om_prod * efficiency *
        hours_per_year)
    total_energy_production = efficiency * hours_per_year * lifetime
    lcoe = total_annual_costs / total_energy_production
    return lcoe

# Storage Technologies with round trip efficiencies
capex_battery_storage = 8.558536 * 1e4
om_annual_battery_storage = 0.126224 * 1e4
om_prod_battery_storage = 3.78e-5 * 1e4
efficiency_battery_storage_round_trip = 0.86
lifetime_battery_storage = 10

capex_pumped_hydro_storage = 103.833246 * 1e4
om_annual_pumped_hydro_storage = 0.735726 * 1e4
om_prod_pumped_hydro_storage = 0.000102 * 1e4
efficiency_pumped_hydro_storage_round_trip = 0.78
```

```
lifetime_pumped_hydro_storage = 55

capex_hydrogen_electricity_storage = 161.181471 * 1e4
om_annual_hydrogen_electricity_storage = 1.368708 * 1e4
om_prod_hydrogen_electricity_storage = 0  # not provided
efficiency_hydrogen_electricity_storage_round_trip = 0.40
lifetime_hydrogen_electricity_storage = 15

capex_hydrogen_storage = 2.1 * 1e4
om_annual_hydrogen_storage = 0.04 * 1e4
om_prod_hydrogen_storage = 0  # not provided
efficiency_hydrogen_storage_round_trip = 0.81
lifetime_hydrogen_storage = 30

# Calculate LCOE for storage technologies
lcoe_battery_storage_round_trip = calculate_lcoe(capex_battery_storage, om_annual_battery_storage, om_prod_battery_storage, efficiency_battery_storage_round_trip, lifetime_battery_storage, discount_rate, hours_per_year)
lcoe_pumped_hydro_storage_round_trip = calculate_lcoe(capex_pumped_hydro_storage, om_annual_pumped_hydro_storage, om_prod_pumped_hydro_storage, efficiency_pumped_hydro_storage_round_trip, lifetime_pumped_hydro_storage, discount_rate, hours_per_year)
lcoe_hydrogen_electricity_storage_round_trip = calculate_lcoe(capex_hydrogen_electricity_storage, om_annual_hydrogen_electricity_storage, om_prod_hydrogen_electricity_storage, efficiency_hydrogen_electricity_storage_round_trip, lifetime_hydrogen_electricity_storage, discount_rate, hours_per_year)
lcoe_hydrogen_storage_round_trip = calculate_lcoe(capex_hydrogen_storage, om_annual_hydrogen_storage, om_prod_hydrogen_storage, efficiency_hydrogen_storage_round_trip, lifetime_hydrogen_storage, discount_rate, hours_per_year)

# Conversion Technologies
capex_biofuel_diesel = 93000
om_annual_biofuel_diesel = 2700
om_prod_biofuel_diesel = 0.131
efficiency_biofuel_diesel = 0.6
lifetime_biofuel_diesel = 20

capex_biofuel_liquids = 516832.0802005012
om_annual_biofuel_liquids = 15534.837092731827
om_prod_biofuel_liquids = 0.00015878395989974935
efficiency_biofuel_liquids = 0.1995  # considering diesel output only as primary
lifetime_biofuel_liquids = 25

capex_hydrogen_liquids = 150000
om_annual_hydrogen_liquids = 9866.666666666667
om_prod_hydrogen_liquids = 0.00035000000000000005
efficiency_hydrogen_liquids = 0.45  # considering kerosene output as primary
lifetime_hydrogen_liquids = 25

capex_biofuel_methanol = 146000
om_annual_biofuel_methanol = 3900
om_prod_biofuel_methanol = 0.00136
efficiency_biofuel_methanol = 0.22
lifetime_biofuel_methanol = 20

capex_biofuel_methane = 214285.71428571433
om_annual_biofuel_methane = 3442.857142857143
om_prod_biofuel_methane = 0.00022857142857142862
efficiency_biofuel_methane = 0.7
lifetime_biofuel_methane = 20

capex_hydrogen_methane = 30000
om_annual_hydrogen_methane = 3440
om_prod_hydrogen_methane = 0  # not provided
efficiency_hydrogen_methane = 1 / 1.21  # considering efficiency from carrier ratios
lifetime_hydrogen_methane = 20

capex_electrolysis = 60862.91306327804
om_annual_electrolysis = 2705.592910547868
om_prod_electrolysis = 0  # not provided
```

```
efficiency_electrolysis = 0.7173333333333334
lifetime_electrolysis = 23.333333333333332

capex_dac = 1592000  # as per tCO2 to energy conversion
om_annual_dac = capex_dac * 0.04
om_prod_dac = 0  # not provided
efficiency_dac = 1 / 50.0  # converting tCO2/MWh to MWh/tCO2
lifetime_dac = 30

