Open Model-based Analyses of Highly Renewable and Sector-coupled Energy Systems

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To my daughter, Rikhia

I believe the world will be a better and happier place when you grow up.

"Hope is a good thing, maybe the best of things, and no good thing ever dies."

The Shawshank Redemption (1994)

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Executive Summary

The Paris Agreement initiated an international framework to keep the increase in global average temperature to well below 2 °C. The EU needs to adapt energy systems based on the smart integration of renewable energy across all sectors to help achieve the ambitious Paris Agreement targets. In recent years, sector coupling has emerged as a new concept in energy and climate policy discussions, which refers to integrating different energy sectors to incorporate more renewable energy sources in the energy system to achieve the target of overall climate neutrality. Decarbonizing the energy sectors depends on state-of-theart techniques such as power-to-heat (P2H) and power-to-gas. These techniques, used in a sector-coupled network, are expected to increase the energy storage capacity and provide additional flexibility to the energy system. The North Sea and its adjacent countries, referred to as the NS region (NSR), are expected to play a vital role in the EU's transition to a sustainable energy system. Examples of RES for planning a future sustainable NSR include offshore wind energy, wave energy, microalgae production, ocean thermal energy conversion, and tidal energy. Furthermore, the intermittent capacity of onshore installments from solar photovoltaics (PV), onshore wind energy, and bioenergy is increasing, alongside advancements in energy efficiencies resulting in changing supply and demand patterns. The NSR also offers the opportunity to deploy Carbon Capture and Storage (CCS) and large-scale bio-CCS. Additionally, the enormous hydropower potential of Norway can be used as a green battery to provide greater flexibility to the European energy system.

Although different approaches allow integrating multiple sectors in energy system models, they lead to an unclear understanding of specific aspects of sector coupling and the relevance of existing approaches to model and analyze such systems. There is no straightforward method to select one or more models from the broad range of available state-of-the-art energy models to portray a comprehensible picture of the energy transition over different temporal and spatial levels. Furthermore, the relationship between P2H and thermal energy storage (TES) for providing flexibility as dispatchable loads need further research. None of the previous studies explicitly characterized, discussed the potential role, and presented the modeling formulations for P2H and TES from the viewpoint of a sector-coupled and carbon-neutral future European energy system. Finally, developing novel methodologies using comprehensive open modeling techniques and applying cross-sectoral holistic approaches is imperative to analyze and investigate policy-relevant research questions for future highly renewable and sector-coupled energy systems. The methods should address aggregated and disaggregated energy systems, ranging from subnational to national levels. In addition, the openness of the model should enable the model users to use, modify, and upgrade the model for performing basic to advanced-level energy system analyses.

The study presents a clear perception of the concept of sector coupling. The review concludes that sector coupling can be advantageous from the perspectives of decarbonization, flexibility, network optimization, and system efficiency. The study uses Oemof as an advanced tool to design a sector-coupled and renewable-based energy system in the NSR. The study identifies electric heat pumps, electric boilers, electric resistance heaters, and hybrid heating systems as the most promising P2H options and groups the most promising TES technologies under four major categories. Low-temperature electric heat pumps, electric boilers, electric resistance heaters, and sensible and latent heat storage show high technology readiness levels to facilitate a large share of the heat demand. After that, the study developed a unique hourly optimization tool using a hybrid approach. The Open Sector-coupled Energy Model (OSeEM) is created using Oemof. Different elements of the OSeEM model include onshore and offshore wind, solar PV, hydro ROR, CHP, ASHP, GSHP, PHS, Li-ion battery, Redox battery, H₂ storage, ACAES, and TES using hot water tanks.

The model validation is performed using two case studies. First, the case study of Schleswig-Holstein shows that the model reaches feasible solutions without additional offshore wind investment. The annual investment cost varies between 1.02 and 1.44 bn \notin /year for the three scenarios. The electricity generation indicates that the curtailment from other renewable plants can be decreased with a high number of biomass-based combined heat and power plants. The model is then further validated using the case study of Germany. The model results show that Germany can use a 100% renewable-based and sector-coupled system for electricity and building heat. The annual investment costs vary between 17.6 – 26.6 bn \notin /yr for volatile generators and 23.7 – 28.8 bn \notin /yr for heat generators. Comparison of OSeEM results with recent studies validates the percentage-wise energy mix composition and the calculated LCOE values from the model. The LCOE for onshore wind is 4.99 \notin cent/kWh, and Biomass ranges between 19.47 – 20.26 \notin cent/kWh. The total LCOE for the OSeEM-DE model ranges between 6.34 – 7.92 \notin cent/kWh. Sensitivity analyses indicate that storage and grid expansion maximize the system's flexibility and decrease investment costs.

The open modeling tool OSeEM paves the pathway towards modeling and analyzing plausible sectorcoupled scenarios for 100% renewable-based national and sub-national energy systems. At the same time, this study shows how different energy mix options, their component-wise investment capacities, and costs can be investigated using the model; hence, Schleswig-Holstein and Germany's cases can be followed for other similar regions to conduct the feasibility analysis of 100% renewable-based sector-coupled systems. The study also reveals that sensitivity analyses can help identify the system's flexibility aspects in future energy infrastructure. Finally, the study proposes future research questions such as (1) detailed grid modeling, (2) inclusion of industrial demand, (3) inclusion of other renewable and storage technologies, (transport sector coupling, (5) demand-side management, and (6) the impact of Nordic hydro expansion on the European energy system.

Keywords: 100% renewable; energy system modeling; energy transition; flexibility; open science; sector coupling; Power-to-Heat; Thermal Energy Storage; P2H Modeling; TES Modeling; Linear Programming; North Sea energy system; Oemof.

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List of Abbreviations

Abbreviation	Elaboration
°C	Degree Celsius
ACAES	Adiabatic Compressed Air Energy Storage
AEE	Agentur für Erneuerbare Energien (Agency for Renewable Energies)
AIV	Annual Investment Cost
ASHP	Air Source Heat Pump
bn	Billion
CAES	Compressed Air Energy Storage
Capex	Capital Expenditure
ccs	Carbon Capture and Storage
CHP	Combined heat and power
CO ₂	Carbon dioxide
COP	Coefficient of Performance
CSP	Concentrated Solar Power
DE	Germany
DHW	Domestic Hot Water
DSM	Demand-side Management
el	Electrical
ENTSO-e	European Network of Transmission System Operators for Electricity
ETS	Electrical Thermal Storage
EU	European Union
EV	Electric Vehicle
FOM	Fixed operation and maintenance
FOR	Feasible Operating Region
GHG	Greenhouse Gas
GSHP	Ground Source Heat Pump
GW	Gigawatt
GWh	Gigawatt-hour
H ₂	Hydrogen
hr	Hour
HRE	Heat Roadmap Europe
HTHP	High-temperature Heat Pump
HTPCM	High-temperature PCM
HVDC	High Voltage Direct Current
ICT	Information and Communications Technology
K	Kelvin
kV	Kilovolt
kW	Kilowatt
kWh	Kilowatt-hour
LAES	Liquid Air Energy Storage
LCOE	Levelized Cost of Electricity
LHS	Latent Heat Storage
Li-ion	Lithium-ion
LP	Linear Programming
LPCM	Low-temperature PCM
MILP	Mixed-integer Linear Programming

mn	Million
MW	Megawatt
MWh	Megawatt-hour
NDE	Northern Germany
NLP	Nonlinear Programming
NPV	Net Present Value
NS	North Sea
NSR	North Sea Region
NTC	Net Transfer Capacity
Oemof	Open Energy Modeling Framework
Openmod	Open Energy Modeling
OSeEM	Open Sector-coupled Energy Model
OSeEM-DE	Open Sector-coupled Energy Model for Germany
OSeEM-SN	Open Sector-coupled Energy Model for Subnational Energy Systems
OTEC	Ocean Thermal-Energy Conversion
P2G	Power-to-gas
P2H	Power-to-heat
P2L	Power-to-liquid
P2X	Power-to-X
PCM	Phase Change Material
PHS	Pumped hydro storage
PJ	Petajoule
PV	Photovoltaic
Redox	Vanadium Redox Flow
RES	Renewable Energy Sources
ROR	Run-of-the-river
SDE	Southern Germany
SH	Schleswig-Holstein
SHS	Sensible Heat Storage
SPCM	Sub-zero Temperature PCM
SSTS	Solid State Thermal Storage
STET	Socio-technical Energy Transition
TCS	Trade, Commerce, and Services
TES	Thermal energy storage
th	Thermal
THS	Thermo-chemical Heat Storage
TIV	Total investment cost
TMS	Thermo-mechanical Heat Storage
TRL	Technology Readiness Level
TTES	Tank Thermal Energy Storage
TW	Terawatt
TWh	Terawatt-hour
UK	United Kingdom
UTES	Underground Thermal Energy Storage
V	Volt
V2G	Vehicle-to-Grid
VOM	Variable Operation and Maintenance
VRE	Variable Renewable Energy
WACC	Weighted Average Capital Cost

WWS	Wind-Water-Solar
yr	Year

Nomenclature

Symbols

t	Timestep	Т	Set of all timesteps
b	Bus	В	Set of all buses
l	Load	L	Set of all loads
v	Volatile generator	V	Set of all volatile generators
h	Heat pump	Н	Set of all heat pumps
S	Storage	S	Set of all storages
т	Transmission line	М	Set of all transmission lines

Variables

Input flow to bus b
Output flow from bus <i>b</i>
Load flow of load l
Flow of volatile generator unit v
Endogenous capacity of volatile generator unit v
Carrier flow of CHP unit chp
Electricity flow of CHP unit chp
Heat flow of CHP unit <i>chp</i>
Electricity flow from the electricity bus for heat pump unit h
Heat flow to the heat bus for heat pump unit h
Energy level of storage unit s
Input flow to storage unit s
Output flow from storage unit s
Energy level of pumped hydro storage unit phs
Output flow of pumped hydro storage unit phs

$x_{phs}^{profile}$	Endogenous inflow profile of pumped hydro storage unit phs
$x_{m,from}^{flow}$	Flow from a bus through the transmission line m
$x_{m,to}^{flow}$	Flow to a bus through the transmission line m

Parameters

$c_l^{profile}$	Exogenous profile of load <i>l</i>
C_l^{amount}	Total amount of load <i>l</i>
$c_v^{profile}$	Exogenous profile of volatile generator v
$c_v^{capacity_potential}$	Maximum capacity potential of volatile generator v
c_{chp}^{beta}	Power loss index of CHP
C ^{electrical_efficiency}	Electrical efficiency of CHP
C ^{thermal_efficiency}	Thermal efficiency of CHP
condensing_efficiency C _{chp}	Condensing efficiency of CHP
C ^{amount} biomass	Absolute amount of biomass commodity
$C_h^{efficiency}$	Conversion efficiency (Coefficient of Performance, i.e., COP) of heat pump unit h
$c_s^{loss_rate}$	Loss rate of storage unit s
$c_s^{eta_in}$	Charging efficiency of storage unit s
$C_s^{eta_out}$	Discharging efficiency of storage unit s
$C_s^{roundtrip_efficiency}$	Round Trip efficiency of storage unit s
$c_s^{capacity}$	Maximum power capacity of storage unit s
$C_{S}^{storage_capacity}$	Maximum energy capacity of storage unit s
$c_{phs}^{loss_rate}$	Loss rate of pumped hydro storage unit phs
$C_{phs}^{efficiency}$	Efficiency of pumped hydro storage unit phs
$c_{phs}^{profile}$	Exogenous inflow profile of pumped hydro storage unit phs
c_m^{loss}	Loss on transmission line m
c ^{marginal_cost}	Marginal cost

c ^{VOM}	Variable operation and maintenance cost
c ^{carrier_cost}	Carrier cost
η	Efficiency
c ^{capacity_cost}	Capacity cost
$c_s^{storage_capacity_cost}$	Energy capacity cost of storage
<i>c</i> ^{annuity}	Annuity cost
c ^{capex}	Capital expenditure cost
c ^{WACC}	Weighted Average Cost of Capital
c ^{FOM}	Fixed operation and maintenance Cost
n	Lifetime
C ^{AIV}	Annual investment cost
C ^{optimized_capacity}	Optimized capacity cost
c^{TIV}	Total Investment cost
c^{LCOE}	Levelized cost of electricity
I_n	Initial cost of investment expenditure
M_n	Sum of all O&M costs
F_n	Sum of all fuel Costs
E_n	Sum of all electrical energy produced
r	Discount rate

Chapter 1 Introduction

Energy transition refers to the global energy sector's shift from fossil-based energy production and consumption to renewable energy sources (RES). The European Union (EU) is a front-runner of this transition and encourages a transformation at the international and national levels to achieve a renewable energy-based system. The Paris Agreement initiated an international framework to keep the increase in global average temperature to well below 2 °C [1]. The 2018 United Nations Climate Change Conference (COP24) in Katowice adopted a clear rulebook for the practical implementation of the Paris Agreement [2]. It delineated a worldwide climate action plan to mitigate climate change by limiting global warming to 1.5 °C, if possible. To accomplish a climate-neutral society with net-zero greenhouse gas (GHG) emissions by 2050, the European Commission stated plans in the European Green Deal to integrate renewables, energy efficiency, and other sustainable solutions [3]. The EU needs to adapt energy systems based on the smart integration of renewable energy across all sectors to help achieve the ambitious Paris Agreement targets [4].

To make the energy transition successful, all the major energy sectors, such as power, heat, transport, and industries, should focus on renewable energies. Sector coupling has emerged as a new concept in energy and climate policy discussions in recent years, which refers to integrating different energy sectors to incorporate more renewable energy sources in the energy system to achieve the target of overall climate neutrality. Sector coupling can make a decisive contribution to the achievement of ambitious climate protection goals through increased use of renewable energy in the heating and transport sectors and industry to substitute fossil fuels. Decarbonizing the energy sectors depends on state-of-the-art techniques such as power-to-heat (P2H) and power-to-gas (P2G). These techniques, used in a sector-coupled network, are expected to increase the energy storage capacity and provide additional flexibility to the energy system [5, Pavičević et al. 2020, p.1]. The modeling of multiple energy sectors, especially power, heat, and transport, is becoming popular in the newer energy models [6, Martínez-Gordón et al. 2021, p.1]. Many researchers analyzed the feasibility of integrating other sectors, especially the heat sector, in 100% renewable energy models in the past decade. These analyses often show that sector coupling decreases the overall system cost; however, further investigations are needed to assess the comprehensive benefits before implementing extensive cross-border transmissions in a sector-coupled EU network [5–8].

The North Sea (NS) and its adjacent countries, together referred to as the NS region (NSR), as shown in Figure 1.1, are expected to play a vital role in the EU's transition to a sustainable energy system [6,9,10]. According to 2019 Eurostat data, 40% of the EU's total population (~200 million) lives in the NSR, whose aggregate gross domestic product is 60% of the EU (~9.6 billion euros) [6, Martínez-Gordón et al., 2021, p.2]. Regarding resource consumption and carbon emissions, the NSR has a massive impact in Europe because of its enormous size, oil and gas production, and industrial development. More than 300 oil and gas fields, 5000 wells, 500 platforms, and a network of around 10,000 km of pipelines are present in the NS offshore [6, Martínez-Gordón et al. 2021, p.2]. The coexistence of well-established gas grids, district heating networks, and large-scale variable renewable energy (VRE) deployment opportunities makes it plausible to examine synergies between activities, supporting strategies for a successful, efficient, and accelerated energy transition [11,12]. In line with European and global policies, current trends show that the NSR will play a pivotal role in decarbonizing the energy sector in the following years due to the extensive deployment of RES. Examples of RES for planning a future sustainable NSR include offshore wind energy, wave energy, microalgae production, ocean thermal energy conversion, and tidal energy. Furthermore, the mainly intermittent capacity of onshore capacities from solar photovoltaics (PV), onshore wind energy, and bioenergy is increasing, alongside advancements in energy efficiencies resulting in changing supply and demand patterns. The NSR also offers the opportunity to deploy Carbon Capture and Storage (CCS) and

large-scale bio-CCS. Additionally, the enormous hydropower potential of Norway can be used as green battery¹ to provide greater flexibility to the European energy system [13, Simensen, 2012, p.11].



Figure 1.1: The North Sea and its adjacent countries. Source: Wikimedia Commons [14].

The impact of carbon emission in the NSR can be realized from the extensive Carbon dioxide equivalent (CO_{2e}) emissions, as shown in Figure 1.2, with historical GHG data by Climate Watch [15].

¹ The idea of using Norwegian hydropower resources to provide flexibility to the European electricity system is widely regarded as the 'green battery' function. A short summary of the studies that analyzed the green battery function is presented in Appendix A.



The NSR countries shown are Denmark, Germany, Norway, Sweden, Netherlands, and the United Kingdom (UK). Although the profile exhibits a declining trend since the 1990s, the aggregated emission of the NSR countries in 2018 was 40% of the total emission by the EU-27 and the UK (1.57 Gt CO_{2e} vs. 3.97 Gt CO_{2e}). The percentage will be much higher (>50%) if Belgium and France's GHG emissions are considered. GHG emissions are driven by high energy demand met by fossil-fueled power plants. Figure 1.3 shows the historical GHG emission in the energy sector by the 6 NSR countries [15]. It is evident from the figure that the countries that are still relying heavily on coal and nuclear for are emitting more (e.g., Germany), and the countries that are using renewables are emitting less (e.g., Denmark, which uses wind as their primary resource).Therefore, the emission by the NSR is very critical from the EU perspective and must be controlled at a significant rate to keep the temperature increment within the Paris Agreement ceiling.



Many previous studies analyzed how the NSR can become a pioneer in leading the European energy transition. For example, Hajer and Pelzer explained the NS's large-scale exploitation for harvesting offshore wind energy using 'techniques of futuring' [16, Hajer and Pelzer (2018), p.222 Hajer and Pelzer]. The North Sea Energy Program's synthesis paper thoroughly investigated the role of offshore energy integration in

the NS energy system [17]. The World Energy Council investigated the decommissioning scenarios and interactions between activities in the NSR, including electrification of gas platforms, P2G conversion in offshore platforms, CCS in offshore fields and caverns, and energy storage [11]. Ørsted's whitepaper presented the prominent and potential RES technologies for a future energy system in the NSR, including hydropower, biomass, biogas and other biofuels, heat pumps, battery storage, power-to-hydrogen, etc. [18]. Martínez-Gordón et al. introduced an integrated and spatially resolved framework for the NSR to support offshore integrated system modeling and spatial analysis [6]. Gusatu et al. discussed challenges and opportunities for offshore wind farm locations in the NSR [10, Gusatu et al. 2020, p.1]. In another paper, Gusatu et al. analyzed the cumulative environmental effects of offshore wind farm development in the NS basin [19, Gusatu et al. 2020, p.1]. These studies validate the case of NSR as a representative region for investigating critical energy transition challenges in Europe. Data, models, tools, and possible solutions from the NSR will constitute essential knowledge and methodologies that can be transferred to other areas in transition. Furthermore, the combined use of different modeling tools and concepts to understand and describe different actors' behavior is essential to provide a coherent picture of the necessary transition process of the energy systems over time and for different spatial levels.