# Calculate LCOE for conversion technologies
lcoe_biofuel_diesel = calculate_lcoe(capex_biofuel_diesel, om_annual_biofuel_diesel, om_prod_biofuel_diesel, efficiency_biofuel_diesel, lifetime_biofuel_diesel, discount_rate, hours_per_year)
lcoe_biofuel_liquids = calculate_lcoe(capex_biofuel_liquids, om_annual_biofuel_liquids, om_prod_biofuel_liquids, efficiency_biofuel_liquids, lifetime_biofuel_liquids, discount_rate, hours_per_year)
lcoe_hydrogen_liquids = calculate_lcoe(capex_hydrogen_liquids, om_annual_hydrogen_liquids, om_prod_hydrogen_liquids, efficiency_hydrogen_liquids, lifetime_hydrogen_liquids, discount_rate, hours_per_year)
lcoe_biofuel_methanol = calculate_lcoe(capex_biofuel_methanol, om_annual_biofuel_methanol, om_prod_biofuel_methanol, efficiency_biofuel_methanol, lifetime_biofuel_methanol, discount_rate, hours_per_year)
lcoe_biofuel_methane = calculate_lcoe(capex_biofuel_methane, om_annual_biofuel_methane, om_prod_biofuel_methane, efficiency_biofuel_methane, lifetime_biofuel_methane, discount_rate, hours_per_year)
lcoe_hydrogen_methane = calculate_lcoe(capex_hydrogen_methane, om_annual_hydrogen_methane, om_prod_hydrogen_methane, efficiency_hydrogen_methane, lifetime_hydrogen_methane, discount_rate, hours_per_year)
lcoe_electrolysis = calculate_lcoe(capex_electrolysis, om_annual_electrolysis, om_prod_electrolysis, efficiency_electrolysis, lifetime_electrolysis, 0.1, hours_per_year)
lcoe_dac = calculate_lcoe(capex_dac, om_annual_dac, om_prod_dac, efficiency_dac, lifetime_dac, 0.07, hours_per_year)

# Collect results
lcoe_storage_round_trip_results = {
    'Battery Storage (Round Trip)': lcoe_battery_storage_round_trip,
    'Pumped Hydro Storage (Round Trip)': lcoe_pumped_hydro_storage_round_trip,
    'Hydrogen Electricity Storage (Round Trip)': lcoe_hydrogen_electricity_storage_round_trip,
    'Hydrogen Storage (Tank) (Round Trip)': lcoe_hydrogen_storage_round_trip
}

lcoe_conversion_results = {
    'Biofuel to Diesel': lcoe_biofuel_diesel,
    'Biofuel to Liquids': lcoe_biofuel_liquids,
    'Hydrogen to Liquids': lcoe_hydrogen_liquids,
    'Biofuel to methanol': lcoe_biofuel_methanol,
    'Biofuel to methane': lcoe_biofuel_methane,
    'Hydrogen to methane': lcoe_hydrogen_methane,
    'Electrolysis': lcoe_electrolysis,
    'dac': lcoe_dac
}
```

B.3.1. Including DAC and electrolysis in the costs

```
# DAC parameters
dac_capex = 15.92 * 1e5  # EUR/tCO2
dac_lifetime = 30  # years
dac_interest_rate = 0.07
dac_annual_op_fraction = 0.04

# Annualize CAPEX for DAC
def annualize_capex(capex, lifetime, discount_rate):
    return capex * (discount_rate * (1 + discount_rate) ** lifetime) / ((1 + discount_rate) ** lifetime - 1)

dac_annualized_capex = annualize_capex(dac_capex, dac_lifetime, dac_interest_rate)
dac_annual_opex = dac_annual_op_fraction * dac_capex
```

```python
# Total annual cost per ton of CO2
dac_total_annual_cost = dac_annualized_capex + dac_annual_opex

# Function to calculate LCOS
def calculate_lcos(capex, om_annual, om_prod, co2_input, efficiency, lifetime, discount_rate=0.05, capacity_factor=1):
    effective_hours_per_year = 8760 * capacity_factor

    # CO2 capture cost per MWh of input energy
    total_co2_cost_per_mwh = co2_input * dac_total_annual_cost / 1e3  # Convert from per ton to per kWh

    # Annualize CAPEX
    annualized_capex = annualize_capex(capex, lifetime, discount_rate)

    # Total annual costs (including CO2 capture)
    total_annual_costs = annualized_capex + om_annual + om_prod * effective_hours_per_year + total_co2_cost_per_mwh * effective_hours_per_year * efficiency

    # Total energy production over the lifetime
    total_energy_production = effective_hours_per_year * lifetime * efficiency

    # Calculate LCOS
    lcos = total_annual_costs / total_energy_production
    return lcos

# Input data for technologies
tech_data = {
    'Biofuel to Liquids': {
        'capex': 516.8320802005012 * 1e4, 'om_annual': 15.534837092731827 * 1e4, 'om_prod': 0.00015878395989974935,
        'co2_input': 0, 'efficiency': 0.299, 'lifetime': 25, 'capacity_factor': 1
    },
    'Hydrogen to Liquids': {
        'capex': 150.0 * 1e4, 'om_annual': 9.866666666666667 * 1e4, 'om_prod': 0.00035000000000000005,
        'co2_input': 2.079831932773109, 'efficiency': 0.75, 'lifetime': 25, 'capacity_factor': 1
    },
    'Biofuel to Diesel': {
        'capex': 93.0 * 1e4, 'om_annual': 2.7 * 1e4, 'om_prod': 0.000131,
        'co2_input': 0, 'efficiency': 0.6, 'lifetime': 20, 'capacity_factor': 1
    },
    'Biofuel to Methanol': {
        'capex': 146.0 * 1e4, 'om_annual': 3.9000000000000004 * 1e4, 'om_prod': 0.00136,
        'co2_input': 0, 'efficiency': 0.22, 'lifetime': 20, 'capacity_factor': 1
    },
    'Hydrogen to Methanol': {
        'capex': 150.0 * 1e4, 'om_annual': 5.3 * 1e4, 'om_prod': 0.000627,
        'co2_input': 1.5950205982446712, 'efficiency': 0.65, 'lifetime': 20, 'capacity_factor': 1
    },
    'Biofuel to Methane': {
        'capex': 214.28571428571433 * 1e4, 'om_annual': 3.442857142857143 * 1e4, 'om_prod': 0.00022857142857142862,
        'co2_input': 0, 'efficiency': 0.7, 'lifetime': 20, 'capacity_factor': 1
    },
    'Hydrogen to Methane': {
        'capex': 30.0 * 1e4, 'om_annual': 3.44 * 1e4, 'om_prod': 0,
        'co2_input': 1.6198347107438018, 'efficiency': 0.65, 'lifetime': 20, 'capacity_factor': 1
    },
    'Electrolysis': {
        'capex': 60.86291306327804 * 1e4, 'om_annual': 2.705592910547868 * 1e4, 'om_prod': 0,
        'co2_input': 0, 'efficiency': 0.7173333333333334, 'lifetime': 23.333333333333332, 'capacity_factor': 1
    }
}

# Calculate LCOS for each technology
lcos_results = {}
```

```
for tech, data in tech_data.items():
    lcos = calculate_lcos(
        capex=data['capex'], om_annual=data['om_annual'], om_prod=data['om_prod'],
        co2_input=data['co2_input'], efficiency=data['efficiency'],
        lifetime=data['lifetime'], capacity_factor=data['capacity_factor']
    )
    lcos_results[tech] = lcos

# Display results in a DataFrame
lcos_df = pd.DataFrame.from_dict(lcos_results, orient='index', columns=['LCOS (EUR/kWh)'])
print(lcos_df)

# Calculate LCOS for Storage Technologies considering round-trip efficiency
storage_data = {
    'Battery': {
        'capex': 10.123820000000002 * 1e4, 'om_annual': 0.126224 * 1e4, 'om_prod': 3.780000000000001e-05,
        'efficiency': 0.86, 'lifetime': 10, 'capacity_factor': 1
    },
    'Pumped Hydro': {
        'capex': 7.357566 * 1e4, 'om_annual': 0.7357260000000001 * 1e4, 'om_prod': 0.00010200000000000001,
        'efficiency': 0.78, 'lifetime': 55, 'capacity_factor': 1
    },
    'Hydrogen Electricity Storage': {
        'capex': 161.18147100000002 * 1e4, 'om_annual': 1.368708 * 1e4, 'om_prod': 0,
        'efficiency': 0.40, 'lifetime': 15, 'capacity_factor': 1
    },
    'Hydrogen Storage': {
        'capex': 2.1 * 1e4, 'om_annual': 0.04 * 1e4, 'om_prod': 0,
        'efficiency': 0.81, 'lifetime': 30, 'capacity_factor': 1
    }
}

# Function to calculate LCOS for storage with round-trip efficiency
def calculate_lcos_storage(capex, om_annual, om_prod, efficiency, lifetime, discount_rate=0.05, capacity_factor=1):
    effective_hours_per_year = 8760 * capacity_factor

    # Annualize CAPEX
    annualized_capex = annualize_capex(capex, lifetime, discount_rate)

    # Total annual costs
    total_annual_costs = annualized_capex + om_annual + om_prod * effective_hours_per_year

    # Total energy production over the lifetime
    total_energy_production = effective_hours_per_year * lifetime * efficiency

    # Calculate LCOS
    lcos = total_annual_costs / total_energy_production
    return lcos

# Calculate LCOS for each storage technology
lcos_storage_results = {}
for tech, data in storage_data.items():
    lcos = calculate_lcos_storage(
        capex=data['capex'], om_annual=data['om_annual'], om_prod=data['om_prod'],
        efficiency=data['efficiency'], lifetime=data['lifetime'],
        capacity_factor=data['capacity_factor']
    )
    lcos_storage_results[tech] = lcos

# Display updated results in a DataFrame
lcos_storage_df = pd.DataFrame.from_dict(lcos_storage_results, orient='index', columns=['LCOS (EUR/kWh)'])
print(lcos_storage_df)