1.1 Problem Statement

The introduction shows that the NSR needs to play a vital role in the EU's energy transition to a sustainable energy system. The possibilities for coupling power, heat, and transport sectors in this region are becoming significant. However, initial findings suggest a knowledge gap in the comprehensive understanding of sector coupling. To envision the future energy transition pathways in the NSR, it is essential to comprehensively understand the sector coupling practices, their potential uses, and benefits.

Flexibility in a sector-coupled energy system can utilize RES-based technologies in high proportions and effectively increase energy efficiency. Adopting P2H (such as electric heat pumps) and P2G technologies (such as Hydrogen storage via electrolysis) can help improve the energy system's flexibility. Flexibility can be offered in multiple ways, for example, shifting the operation of electric heat pumps or electric vehicle loads in private households and even shifting the energy consumption in industries as a part of a sector-coupled network. However, the energy flow should be smartly and effectively managed between the sectors to stabilize the network operation while keeping the system flexible and efficient. P2H technologies refer to applications in which electrical energy generates heat mainly for the built environment or industrial processes. P2H offers many advantages to drive the energy transition. P2H, coupled with thermal energy storage (TES), can be a promising option for integrating renewable energy, improving operational efficiency, providing demand-side flexibility and sector coupling.

Modeling methods and tools play a crucial role in providing insights into the energy transition. The combined use of different modeling tools and concepts to understand and describe diverse actors' behavior is essential to give a coherent picture of the necessary transition process of the energy systems over time and for different spatial levels. However, the modeling methodologies often ignore the details of small energy systems. Aggregated models provide more holistic pictures but cannot absorb the regional specifics and often fail to deliver meaningful results at lower spatial scales, including demand behavior. In general, models need not be necessarily larger and more complex; instead, using model collaboration, different approaches and tools are used in conjunction. Aggregated modeling should have proper parameterization and level of detail to capture the main system aspects and interactions. Likewise, disaggregated models should have proper interlinkages with potential developments and system changes across scales. The linkages between small- and large-scale energy systems need to be addressed better in energy system models.

The following research problems are identified after a thorough background study on sector coupling with a focus on the NSR from an energy system modeling perspective:

- 1. Although different approaches allow integrating multiple sectors in energy system models, they lead to an unclear understanding of specific aspects of sector coupling and the relevance of existing approaches to model and analyze such systems.
- 2. There is no straightforward method to select one or more models from the broad range of available state-of-the-art energy models to portray a comprehensible picture of the energy transition over different temporal and spatial levels.
- 3. The relationship between P2H and TES for providing flexibility as dispatchable loads need further attention in energy research. None of the previous studies explicitly characterized, discussed the potential role, and presented the modeling formulations for P2H and TES from the viewpoint of a sector-coupled and carbon-neutral future European energy system.
- 4. It is imperative to develop novel methodologies using comprehensive open modeling techniques and applying cross-sectoral holistic approaches to analyze and investigate policy-relevant research questions for future highly renewable and sector-coupled energy systems. The methods should address both aggregated and disaggregated energy systems, ranging from subnational to national levels. In addition, the openness of the model should enable the model users to use, modify, and upgrade the model for performing basic to advanced level energy system analyses.

1.2 Research Question

Based on the problem statement, the following main research questions are formulated. The sub-research questions are also presented along with the main research questions.

- 1. How can sector coupling be defined and realized from the far-reaching perspective of energy system modeling?
- 2. Which state-of-the-art tools are accessible to model sector-coupled energy systems?
 - How to choose an appropriate tool based on specific rationales?
- 3. Which P2H and TES technologies will play a significant role in the carbon-neutral future European energy system?
 - What are their classifications and potential roles in the European energy transition?
 - How to mathematically formulate the identified technologies for large-scale energy models?
- 4. How to develop methodologies for building open models of highly renewable-based energy systems within the sector-coupled networks for the NS countries?
 - How to integrate state-of-the-art technologies into the models and quantify their impacts?
 - How to utilize the models to investigate policy-relevant research questions from both subnational and national perspectives?

1.3 Research Objective

The main research objective is to develop an open-source energy model to investigate highly renewablebased and sector-coupled energy systems, focusing on the NSR. In pursuing the broad goal, the research addresses the following sub-objectives:

1. To understand the definition of sector coupling and its potential role and applicability in the energy transition.

- 2. To comprehend the progression of state-of-the-art energy system models and select appropriate modeling tools based on the research rationale.
- 3. To identify the vital P2H and TES technologies for the energy transition, classify them, discuss their potential roles, and formulate them for large-scale energy models.
- 4. To design and develop a novel open modeling method and tool using one or more of the selected tools for analyzing highly renewable and sector-coupled energy systems.
- 5. To validate the tool using case studies of subnational and national levels by answering policyrelevant research questions.

1.4 Scope of Research

Answering the first two research questions requires a comprehensive literature review focusing on sector coupling and energy system modeling. Since there has been a significant evolution of research in these topics in different periods, the review findings are presented according to analysis performed in different decades. Scholar databases are screened for articles mentioning the following keywords—sector coupling, energy system modeling, North Sea energy, energy transition, 100% renewable, power-to-heat, and power-to-gas. The literature review investigates sector coupling practices for the energy transition in energy systems, presents the development of energy system models to date, followed by a list of the up-to-date energy system models that are open or free for educational use. The study then formulates the selection of appropriate tools based on the rationales of the research. The resolutions provide a detailed understanding of the concept of sector coupling and indicate how sector coupling can be advantageous in terms of decarbonization, flexibility, network optimization, system efficiency, and clarify how to solve the sector coupling barriers. The study also presents how a list of appropriate tools for model collaboration can be picked up methodologically from an available wide range of models and suggest an advanced tool to design a sector-coupled and renewable-based energy system in the NSR.

To answer the third research question, scholarly databases were screened for power-to-heat, thermal energy storage, combined heat and power (CHP), and modeling these three components. Additionally, several important articles and reports from different projects were reviewed. CHP is included as it is expected to play an essential role in coupling the power and heat sectors, especially district heating. Based on the findings, the significant P2H and TES technologies, their classifications, the potential role of these technologies in the energy transition, and modeling equations are presented in this thesis. The review describes the main P2H and TES technologies that are technologically innovative and economically viable, improve energy efficiency, and reduce CO₂ emissions. The classifications are sketched out, with precise representations of the most promising technologies under different categories. Finally, the study presents the mathematical models using the most preferred and suitable modeling approaches.

The fourth research question is answered by designing and developing an innovative approach to facilitate energy systems with 100% renewable penetration and sectoral integration. The modeling is conducted using one of the selected tools based on the literature review and considers the state-of-the-art technologies in the model. The model is then validated under different scenarios using the case study of Schleswig-Holstein (SH) in Germany as a subnational region. Finally, the model is adapted to answer policy-relevant research questions for a German energy system. The study presents a source-rich and flexible tool for modeling highly renewable and sector-coupled energy systems. The model's openness allows other users to actively develop the tool and modification for specific purposes to answer research questions. The model uses a straightforward approach to answer energy transition-related questions and examine different pathways to help researchers and policymakers. The case studies use the model to analyze the feasibility of 100% renewable and sector-coupled energy systems and other relevant research questions for SH and

Germany. The results are then validated by comparing results from similar studies. Finally, the model provides scopes for further upgradation to adapt to diverse contexts.

1.5 Research Methodology

The research is carried out in five steps. First, the background and the research problem are stated. Based on the problem statement, the research questions are formulated, leading to the main objectives of the research. Then the scope explains the extent to which the research area will be explored in the thesis. The research methodology presents how the subsequent phases of the research are conducted step by step.

The second part of the thesis consists of a comprehensive literature review on three topics: sector coupling, energy system modeling, and P2H and TES. All topics are discussed based upon the previous literature, and the current status and prospects are analyzed. The literature review helps to understand the research background in detail, aids with a list of tools used for modeling the NS energy system and indicates how an appropriate model can be selected based on rationales. This part is significant for the model development part of the thesis. Additionally, the review also helps understand the classification, potential role, and modeling equations of P2H and TES, two vital components of the future sector-coupled energy networks in Europe.

In the third part of the research, the energy model is developed using one of the selected tools based on the literature review. First, the model architecture and the components of the model are presented. Block diagrams and flowcharts are used to explain the model dynamics. Then the mathematical formulations are presented in detail. The relevant equations for each model component are presented. Finally, it is shown how the model data are prepared and handled to input and interpret the model outputs. The third part of the research helps to understand the model design, development, and data handling, leading to a complete understanding of how to perform a model-based analysis.

The fourth part of the research presents the model application for two case studies representing two NSR regions. The first case study shows how the model is used to design a subnational energy system. Three scenarios are developed and analyzed for the sector-coupled network of Schleswig-Holstein. The results are visually represented and interpreted to show how the model can answer diverse research questions. The second case study shows how the model scope can be extended to fit a larger-scale energy system. The case of Germany, divided into two parts, is investigated using the model. Critical current research questions regarding the future German energy system are analyzed in detail.

The concluding part discusses the model results in light of the case studies and presents the main findings. The discussion leads to understanding how the model can be used for different contexts, ranging from small to large scale energy systems, and how the model results can be used to shape policy recommendations. The current limitations and model upgradation plans are also presented in detail. Finally, the novelty, contributions, and future recommendations of the thesis are presented. The research methodology is presented in Figure 1.4.



Figure 1.4: Research Methodology

1.6 Thesis Outline

The thesis is presented as a composition of seven chapters. Chapter 1 is the introduction, which shows the research problem, questions, objectives, scope, and methodology. Then the literature review of the thesis is divided into two chapters. Chapter 2 presents the study on sector coupling and energy system modeling, which elaborates on sector coupling, energy models, prospective models for analyzing the NSR, and an appropriate tool selection. Chapter 3 presents the definition, classification, characterization, and potential role of power-to-heat and thermal energy storage technologies in the future European energy system. It also shows the P2H and TES modeling equations based on existing reviews. Chapter 4 presents the design and development of the model, including the model architecture, detailed modeling equations, data preparation, and handling of data in the model. The application of the model for two different cases is presented in the following two chapters. Chapter 5 presents the case of Schleswig-Holstein, and Chapter 6 presents the case of Germany. Both cases investigate the capacities, investment costs, and flexibility aspects for the respective regions so that the feasibility of a 100% renewable and sector-coupled energy system can be determined. Finally, Chapter 7 concludes the thesis with a discussion on main findings of the study, model limitations, novel contributions of the thesis, and future research scopes.

Chapter 2 Sector Coupling and Energy System Modeling

2.1 Sector Coupling

Sector Coupling (also known as sector integration) represents replacing fossil fuels with RES in every endconsumption sector, such as electricity, heat, transport, and industries. It supports installing 100% RESbased systems, improves flexibility, and provides storage and distribution options. Though sector coupling is getting popular among energy system researchers and policymakers, the definition and scope of the approach are still not clear. This section aims to provide a thorough understanding of the sector coupling concept using a detailed literature review in two timelines.

2.1.1 Definition of Sector Coupling

Sector coupling indicates the concept of combining different energy-consuming sectors—such as electricity with heating, cooling, transportation, etc. The integration of various sectors can provide flexibility and reliability to the system. For example, electricity can be used for district heating or producing hydrogen and synthetic gas. The gas can be stored to either fuel vehicles or to provide backup for electricity or heat conversion in peak times. Another example is biofuels, which can stimulate the decarbonization of heating and transport industries [20].

In the heating sector, P2H technologies hold great opportunities for the energy transition. Important examples are the heat pumps that use electricity to absorb existing heat from the Earth, compact it, and then use it to operate the heating system. It is also efficient; for example, in energy-efficient buildings, a good heat pump with a Coefficient of Performance (COP) 3 can produce 3 kWh thermal energy by consuming 1 kWh of electricity. However, it is necessary to mention here that COP 3 does not indicate the efficiency of 300%, which is thermodynamically impossible. Instead, it suggests that 1 kWh of electricity can run the compressor and require pumps to transfer the energy from environmental heat sources to a building [21].

The transportation sector is another primary consumer sector of electricity. It is possible to electrify the transport sector in many areas. For example, electric cars and trains are already in use in Europe in many countries. It is essential to expand the charging infrastructure for the extended use of electricity in these areas. Overhead lines for heavy trucks are also being tested. Besides electricity, hydrogen can be another option for making the transport sector more environmentally friendly. Electrolysis can be used for this P2G technology, which is a reversible process. Biofuel is another attractive fuel option in the transport sector because of its energy density, easy distribution system, and adaptability with current motor engines [22].

The idea of sector coupling is visualized in Figure 2.1, adapted from [23, Brennig 2018, p.12]. The figure illustrates only the primary RES and the three main energy sectors. P2H, P2G, and power-to-liquid (P2L) are often referred to as power-to-X (P2X). Nevertheless, the integration of different sectors is more complex than shown in this figure and includes more resources and sectors.



Figure 2.1: Coupling of power, heat, and transport sectors. Adapted from [23, Brennig 2018, p.12].

2.1.2 Sector Coupling Studies: 2001 – 2010

Early research on sector coupling can be traced back to the short report of Lehmann on 'Energy Rich Japan' [24]. They used six different scenarios to illustrate how Japan can transition towards a renewable-based energy system using efficient energy technologies across residential, transport, industrial, and commercial sectors. Later, Lund and his co-authors described the Danish perspective on sector coupling in many papers. For example, in one article, Lund and Mathiesen presented the possibility for a 100% renewablebased energy supply in Denmark [25, Lund and Mathiesen 2009, p.524]. They considered several alternatives such as wind, biomass, and hydrogen. They concluded that some of the energy carriers could also cause inefficiency in the system's design, and we can avoid this if we take specific measures beforehand. Lund et al. investigated the possible use of district heating and heat pumps in Denmark in another research work [26, Lund et al. 2010, p.1381]. They recommended that the district heating networks in Denmark be expanded from 46% to 63%-70%, and individual heat pumps to provide the optimal solution in the future energy system [26, Lund et al. 2010, p.1388]. Furthermore, Lund and Kempton discussed the concept of including electric vehicles (EV) and vehicle-to-grid (V2G), where they identified that including EV and V2G in the system allows the inclusion of more wind electricity without surplus production, and thus reduces the carbon emissions [27, Lund and Kempton 2008, p.3578]. Madlener et al. suggested descriptive renewable-focused energy scenarios developed in guantitative and gualitative terms for Austria [28, Madlener et al. 2007, p.6060].

Some studies consider using hydrogen as a convenient technique to aid sector coupling. For example, Sørensen discussed having hydrogen as an alternative in sector-coupled electric and heat sectors and projected that hydrogen could also supply fuel for half of the German cars [29, Sørensen 2007, p.496]. Krajačić et al. presented similar research outcomes and concluded that hydrogen is a secure and technically expedient energy supply [30, Krajačić et al. 2008, p.1091]. Kim and Moon reported in their research that carbon-emission reduction and energy-efficiency gain are possible through hydrogen in the

energy system of Korea [31, Kim and Moon 2008, p.7326]. Mason et al. suggested energy demand management, biomass gasification, load shifting, and transport sector electrification for New Zealand [32, Mason et al. 2010, p.3973]. Zervos et al. presented different perspective literature on sector-coupled European energy systems, which sketches out a way forward for 2030 and 2050, mainly focusing on policy recommendations to overcome the non-technical obstacles of coupling electricity, heating, cooling, and transportation sectors [33, Zervos et al. 2010, p.6].

2.1.3 Sector Coupling Studies: 2011 - Present

Significant research has been carried out on sector coupling of national energy systems in the past decade. Connolly et al. presented the 100% renewable-based energy system for Ireland [34, Connolly et al. 2011, p.502]. He equipped the heating sector with district heating and heat pumps and the transport sector with electricity, hydrogen, and biomass. In another research work, Krajačić et al. planned a 100% self-sufficient energy system using renewables for Croatia [35, Krajačić et al. 2011, p.2073]. Liu et al. analyzed the Chinese energy system, where they recommended changing the current infrastructure to match the power supply and demand with renewables [36, Liu et al. 2011, p.518]. Ćosić et al. proposed a 100% renewablebased Macedonian energy system with a high share of solar, wind, and biomass, along with various storage technologies [37, Ćosić et al. 2012, p.80]. Henning and Palzer modeled the sector-coupled future energy system for Germany consisting of electrical and heating, and storage components and analyzed the system's cost and performance values [38, Henning and Palzer 2014, p.1003]. In the second part of their research, they concluded that 100% renewable energy could feed the power and heat demands (space and hot water) of the entire building sector in Germany [39, Palzer and Henning 2014, p.1019]. Garmisri et al. examined the gas sector electrification of Canada, where they considered the plausible benefits of P2G, using excess power from the wind to generate hydrogen [40, Garmisri et al. 2014, p.2506]. In another research work relevant to the P2G method, Qadrdan et al. showed that the overall operating cost of Great Britain's power-gas network could be reduced by producing hydrogen from electricity [41, Qadrdan et al. 2015, p.5763]. Teng et al. investigated the coupling of power, heat, and transport in the future United Kingdom (UK) energy system by using an advanced stochastic analytical framework [42, Teng et al. 2016, p.420]. Another prospective national sector-coupling example is from Guandalini et al., who evaluated the remote future P2G potential for Italy and concluded that excess energy recovered from renewables could be used for 7% of Italy's current fuel consumption [43, Guandalini et al. 2017, p.13389].

Delucchi and Jacobson analyzed the feasibility of integrating power, heat, and transport sectors from 100% renewables worldwide and concluded that the barriers are not economic or technological, rather predominantly social and political [44, Delucchi and Jacobson 2011, p.1170]. Connolly and Mathiesen showed that renewable energy's techno-economic potential depends on resource availability and fuel imports [45, Connolly and Mathiesen 2014, p.7]. They indicated that the transition needs to start soon, is plausible without any additional system costs, and can positively impact local jobs [45, Connolly and Mathiesen 2014, p.22]. In other analogous research, Mathiesen et al. suggested that creating smart energy systems with smart infrastructures enables the proper utilization of flexible components in a system, such as storage, heat pumps, and EVs [46, Mathiesen et al. 2015, p.139]. Their smart energy systems integrated electricity, heat, and gas grids to realize 100% RES. They presented biomass in a limited and sustainable way and concluded that energy transition towards a bioenergy free sector coupled system is possible via smart energy systems [46, Mathiesen et al. 2015, p.151]. Nastasi and Lo Basso analyzed an aggregated energy model, which considered P2G as a solver of dispatch issues relevant to the storage and energy market [47, Nastasi and Lo Basso 2016, p.5]. Samsatli et al. presented an optimal design and operation of the wind-hydrogen-electricity network [48, Samsatli et al. 2016, p.447]. Rogge et al. investigated the electrification of public transport with fast-charging batteries [49, Rogge et al. 2015, p.4587].