#adding the electrolysis costs to the hydrogen to liquids, hydrogen to methane and hydrogen to methanol
combined_lcos_df.loc['Hydrogen to Liquids'] = combined_lcos_df.loc['Hydrogen to Liquids'] + combined_lcos_df.loc['Electrolysis']
```

```
combined_lcos_df.loc['Hydrogen␣to␣Methane'] = combined_lcos_df.loc['Hydrogen␣to␣Methane'] + combined_lcos_df.loc['Electrolysis']
combined_lcos_df.loc['Hydrogen␣to␣Methanol'] = combined_lcos_df.loc['Hydrogen␣to␣Methanol'] + combined_lcos_df.loc['Electrolysis']
```

B.3.2. Weighted cost calculation

```
# Define the relevant technologies for each sector coupling group with corrected column names in order to calculate the weights for the weighted average LCOS
heating_cooking_techs = [
    "hydrogen_to_methane_nameplate", "chp_biofuel_extraction_nameplate",
    "chp_methane_extraction_nameplate", "chp_wte_back_pressure_nameplate",
    "biofuel_to_methane_nameplate"
]

transport_techs = [
    "biofuel_to_liquids_nameplate", "hydrogen_to_liquids_nameplate",
    "biofuel_to_diesel_nameplate"
]

# Sum the capacities for each technology across all rows
total_capacities = merged_df.sum()

# Calculate the total capacity for each group
total_capacity_heating_cooking = total_capacities[heating_cooking_techs].sum()
total_capacity_transport = total_capacities[transport_techs].sum()

# Calculate the weight for each technology
weights_heating_cooking = total_capacities[heating_cooking_techs] / total_capacity_heating_cooking
weights_transport = total_capacities[transport_techs] / total_capacity_transport

# Convert the weights to a dictionary using concat
weights_dict = pd.concat([weights_heating_cooking, weights_transport]).to_dict()

# Example DataFrame (with Electrolysis already removed)
combined_lcos_df = pd.DataFrame({
    'LCOS␣(EUR/kWh)': [
        7.972615, 17.219606, 0.966769, 4.051632, 16.832475,
        1.682803, 16.061731, 0.190790, 0.030087, 3.223156,
        0.254000, 5.075000, 0.250000, 0.250000, 0.250000
    ],
    'Group': [
        "TRANSPORT_SECTOR_COUPLING", "TRANSPORT_SECTOR_COUPLING", "TRANSPORT_SECTOR_COUPLING",
        "TRANSPORT_SECTOR_COUPLING", "HEATING_COOKING_SECTOR_COUPLING", "HEATING_COOKING_SECTOR_COUPLING",
        "HEATING_COOKING_SECTOR_COUPLING", "STORAGE", "STORAGE", "STORAGE",
        "EV_PEN", "TRANSMISSION", "HEATING_COOKING_SECTOR_COUPLING", "HEATING_COOKING_SECTOR_COUPLING",
        "HEATING_COOKING_SECTOR_COUPLING"
    ]
}, index=[
    "Biofuel␣to␣Liquids", "Hydrogen␣to␣Liquids", "Biofuel␣to␣Diesel",
    "Biofuel␣to␣Methanol", "Hydrogen␣to␣Methanol", "Biofuel␣to␣Methane",
    "Hydrogen␣to␣Methane", "Battery", "Pumped␣Hydro",
    "Combined␣Hydrogen␣Storage", "EV", "transmission",
    "chp_biofuel_extraction_heat", "chp_methane_extraction_heat",
    "chp_wte_back_pressure_heat"
])

# Map weights to technologies
weight_mapping = {
    "Biofuel␣to␣Liquids": weights_dict.get("biofuel_to_liquids_nameplate", 0),
    "Hydrogen␣to␣Liquids": weights_dict.get("hydrogen_to_liquids_nameplate", 0),
    "Biofuel␣to␣Diesel": weights_dict.get("biofuel_to_diesel_nameplate", 0),
    "Biofuel␣to␣Methanol": 0,  # No weight for this technology
    "Hydrogen␣to␣Methanol": weights_dict.get("hydrogen_to_methane_nameplate", 0),
    "Biofuel␣to␣Methane": weights_dict.get("biofuel_to_methane_nameplate", 0),
    "Hydrogen␣to␣Methane": weights_dict.get("hydrogen_to_methane_nameplate", 0),
```

```
    "chp_biofuel_extraction_heat": weights_dict.get("chp_biofuel_extraction_nameplate", 0),
    "chp_methane_extraction_heat": weights_dict.get("chp_methane_extraction_nameplate", 0),
    "chp_wte_back_pressure_heat": weights_dict.get("chp_wte_back_pressure_nameplate", 0)
}

# Assign weights to the DataFrame
combined_lcos_df['Weight'] = combined_lcos_df.index.map(weight_mapping).fillna(0)

# Normalize weights within each group
sector_coupling_groups = ["TRANSPORT_SECTOR_COUPLING", "HEATING_COOKING_SECTOR_COUPLING"]
for group in sector_coupling_groups:
    total_weight = combined_lcos_df[combined_lcos_df['Group'] == group]['Weight'].sum()
    combined_lcos_df.loc[combined_lcos_df['Group'] == group, 'Normalized␣Weight'] =
        combined_lcos_df.loc[combined_lcos_df['Group'] == group, 'Weight'] / total_weight