Buttler and Spliethoff reviewed the role of water electrolysis coupling electricity, heat, transport, and chemical sectors via P2G and P2L [50, Buttler and Spliethoff 2018, p.2440]. An exciting revelation from their paper is that water electrolysis is likely to play an essential role in providing flexibility to large energy storage applications. However, there is a need for more investigation and advanced optimization to integrate the electrolysis process in different sectors. Schaber presented an elaborated least-cost optimization energy model for Germany [51, Schaber 2013, p.21]. The research compared sector-coupling options and their economic impact with electric storage via two different scenarios. The research results suggest that long-term hydrogen or gas storage becomes debatable when the heat sector is electrified using renewables [51, Schaber 2013, p.147–149]. The model also showed that grid extension from North to South is necessary to electrify the heat sector in Southern Germany in long-term scenarios [51, Schaber 2013, p.65]. They concluded that sector coupling with VRE integration could improve the economic efficiency of the German energy system [51, Schaber 2013, p.154]. Gils et al. presented a 100% system for Brazil with sector-coupling options and revealed that solar and wind could be more cost-effective than installing new hydroelectric plants [52, Gils et al. 2017, p.1]. Their model results indicate transition towards a 100% system requires coupling of electricity, heat, and transport sectors via P2H, EV, and hydrogen options. The change is also heavily dependent on local development, public perception, and industrial policies. Liu et al. discussed the concept of integrating the transport sector using different EVs and assessed the ability to include more fluctuating wind power in the energy system in Inner Mongolia in China [53, Liu et al. 2013, p.445]. They also recommended the inclusion of heat pumps and pumped storage in the energy system to enhance benefits. In another paper, Liu et al. recommended mitigating individual transport demands, improving the efficiency of vehicles, and increasing alternative fuels from renewables to provide a long-term solution in China [54, Liu et al. 2013, p.347].

Mathiesen et al. showed that 100% RES-based systems could impact socio-economic actions positively while creating more job opportunities leading to extensive export incomes [55, Mathiesen et al. 2011, p.488]. They also revealed that the 100% systems would be competitive in the future compared to the current plans, based on climate change and economic development challenges. Lund et al. discussed the concept of adding smart thermal grids to implement fossil-fuel-free heat supply in future smart and sustainable energy systems [56, Lund et al. 2014, p.1]. In another paper, Lund et al. explained the need for smart energy systems. They recommended that the VRE integration in the power sector be harmonized with the heat and transport sectors, focusing on energy efficiency [57, Lund et al. 2012, p.96]. This study also described the importance of CHP in providing flexibility for power supply-demand balance and stabilization of electrical grids. Connolly et al. discussed the idea of decarbonizing the heat sector via district heating and heat pumps in the Heat Roadmap Europe [58, Connolly et al. 2014, p.475]. Their heat strategy indicates a significant reduction in heating and cooling costs and recommends considering environmental pollution and policy impact parameters while integrating the transport sector in the future decarbonization approaches. In a similar strategic paper on Heat Roadmap China, Xiong et al. revealed the idea of district heating as a long-term solution to reduce dependency on fossil fuels and to decrease system costs [59, Xiong et al. 2015, p.274]. David et al. discussed the role of large-scale heat pumps in future energy systems and concluded the replication of heat pumps throughout Europe is technically feasible [60, David et al. 2017, p.1].

Connolly et al. presented a 100% EU energy system pathway by 2050 in nine transitional steps [61, Connolly et al. 2016, p.1634]. They stated that the transition towards a 100% system in the EU depends more on politics and societal abilities rather than on cost-effective energy solutions. Electricity storage is not the optimal solution to integrate large inflows of fluctuating renewable energy since more efficient and cheaper options can be found by combining the electricity sector with other parts of the energy system and creating a smart energy system. Lund et al. presented the idea of sector coupling in smart energy systems as a more efficient and cheaper option than integrating energy storage [62, Lund et al. 2016, p.3]. However,

they did not recommend excluding energy storage from the system since they provide other usabilities in future energy systems. The feasibility of 100% RES-based systems was further validated in a paper by Brown et al., where the authors demonstrated that 100% renewable systems are viable [63, Brown et al. 2018, p.834]. They presented a comprehensive list of 100% RES-based systems covering the globe and its continents, sub-continents, countries, regions, and sub-regions. Lund et al. reviewed the concept of smart energy systems and stated that the term 'smart energy system' can signify sectoral integration instead of considering individual sectors [64, Lund et al. 2017, p.556]. They concluded that the idea of smart systems could provide plausible, efficient, and achievable solutions. Another paper from Lund compared the concepts of smart grids with smart energy systems and concluded that the latter with sector coupling can be implemented with relatively lower investments with a minimum extension of grids and storage facilities [65, Lund 2018, p.94].

Several recent papers present the most advanced prominent research on sector coupling in Europe. Robinius et al. analyzed the potential of sector coupling and linked the electricity and transport sectors on national, continental, and global levels [66, Robinius et al. 2017, p.1]. The follow-up paper outlined an approach for the modeling, mainly focusing on Germany's power and transport sectors [67, Robinius et al. 2017, p.1]. The model results were presented using excess power, electrolysis application, hydrogen infrastructure, and economic analysis to show the potential benefits of sector coupling. Brown et al. considered two concepts in his renewable-based model, electrification of heating and transport sectors and reinforcement of the inter-continental transmission network in Europe [68, Brown et al. 2018, p.720]. Their scenarios concluded that while the battery electric vehicles can balance solar power variation, P2G and TES can balance long-term variations in supply and demand. They also concluded that the system cost could be reduced by expanding the transmission network, but only when the sectors are weakly coupled. Pavičević et al. suggested cross-sector coupling to avoid curtailment and load shedding in a high VREbased system [5, Pavičević et al. 2020, p.1]. They recommended pumped hydro storage (PHS) and gridconnected EV storage for improving system flexibility. In addition, they suggested using TES to prevent overcapacity of thermal units and provide load shifting alternatives to couple power and heat sectors. Fridgen et al. proposed a holistic understanding of sector coupling to reduce spatial energy-transportation losses [7, Fridgen et al. 2020, p.1]. They suggested a framework to align energy goals and economic incentives for individual actors in the complex energy network. Koivisto et al. showed that sector coupling could boost offshore wind power in the NSR as electricity consumption rises [69, Koivisto et al., 2020, p.1705]. They also found that VRE curtailment decreases significantly with sector coupling as the energy system's flexibility increases.

2.2 Energy System Modeling

This section presents an overview of energy system models and a list of appropriate open-source energy models, which can be helpful for the scientific community working on modeling large RES-based systems.

2.2.1 Energy System Modeling: 1970 – 2000

The earliest review of energy models can be traced back to the research reports by Charpentier et al., in which they described 14 energy models and classified them in terms of substance and geographical applicability [70, Charpentier et al. 1975, p.9]. Beaujean et al. developed the first global and international energy models survey based on earlier reviews by Charpentier et al. [71, Beaujean et al. 1977, p.153]. Meier, in his book, contrasted different energy models and proposed a categorization taxonomy for developing countries [72]. Markandya focused on power system planning models, focusing on environmental concerns and developing countries [73]. Grubb et al. classified energy models based on six dimensions: bottom-up and top-down, temporal horizon, sectoral scope, simulation and optimization, aggregation level, and geographical scope [74, Grubb et al. 2993, p.397]. Shukla compared energy models

and evaluated the bottom-up and top-down approaches [75, Shukla 1995, p.677]. Bhattacharyya undertook a comparison between equilibrium energy models [76, Bhattacharyya 1996, p.145]. Krause presented different energy models to reduce CO₂ emissions in future European energy systems [77, Krause 1996, p.899]. Hourcade and Robinson determined three objectives for energy system models: forecast, backcast, and scenario development [78, Hourcade and Robinson 1996, p.863]. Kelly and Kolstad contrasted between the evaluation models for controlling climate change in [79]. Van Beeck presented the classification of energy models and the selection of an energy model for regional planning in his book [80].

2.2.2 Energy System Modeling: 2001 – 2010

Between 2001 and 2010, there were two elaborated energy-model reviews. The first one was by Jebaraj and Iniyan [81, Jebaraj and Iniyan 2006, p.281]. They reviewed a list of energy models, including planning models, supply-demand models, forecast models, renewable models, emission reduction models, optimization models, neural network models, and fuzzy theory models. Another detailed review was by Connolly et al. [82, Connolly et al. 2010, p.1059]. They presented 68 different computer tools that can be useful to model renewable-based systems to meet various objectives needed for the energy transition. Among other notable reviews, Pandey suggested incorporating the features of developing countries in energy-policy modeling and discussed the transition dynamics and barriers [83, Pandey 2002, p.97]. Bahn et al. reviewed the modeling approaches for presenting, understanding, and controlling the synergy between regional economies, energy systems, and environmental impacts [84]. Nakata addressed different energy-economic model issues and application of the model in concurrence with renewable energy systems, national policies, and the environment [85, Nakata 2004, p.417]. Ventosa et al. focused on market modeling for electricity production to aid identification, classification, and characterization of approach divergence [86, Ventosa et al. 2005, p.897]. Urban et al. analyzed the performance of models dealing with developing country aspects [87, Urban et al. 2007, p.3473]. Hiremath et al. explained why decentralized planning is needed for energy systems and how energy models can be accommodated at the decentralized level [88, Hiremath et al. 2007, p.729]. Sensfuß et al. reviewed agent-based models that can be used to investigate market power and designs [89, Sensfuß et al. 2007, p.729]. Van Ruijven et al. discussed the compatibility of global energy models for developing countries [90, Van Ruijven et al. 2008, p.2801]. Möst and Keles presented approaches via stochastic modeling for liberalized electricity markets [91, Möst and Keles 2010, p.543]. Foley et al. provided techniques for electricity modeling and examined a few USA- and Europe-based power system models [92, Foley et al. 2010, p.4522]. Bhattacharyya and Timilsina discussed a comparison of existing energy models and investigated the suitability of models for analyzing energy, environmental, and climate change-related policies of the developing countries [93, Bhattacharyya and Timilsina 2010, p.494].

2.2.3 Energy System Modeling: 2011 – Present

There is significant literature on energy system modeling focusing on the latest trends and developments in the modern energy systems and looking forward to the energy transition. For example, Bazmi and Zahedi presented optimization modeling as a helpful tool in renewable-based energy systems [94, Bazmi and Zahedi 2011, p.3480]. They also assessed the long-term potential of P2G, the foreseeable change in the demand pattern, and the penetration of photovoltaics (PV) and wind in a national energy system in their research. Keirstead et al. discussed the critical areas of urban energy systems, which are the design of technologies, buildings and systems, urban climate, assessment of policies, use of land, and modeling of transportation systems [95, Keirstead et al. 2012, p.3847]. DeCarolis et al. reviewed energy economic optimization models [96, DeCarolis et al. 2012, p.1845]. They provided recommendations regarding a sustainable software framework for repeatable analysis. They suggested that models should be open through cross-examination of open code and data, and everyone should be able to verify the model results by running the model. Suganthi and Samuel reviewed energy demand forecasting models [97, Suganthi

and Samuel 2012, p.1223]. The models are characterized by traditional and computational methods, support vector regression, ant colony, particle swarm optimization, and bottom-up approaches. Hedenus et al. reviewed policy process models and analyzed their mechanisms [98].

While revealing the 21st-century challenges for energy system modeling, Pfenninger et al. divided the models into four categories: optimization models, simulation models, market models, and qualitative and mixed-method scenarios [99, Pfenninger et al. 2014, p.76]. According to their research, the four key challenges are (1) the temporal and spatial resolution, (2) the balance of transparency and uncertainty, (3) recognizing the increasing complexity of energy systems and incorporating people's behavior, and (4) associated social risks and opportunities. Olanrewaju and Jimoh analyzed an integrated model to evaluate the possibility of energy efficiency in the industries [100, Olanrewaju and Jimoh 2014, p.661]. Li et al. introduced socio-technical energy transition (STET) and analyzed the STET models and their operations for three sectors: energy supply, transportation, and buildings [101, Li et al. 2015, p.290]. Sinha and Chandel reviewed the recent optimization techniques for hybrid (PV-wind) renewable-energy systems [102, Sinha and Chandel 2015, p.755]. Després et al. abstracted a typology of long-term energy system and power system tools [103, Després et al. 2015, p.486]. Multi-energy systems models on the city level were summarized by Van Beuzekom, who concluded that none of them provide practical grid feasibility perspectives [104, Van Beuzekom 2015, p.1]. Hall and Buckley presented a systematic approach to identify the established modeling tools via literature reviews and policy papers [105, Hall and Buckley 2016, p.607]. Tools for modeling EVs and their characteristics were reviewed by Mahmud and Town [106, Mahmud and Town 2016, p.337].

The latest developments in energy system modeling and their detailed overview can be found in the research papers by Sola et al., Ringkjøb et al., and Lopion et al. [107–109]. While the perspective of Sola et al. was to implement the current co-simulation methods for city-scale energy system models [107, Sola et al. 2018, p.1], Ringkjøb et al. presented a detailed review of 75 recent energy system modeling tools which consider renewables as primary generating resources [108, Ringkjøb et al. 2018, p.441–442]. Lopion et al. reviewed 24 national-level energy models, which included all the energy sectors [109, Lopion et al. 2018, p.156. A list of open energy modeling tools can also be found in [110], where energy models published under open-source licenses are frequently added and updated by the Open Energy Modelling (openmod) community.

2.2.4 Appropriate Tool Selection: Open Energy System Modeling

Promoting open energy system modeling, in which the source code is available freely for studies, modification, and improvement by the users is getting popular. The process increases transparency, reliability, reproducibility, and networking among the energy system modelers and the users. It also avoids repetitive work and enhances education and public engagement. The open energy modeling process is shown in Figure 2.2, adapted from [111, Pfenninger et al. 2018, p.64].



Figure 2.2: Open Energy Modeling Process. Adapted from [111, Pfenninger et al. 2018, p.64].
The energy system transition towards carbon neutrality needs to perceive the idea of open energy system modeling. The models need to be transparent and openly accessible to align with the policy relevance. The significant steps to consider have been addressed by Pfenninger et al., where the authors discussed the strategies regarding code, data, intellectual property, license, modeling languages, supports, and community building [111, Pfenninger et al. 2018, p.63–71].

2.2.4.1 Rationale-Based Tool Selection

Because of the eminent essentiality for open science required by the global energy system transition, the idea of open energy modeling has been considered as the key criterion in this research to select several tools to model an energy system. A preliminary list of recent energy system modeling tools (open and non-open) can be drafted by combining the 75 tools presented by Ringkjøb et al. [108, Ringkjøb et al. 2018, p.441–442] and tools listed by the openmod community [110]. The number of tools then narrows down to 59, which are open or accessible for energy modeling and educational use. The tools and their geographical scopes can be found in Appendix B (Table B.1). The list is then further shortened to accommodate the modeling of the sector-coupled renewable-based system. The rationale used further shortening the list is shown in Figure 2.3. The rationales used for shortening the list is stated below:

- 1. The model openly shares the code and data.
- 2. The model either provides all proven renewable components, or the users have access to code to build and modify different elements.
- 3. The model lets the user realize and integrate different energy sectors (e.g., electricity, heat, and transport).
- 4. Energy storage is present, or the user can add it to the model
- 5. The users can replicate the model for any geographical contexts.
- 6. The model horizon varies from sub-national to global levels to allow for modeling from different resolution aspects.
- 7. The model allows grid modeling.



Figure 2.3: Rationales used for selecting tools to design RES-based and sector-coupled energy systems

Based on these rationales, the list narrows down to 16 tools. Some of the omitted tools can also model RES-based sector-coupled energy systems with additional adjustments. However, this research focused on models which fulfill all the selected criteria explicitly. Table 2.1 shows the shortlist of 16 tools along with their methodology, temporal resolution, sectoral coverage (electricity, heat, and transport), and demand response consideration.

SI.	ΤοοΙ	Methodology	Temporal Resolution	Sectoral Coverage	Demand Response		
1	Calliope	Linear Programming (LP)	User-defined	-	\checkmark		
2	DESSTinEE (Demand for Energy Services, Supply and Transmission in Europe)	Simulation	Hourly	-	-		
3	Dispa-SET (Unit commitment and Dispatch model. SET refers to the European Strategic Energy Technology Plan)	LP, Mixed-Integer Linear Programming (MILP)	Hourly	\checkmark	\checkmark		
4	ELMOD (Electricity Sector Model Family)	LP, MILP	Hourly	\checkmark	-		
5	ficus	MILP	15 Minutes	\checkmark	-		
6	LEAP (Long-range Energy Alternatives Planning)	Simulation and Optimization	Yearly	\checkmark	-		
7	LUSYM (Leuven University System Modeling)	MILP	15 Minutes, Hourly, Daily, Weekly	-	\checkmark		
8	MEDEAS (Modelling the Energy Development under Environmental and Social Constraints)	Mixed	Yearly	√	-		
9	Oemof (Open Energy Modeling Framework)	LP, MILP, Partial Equilibrium	User-defined	\checkmark	\checkmark		
10	OSeMOSYS (Open Source Energy Modeling System)	LP	User-defined	-	\checkmark		
11	PowerGAMA (Power Grid and Market Analysis)	Simulation, LP	Hourly	-	-		
12	PyPSA (Python for Power System Analysis)	LP	User-defined	\checkmark	\checkmark		

Table 2.1: Rationale-based tools for modeling RES-based and sector-coupled energy systems

13	RETScreen (RET refers to Renewable- energy and Energy-efficient Technologies)	Simulation	Daily, Monthly, Yearly	-	-
14	SIREN (SEN Integrated Renewable Energy Network. SEN refers to the Organization 'Sustainable Energy Now Inc.')	Simulation	Hourly	-	-
15	SWITCH (Solar, Wind, Transmission, Conventional Generation and Hydroelectricity)	MILP	Hourly	\checkmark	\checkmark
16	urbs (Urban Energy Systems)	LP	User-defined	\checkmark	\checkmark

2.2.4.2 Short Description of the Selected Tools

This section provides a short description of the 16 selected tools. The idea of open science is the core focus for preparing the list. Nevertheless, modelers who want to develop RES-based and sector-coupled energy systems can use these tools and other tools based on the additional rationales of research to portray different aspects of the energy system. Appendix B (Table B.2) provides a detailed comparison of the selected tools.