# Calculate weighted average LCOS for each group
weighted_avg_cost = combined_lcos_df.groupby('Group').apply(lambda x: (x['LCOS␣(EUR/kWh)'] *
    x['Normalized␣Weight']).sum())

# Convert to DataFrame for better readability
weighted_avg_cost_df = pd.DataFrame(weighted_avg_cost, columns=['Weighted␣Average␣LCOS␣(EUR/
    kWh)'])

# Display the weighted average costs per group
print(weighted_avg_cost_df)
```

B.3.3. Cost reduction

```
# Example data points
years = np.linspace(2000, 2100, 100)

# Polynomial cost reduction function
def polynomial_costs(years, a, b, c, cost_2050):
    return cost_2050 * (a + b * (years - 2050) + c * (years - 2050)**2)

# Coefficients for the polynomial
a = 1
b = -0.02
c = 0.0002
# Costs in 2050 for different technologies
costs_2050 = {
    "EV_PEN": 0.254,
    "HEATING_COOKING_SECTOR_COUPLING": 8.516646,
    "TRANSMISSION": 5.075,
    "TRANSPORT_SECTOR_COUPLING": 15.606501,
    "STORAGE␣(Battery)": 0.190790,
    "STORAGE␣(Pumped␣Hydro)": 0.030087,
    "STORAGE␣(Combined␣Hydrogen)": 3.223156
}
```

```
* Define Sets
*-------------------------------------------------------------------------------
$ifthen %phase%=='sets'

* Define flexibility bins
set Flex_Bin 'Flexibility bins' /0*8/;

* Define storage technologies
set j  'technologies' /
str_phes    # Pumped Hydro Electrical Storage
str_lib     # Lithium-ion batteries
str_h2_pem  # Accumulator hydrogen storage
str_meth    # Methane storage
str_caes
str_h2_soec
elpv        # Photovoltaic technology
elwindon    # Onshore wind technology
elwindoff   # Offshore wind technology
elgastr_old
elgastr_new
```

```
elgasccs
elhydro_old
elhydro_new
elpb_new
elpb_old
elbigcc
plg_hybrid
edv
/;

set jreal(j) /
str_phes
str_lib
str_h2_pem
str_meth
str_caes
str_h2_soec
elpv
*elwindon
*elwindoff
/;

set jel(jreal) /
str_phes
str_lib
str_h2_pem
str_meth
str_caes
str_h2_soec
elpv
*elwindon
*elwindoff
/;

set j_stor_jt(j) 'storage technologies' /
str_phes
str_lib
str_h2_pem
str_meth
str_caes
str_h2_soec
/;

set jreal_stor_jt(jreal) /
str_phes
str_lib
str_h2_pem
str_meth
str_caes
str_h2_soec
/;

set jel_stor_jt(jel) /
str_phes
str_lib
str_h2_pem
str_meth
str_caes
str_h2_soec
/;

* Define subsets for short-term and long-term storage
set j_sts(j) 'short-term storage technologies' /
    str_phes
    str_lib
/;

set j_lts(j) 'long-term storage technologies' /
    str_meth
    str_h2_pem
/;
```

```
* Define other flexibility measures
set flexibility_vars 'Flexibility measures' /
    transmission                        # Transmission expansion
    ev_pen                              # Penetration of electric vehicles
    flexible_techs                      # Flexible generation
    heating_cooking_sector_coupling     # Residential sector coupling
    transport_sector_coupling           # Transport sector coupling
    storage                             # Energy storage
    hydropower
/;

set j_curt(j) 'technologies producing curtailment' /  /;

set curt_type 'curtailment type' /
seasonal
short-term
/;

set j_pv_j(j) 'pv technologies' / elpv /;

set j_wind_j(j) 'wind technologies' / elwindon, elwindoff /;

set j_flex(j) 'flexible technologies'/
elgastr_old
elgastr_new
elgasccs
elhydro_old
elhydro_new
elpb_new
elpb_old
elbigcc
/;

set j_flex_ev(j) 'ev cars that can be used for flexibility'/
plg_hybrid
edv
/;


set jel_firm(jel) 'Firm, non intermittent technologies' /
    elpc_new, elpc_old, elpc_late elcigcc, elpc_ccs, elpc_oxy, eloil_new, eloil_old,
        elgastr_new,
    elgastr_old, elgasccs, elhydro_new, elhydro_old /;


set z_all 'All demand sectors, including transport and road transport' /
    commercial
    industry
    transport
    residential
    agriculture
    non_energy
    road_trans
/;
set z(z_all) 'Demand sectors' /
    commercial
    industry
    transport
    residential
    agriculture
    non_energy
/;
alias(z,z2)

set ener_ab 'Coefficients of enerdata MACCs'/
    a
    b
/;

set fr 'Demand Fuels' /
```

```
    biogas
    coal
    gas
    oil
    trbiofuel
    waste
    wbio
    electricity
    geotherm
    heat
    solar
/;

*--------------------------------------------------------------------------------
* Define Parameters
*--------------------------------------------------------------------------------
$elseif %phase%=='include_data'

* Define decay rate for storage costs
parameter storage_cost_reduction_rate(jreal_stor_jt) 'Cost reduction rate for storage
    technologies' /
    str_phes    0.03
    str_lib     0.05
    str_h2_pem  0.10
    str_meth    0.10
/;

* Define decay rate for sector coupling costs (transmission lower, because mature technology)
parameter cost_reduction_rate(flexibility_vars) 'Cost reduction rate for flexibility measures
    ' /
    transmission                        0.03
    ev_pen                              0.05
    flexible_techs                      0.05
    heating_cooking_sector_coupling     0.05
    transport_sector_coupling           0.05
    storage                             0.05
    hydropower                          0.00
/;

* Define storage costs (change to dollars)
parameter storage_costs(flexibility_vars) 'Levelized costs of storage [T$/TWh]' /
    transmission                        0.0
    ev_pen                              0.0
    flexible_techs                      0.0
    heating_cooking_sector_coupling     0.0
    transport_sector_coupling           0.0
    storage                             3.22e-3
    hydropower                          0.0
/;

* Define 2050 costs for storage technologies
parameter storage_costs_2050(jreal_stor_jt) 'Costs for storage technologies in 2050 [T$/TWh]'
     /
    str_phes    0.03e-3
    str_lib     0.19e-3
    str_h2_pem  3.22e-3
    str_meth    3.22e-3
    str_caes    3.22e-3
    str_h2_soec 3.22e-3
/;

* Define power to energy ratio to calculate the yearly costs
parameter power_to_energy_ratio(flexibility_vars) 'Power to energy ratio for flexibility
    measures' /
    transmission 1                          # No power to energy ratio so 1
    ev_pen 1                                # No power to energy ratio so 1
    flexible_techs 2000                     # Assumed number of hours
    heating_cooking_sector_coupling 2000    # Assumed number of hours
    transport_sector_coupling 2000          # Assumed number of hours
    storage 0
    hydropower  1
```

```
/;

* Define power-to-energy ratio for storage technologies
parameter power_to_energy_ratio_storage(jreal_stor_jt) 'Power to energy ratio for storage
    technologies' /
    str_phes    1544
    str_lib     1148
    str_h2_pem  77
    str_meth    4400
    str_caes    0
    str_h2_soec 0
/;


* Define 2050 costs for flexibility measures
parameter costs_2050(flexibility_vars) 'Costs for flexibility measures in 2050 [T$/TWh]' /
    transmission                          5.1e-3
    ev_pen                                0.25e-3
    flexible_techs                        0.08e-3
    heating_cooking_sector_coupling       8.50e-3
    transport_sector_coupling             15.60e-3
    storage                               0
    hydropower                            0.0e-3
/;

* Define parameters for flexibility boxes data
parameter outer_value(Flex_Bin) 'Outer values of flexibility boxes' /
    0 1.45
    1 1.84
    2 2.22
    3 2.60
    4 2.98
    5 3.36
    6 3.74
    7 4.12
    8 4.51
/;

parameter allocation(flexibility_vars, Flex_Bin) 'Allocation of flexibility variables within
    boxes' /
    'transmission'.0 5.10e-02
    'transmission'.1 2.44e-01
    'transmission'.2 4.31e-01
    'transmission'.3 6.18e-01
    'transmission'.4 7.96e-01
    'transmission'.5 9.75e-01
    'transmission'.6 1.16e+00
    'transmission'.7 1.35e+00
    'transmission'.8 1.54e+00
    'ev_pen'.0 5.59e-01
    'ev_pen'.1 6.06e-01
    'ev_pen'.2 6.50e-01
    'ev_pen'.3 6.94e-01
    'ev_pen'.4 7.36e-01
    'ev_pen'.5 7.78e-01
    'ev_pen'.6 8.21e-01
    'ev_pen'.7 8.65e-01
    'ev_pen'.8 9.09e-01
    'flexible_techs'.0 1.50e-02
    'flexible_techs'.1 1.76e-02
    'flexible_techs'.2 2.00e-02
    'flexible_techs'.3 2.24e-02
    'flexible_techs'.4 2.47e-02
    'flexible_techs'.5 2.70e-02
    'flexible_techs'.6 2.94e-02
    'flexible_techs'.7 3.18e-02
    'flexible_techs'.8 3.42e-02
    'heating_cooking_sector_coupling'.0 2.13e-03
    'heating_cooking_sector_coupling'.1 1.26e-02
    'heating_cooking_sector_coupling'.2 2.32e-02
    'heating_cooking_sector_coupling'.3 3.39e-02
```