1. Calliope

Calliope is an energy-planning tool for systems ranging from districts to continents [112]. The main focus of Calliope is flexibility, spatial and temporal resolution, and separate code-data platforms. Pre-defined systems can be tested for different modes in calliope. Text files are used to define technologies, geographical location, and possible sources. The model then creates an optimization problem based on the files, provides a solution, writes the results in dataset formats to be easily converted into Pandas structures. It helps a simple analysis using either endogenous Calliope or Python data-processing tools.

2. DESSTinEE

DESSTinEE is developed as a futuristic energy system model for 2050 in the European context [113]. The model is used mainly for testing electricity transmission assumptions and the economic obstacles that arise with the modeling. Forty countries have been included in the model with ten primary- and secondary-energy forms. The technique used in the model is a predictive simulation. When the user provides data and assumptions into the model, it gives a set of answers as simulation results.

3. Dispa-SET

The *Dispa-SET* model is developed using the General Algebraic Modeling System (GAMS) and Python. The model uses simple comma-separated values (CSV) files as input data [114]. The model's methodology is based on linear programming (LP) or mixed-integer linear programming (MILP) and depends on accuracy and complexity levels. There are two types of variables in the model. The continuous variables indicate power dispatch units, load shedding, and curtailed power generation. Binary variables indicate unit commitment status. The model solves the unit commitment problem by considering a central operator with complete information. However, the unit commitment problem excludes optimal power flow calculations.

The problem is subdivided into unit scheduling and economic dispatch problems. The goal of the unit commitment is to minimize the total system cost.

4. ELMOD

ELMOD consists of several spatial optimization models and demonstrates details of the European power sector, including generation and transmission networks [115]. The modeling approach is bottom-up and considers different engineering and economic parameters of the system. The models consider power flow in high-voltage grids and features of the generating units and results in minimum-cost or maximum-welfare dispatches. Market design, network congestion, and investment problems can be solved using ELMOD. ELMOD's several versions are ELMOD (Europe), ELMOD-DE (Germany), stELMOD (stochastic multi-market model), and dynELMOD (multi-period investment model).

5. ficus

The *ficus* model is based on MILP and is mainly used for expanding system capacities or solving unit commitment problems for local energy systems [116]. The model was originally developed for factories. If a demand time series is provided, the model finds the least-cost solution for commodities like electricity and heat. The model considers cost time-series, peak demand charges, etc. The model can be converted into an LP model by deselecting equations. The model can deal with multiple numbers of inputs and outputs for energy conversion and considers relevant efficiencies.

6. LEAP

LEAP is a popular scenario-based modeling tool that includes energy generation, consumption, and all economic sectors. GHG emissions can be tracked for all areas [117]. LEAP can analyze air pollutants and greenhouse gases (GHGs) leading to local pollution reduction. Although LEAP does not represent a particular energy system, the users can use it to develop different energy system models with unique data structures. A broad range of modeling techniques can be supported by LEAP, including top-down and bottom-up modeling. There are also unique methods to realize transport planning. LEAP provides both simulation and optimization techniques to model power sectors and capacity expansions. The models are transparent, flexible, and adaptable to other models.

7. LUSYM

LUSYM is a MILP-based unit commitment model developed by the University of Leuven (KU Leuven) [118]. It selects the optimized scheduling from several power plants to satisfy the electrical demand and considers all the system's operational parameters. The mathematical formulations include power station limitations, load flexibility, curtailment of RES, storage options, grid parameters and limitations, spinning reserves, and must-run scenarios. LUSYM can be used for large-scale systems within reasonable simulation times. Through compact formulation, efficient data handling, and MILP solvers, the simulation times are reduced in LUSYM.

8. MEDEAS

The objective of *MEDEAS* is to develop a model to structure the futuristic energy system in Europe while considering the technical and social constraints [119]. The renewable-based transition in Europe and the required policies can be tested using the MEDEAS model. It considers various other tools, for example, WoLim (World Limits Model), TIMES (The Integrated MARKAL-EFOM System), and LEAP. MEDEAS considers input-output analysis to realize the socio-economic and environmental impacts. The design is

modular so that the system is flexible and engages stakeholders from different categories. The model also provides high spatio-temporal resolution and involvement of sectors.

9. Oemof

Oemof is a framework for developing energy system models and different applications to perform energy system analysis [120–122]. The model generator of Oemof can be used for solving investment, dispatch optimization, and unit commitment problems. Oemof provides detailed component-based modeling using mathematical formulation and includes heat components such as CHP, heat pump, heat storage, etc. The grids can be modeled via two approaches, either by transshipment or by linear optimal power flow. Oemof as an advantageous tool for open model-based analysis is further discussed in Section 2.2.5.

10. OSeMOSYS

OSeMOSYS assesses long-term energy planning scenarios on different geographical scales (from continents to villages) [123]. The tool is ready to use by scientists and policymakers for its rapid learning curve and minimum run-time requirement. The tool balances energy supply and demand and minimizes the total cost. The tool includes sectoral integration as well as operating in different spatio-temporal levels. The energy resource component details incorporate technical and economic parameters, technology potentials, and system costs. Real issues like techno-economic constraints or emissions can be addressed via policy scenarios. The tool is a deterministic, LP, long-term modeling framework, which is also adaptable to MILP for including complex functions.

11. PowerGAMA

PowerGAMA is a simple simulation tool for analyzing RES integration in large-scale power systems [124]. The tool is based on Python and provides high-level analysis for a dispatchable generation. The optimization is based on marginal costs for user-given timesteps. The tool considers the variability of RES and demand. Another critical feature of PowerGAMA is that it considers alternating current (AC) grid power flows based on physical equations. PowerGAMA can address the flexibility assessment via storage inclusion, optimum energy mix, associated costs, and network congestion problems.

12. PyPSA

PyPSA is a tool for the simulation and optimization of modern power systems. The tool considers various features, for example, conventional generation with unit commitment, variable renewable generation, storage inclusion, sector coupling, and mixed AC-direct current (DC) networks [125–127]. PyPSA can be used for large-scale networks with a long time series. It can solve static and linear optimal power flow, least-cost optimization problems. The static power flows can be calculated using linear and nonlinear equations. Linear optimal power flow addresses minimum cost optimization of power and storage dispatching units using linear equations. Additionally, security-constrained linear optimal power flow can also be performed. The total system cost optimization can be undertaken using linear equations for optimizing generation and storage unit dispatch and considers investment in generation, transmission, storage, and other infrastructural capacities.

13. RETScreen

RETScreen is a popular pre-feasibility analysis tool for renewable energy projects [128]. It can be used for energy efficiency, renewable integration, and cogeneration for addressing the feasibility of an upcoming or ongoing project. There are two different versions of RETScreen, excel-based and graphical user interface-based (RETScreen Expert). The tool is easy to use and can be used by scientists and policymakers to

determine, evaluate and optimize the techno-economic feasibility of clean energy projects. The tool also allows measuring and verifying an energy project's performance and helps determine the plausible savings opportunities. The tool is available in 36 languages, which enhances the versatile use of the tool. Both conventional and renewable technologies are incorporated in RETScreen, including their efficiencies, sectoral integration, etc. The tool can be connected to the central databases for obtaining different input parameters. Several available projects also simplify the understanding of RETScreen based clean energy projects and their implementation strategies.

14. SIREN

SIREN is a toolkit that uses the 'System Advisor Model (SAM)' for energy calculations [129]. SIREN provides scenario building provisions for the preferred energy mix. A map can be chosen to build a scenario that addresses the current local electrical network in the map and allows additional stations by the user. The user can also obtain relevant data from other resources to put into the model. The result from the model is listed as shortfalls and is uploadable into the power balance component of the SIREN toolkit. This way, the cost of dispatchable generation, storage, and emissions can be quantified. The outcome is a complete RES-based scenario reflecting the expenses.

15. SWITCH

SWITCH can be used for energy transition planning to modern energy systems to satisfy state-of-the-art grid requirements [130]. Investment and operational planning, including renewable integration, can be performed using this tool. SWITCH has several applications, such as resource planning via integration, fundamental research, techno-economic analysis, policy evaluation, etc. The electrical elements of SWITCH consider unit commitment, efficiency, supply curves, planning and operational reserves, storage provisions, demand response activities, hydropower networks, and policy limitations. The flexible architecture of SWITCH allows a user to choose reference models and write their customized models.

16. urbs

The model *urbs* consists of various model entities [131]. The entities are commodities, processes, transmission, and storage. Intermittent supply and demand datasets can be modeled in urbs using time series. This model can generate linear optimization models for energy systems. The tool uses linear programming and can be used for capacity expansion planning and solving unit commitment problems in distributed systems. The model can be adapted for varying geographical scales, from continental to local levels. The tool focuses on the optimized sizing of storages and their usage. It looks for the cost-optimal solution for the given time series for multiple commodities. The model generally considers hourly time steps and incorporates reporting and plotting features.

2.2.5 Oemof for Open Model-based Analyses

Most energy system model reviews provide a general overview of the tools and are often classified based on their functionalities. So far, the study has described the evolution, current challenges, and available tools for energy system modeling. Then it proceeded with the idea of finding a suitable model based on several rationales. This list of 16 tools does not predicate a 'must choose from' obligation; instead, it helps a user realize and justify which tools are suitable for a sector-coupled RES-based open system modeling. Hence, a user can select any of the 16 tools described in the previous section, combine them, and even select an additional model that is not listed here. This section discusses Oemof as one of the advanced tools to model sector-coupled and highly renewable open energy models for the NSR. Energy system modeling challenges increase with the growing complexities of the largely renewable-based energy systems and their strong weather dependance. Hilpert et al. addressed the critical challenges of energy system modeling: complexities, uncertainties, interdisciplinary modeling, scientific standards, and model utilization. They introduced the concept of the modeling framework Oemof as a contemporary approach for modeling energy systems [120, Hilpert et al. 2018, p.16]. They explained how Oemof could be used to tackle the challenges of modern energy systems. The following parts briefly discuss the applicability, concept, and simple examples of using Oemof to model the NS energy system.

2.2.5.1 Addressing Energy Modeling Challenges using Oemof

Oemof can significantly contribute to open science through its free and open-source software, collaborative development, and modular structural representation. Oemof's open philosophy can address the critical challenges of complex energy systems [120, Hilpert et al. 2018, p.16]. Some of the significant features of Oemof to address the energy system modeling challenges are:

- 1. Oemof can create flexible energy system models due to its easily integrable generic structures and object-oriented approach.
- 2. Oemof addresses the uncertainty through collaborative modeling to look deep into various decisive features of energy systems.
- 3. Oemof allows interdisciplinary modeling to understand common research problems in energy systems.
- 4. Oemof follows strict scientific standards via different levels of control mechanisms to ensure transparency and reliability. Oemof also allows repeatability, reproducibility, and scrutiny of the model.
- 5. The open-source, open data approach of Oemof also allows communication between modelers, policymakers, and other stakeholders, enhancing the understanding of energy systems and accelerating the energy transition.

An investigation into the details of Oemof and its applications and usage suggests that it can include all the conventional and renewable generations of the NS energy system. Most of the proven components of an energy system are already available in the Oemof framework. In addition, Oemof makes provisions to include different kinds of storage and dispatchable loads. The Oemof framework has cross-sectoral modeling opportunities, including heat and transport.

2.2.5.2 The Oemof Concept

The acronym Oemof is derived from the 'Open Energy System Modeling Framework.' Oemof provides an energy modeling toolbox that is open-source, free and has excellent documentation. Python is its base language, and it has a modular structure with various packages linked via specific interfaces. Hilpert et al. discussed the scientific contribution, concept, architecture, implementation, and usage of Oemof [120, Hilpert et al. 2018, p.16–25]. Figure 2.4 presents a graphical representation of how to describe an arbitrary energy system using Oemof [120, Hilpert et al. 2018, p.19].



Figure 2.4: Schematic illustration of an energy system represented as an Oemof network. Source: [120, Hilpert et al. 2018, p.19].

In Oemof, the energy system is represented by a network of Nodes connected via Flows. Nodes represent either balance spaces or entities of an energy system, and Flows represent energy flows. There are two types of Nodes in Oemof: Components and Buses. Every Component has to be connected with one or more Buses. While Buses (e.g., electricity bus, heat bus) connect the Components, the Components (e.g., power plants, storage units, loads) indicate generators and consumers in the energy system. The connection between a Component and a Bus is the Flow. Flows (e.g., electricity, heat) are used to represent the inputs-outputs of the Components. The Components of Oemof can be directly used or can be modified according to modeling needs [120, Hilpert et al. 2018, p.20-21]. The main Components of Oemof are Sources, Sinks, and Transformers [120, Hilpert et al. 2018, p.19]. The Sources have only outflows. For example, solar PV, wind turbines, and biomass commodities are modeled as Sources. The Sinks only have inflows. Consumer demands such as electricity or heat loads are modeled as Sinks. Transformers have both inflows and outflows. For example, heat pumps can be modeled as Transformers, which receive electricity inflow and convert it to heat outflow. There are also other components, such as ExtractionTurbineCHP, GenericCHP, Link, GenericStorage, GenericCAES, SinkDSM, etc., which are designed in the Oemof Solph package [132, Krien et al. 2018, p.1-4]. Figure 2.5 shows a simple Oemofbased energy system [133, Oemof Documentation v0.2.3 2018, p1]. The Source provides the demand of Sink 1 through Bus 1 and the demand of Sink 2 via a Transformer and Bus 2.



Figure 2.5: Oemof Components. Adapted from Oemof Documentation [133, Oemof Documentation v0.2.3 2018, p1].

2.2.5.3 Using Oemof to Model Energy Systems

There are three ways to create an optimization problem based on Oemof [133, Oemof Documentation v0.2.3 2018, p15]:

- 1. The energy system describes a graph with flows on its edges by combining necessary *Components* and *Buses*;
- 2. The basic energy system is adapted by defining additional constraints on top of the aforementioned graph logic; and
- 3. Custom components are added to a model by subclassing from the core or creating from scratch.

The use cases can be separately or combinedly used in an energy model, allowing maximum flexibility. Oemof provides existing functionalities to build energy models for varying scales. In addition, it enables the combination and adaptation of different energy models to create tools with specific research objectives. Oemof libraries can be combined to write an application to model an energy system. The current Oemof libraries are *network*, *solph*, *outputlib*, *feedinlib*, and *demandlib* [133, Oemof Documentation v0.2.3 2018, p15]. The solph library can solve optimization problems like LP and MILP. The *outputlib* collects the results of optimization, which can be visualized using any plotting library. *Feedinlib* and *demandlib* can be installed additionally to calculate feeding time series and load profiles. A *Source* has one output, a *Sink* has one input, and a *Transformer* can have multiple inputs and outputs. For example, a CHP plant can get gas from the *Gas Bus* and provide electricity and heat demand via two different *Buses*. *Transformers* can also be used to model transmission lines in the energy system [133, Oemof Documentation v0.2.3 2018, p43].

To create an Oemof-based model, an empty energy system object is constructed, which contains the *Nodes* and sustains information. Different scenario provision and node-handling capabilities are also provided in this step. The next step involves the population of the energy system *Nodes* and *Flows*. After that, the model is optimized using a solver. The final results are then processed using the output library in the last step [133, Oemof Documentation v0.2.3 2018, p44–46]. The usage can be separate or within one single model. Thus, a developer of Oemof can easily switch between economic dispatch, unit commitment, and investment modes by making minor changes depending upon the application developed. Figure 2.6 shows a more detailed example of an Oemof-based energy system where PV, Wind and a Gas plant are used as *Sources*, a CHP is used representing a Transformer, a storage *Component* is connected to the *Electricity*

Bus, and electricity and heat loads are representing *Sinks*. There are three *Buses* in the energy system: *Electricity, Heat* and *Gas*.



Figure 2.6: Example of Oemof-based Renewable Energy System. Own Illustration.

Many projects have used Oemof to investigate various energy system research questions. For example, *renpass* simulates power supply in Germany and Europe with high temporal and regional resolution, *openMod.sh* couples the electricity, heat, and gas sectors of Schleswig-Holstein, and *reegis*^{hp} models local heat and power systems [134–136]. These applications validate Oemof's usability to investigate diverse research questions of large and complex energy systems. Figure 2.7 shows an Oemof application adapted from Hilpert et al. [120, Hilpert et al. 2018, p.23].



Figure 2.7: Example of Oemof-based sector-coupled energy system. Adapted from [120, Hilpert et al. 2018, p.23].

2.3 Summary

Chapter 2 details the role of sector coupling in the global context with its definition, the basic idea of integrating the heat and transport sectors into the power sector, and the hypothesis of P2X required by the sectoral integration. The literature review on sector coupling was divided into two different timelines. The first timeline (2001 – 2010) presents national schemes for potential pathways towards a sector coupled with future energy society and includes research examples from Japan, Denmark, Austria, Germany, Korea, and New Zealand. The second timeline (2011 – present) presents the more recent trends in sector coupling and demonstrates examples from Ireland, Brazil, Mongolia, Croatia, China, Macedonia, Germany, Canada, Great Britain, the UK, and Italy. Both the timelines include the potential of various renewable resources, district heating, heat pumps, P2X, and hydrogen. Additionally, issues like the usage of smart grids, electrification of all the sectors, and optimal operation of the sector-coupled network are also vital factors of the prominent research into sector coupling.

Evaluating the different studies for sector coupling has shown a lack of a uniform view in science and politics and a definite need for a clear understanding. While some studies discuss only the transformation of renewable electricity to heat, gases, or liquids, other studies show integrating all energy sectors. Hence, a unique understanding of sector coupling can refer to the progressive process of substituting fossil fuels through the use of known cross-sectoral applications using renewable resources. While electricity can be generated directly from renewables, heating, cooling, and transportation are possible via P2X. Sector coupling refers to supply-demand relations and considers the interlinkage between the consumption sectors like households, commerce, trade, services, industries, transports, etc. While the main objective of sector coupling is to reduce GHG emissions by substituting fossil fuels, the secondary aim is to provide flexibility, network optimization, and increased efficiency to the energy systems. In summary, sector coupling challenges are composed of techno-economic, social, and political challenges, which should be solved together for the energy transition.