```
    'heating_cooking_sector_coupling'.4 4.40e-02
    'heating_cooking_sector_coupling'.5 5.41e-02
    'heating_cooking_sector_coupling'.6 6.47e-02
    'heating_cooking_sector_coupling'.7 7.53e-02
    'heating_cooking_sector_coupling'.8 8.59e-02
    'transport_sector_coupling'.0 2.31e-03
    'transport_sector_coupling'.1 1.46e-02
    'transport_sector_coupling'.2 2.71e-02
    'transport_sector_coupling'.3 3.96e-02
    'transport_sector_coupling'.4 5.16e-02
    'transport_sector_coupling'.5 6.36e-02
    'transport_sector_coupling'.6 7.61e-02
    'transport_sector_coupling'.7 8.87e-02
    'transport_sector_coupling'.8 1.01e-01
    'storage'.0 5.41e-01
    'storage'.1 6.87e-01
    'storage'.2 8.20e-01
    'storage'.3 9.53e-01
    'storage'.4 1.08e+00
    'storage'.5 1.21e+00
    'storage'.6 1.34e+00
    'storage'.7 1.47e+00
    'storage'.8 1.61e+00
    'hydropower'.0 5.58e-02
    'hydropower'.1 5.59e-02
    'hydropower'.2 5.58e-02
    'hydropower'.3 5.58e-02
    'hydropower'.4 5.58e-02
    'hydropower'.5 5.58e-02
    'hydropower'.6 5.58e-02
    'hydropower'.7 5.58e-02
    'hydropower'.8 5.58e-02
/;


parameter storage_ratios(j) 'Ratios of different storage technologies' /
    str_lib 0.027
    str_phes 0.055
    str_h2_pem 0.158
    str_meth 0.76
    str_h2_soec 0
    str_caes 0
/;

parameter cost_switch(flexibility_vars) 'Switch between storage and other flexibility
    measures costs';
cost_switch(flexibility_vars) = 0;
cost_switch('storage') = 1;

* Replace variable definition with parameter definition
parameter k_en_flex_dist(flexibility_vars, t, n) 'Flexibility provided by each measure [TWh
    ]';

parameter vre_penetration(t,n)'VRE capacity [TW]';
*--------------------------------------------------------------------------------
* Compute data
*--------------------------------------------------------------------------------
$elseif %phase%=='compute_data'

set j_curt(j) 'technologies producing curtailment' / elwindon, elwindoff, elpv /;

parameter historical_costs(flexibility_vars, t, n) 'Historical costs for flexibility measures
     over time';
historical_costs(flexibility_vars, t, n) =
    max(0, costs_2050(flexibility_vars) * (1 -0.01  * max(year(t) - 2050, 0) + 0.0001 * max(
        year(t) - 2050, 0)**2));

parameter historical_storage_costs(jreal_stor_jt, t, n) 'Historical costs for storage
    technologies over time';
historical_storage_costs(jreal_stor_jt, t, n) =
    max(0, storage_costs_2050(jreal_stor_jt) * (1 -0.01  * max(year(t) - 2050, 0) + 0.0001 *
```

```
        max(year(t) - 2050, 0)**2));
*------------------------------------------------------------------------------
* Define Variables
*------------------------------------------------------------------------------
$elseif %phase%=='vars'
*positive variable VRE_PENETRATION(t,n) 'Total capacity of VRE technologies';
*loadvarbnd(VRE_PENETRATION,'(t,n)',1e-5,0,inf);

positive variable SHARE_EL_VRE(t,n) 'Total share of VRE technologies over el';
loadvarbnd(SHARE_EL_VRE,'(t,n)',1e-5,0,1);

positive variable K_EN_FLEX(t,n) 'Predicted total flexibility [EJ]';
loadvarbnd(K_EN_FLEX, '(t,n)', 1e-5,0,+inf);

positive variable COSTS_FLEX(t, n) 'Total flex costs[T$]' ;
loadvarbnd(COSTS_FLEX, '(t,n)', 1e-5,0,+inf);

positive variable DELTA_K_EN_FG(t,n) 'Additional Electricity capacity needed from flexible generation technologies [TW]';
loadvarbnd(DELTA_K_EN_FG, '(t,n)', 1e-5,0,+inf);

positive variable DELTA_Q_EN_FEV(t, n) 'Capacity of EV batteries [TWh]';
loadvarbnd(DELTA_Q_EN_FEV, '(t,n)', 1e-5,0,+inf);

positive variable DELTA_K_EN_GRID(t,n) 'Additional electricity transmission capacity needed [TW]';
loadvarbnd(DELTA_K_EN_GRID, '(t,n)', 1e-5,0,+inf);

positive variable Q_EN_BC(j_curt,t,n) 'Electricity generation before curtailment from VRE technologies [TWh]';

*------------------------------------------------------------------------------
* Equations
*------------------------------------------------------------------------------
$elseIf %phase%=='eql'

*eq_vre_penetration_%clt%
eq_flexibility_prediction_%clt%
eq_costs_flex_%clt%
eq_delta_k_en_fg_%clt%
eq_delta_q_en_fev_%clt%
eq_delta_k_en_grid_%clt%

*------------------------------------------------------------------------------*------------------------------
* Define equations
*------------------------------------------------------------------------------
$elseIf %phase%=='eqs'
*eq_vre_penetration_%clt%(t,n)$(mapn_th('%clt%') and year(t) ge 2020)..
*    VRE_PENETRATION(t,n) =e= K_EN.l('elpv',t,n) + K_EN.l('elwindon',t,n) + K_EN.l('elwindoff',t,n);

* Equation to predict total flexibility based on EJ
eq_flexibility_prediction_%clt%(t, n)$(mapn_th('%clt%') and year(t) ge 2020)..
    K_EN_FLEX(t, n) =e= 0.702711 + 1.436179 * vre_penetration(t, n);

eq_delta_k_en_fg_%clt%(t,n)$(mapn_th('%clt%') and year(t) ge 2020)..
    DELTA_K_EN_FG(t,n)=e= max(0,k_en_flex_dist('flexible_techs', t, n) - sum(jel_firm, K_EN.l(jel_firm,t,n)));

eq_delta_q_en_fev_%clt%(t,n)$(mapn_th('%clt%') and year(t) ge 2020) ..
    DELTA_Q_EN_FEV(t,n) =e= max(0, 1e3 * (k_en_flex_dist('ev_pen', t, n) - (Q_EN.l('edv', t, n) + Q_EN.l('plg_hybrid', t, n))));

eq_delta_k_en_grid_%clt%(t,n)$(mapn_th('%clt%') and year(t) ge 2020)..
    DELTA_K_EN_GRID(t,n) =e= max(0,(k_en_flex_dist('transmission', t, n)-k_en_flex_dist('transmission', t-1, n)) - (K_EN_GRID.l(t,n)-K_EN_GRID.l(t-1,n)));

eq_costs_flex_%clt%(t, n)$((map_clt_n('%clt%',n) and (not tfix(t)) and (year(t) le yeoh))and year(t) ge 2020)..
    COSTS_FLEX(t, n) =e= 10e-3 *
```

```
        ((sum(flexibility_vars$((not sameas(flexibility_vars, 'flexible_techs')) and (not
            sameas(flexibility_vars, 'ev_pen')) and (not sameas(flexibility_vars, '
            transmission')) and (not sameas(flexibility_vars, 'storage'))),

            k_en_flex_dist(flexibility_vars, t, n) * power_to_energy_ratio(flexibility_vars)
                *
            historical_costs(flexibility_vars, t, n)))

        + sum(jreal_stor_jt,
            k_en_flex_dist('storage', t, n) * storage_ratios(jreal_stor_jt) *
            power_to_energy_ratio_storage(jreal_stor_jt) * historical_storage_costs(
                jreal_stor_jt, t, n))

        + delta_k_en_fg.l(t, n) * power_to_energy_ratio('flexible_techs') *
              historical_costs('flexible_techs', t, n)

        + delta_q_en_fev.l(t, n) * power_to_energy_ratio('ev_pen') *
              historical_costs('ev_pen', t, n)

        + delta_k_en_grid.l(t, n) * power_to_energy_ratio('transmission') *
              historical_costs('transmission', t, n));
*------------------------------------------------------------------------------
* Fix Variables
*------------------------------------------------------------------------------
$elseif %phase%=='fix_variables'
tfixvar(SHARE_EL_BC_VRE,'(t,n)')
tfixvar(SHARE_EL_VRE, '(t,n)')
tfixvar(K_EN_FLEX, '(t,n)')
tfixvar(COSTS_FLEX, '(t,n)')
tfixvar(DELTA_K_EN_FG, '(t,n)')
tfixvar(DELTA_Q_EN_FEV, '(t,n)')
tfixvar(DELTA_K_EN_GRID,'(t,n)')
*tfixvar(VRE_PENETRATION,'(t,n)')'

$elseif %phase%=='before_solve'
* Loop through each time period and region to determine the flex bin and assign allocation
loop(flexibility_vars,
    loop((t,n),
* put it in after solve phase
        loop(Flex_Bin,
            if (K_EN_FLEX.l(t, n) <= outer_value(Flex_Bin),
                k_en_flex_dist(flexibility_vars, t, n) = allocation(flexibility_vars,
                    Flex_Bin);
                break;
            );
        );
    );
);

vre_penetration(t,n) = K_EN.l('elpv',t,n) + K_EN.l('elwindon',t,n) + K_EN.l('elwindoff',t,n);
*------------------------------------------------------------------------------
* GDX Items
*-----------------------------------------------------------------------------

$elseif %phase%=='gdx_items'
* Sets
Flex_Bin
j
jreal
jel
j_stor
jreal_stor_jt
jel_stor
j_sts
j_lts
flexibility_vars
j_curt
curt_type
j_wind_j
j_pv_j
j_flex
```

```
j_flex_ev

* Parameters
lifetime
storage_costs
power_to_energy_ratio
outer_value
allocation
storage_ratios
cost_switch
k_en_flex_dist

* Variables
*VRE_PENETRATION
K_EN_FLEX
COSTS_FLEX
DELTA_K_EN_FG
DELTA_Q_EN_FEV
DELTA_K_EN_GRID

$endif
```