The literature review on energy system models is divided into three different timelines to understand the evolution, availability, and capabilities of energy system models. The first timeline (1970 – 2000) presents the early energy modeling tools and their classification approaches. It is revealed from the review that some of the old modeling tools addressed carbon emission reduction, and some of the models were modified at a later stage to cope up with the transition in the energy systems. The second timeline (2001 – 2010) gives more attention to the use of renewable energy required by the energy transition and addresses other important energy modeling issues such as national policies, environment, electricity market, regional economies, decentralized planning, etc. Finally, in the third timeline (2011 – Present), the idea of sector coupling has been considered by many of the models. The latest trends in energy modeling also include the concepts of P2X, electric vehicles, open science; and addresses challenges such as temporal and spatial resolution, the increasing complexity of the energy systems, societal barriers, etc.

One of the conclusions from the review of energy system modeling studies is a shortcoming in the purposeful and efficient combination of different modeling approaches and viewpoints and collaboration between modeling tools on various aggregation and spatial levels. Combining tools and ideas is necessary to provide a coherent picture of the required transition process of large-scale energy systems like the NS region. Furthermore, linking these tools will translate the techno-economic, social, and environmental aspects of various strategies and scenarios. Another conclusion concerns the resolution aspects of energy system modeling. For example, when modeling from a national perspective, the aggregated models only provide more holistic pictures. Still, they cannot portray regional or sub-regional specifics, which results in meaningless results at lower spatial scales, including demand response. Hence it is imperative to address the energy system modeling from smaller to larger spatial levels, in which different aspects of the energy systems, for example, technology components and their deployment potential, infrastructure, demand response, the participation of society, market behavior, costs, etc. are more specific and influential. Both of the spectrums, local and global, and the linkages between them are important to address the challenges of energy system modeling. The paragraph can be summarized into two main points: (1) the collaboration of modeling strategies and tools is still not very practiced, but is essential, and (2) both aggregated and disaggregated level analyses are important to address the complex challenges of energy system modeling.

The next obvious question is, what is already there on the table, and how to choose one or many tools from this broad range of models. The answer is that selecting an appropriate tool can be based on the rationale of a project. For example, one key objective of this study is to model an open-data, open-source, 100% RES-system with sector coupling options in the NSR. Hence based on these rationales, an example of shortening the list is presented, where a list of 59 open energy modeling tools is shortened to 16 tools. It can be presumed that most sub-regional to large-scale challenges of the energy system transition and

sector-coupling can be assessed using a combination of these tools. However, other models that are not present in this list can also co-act to portray different specifics of an energy system from different contexts.

An additional realization from the studies is that there is a need to include social and political aspects of the energy system models. The energy system modelers should not focus on least-cost optimization only; instead, they should try to look for near-optimal solutions, including political and social processes. For example, establishing a new wind-power plant or transmission line may be accepted, actively taken up, or resisted by the local citizens, and these issues should be dealt with from social or political perspectives. Hence, the collaboration of modeling tools needs to consider the insights of policies and investment planning to finalize the strategies for a smooth energy transition.

One of the promising tools to address the modern energy system challenges is Oemof, which is becoming widely popular and is capable of understanding complex energy systems. Therefore, the concept of Oemof is presented, followed by the hypothesis behind Oemof, its core structure and components, and the usage of Oemof to design simple to complex energy systems. Based on the basic understanding of the Oemof modelling framework, it is taken from the analysis that Oemof can be used as an advantageous tool to design the sector-coupled and 100% RES-based future energy system for the NSR.

In Chapter 3, the literature review is extended to include a coherent idea of P2H and TES as promising technology alternatives for the ongoing European energy transition. Besides defining, classifying, and discussing the potential roles of the technologies, Chapter 3 presents the modeling equations for realizing and implementing the technologies as components of large-scale energy optimization models.

Chapter 3 Power-to-Heat and Thermal Energy Storage

3.1 Background

Sustainable heating and cooling strategies are expected to play a significant role in achieving the ambitious Paris Agreement target in Europe. Heating and cooling in buildings and industries account for half of the total final energy demand in the EU, of which 80% is industrial process heating [137]. In the EU households, space and water heating account for 79% of the total final energy use [138,139]. Over the years 2003-2018, the share of energy from renewable sources for heating and cooling in these two sectors has steadily grown from 10% to almost 20% in the EU-27 and the UK [140]. Figure 3.1 shows the share of renewable energy as a percentage of gross final energy consumption for heating and cooling in European countries in 2018. In Sweden, Latvia, Finland, and Estonia, renewable energy accounted for more than 50% of the energy consumption for heating and cooling. On the other hand, the shares are less than 10% in Ireland, the Netherlands, Belgium, and Luxembourg.



Figure 3.1: Share of renewable energy for heating and cooling in European countries in 2018. Data Source: Eurostat [140].

Power-to-Heat technologies, often abbreviated as PtH or P2H, refer to applications in which electrical energy generates heat, which is mainly used in the built environment or industrial processes. P2H offers many advantages to drive the energy transition. For example, P2H using excess VRE helps energy regulation and reduces the use of fossil fuels. With more VRE penetration on the European grid, the power system's voltage, transient, small-signal, and frequency stabilities are increasingly challenged [141, Impram et al. 2020, p.1]. For this reason, grid operators occasionally switch off some of the (inverter based) VRE plants (e.g., wind turbines), leading to the curtailment of a large amount of renewable energy. Using P2H, the total load can be increased during high VRE production and low load, thus limiting the rise of the instantaneous VRE penetration, and keeping the power system more stable with less curtailment of renewable energy. Besides, P2H offers additional flexibility in the electricity market by using and balancing energy in times of low or negative electricity prices. When there is a negative electricity price, fossil-fueled power plants may not leave the market because it might not be profitable, e.g., they reserve capacity for the balancing energy market. P2H can provide this service at a comparatively low cost and thereby reduce carbon dioxide emissions. Efficient P2H systems can ensure the energy supply system's stability and contribute to the decarbonization of the heating sector using green electricity, and thus actively supporting the energy transition.

A heat pump is an efficient P2H application that can extract and provide heat from a medium (water or air) with much less electrical energy use, i.e., one electricity energy unit of input typically produces more than one or two heat energy units of output. Another typical application of P2H is domestic hot water production by using electric boilers or instantaneous water heaters. P2H applications also include room heating using direct electric heaters such as storage heaters or radiant heaters. For the central provision of large amounts of heating energy, auxiliary P2H applications sometimes support district heating grids. Hybrid systems are becoming increasingly popular for increased flexibility in large-scale power systems, where the P2H technologies integrate with other heating technologies or a CHP plant. The integration of heat storage tanks in hybrid systems further enhances flexibility. Because of high efficiency and comparatively low cost, P2H from renewable sources is a matter of growing interest across Europe. Studies and projects on P2H present potentials and opportunities for applying P2H in different sectors of the EU energy system [142,143]. P2H applications, especially in hybrid systems or combined with heat storage, support VRE integration in the energy system in the following ways [144]:

- 1. Reduce VRE curtailments;
- 2. Increase demand-side flexibility through load shifting;
- 3. Provide grid services via aggregators to optimize heating costs for consumers and provide grid balancing services to the national grid; and
- 4. Increase self-consumption from local renewable-based generation.

Heat pumps, electric boilers, and electric resistance heaters are generally identified as the three most promising P2H applications. A combination of two or more heating options is also possible, typically presented as a hybrid heating system.

Heat pump is an outstanding technology to provide flexibility to the power system while providing efficient heating and cooling solutions. Using external energy, they use a refrigerant through insulated pipes to transfer heat from a low-temperature source to a high-temperature sink. Heat pumps are used for space and water heating, air conditioning, and diverse industrial applications. The technology is advantageous because of its high efficiency, low energy cost, easy installation, minimum maintenance requirement, and high safety standard compared to other heating technologies.

Electric boiler is another popular P2H application widely used in utility-related processes to produce hot water and steam. The technology is advantageous because of its low initial cost, robust and compact design, flexibility, no stack requirements, zero carbon emission if provided with renewable electricity, quiet

operation, high efficiency, and ease of maintenance. Two installations are typical: electrical resistance boiler and electrode boiler. In addition, there are also small-scale infrared and induction-type electric boilers. While electric resistance boilers are connected at low voltages, electrode boilers are connected at medium voltage levels. Industrial processes use electrode boilers for producing superheated steam at high pressure.

Electric resistance heating systems convert electric current directly into heat. The heating units may have internal thermostats or external control systems and sometimes even use smart technologies (e.g., programmable scheduled heating) to regulate the temperature. Electric resistance heaters start quicker than heat pumps and require less space and investment costs. However, heat pumps have higher efficiency.

In this study, hybrid heating systems refer to heat pumps coupled with an electric boiler or electric resistance heater. The output of air heat pumps is highly dependent on the outside temperature. When the outside temperature is low, the heat pump performs with lower efficiency as it needs to extract the same amount of heat from cooler air. An electric boiler or resistance heater in tandem with a heat pump helps reduce the problem. Hybrid heating systems can be a promising alternative in terms of flexibility (e.g., heat pump technologies and electric boiler) but require higher installation costs than the individual technologies.

CHP plants consume fuel to produce both power and heat. A recent cross-country analysis using data from 35 countries showed that the CHP share in total electricity generation increases with rising VRE shares [145, Kim et al. 2019, p.1]. Therefore, CHP is a prominent candidate for bridging between power and heat sectors in the energy transition process. In addition to increased energy efficiency, CHPs offer cost-saving in operation, reduced air pollution, high reliability, improved power quality, and higher productivity. However, it may become difficult for the CHP plants to get enough full load hours when the share of VRE grows. Thus, they will benefit if they are profitable to run also at reduced full load hours and if they can start up and shut down flexibly, operate at low loads, and change the ratio of the heat and power outputs [146, Helistö et al. 2018, p.718]. It should be mentioned here that CHP often has a substantial 'must run' component, which may make it difficult to complement VREs. This can only be bridged by thermal energy storage.

The technology readiness level (TRL) of most P2H devices indicates that it is feasible to electrify the heating sector rapidly. However, with the increase of P2H devices, there will be an additional burden on the infrastructure. Most distribution grids are not sufficiently strong to incorporate a surge in both P2H devices and electric vehicles. Similarly, wirings and switchgear in buildings may not be sufficient.

Thermal Energy Storage, abbreviated as TES in this study, can play a significant role in achieving future decarbonization goals in Europe, especially in a highly renewable energy integrated system. P2H, coupled with TES, can be a promising option for integrating renewable energy, improving operational efficiency, and providing demand-side flexibility and sector coupling. TES can store energy to be used later for heating, cooling, or electricity generation. Large TES with a district heating network can store more heat and supply heat for long periods, offering better flexibility in the sector-coupled system. TES can help to tackle the following three main challenges [147]:

- 1. VRE and varying demand patterns of P2H technologies cause additional strain on the electricity grid. TES can mitigate this challenge by storing heat;
- 2. Solar-based heaters generate heat only during the daytime and mostly in summer. Short-term TES can provide stored heat during nighttime, and long-term TES can provide heat during winter, which can help reduce this time-constraint problem; and
- 3. TES can store thermal energy on large scales to help address daily and seasonal variability in supply and demand for electricity, heating, and cooling. It can help balance the mismatches between CHP operation and the needs of the electricity sector.





Figure 3.2: The key P2H and TES Technologies for the European Energy Transition. Own Illustration.

Implementing P2H in energy systems will benefit from technical advancements (both hardware and software), changes in policies and regulations, and proactive roles by the involved stakeholders. Improvements in hardware includes improving the different system components, upgrading and enhancing network infrastructures (electrical and district heating), and better control and metering systems. On the other hand, software advancements include designing, developing, and enhancing optimization, aggregation, and real-time communication energy system models [144].

The mathematical formulation for some of these P2H and TES technologies are available in different energy models. These formulations vary based on various objectives, such as cost minimization, welfare maximization, residual load variability minimization, or flexibility maximization. Most of the models follow cost minimization objectives, assume perfect competition, and use LP or MILP to carry out the optimization [148]. Some of these models exhibit explicit mathematical equations representing different P2H and TES technologies. These modeling methodologies will be examined in the latter part of this paper.

Several recent studies review the potential of P2H. Schweiger et al. studied the possibility of P2H in Swedish district heating systems [142, Schweiger et al. 2017, p.661]. They estimated the P2H potential of Sweden to be 0.2 - 8.6 TWh. Similarly, Böttger et al. studied the P2H potential of German district heating

grids [149, Böttger et al. 2014, p.250]. According to their estimation, the maximum theoretical P2H potential of the German district heating grid is 32 GWel. Hers et al. presented the prospect of P2H in district heating, industry, and horticulture in the Netherlands [143, Hers et al. 2015, p.4]. They concluded that the technoeconomic potential for P2H application in the mentioned sectors could be as high as 3.1 GW. Yilmaz et al. analyzed the future economic potential of flexible P2H in Europe [150, Yilmaz et al. 2018, p.6]. In another study, Yilmaz et al. analyzed how P2H can increase the flexibility of the European electricity system until 2030 [151, Yilmaz et al. 2017, p.1]. Bloess et al. reviewed the residential P2H technologies and presented their model-based analyses and flexibility potentials [148, Bloess et al. 2018, p.1611]. They pointed out that P2H technologies could cost-effectively contribute to replacing fossil fuel, integrating renewable energy, and decarbonizing the energy system. Ehrlich et al. analyzed the decentralized P2H as a flexible option for the German electricity system [152, Ehrlich et al. 2015, p.417]. Leitner et al. presented a method for the technical assessment of P2H to couple the electricity distribution systems with local district heating [153, Leitner et al. 2019, p.729]. Kirkerud et al. analyzed how the use of P2H in the district heating system impacts the VRE resources of the Northern European power system [154, Kirkerud et al. 2017, p.776]. Their results showed a significant increase in VRE market value with an increased installed P2H capacity. Kuprat et al. presented the role of P2H as a flexible load in the German electricity network [155, Kuprat et al. 2017, p.135]. Gjorgjevski et al. gave an empirical review of the P2H demand response potential of 34 large-scale projects worldwide [156, Gjorgievski et al. 2021, p.1]. Besides P2H, Sarbu and Sebarchievici presented a comprehensive review of TES [157, Sarbu and Sebarchievici 2018, p.1]. They described the principles of various energy storage techniques and the analysis of storage capacities. Pfleger et al. gave an overview of TES in their study [158, Pfleger et al. 2015, p.1487], while Enescu et al. reviewed the emerging trends of TES for grid applications [159, Enescu et al. 2020, p.1]. Enescu et al. also addressed the TES models, their characteristics, parameters, and deployment in VRE-based energy systems.

The potential of P2H is hardly discussed from the perspective of interconnected future European energy systems with a high share of VRE; instead, it is often addressed from a national point of view. The relationship between P2H and TES for providing flexibility as dispatchable loads need further attention in energy research. Only a few studies characterized the P2H technologies. Bloess et al. classified the residential P2H options [148, Bloess et al. 2018, p.1612]. Pieper presented a general overview of household and industrial P2H based on Beck and Wenzl [160, Pieper 2018, p.100] [161]. Schüwer and Schneider presented a similar classification focusing on the industrial sector [162, Schüwer and Schneider 2018, p.412]. Den Ouden et al. characterized P2H for process industries [163, Den Ouden et al. 2019, p.57-59]. However, none of these studies explicitly illustrated P2H for all end-use energy sectors.

The most prominent and recent research on model-based analyses of P2H and their modeling formulations is presented in the study by Bloess et al. [148, Bloess et al. 2018, p.1614–1620]. They provided a rich set of analytical approaches to implement P2H technologies in power systems and market models. However, their review focused on only residential P2H options. The scope needs to be broadened by including the P2H and TES technologies across all sectors and modeling them in energy systems to provide further insights on alternative or complementary decarbonization and flexibility potentials. Also, it is necessary to characterize these technologies and understand their potential roles before presenting these technologies' general mathematical formulations. The presentation of modeling formulations is limited to optimization-based energy models because of their quick and efficient objective seeking within highly complex systems and their ability to capture sectoral interactions leading to cross-cutting insights [164, DeCarolis et al. 2017, p.184].

Based on the research scope, the main contributions of this Chapter are as follows:

1. It identifies and classifies the main P2H and TES technologies looking across all sectors of the future carbon-neutral European energy system;

- 2. It briefly describes the technologies and addresses the potential roles in the European context; and
- 3. It presents the optimization energy modeling equations of these technologies suitable for largescale energy models.

The screening includes journal articles from Energy, Energies, Applied Energy, Energy Policy, International Journal of Energy Research, Applied Thermal Engineering, Renewable and Sustainable Energy Reviews, Sustainability, International Journal of Sustainable Energy Planning and Management, and Energy Economics. Additionally, several important articles and reports from different projects in the field of energy systems were reviewed. The modeling equations are mainly presented for large-scale energy models, which can be modified to suit smaller energy systems. The study does not include a detailed analysis of all available TES technologies; instead, it focuses on thermal storage technologies coupled with P2H technologies. Since CHP may have a considerable impact on linking power and heat sectors, it is considered part of the study. Nevertheless, the study does not claim to deliver a complete account of all published research on P2H, TES, and CHP. Instead, the study aims to present a comprehensive understanding of significant findings and possible approaches to modeling P2H and TES components in a highly renewable European energy system.

The rest of the Chapter is structured as follows. Section 3.2 presents classifications of P2H and TES technologies. Section 3.3 provides a short description of the main identified P2H and TES technologies and discusses their potential role in the context of the European energy transition. Section 3.4 provides the modeling formulation for the key P2H and TES technologies for large-scale optimization energy models. Finally, section 3.5 summarizes the Chapter and concludes with some remarks. Furthermore, Appendix C presents the relevant studies, merits, and demerits of the P2H and TES technologies.

3.2 Classification of Power-to-Heat and Thermal Energy Storage

In this section, the P2H and TES technologies are classified based on existing studies. First, the P2H technologies are categorized based on sectors and temperature levels. Next, TES is classified based on technologies, storage materials, applications, and end-users. The key technologies are discussed in brief after both classifications.

3.2.1 Power-to-Heat Classification

Bloess et al. proposed a new classification of residential power-to-heat [148, Bloess et al. 2018, p.1612]. They divided the built environment technologies into centralized and decentralized options. The centralized options use district heating, and the decentralized options use individual or community-based local networks. Their classification also indicates storage provisions. For example, centralized P2H comes with storage options, while decentralized P2H may or may not come with storage. Storage can be internal or external hot water tanks. Apart from active thermal energy storage, there can also be passive thermal storage where building mass or interiors store energy. Pieper described an overview of P2H technologies based on Beck and Wenzl, where he identified thermal energy storage as an integral part of P2H to supplement and simplify the operations [160, Pieper 2018, p.100] [161]. Schüwer and Schneider classified the P2H options based on household, trade, commerce, and service (TCS), and industrial heat applications [162, Schüwer and Schneider 2018, p.412]. Household and TCS applications included resistance heating systems, electrode boilers, electric heat pumps, and hybrid heating systems. Industrial P2H had conductive resistance heating, inductive heating, high-frequency heating, magnetic direct current heating, electrical infrared heating, electrode boiler (with and without CHP), and electric heat pumps. Den Ouden et al. presented the electrification strategies and promising technologies for the Dutch process industries [163, Den Ouden et al. 2019, p.57-59]. According to their research, while some technologies are already

commercially available, other promising technologies are currently in the research phase. Still, they are likely to play essential roles in industrial P2H options.



Figure 3.3: P2H classification

Figure 3.3 illustrates the state-of-the-art classification of different P2H technologies based on the review. First, the P2H technologies are categorized by three sectors: households and TCS, industry and process heat, and district heating. The second classification level is based on temperatures. Garcia et al. presented three temperature levels: (i) low (<120 °C), (ii) medium (120 – 1000 °C), and (ii) high (>1000 °C) [165, Garcia et al. 2012, p.19, p.28]. However, the classification of this thesis assumes 100 – 1000 °C as the range for medium temperature. On the third classification level, the technologies are characterized as available technologies. Electric heat pumps and electric boilers are most common. Electric resistance heaters are available mainly in household applications. The medium-temperature applications require high-temperature heat pumps. Large-scale implementations of electric heat pumps are available in district heating applications. Electrode boilers are used in medium and high-temperature applications, especially in high-temperature industrial process heating applications. Hybrid heating systems by combining different P2H technologies can be used in all sectors for different temperature levels. Industries sometimes require special process heaters for high-temperature applications, shown as subtypes in Figure 3.3.

Heat pumps appear as one of the most promising P2H technologies². High-temperature and large-scale heat pumps are also becoming popular in industrial process heating and district heating applications. Electric heat pumps can be distinguished as monovalent, mono-energetic, and bivalent options. The monovalent systems have only heat pumps, the mono-energetic systems consist of heat pumps and heating elements, and the bivalent systems consist of heat pumps and auxiliary boilers [148, Bloess et al 2018, p.1613]. Several studies review different heat pump configurations and their design, operation, recent developments, and application potentials to characterize various aspects of heat pump technology. For example, Staffell et al. reviewed the residential heat pumps, focusing primarily on air and ground heat pumps from the UK and Germany [166, Staffell et al. 2012, p.1]. Chua et al. reviewed the recent developments in heat pump systems and analyzed their suitability for various applications [167, Chua et al. 2010, p.3611]. Fischer et al. presented model-based flexibilities of domestic heat pumps [168, Fischer et al. 2017, p.853]. Arpagaus et al. presented a study on high-temperature heat pumps, where they reviewed the market and application potentials in detail [169, Arpagaus et al. 2018, p.990]. The vapor compression electric heat pump is the most widely used technology among different heat pump configurations, especially for low-temperature applications because of its simple structure and low initial cost. There are four main components in a vapor compression heat pump: evaporator, compressor, heat exchanger (condenser), and an expansion device. First, the liquid working fluid (i.e., the refrigerant) gets evaporated in the evaporator at low pressure using the heat source (e.g., air, ground, water). Then the vapor is compressed in the electricity-driven compressor, increasing the temperature and pressure of the steam. After that, the high temperature and high-pressure steam enter the heat exchanger, where the heat transfers to the sink. Finally, the condensed vapor goes through the expansion device, where it returns to liquid form, and the cycle repeats. A commonly used indicator for measuring heat pumps' performance is the Coefficient of Performance (COP), calculated from the ratio of heat output and electrical input. COP represents the steady-state performance under a set of controlled conditions with defined input and output temperatures [166, Staffell et al. 2012, p.1].

The second promising option for P2H is an electric boiler². It can be used as simple direct heating resistance boilers in low-temperature cases and complex three-phase electrode boilers in medium and high-temperature cases. Both cases have been widely analyzed. Electrical resistance boilers use an electric heating element that acts as resistance. Electrode boilers use the conductive and resistive properties of water. Other than these two, there are also small-scale infrared and induction-type electric boilers.

Electric resistance heating is another promising P2H option². Electric resistance heating systems use heating elements to generate heat using the Joule effect, where the energy of an electric current is converted into heat as it flows through a resistance. As opposed to electric boilers, no hot water or steam

² Please check Appendix C for all relevant references.

is used. These P2H heaters are used in households and industrial heating systems using conductive, inductive, high frequency, and infrared processes.

Hybrid heating systems generally refer to combining a heat pump with an electric boiler or an electric resistance heater. This combination is typical for low-temperature hybrid heaters in households. However, a different combination of other P2H technologies is also possible. For example, electrode boilers are often combined with CHPs to form hybrid heating systems in district heating systems. Supplementing the heat pump with a gas boiler is another plausible solution. In this way, we can reduce the cost (compared to CHP) and improve the flexibility (compared to direct electric heaters). Furthermore, we can replace gas with electro fuels to avoid emissions in the future.

In addition to the P2H technologies mentioned above, five different industrial process heating systems are identified: conductive heating, inductive heating, high-frequency heating, magnetic direct current heating, and electrical infrared heating [160–163]. Detailed descriptions of other commercial and research-phase process heating systems can be found in [163, Den Ouden et al. 2019, p.57–59].

CHP is a mature and proven technology that currently plays a vital role in integrating power and heat sectors and is likely to be widely used in medium to high-temperature cases in future energy systems². Generally, the two main types of steam turbines in CHP are the non-condensing or backpressure turbine and the condensing or extraction turbine. The backpressure turbine CHP produces electricity and heat with a fixed ratio. The second type is the extraction turbine, where the ratio of electricity and heat can be altered by varying the amount of heat taken from the extraction valve and the amount of energy directed to a lowpressure turbine. Therefore, extraction turbines can offer more flexibility to the system and for the plant operator [170, Kavvadias et al. 2018, p.8]. Other configurations such as CHP plants with turbine bypass systems are also possible.

3.2.2 Thermal Energy Storage Classification

Thermal Energy Storage is a proven concept used to balance supply and demand for electricity, heating, and cooling. The integration of TES with P2H and CHP applications can provide flexibility and increase the power system's reliability. Most P2H technologies generally combine with external TES. The electric resistance heating systems and some industrial process heating systems that use direct electricity conversion to heat do not need any storage. TES is classified and discussed in most of the literature based on the technologies: sensible heat storage (SHS), latent heat storage (LHS), and thermo-chemical heat storage (THS)². In addition to these three, a study by IRENA identifies thermo-mechanical energy storage (TMS), also known as mechanical-thermal coupled storages, as another promising TES technology [171, IRENA 2020, p.53].

SHS is the most widely used TES form, which stores heat by heating solid or liquid mediums such as water, molten salt, rocks, sand, etc. The term 'sensible' indicates that the medium's heat causes a change in its temperature. Hot water based SHS is the most used TES because of its low cost, compactness, scalability, maturity, availability, usability, and non-toxicity [157, Sarbu and Sebarchievici 2018, p.4].

LHS is another popular TES that uses phase change materials (PCM) to absorb and release energy with a physical state change. Promising and commonly used PCMs for TES applications include salt hydrates, fatty acids and esters, and various kinds of paraffin [157, Sarbu and Sebarchievici 2018, p.11]. The term 'latent' indicates that the storage material changes its state (e.g., solid to liquid) for the addition or removal of heat. Using the LHS system with PCM has the advantage of high energy storage density and the isothermal nature of the storage process [157, Sarbu and Sebarchievici 2018, p.10]. Therefore, integrating the heat pump with latent TES can be advantageous, providing constant temperature and compactness to the system.

THS uses thermochemical materials to store and release heat by a reversible endothermic or exothermic reaction process. The most prominent THS materials are water paired with silica gel, magnesium sulfate, lithium bromide, lithium chloride, and sodium chloride. THS can be used to control heat and humidity by using the thermo-chemical adsorption process [157, Sarbu and Sebarchievici 2018, p.28]. This technology is potentially highly efficient (up to 100%) [147].

TMS is based on mechanical and thermal energy transformations, where the TES is internally combined with mechanical energy storage. TMS includes standard mechanical components such as heat exchangers, compressors, or turbines, sometimes with necessary modifications [172, Steinmann 2017, p.206]. The benefits of TMS include the provision to electric and heat storage, high integrability with other heat sources and power generation systems, lower geographic constraints and environmental impacts, and a long lifetime [173, Olympios et al., p.3].



Figure 3.4 shows the TES classification adapted from [171,174,175].

Figure 3.4: TES Classification. Adapted from [171,174,175].

Furthermore, based on the IRENA study, thirteen promising TES technologies are identified which can help integrate more VRE into the energy system, as shown in Figure 3.5 technology [171, IRENA 2020, p.53]. Tank Thermal Energy Storage (TTES) uses water as the storage medium. Solid State Thermal Storage (SSTS) uses ceramic bricks, rocks, concrete, or packed beds as storage medium. Molten salts are inorganic chemical compounds. Underground Thermal Energy Storage (UTES) uses geological strata made up of soil, sand or solid bedrock, or water in artificial pits or aquifers. Ice Thermal Storage (ITS) uses cold energy in ice. Sub-zero Temperature PCMs (SPCM) are single components or are composed of a mixture, such as eutectic mixtures (e.g., salt-water). Low-temperature PCM (LTPCM) uses paraffin waxes and inorganic salt hydrates. High-temperature PCM (HTPCM) uses inorganic salts with high phase-change temperatures. Chemical looping is primarily identified as a potential carbon capture technology using calcium. Salt hydration absorbs and releases energy through hydration and dehydration of solid salts such as magnesium chloride and sodium sulphide. Absorption systems are based on the principle of a concentrated refrigerant solution. In Compressed Air Energy Storage (CAES), the air is stored at high pressure, and in Liquid Air Energy Storage (LAES), it is stored in a liquid form. Adiabatic CAES systems can improve the overall efficiency where an additional high-temperature TES is added.



Figure 3.5: Promising TES for VRE integration. Based on [171, IRENA 2020, p.53].

Many studies also considered and modeled passive heat storage using the buildings' thermal mass, and electrical thermal storage (ETS) using insulated thermal bricks (i.e., electric storage heaters). Passive heat storages can store heat in the building's enclosed structure [159, Enescu et al. 2020, p.13] and directly influences the operation of P2H applications (e.g., heat pumps) in the built environment. On the other hand, ETS is mature and advantageous because of its easy management with dynamic charging and comparatively lower cost than batteries [159, Enescu et al., p.10]. Generally, Passive heat storage and ETS store the medium's heat without phase transition and therefore belong to SHS. However, Heier et al. showed that passive TES in buildings can store heat in latent thermal mass [176, Heier et al. 2015, p.1309].

3.3 Potential of Power-to-Heat and Thermal Energy Storage

Technology readiness levels can help understand the potential of technologies required by the energy transition [160, Pieper 2018, p.16]. Figure 3.6 shows the TRLs of prominent P2H and TES technologies based on data from [160, Pieper 2018, p.100, p.160]. The ranking scales range from 1 to 9, where level 1 indicates that the technology is in the elemental level of research, and level 9 indicates that the technology is thoroughly tested and proven. Appendix D presents a brief definition of all technology readiness levels. Low-temperature electric heat pumps (<90°C), electric boilers (resistance and electrode types), and electric resistance heaters are established technologies and are fully technologically ready (TRL 9). For heat pumps over 90°C, the TRL levels decrease from 9 to 3 as the output temperature increases from <90°C to <160°C. Although sensible and latent heat storages have a high TRL (TRL 9), the LHS technology is relatively immature in the domestic segment. On the other hand, thermo-chemical heat storages are still in the early stages of development (TRL 4). In the following subsections, the potential roles of prominent P2H and TES technologies in the EU are briefly discussed.



Figure 3.6: Technology readiness levels of P2H and TES technologies. Data Source: [160, Pieper 2018, p.100, p.160].

3.3.1 Heat Pump

The growing potential of heat pumps is observable in Figure 3.7, which shows its sales from 2008 to 2020 in the EU, including the UK (21 countries) [177]. However, the adoption of the different heat pump technologies varies across European countries. The data in Figure 3.6 includes all heat pump technologies providing heating, cooling, sanitary hot water and process heat. The graph shows an upward trend in heat pump sales achieving more than, on average, 12% growth per annum in the last six years. According to

IRENA, heat pumps will supply 27% of the total heat demand in the EU by 2050, when the total installation rises to 250 million units in the building sector and 80 million units in the industry sector [144, IRENA 2019, p.6].



Figure 3.7: Heat pump sales development in the EU. Source: European Heat Pump Association [177].

High-temperature heat pumps (HTHPs) are becoming increasingly popular in relevance to industrial heating processes. The closed-cycle compression heat pumps are the most widely used HTHPs, while thermally driven sorption cycles and hybrid absorption-compression heat pumps are the other relevant HTHP technologies. Figure 3.8 gives an overview of industrial processes in different industrial sectors identified as suitable for integrating heat pumps. Four color bands indicate four different TRL for the available heat pump technologies. Overall, the food, paper, and chemical industries show promising potential for HTHPs. While drying, pre-heating, boiling, and pasteurization applications can already use commercially available HTHPs (<100 °C), higher temperature heat pumps (>100 °C) are expected to be technologically ready within the next few years [169, Arpagaus et al. 2018, p.990].

Sector	Process Temperature																					
		20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170	180	190	200		[°C]
Paper	Drying																					90 - 240
-	Boiling																					110 - 180
	Bleaching																					40 - 150
	De-inking																					50 -70
Food & Beverages	Drying																					40 - 250
	Evaporation																					40 -170
	Pasteurization																					60 - 150
	Sterilization																					100 - 140
	Boiling																					70 - 120
	Distillation																					40 - 100
	Blanching																					60 - 90
	Scalding																					50 - 90
	Concentration																					60 -80
	Tempering																					40 - 80
	Smoking																					20 - 80
Chemicals	Distillation																					100 - 300
	Compression																					110 - 170
	Thermotorming																					130 - 160
	Concentration																					120 - 140
	Boiling																					80 -110
	Bioreactions																					20 - 60
Automotive	Resin molding																					70 - 130
Metal	Drying																					60 - 200
	Pickling																					20 - 100
	Degreasing																					20 - 100
	Electroplating																					30 - 90
	Phosphating																					30 - 90
	Chromating																					20 - 80
	Purging																					40 - 70
Plastic	Injection molding																					90 - 300
	Pellets drving	,																				40 - 150
	Preheating																					50 - 70
Mechanical Engineering	Surface treatmen	+																			<u> </u>	20 - 120
Weenanical Engineering	Cleaning	ii.																				40 00
Tautilaa	Calaurian																					40 - 90
lextiles	Colouring																					40 - 160
	Drying																					60 - 130
	Washing																					40 - 110
	Bleaching																					40 -100
Wood	Glueing																					120 - 180
	Pressing																					120 - 170
	Drying																					40 - 150
	Steaming																					70 - 100
	Cooking																					80 - 90
	Staining																					50 - 80
	Pickling																					40 - 70
Others	Hot water																					20 - 110
	Preheating																					20 - 100
	Washing/Cleanin	g																				30 - 90
	Space heating																					20 - 80
Technology Readiness Level (TRL) of Heat Pumps																						
	Conventional HD	< 80 °	°C+	ablic	hedi	n indi	istry															
	Commercially ar	ailabi	с, сі 2 µт		ncu II 1-100	n nuu	23CI Y	char														
	Drototormo etchi	und Ul	e mil bnel			, C, K	ey it	ланно тип	100 100	110 0	c											
	laboration and a received of the second state of access to 1710 state of																					
	Laboratory scale research, functional models, proof of concept, HTHP >140 °C																					

Figure 3.8: Overview of industrial processes suitable for heat pumps. Source: [169, Arpagaus et al. 2018, p.990].

Recent studies showed a large market potential for industrial heat pumps. Nellissen and Wolf estimated a technical potential of 626 PJ in Europe³, of which 113 PJ is accessible by industrial HTHPs (100 – 150 °C) [178, Nellissen and Wolf 2015, p.10]. A model-based analysis by Wolf and Blesl showed that the technical potential of heat pumps across the industrial sector in EU-27 and the UK is 1717 PJ [179, Wolf and Blesl 2016, p.485]. However, because of economic considerations, only 15% of the potential (270 PJ) is accessible [179, Wolf and Blesl 2016, p.485]. Another study by Marina et al. estimated that industrial heat pumps up to 200 °C can cover 641 PJ of the process heat demand of EU-27 and the UK [180, Marina et al. 2021, p.13].

3.3.2 Electric Boiler

Electric resistance boilers are usually connected at low voltages (e.g., 400 V) and have a low capacity (<5 MW). Electrode boilers are generally connected at medium voltage levels (e.g., 10 kV) and have a higher capacity (3–70 MW). They can produce superheated steam with high temperature (>350 °C) and high pressure (>70 bar). Both types of electric boilers have high efficiency ranging from 95 to 99.9% [163, Den Ouden et al. 2019, p.57]. Table 3.1 shows the industrial applications of electric boilers according to various temperature levels.

Applications	Temperature Level	Use in industries
Low-temperature	<120 °C	Food and beverages, chemicals, textiles, dairy, breweries, mineral oil, etc.
Medium-temperature	120 – 1000 °C	Drying, production of plastic materials, plasterboards, bitumen, asphalt, etc.
High-temperature	>1000 °C	Process heating such as the production of iron, steel, bricks, cement, etc.

Table 3.1: Temperature-wise industrial applications of electric boilers. Source: [151, Yilmaz et al. 2017, p.51].

In the residential sector the electric boilers are often identified as a supplementary option [148, Bloess et al. 2018, p.1618], however, they have a higher potential in district heating networks and industries [181, Wietschel et al. 2020, p.11]. No study could be found that estimated the potential of electric boilers using energy models. Nonetheless, the rising trend of electric boiler usage in the past few years can be seen from Eurostat data [182]. As shown in Figure 3.9, the electricity consumption by electric boilers for all sectors increased from 243 GWh to 697 GWh in the last ten years (EU-27 and the UK) [182]. The trend indicates plausible higher usage of electric boilers in the future, especially in an energy system with a highly electrified industrial sector.

³ However, this is only 8% of the total industrial heat demand (8150 PJ) as estimated by Naegler et al. (2015). DOI: https://doi.org/10.1002/er.3436





3.3.3 Electric Resistance Heater

For households, electric resistance heating using only heating elements can be supplied by radiant heaters, baseboard heaters, wall heaters, underfloor heating systems, and electric furnaces. Heating elements can also be associated with internal ceramic blocks, known as electric storage heaters. An electric storage heater is a flexible P2H application that can reduce the peak demand by storing heat in ceramic blocks at low price times.

In industrial processes, an electric process heater is a form of resistance heating that is technologically matured and can be used in high temperature and pressure applications. These heaters use several heating elements across which the working fluid flows lengthwise and crosswise to be heated up to 600 °C. Electric arc furnaces and the Hall-Héroult process are proven conductive heating processes for metallurgy applications [160, Pieper 2018, p.100].

Besides conductive heating, inductive, high-frequency, and infrared heating systems are also popular and proven in electrifying industrial processes. Inductive heating uses electromagnetic induction to generate heat and is available for several applications such as furnaces for heating metals, welding, cooking, brazing, sealing, heat treatment, and plastic processing. High-frequency heating, also known as microwave or radiofrequency heating, is also commonly used in textiles, paper, food, plastic and chemical industries. Finally, infrared heating is another commercially available P2H application used in various industrial processes such as drying, curing, welding, and coating.

The use of electric resistance heating depends heavily on the energy sources and the countries' energy policies. For example, in countries with a high share of nuclear power, electric storage heaters can store heat using electricity in times of excess generation. We can expect the same for countries with high VRE shares. On the other hand, direct electrical heating is also widespread in countries with high hydropower

resources or fewer wintery days. Installing decentralized and relatively cheaper electrical heating systems in such countries is more cost-effective than investing in expensive heat pumps or electric boilers. In the future, the development of smart grids and grid interaction with direct electric heaters may lead to positive technology advancements [151, Yilmaz et al. 2017, p.52].

3.3.4 Combined Heat and Power

Combined Heat and Power is known as the most efficient technology that can deliver both heat and power simultaneously and can utilize waste and biomass resources [183]. Based on the Eurostat statistics for 2018 in EU-27 and the UK, CHP electricity generation was 327 TWh, and total CHP heat production was 2787 PJ [184]. An optimal combination of CHP with P2H and TES technologies in district heating systems can facilitate flexible sector coupling of power and heat and shows excellent potential to increase renewable shares in the energy system [185,186]. In addition to district heating, CHP can also be used to supply industrial process heating. The JRC policy report in 2017 states that the conversion of existing power plants to CHPs will increase the overall efficiency of the European energy system, which is otherwise limited to 50% [170, Kavvadias et al. 2018, p.26]. According to the Heat Roadmap Europe (HRE) 2050 scenarios, district heating should include various sources to ensure flexibility and low emission levels. Figure 3.10 shows the distribution of district heating source shares in HRE 2050 for 14 countries in the EU, where CHP covers a significant portion (38%) of the total district heating [187, AAU HRE4 2020, p.12].



Figure 3.10: Share of district heating sources according to HRE 2050. Adapted from [187, AAU HRE4 2020, p.12].

A recent study published by Artelys finds that CHP will play a fundamental role in achieving total decarbonization in Europe by 2050 [188]. According to their analysis, CHPs can maximize system efficiency and flexibility to complement high VRE generation. An optimized CHP deployment can save over €8 billion compared to a lower CHP deployment solution, allowing an annual CO₂ emission reduction of up to 5 metric tons [188, Artelys 2020, p.23]. They also found that CHP is suitable in all economic sectors, and it can foster a higher use of biomass resources [188, Artelys 2020, p.38].

3.3.5 Thermal Energy Storage

TES is considered an essential tool for smart heating and cooling concepts, playing significant roles in different applications. Residential TES can be used as a demand response tool for energy arbitrage, load variability reduction, and reserve provisions [189, Anwar et al. 2019, p.4151]. The flexibility of using residential TES (e.g., smart electric thermal storage) can facilitate the consumers to maximize their local RES usage. The integration of TES in district heating systems can significantly increase system flexibility and facilitate the smooth coupling of P2H technologies in the energy system [142, Schweiger et al. 2017, p.661]. TES can improve the overall storage capacity and enhance operational strategies in smart community-based energy systems [159, Enescu et al. 2019, p.15]. Mobile TES offers additional flexibility by making heat available at remote locations [190,191]. Waste heat storage in TES can increase industrial processes' efficiency and operational flexibility. Furthermore, the combination of TES with HTHP can increase the overall energy efficiency, reduce VRE curtailments, reduce system cost, and improve environmental footprint [190–192]. The thirteen promising TES technologies for 2050, identified by IRENA, can be distributed according to their applications across different sectors as shown in Figure 3.11 [171].



Figure 3.11: Most promising TES technologies for 2050 and their sectoral distribution according to applications. Based on [171].

According to a recent study by LUT and EWG, TES⁴ will emerge as the most relevant heat storage technology across all sectors in Europe with around 40-60% of heat storage output from 2030 until 2050 [193, Ram et al. 2018, p.3]. Gas storage is expected to cover the rest of the demand.

3.4 Modeling of Power-to-Heat and Thermal Energy Storage

Three modeling approaches are prominent in energy system optimization models: Linear Programming, Mixed-integer Linear Programming, and Nonlinear Programming (NLP). Most energy system models use LP because of its inherent computational advantages. In large-scale energy systems with numerous components, LP can serve as a simple, fast, scalable, and straightforward method. Although MILP and NLP allow more accurate modeling results than LP, they can be impractical for large-scale models due to higher computational times. Ommen et al. compared LP, MILP, and NLP in energy models [194], where they concluded that MILP is the most suitable option considering model runtime and accuracy. Nevertheless, when it comes to large-scale energy systems with detailed characteristics from individual components, LP is a more preferred alternative by most researchers. It is also possible to combine LP results with MILP so that MILP is used for analyzing a minor part of the large-scale energy system in detail [195]. This section presents the mathematical models⁵ for the P2H and TES technologies. Through this section, we use capital letters to denote parameters and small letters to represent variables.

3.4.1 Heat Pump

While modeling heat pumps, it is essential to acknowledge the difference in temperatures of the source and the sink [148,196–199]. The theoretical maximum COP formulates as:

$$COP_{Theory}(t) = \frac{Q_H(t)}{Q_H(t) - Q_L(t)} = \frac{T_H(t)}{T_H(t) - T_L(t)} \quad \forall t$$
 (3.1)

where Q_H denotes the heat supplied to the high temperature reservoir (sink), Q_L denotes the heat supplied from the low temperature reservoir (source), T_H denotes the sink temperature, T_L indicates the source temperature, and COP_{Theory} represents the maximum theoretical COP (i.e., Carnot COP without any loss).

The relationship between the maximum theoretical COP and the actual COP after loss depends upon the efficiency η_{HP} of the heat pump. The actual COP is calculated as:

$$COP(t) = \eta_{HP} \cdot COP_{Theory}(t) \quad \forall t$$
 (3.2)

In reality, the sink temperature of a heat pump is directly affected by the heat flow \dot{q}_{HP} . Therefore, the heat pump is modeled as:

$$\dot{q}_{HP}(t) = p_{HP}(t) \cdot COP(t) \quad \forall t$$
(3.3)

where p_{HP} represents the electrical power input of the heat pump.

The formulation in (3.3) is the most widely used model in the academic literature on heat pumps in the energy system [148, Bloess et al. 2018, p.1617–1618]. The heat pump can operate between a minimum P_{HP} and maximum $\overline{P_{HP}}$ electric power input (3.4). The heat output is constrained by an upper limit $\overline{Q_{HP}}$

⁴ TES here refers to all possible thermal energy storage technologies.

⁵ The mathematical models Equations (3.1) – (3.31) of the P2H and TES technologies are generalized forms of large-scale optimization models, which the author adapted from various studies. Please check the relevant references for each of the technologies. For further details, please check the review paper by Maruf et al. (2022). DOI: <u>https://doi.org/10.1016/j.seta.2022.102553</u>

(3.5). A binary variable⁶ u is introduced to model non-linear costs (e.g., no-load cost, start-up cost) and the minimum output [200, Morales-España et al. 2013, p.4897].

$$\underline{P}_{HP}.u(t) \le p_{HP}(t) \le \overline{P}_{HP}.u(t) \qquad \forall \quad t$$
(3.4)

$$\dot{q}_{HP}(t) \leq \overline{Q}_{HP} \cdot u(t) \quad \forall t$$
(3.5)

$$\dot{q}_{HP}(t) \ge 0 \qquad \forall \quad t$$
(3.6)

If we consider a variable temperature window for the sink (such as 18 - 22 °C for comfort level), the heat pump can provide flexibility to the system. In that case, the sink temperature T_H becomes a variable, and equation (3.1), which is embedded in equations (3.2) and (3.3), becomes nonlinear. Similarly, T_L often depends on the weather, which can be considered when modeling the COP. However, in large-scale aggregated energy models, it is common to assume a constant COP. Demand response through load shifting can be applied to provide flexibility in the heat pump-based system, which can be modeled using formulations from Morales-España et al. by supplying a given demand in a given maximum delay time window [201].

In the case of reversible heat pumps for air conditioning or refrigeration, the relationship between maximum theoretical COP for cooling $COP_{Theory}^{Cooling}$ and the source and sink temperatures is expressed as [202,203]:

$$COP_{Theory}^{Cooling}(t) = \frac{Q_L(t)}{Q_H(t) - Q_L(t)} = \frac{T_L(t)}{T_H(t) - T_L(t)} \quad \forall \quad t$$
(3.7)

where Q_L denotes the heat extracted from the low temperature reservoir (i.e., the cooling load), $Q_H - Q_L$ indicates the work required for cooling, T_L represents the sink temperature (low temperature reservoir), and T_H indicates the source temperature (high temperature reservoir).

Other comprehensive heat pump formulations to address the temperature dependence of COP can be found in various studies. For example, Verhelst et al. suggested four different empirical approximations of the physical laws governing heat pump operation based on the data from the heat pump manufacturer [204]. Heinen et al. suggested pre-computing the heat pump dependence on temperature using a linear equation [205]. They determined the slope of the equation from heat pump performance data, assumed a constant ambient temperature of 280.15 K (7 °C) according to EU performance regulations, and fit the relation to a constant COP. Georges et al. presented piecewise linearization of the nonlinear problem from Verhelst et al., requiring empirical manufacturer data and considering nominal conditions [206]. Heat pump formulations by Salpakari et al. involve district heating integration and are limited to a supply temperature of 90 °C [207]. According to Lyden and Tuohy, Staffell et al. proposed a generic regression performance map for modeling COP variance, which used surveys of industrial data sheets and field trials. Their formulations apply to household-scale heat pumps as well as large scale industrial heat pumps [208]. Fischer et al. followed a similar approach in [168], which has been applied to manufacturer data under different temperature conditions by Ruhnau et al. in [209]. To summarize, comprehensive heat pump modeling based on available data is another viable alternative, as it has been used by many researchers. Such methods are preferred in comparatively small-scale and complex heat pump models, such as capturing higher efficiency in varying load modes or allowing higher flexibility in variable speed heat pumps.

⁶ Please check the study by Morales-España et al. [200, Morales-España et al. 2013, p.4897] for more information on modeling of non-linear costs.

3.4.2 Electric Boiler and Electric Resistance Heater

The relationship between electric power input p_{EB} and heat output \dot{q}_{EB} in an electric boiler is widely modeled as [210,211]:

$$\dot{q}_{EB}(t) = \eta_{EB} \cdot p_{EB}(t) \qquad \forall t$$
(3.8)

where η_{EB} indicates the efficiency of the electric boiler. The electric boiler usually operates between a minimum P_{EB} and maximum $\overline{P_{EB}}$ electric power input (3.9). The heat output is constrained by an upper limit $\overline{Q_{EB}}$ (3.10) [212]. The binary variable⁶ u is used to model non-linear costs and the minimum output.

$$P_{EB}.u(t) \le p_{EB}(t) \le \overline{P_{EB}}.u(t) \qquad \forall \quad t$$
(3.9)

$$\dot{q}_{EB}(t) \leq \overline{Q}_{EB} \cdot u(t) \quad \forall t$$
(3.10)

$$\dot{q}_{EB}(t) \ge 0 \qquad \forall \quad t \tag{3.11}$$

Electric boilers and electric resistance heaters are capable of transitioning from no-load to full-load state within minutes or even seconds. Nielsen et al. did not consider any start-up costs and ramping constraints for electric boilers [213]. The modeling of electric boilers can be more complex taking the thermal stratification effect into account. Thermal stratification in electric boiler storage tanks indicates different temperature levels in several layers inside the tank. In energy system models, many approaches are used to address the thermal stratification effect. Campos Celador et al. used three techniques to model hot water storage tanks: actual stratified, ideal stratified, and fully-mixed [214, Campos Celador et al. 2011, p.189]. Farooq et al. presented experimental results of a low-pressure domestic electric boiler with eight stratification layers [215, Faroog et al. 2015, p.257]. De Cesaro Oliveski et al. introduced a numerical and empirical analysis of temperature and velocity inside the hot water tank using one-dimensional and twodimensional models [216, De Cesaro Oliveski et al. 2003, p.121]. Diao et al. tested electric boilers' response with various control strategies and considered two modes in a comprehensive model: one-node and twonodes [217, Diao et al. 2012, p.1]. Han et al. presented a review of different types of thermal stratification tanks, their research methods, and compared their efficiencies [218, Han et al. 2009, p.1014]. In electric boiler modeling, single mass, one-node, or fully mixed tank models are widely used because of their simple formulation. These models consider that the tank's water is mixed and has a uniform temperature without any thermal stratification. This study considered the single mass system without any thermal stratification for modeling in energy systems. The readers are suggested to go through the references [219-222] for a detailed formulation of stratified boilers.

Electric resistance heaters can be modelled using the same equations (3.8)–(3.11), where the ratio between heat production and electricity has different values.

3.4.3 Hybrid Heating Systems

In the case of hybrid heating systems, each technology is modeled individually. For example, if a supplementary equipment complements the heat pump, the relation between the total power required by the hybrid system p_{HB} is the sum of electric power required by the heat pump p_{HP} and the electric power required by the supplementary system p_{SUP} :

$$p_{HB}(t) = p_{HP}(t) + p_{SUP}(t) \quad \forall t$$
(3.12)

Equations (3.1)–(3.5) are used to model the heat pump, and (3.7)–(3.11) are used to model the supplementary equipment, which is either an electric boiler or an electric resistance heater. Patteeuw et al. modeled hybrid heating systems using such approach [197, Patteeuw et al. 2015, p.4]. The heat from P2H technologies is part of the total heat demand Q of the system (which can be an exogenous parameter), as shown in (3.13):

$$\dot{q}_{HP}(t) + \dot{q}_{SUP}(t) + \dot{q}_{GB}(t) \ge Q(t) \quad \forall \quad t$$
(3.13)

Where \dot{q}_{GB} denotes the heat from a gas boiler. For the sake of completeness, we assume that there is a gas boiler in combination with the heat pump and the supplementary system. Flexibility to such hybrid systems can be provided either by shifting the sources (e.g., from electricity to gas) or by shifting in time. Time shifting can be enabled by TES, which allows stored energy to be used later, or by a specific technology, such as heat pumps, which can provide shifting in time through demand response formulations, as presented in [201].

3.4.4 Combined Heat and Power

In CHPs, power, heat, and cost depend on each other resulting in a convex feasible operating region (FOR) as shown in Figure 3.12 [223, Rong and Lahdelma 2007, p.415].



CHP characteristic

Figure 3.12: Feasible Operating Region (FOR) of a convex CHP plant. Source: [223, Rong and Lahdelma 2007, p.415].

The operation of a single CHP unit as a convex combination of the extreme points C_j , P_j , Q_j of the characteristic surface is expressed using (3.14)–(3.18) [183,223,224]. C_j , P_j , Q_j indicate the production cost, power production and heat production at characteristic point $j \in J$, respectively. Characteristic points are the extreme points of the operating region of the plant. Variable x_j is used to encode the operating region as a convex combination of extreme points (3.14)–(3.16). Variable u indicates the commitment status of the unit for hour t, which is equal to 1 if the unit is online and 0 if offline. Parameter p_{CHP} indicates the net power production, q_{CHP} indicates net heat production, and c_{CHP} indicates the production cost of the convex plant. The production cost mainly indicates the fuel cost, however, other variable costs (e.g., maintenance costs) can be included.

$$c_{CHP}(t) = \sum_{i \in I} \quad C_j x_j(t) \quad \forall \quad t$$
(3.14)

$$p_{CHP}(t) = \sum_{j \in I} P_j x_j(t) \quad \forall t$$
(3.15)

$$q_{CHP}(t) = \sum_{j \in J} \quad Q_j x_j(t) \qquad \forall \quad t$$
(3.16)

$$\sum_{j \in J} \quad x_j(t) = u(t) \quad \forall \quad t$$
(3.17)

$$x_i(t) \ge 0, j \in J \quad \forall \quad t \tag{3.18}$$

The following constraints ensure that the unit operates within the ramp rate limits [200]:

. .

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$$p_{CHP}(t) - p_{CHP}(t-1) \le RU \quad \forall t$$
(3.19)

$$-p_{CHP}(t) + p_{CHP}(t-1) \le RD \quad \forall \quad t$$
(3.20)

Where RU is the ramp-up rate, and RD is the ramp-down rate of the unit. The model can be easily expanded to include spinning reserves [200]. The start-up cost of CHP $c_{CHP,g}^{SU}$ is constrained by the online

status of the unit in two consecutive time steps and the start-up cost parameter C_{CHP}^{SU} as shown in (3.21):

$$c_{CHP}^{SU}(t) \ge \left(u(t) - u(t-1)\right) \cdot C_{CHP}^{SU} \quad \forall \quad t$$
(3.21)

Morales-España et al. provide other constraints such as minimum uptime and downtime, startup and shutdown capability, variable startup cost, etc., that can apply to this model [200]. CHP units can also be modeled using multiple conversion components, particularly when the plant has more operating modes and offers more flexibility [192,225]. Helistö et al. present a more generic formulation where the unit can have multiple inputs and outputs [226]. It also allows chaining of units to present more complicated plants. Nevertheless, the convex FOR is usually simplified using fewer parameters, as discussed in the following subsections that present formulations for backpressure and extraction turbines.
3.4.4.1 Backpressure Turbine

The FOR of a backpressure turbine CHP plant is presented in Figure 3.13 [170, Kavvadias et al. 2018, p.8], [212, Dimoulkas et al 2017, p.852]. The FOR is expressed as (3.22)–(3.23), where σ is the fixed power-toheat ratio, $\overline{P_{CHP}}$ is the maximum power generation, and $\underline{P_{CHP}}$ is the minimum power generation of the backpressure unit [170, Kavvadias et al. 2018, p.8].



Figure 3.13: Feasible operation region (FOR) of CHP with a backpressure turbine. Source: [170, Kavvadias et al. 2018, p.8].

$$p_{CHP}(t) = \sigma. q_{CHP}(t) \quad \forall \quad t$$
(3.22)

$$\underline{P_{CHP}}.u(t) \le p_{CHP}(t) \le \overline{P_{CHP}}.u(t) \qquad \forall \quad t$$
(3.23)

Limiting heat generation is not required in CHP mode because it is achieved by the fixed power-to-heat ratio (3.22) together with (3.23). In the case of large-scale energy models, u can be relaxed (i.e., a continuous variable between 0 and 1) resulting in an LP approximation of the problem [227].

3.4.4.2 Extraction Turbine

The FOR of an extraction turbine CHP plant is presented in Figure 3.14, where A-B and E-D indicate the power-loss limits (iso-fuel lines at maximum and minimum production), D-C indicates the maximum heat limit for a given amount of power, and B-C indicates the maximum possible heat extraction [170, Kavvadias et al. 2018, p.9], [212, Dimoulkas et al 2017, p.852].



Figure 3.14: FOR of CHP with an extraction turbine. Source: [170, Kavvadias et al. 2018, p.9].

Therefore, the FOR of the extraction turbine is modelled as [170, Kavvadias et al. 2018, p.9]:

$$p_{CHP}(t) \ge \sigma. q_{CHP}(t) \quad \forall \quad t$$
(3.24)

$$q_{CHP}(t) \le \overline{Q_{CHP}}. u(t) \quad \forall t$$
(3.25)

$$p_{CHP}(t) \le \overline{P_{CHP}}.u(t) - \beta.q_{CHP}(t) \quad \forall t$$
(3.26)

$$p_{CHP}(t) \ge \underline{P_{CHP}}.u(t) - \beta.q_{CHP}(t) \quad \forall t$$
(3.27)

where $\overline{Q_{CHP}}$ is the maximum heat generation and β is the power loss index (ratio between lost power generation and increased heating generation). Following the FOR of Figure 3.13, (3.24) imposes the limit indicated with the points D-C, (3.25) imposes the limit B-C, (3.26) imposes the limit A-B, (3.27) imposes the limit E-D, and the limit A-E is imposed by the variables being defined non-negative. A collection of typical parameter values from various literature references for this model can be found in [170, Kavvadias et al. 2018, p.34].

3.4.5 Thermal Energy Storage

The generic formulations for TES, notably for hot water tanks (sensible heat storage), are presented here. The tank is assumed to be perfectly stirred; therefore, it has the same temperature range in every layer. In addition, the storage losses are generally taken into account either as only stationary losses [38,152,198,205,213,228], or stationary and dynamic losses [229]. As a result, TES balance is expressed using (3.28)–(3.31):

$$s(t) = (1 - L_s) \cdot s(t - 1) + (1 - L_D) \cdot \dot{q}_C(t) - (1 - L_D) \cdot \dot{q}_D(t) \qquad \forall \quad t$$
(3.28)

$$s(t) \le S_{cap} \qquad \forall \quad t \tag{3.29}$$

$$\dot{q}_{c}(t) \leq \overline{Q_{FLOW}} \quad \forall t$$
(3.30)

$$\dot{q}_D(t) \le \overline{Q_{FLOW}} \quad \forall t$$
(3.31)

where *s* is the heat storage level, L_s is the stationary heat loss, L_D is the dynamic heat loss, \dot{q}_C is the heat flow to the storage (i.e., charging), \dot{q}_D is the heat flow from the storage (i.e., discharging), S_{cap} is the capacity of the heat storage, and $\overline{Q_{FLOW}}$ is the maximum allowable heat flow from and to the storage. In addition, *s* is defined non-negative.

These formulations neglect the temporal variation of heat storage losses. Stationary heat loss depends upon the temperature difference between the storage and the environment, which is sometimes neglected in large-scale storage [207,213]. Henning and Palzer suggested calculating the stationary heat loss using storage tank parameters and the temperature difference between the storage and the environment [38]. Similarly, the dynamic losses can also be calculated if the pipe parameters and the temperature differences are known. However, for simplicity both heat losses are often used as constant parameters, either as a percentage or assuming constant temperature difference over time. Salpakari et al. and Hedegaard et al. used such formulation with negligible losses to model TES in large-scale aggregated models [207,229]. The heat storage capacity S_{cap} can be pre-calculated using formulations by Heinen et al., which considers specific heat capacity and density of water, temperature difference and volume of the storage tank [205, Heinen et al. 2016, p.910]. This study has not presented the modeling of buildings and their thermal characteristics. Rasku and Kiviluoma presented a lumped capacitance model used to describe the thermal dynamics of the detached housing stock [230, Rasku and Kiviluoma 2019, p.8]. The same approach could also be taken to represent stratification in TES and industrial heating processes.

3.5 Summary

Chapter 3 describes the principal P2H and TES technologies that are technologically innovative and economically viable and can improve energy efficiency and reduce CO₂ emissions. Based on the literature, classifications of P2H and TES technologies have been sketched out. The most efficient and technologically matured P2H technologies for the European energy system are electric heat pumps, electric boilers, electric resistance heaters, and hybrid heating systems. Furthermore, the role of CHP in coupling power and heat sectors, especially in district heating, has been discussed. Among TES technologies, sensible and latent heat storages are mature and cost-effective technologies. However, other technologies such as thermo-chemical heat and thermo-mechanical heat storage are also prospective. Finally, the study presents thirteen most promising technologies under these four TES categories.

Low-temperature electric heat pumps, electric resistance and electrode boilers, electric resistance heaters, and sensible and latent heat storages have a high TRL. Therefore, they can facilitate a large share of the heat demand. Besides low-temperature heat pumps for household heating, high-temperature heat pumps show promising potential in the food, paper, and chemical industries. Electric resistance boilers are suitable

for low-temperature applications such as food and chemical industries. Electrode boilers are ideal for hightemperature process heating such as steel and cement industries. Electric resistance heating for residential households is available as radiant heaters, baseboard heaters, wall heaters, underfloor heating systems, and electric furnaces. High-temperature industrial applications can use electric process heaters, besides conductive, inductive, high-frequency, magnetic direct current, and electrical infrared heating systems. Hybrid heating systems combining heat pumps with electric or gas boilers are also an essential solution. CHP plays a vital role in coupling power and heat sectors by supplying district and industrial process heating. An optimal combination of CHP with other P2H and TES technologies in district heating systems can facilitate flexible sector coupling of power and heat and shows excellent potential to increase renewable shares in the energy system. TES is considered an essential flexibility tool for smart energy systems to aid the smooth coupling of P2H and is expected to cover 60% of total heat storage in 2050.

Heat pumps are modeled using COP formulations and taking the effect of temperature into account. Electric boilers and electric resistance heaters are modeled using similar equations but different power-to-heat ratios. Heat pump and electric boiler modeling considers the unit's operational status and power consumption limits. The electric boiler model avoids stratification effects. In the case of hybrid heating systems, each technology is modeled individually. Flexibility to such hybrid systems can be provided, either shifting the sources or shifting in time. CHP modeling formulations are presented for a generic case for backpressure and extraction turbines. Thermal energy storage is modeled using generic equations focusing on sensible hot water storage.

When the technology's performance depends on environmental temperatures, such as heat pumps and TES in insulated thermal mass, the effect of climate change is to alter the long-term weather averages and max/min values used for linear modeling of the technologies. Therefore, this feedback from the climate should be considered in large-scale energy system models.

Future promising research scopes include the role of P2H in other geographical contexts, the combination of P2H, P2Gs, and other options in an entirely sector-coupled energy system, and policy and regulatory behaviors in energy models to reflect on a more realistic analysis besides optimization models.

Based on the literature reviews, Chapter 4 discusses the elements of the Oemof-based model, mathematical formulations of the model elements, and architecture of the model to clarify its inputs, outputs, and the workflow.

Chapter 4 Model Development

4.1 Model Elements

The study developed a unique hourly optimization tool using a hybrid approach. The technological capacities are exogenously set, and the investment capacities are endogenously resolved. Technical limits set the boundary of the system so that the solutions are realistic. The Open Sector-coupled Energy Model (OSeEM) is created using Oemof Tabular [231, Hilpert et al. 2020]. Figure 4.1 illustrates the OSeEM energy model.



Figure 4.1: Simplified block diagram of the Open Sector-coupled Energy Model (OSeEM)

The model presents a self-sufficient energy system, where the demands are met using its renewable resources. The model's volatile components are Onshore wind, Offshore wind, Solar PV, and Hydro Runof-the-River (ROR) plants. The fuel input of the CHP plants comes from biomass resources. In addition to CHPs, two types of heat pumps are used to supply heat loads in the model: Air Source Heat Pump (ASHP) and Ground Source Heat Pump (GSHP). The state-of-the-art GSHPs are becoming cost-competitive compared to ASHPs and offer a more energy-efficient solution because of their use of consistent ground temperatures. The storage options are Pumped Hydro Storage (PHS)⁷, Lithium-ion (Li-ion) battery, Vanadium Redox (Redox) flow battery, Hydrogen (H₂) storage, and ACAES. The heat storage option is TES using hot water tanks.

Other energy systems can be connected using a transmission line (transshipment approach), which uses the Oemof class *Link*. The nodes (i.e., components and buses) of the OSeEM model, according to the Oemof Classes, are presented in Table 4.1.

Oemof Class	Nodes	Remarks
Bus	Electric Bus	Represents grid or network without losses.
	Heat Bus	
	Fuel Bus	
Sink	Electricity	Represents the electricity and building heat
	Space Heat	demands in the energy system.
	Domestic Hot Water	
Source	Offshore Wind	Represents the volatile generators of the
	Onshore Wind	energy system.
	Solar PV	
	Hydro Run-of-the-river	
	Biomass	Represents the biomass commodities which are fed into the CHP plants.
ExtractionTurbineCHP	Combined Heat and Power	Represents the heat generators of the energy system. The OSeEM model uses extraction turbines and uses only biomass as the fuel.
Transformer	Air Source Heat Pump	Complements CHP for meeting heating
	Ground Source Heat Pump	demands.
GenericStorage	Li-ion	Represents batteries.
	Vanadium Redox Flow	
	Adiabatic Compressed Air Energy Storage	Simplified model as Generic Storage.
	Hydrogen	Fresents electricity storage.
	Pumped Hydro Storage	Storage units with constant inflow and possible spillage. The storage capacity is not expandable.

Table 4.1: List of all components and buses of OSeEM

⁷ In Oemof.Tabular, a set of connected oemof.solph components is required to model reservoir storages with an inflow and possible spillage. To simplify modeling, the Reservoir facade bundles these components and provides a high-level API access to a more complex underlying model. Further details are available at Hilpert et al. (2021), p.3-5. DOI: <u>http://doi.org/10.5334/jors.320</u>

	Thermal Energy Storage	Simplified model as Generic Storage. Presents heat storage in sensible hot water tanks.
Link		Bi-direction link for two buses (e.g., to model transshipment)

4.2 Mathematical Formulation

The OSeEM model uses Oemof Solph [132, Krien et al, 2020], following the formulation by Hilpert [232, Hilpert 2020, p.4–6], where the maximum potential constrains the renewable sources, total biomass amount, and storage capacities. The upper limit for the P2H technologies are subject to optimization but depends on the availability of electricity. OSeEM uses a perfect foresight approach; hence all timesteps of the model time horizon are read by the solver at once. Also, the weather and the renewable supply data is known in advance. The model optimizes the operating and investment costs of all the volatile generators, CHP, heat pumps, and storages. x and c present the endogenous variables and exogenous parameters as listed in Table 4.2.

Variables/Parameters	Description	Technology
x_v^{flow}	Flow of volatile generator unit v	Offshore Wind Onshore Wind
$x_v^{capacity}$	Capacity of volatile generator unit v	Solar PV Hydro ROR
$c_v^{marginal_cost}$	Marginal cost ⁸ of volatile generator unit v [232]	
$c_v^{capacity_cost}$	Capacity cost ⁹ of volatile generator unit v [232]	
x_{chp}^{flow}	Flow of CHP unit <i>chp</i>	СНР
$x_{chp}^{capacity}$	Capacity of CHP unit <i>chp</i>	
c ^{marginal_cost} c _{chp}	Marginal cost of CHP unit <i>chp</i>	
c ^{capacity_cost} c _{chp}	Capacity cost of CHP unit <i>chp</i>	
x_h^{flow}	Flow of heat pump unit h	ASHP GSHP
$x_h^{capacity}$	Capacity of heat pump unit h	
$c_h^{marginal_cost}$	Marginal cost of heat pump unit h	
$c_h^{capacity_cost}$	Capacity cost of heat pump unit h	

Table 4.2: Variables and parameters for cost optimization

⁸ The marginal costs are calculated based on variable operation and maintenance costs, carrier costs, and the efficiency.

⁹ The capacity costs are calculated based on fixed operation and maintenance costs and the annuity.

x_s^{flow}	Flow of storage unit <i>S</i>	Li-ion Redox		
$x_s^{capacity}$	Capacity (power) of storage unit s	ACAES H2 PHS (No Investment)		
$x_s^{storage_capacity}$	Storage capacity (energy) of storage unit s	TES		
$C_{S}^{marginal_cost}$	Marginal cost of storage unit s			
$c_s^{capacity_cost}$	$c_s^{capacity_cost}$ Capacity cost (power) of storage unit s			
$c_s^{storage_capacity_cost}$	Storage capacity cost (energy) of storage unit S			
$x_{m,from}^{flow}$	Flow from a bus through the transmission line m	Link		
$x_{m,to}^{flow}$ Flow to a bus through the transmission line m				
c_m^{loss}	Loss on transmission line m			

Equations (4.1)-(4.24) in the next subsections follow the mathematical formulations by [232, Hilpert 2020, p.4–6].

4.2.1 Bus

There are three types of buses in the energy model: electrical, heat, and fuel bus. Since all flows into and out of a bus are balanced, for the set of all buses $b \in B$, sum of all input flows $x_{b,in}^{flow}$ to a bus *b* must be equal to the sum of all output flows $x_{b,out}^{flow}$:

$$\sum x_{b,in}^{flow}(t) = \sum x_{b,out}^{flow}(t) \qquad \forall t \in T, \forall b \in B$$
(4.1)

4.2.2 Load

Two types of loads are considered in the energy model: electricity and heat. The heat load consists of space heat and domestic hot water. For the set of all loads $l \in L$, the load flow x_l^{flow} at every time step t must be equal to the product of two exogenously given inputs: profile value of the load $c_l^{profile}$ at time step t, and the total amount of the load c_l^{amount} :

$$x_l^{flow}(t) = c_l^{profile}(t) \cdot c_l^{amount} \quad \forall t \in T, \forall l \in L$$
(4.2)

4.2.3 Volatile Generator

The volatile generators in the model are onshore and offshore wind, solar PV, and hydro ROR. These components are connected to electricity buses. For all the volatile generators $v \in V$, the flow x_v^{flow} at every time step *t* must be equal to the product of the capacity $x_v^{capacity}$ and the profile value of the volatile generator $c_v^{profile}$:

$$x_{v}^{flow}(t) = x_{v}^{capacity}(t). c_{v}^{profile}(t) \qquad \forall t \in T, \forall v \in V$$

$$(4.3)$$

The endogenously obtained capacity of the generator $x_v^{capacity}$ at every time step *t* must be less than or equal to the maximum capacity potential of the volatile component $c_v^{capacity_potential}$:

$$x_{v}^{capacity}(t) \le c_{v}^{capacity_potential} \qquad \forall t \in T, \forall v \in V$$
(4.4)

4.2.4 Combined Heat and Power

Since the model is 100% RES-based, the CHP plants use only biomass resources as fuel. Thus, biomass goes into the fuel bus, which later goes as the input of CHP, as shown in Figure 4.1. The CHP runs in extraction turbine mode, as shown by (4.5)–(4.7), according to Mollenhauer et al. [233]. Equation (4.5) shows the relation between the input carrier flow $x_{chp}^{flow,carrier}$ and the two output flows: electrical output flow $x_{chp}^{flow,electricity}$ and heat output flow $x_{chp}^{flow,heat}$, at every time step *t*. Equation (4.6) shows the relationship between the two output flows. c_{chp}^{beta} is the power loss index, which is derived using (4.7). $c_{chp}^{electrical_efficiency}$, $c_{chp}^{thermal_efficiency}$ and $c_{chp}^{condensing_efficiency}$ denote the electrical, thermal and condensing efficiencies of the CHP unit, respectively.

$$x_{chp}^{flow,carrier}(t) = \frac{x_{chp}^{flow,electricity}(t) + x_{chp}^{flow,heat}(t) \cdot c_{chp}^{beta}}{c_{chp}^{condensing_efficiency}} \quad \forall t \in T$$

$$(4.5)$$

$$x_{chp}^{flow,electricity}(t) \ge x_{chp}^{flow,heat}(t) \cdot \frac{c_{chp}^{electrical_efficiency}}{c_{chp}^{thermal_efficiency}} \quad \forall t \in T$$
(4.6)

$$c_{chp}^{beta} = \frac{c_{chp}^{condensing_efficiency} - c_{chp}^{electrical_efficiency}}{c_{chp}^{thermal_efficiency}}$$
(4.7)

Equation (4.8) models the limited availability of biomass commodities where the aggregated inflows are constrained by the absolute amount of the biomass commodity $c_{biomass}^{amount}$:

$$\sum x_{chp}^{flow,carrier}(t) \le c_{biomass}^{amount} \quad \forall t \in T$$
(4.8)

4.2.5 Heat Pump

Oemof Solph's conversion component, which converts power to heat, is used for modeling both GSHP and ASHP. Therefore, a conversion process of one input flow $x_{h,from}^{flow}$ (electricity flow from the electricity bus) and one output $x_{h,to}^{flow}$ (heat flow to the heat bus) and a conversion factor $c_{h,to}^{efficiency}$ (conversion efficiency i.e., coefficient of performance of the heat pump) at every time step *t* models all the heat pumps $h \in H$:

$$x_{h,to}^{flow}(t) = x_{h,from}^{flow}(t) \cdot c_{h,to}^{efficiency} \quad \forall t \in T, \forall h \in H$$
(4.9)

4.2.6 Storage

In addition to PHS, the other electricity storage technologies used in the model are Li-ion and Redox batteries, ACAES, and H₂ storage. Hot water-based TES is the only heat storage component. Oemof Solph's generic storage formulations are used to model all the storage components except PHS. For all these storages $s \in S$, the mathematical model includes the input and output flows and the storage level:

$$x_s^{level}(t) = x_s^{level}(t-1).\left(1 - c_s^{loss_rate}\right) + c_s^{eta_in}. \ x_s^{flow,in}(t) - \frac{x_s^{flow,out}(t)}{c_s^{eta_out}} \quad \forall t \in T, \forall s \in S$$
(4.10)

where x_s^{level} indicates the storage energy level, $c_s^{loss_rate}$ marks the loss rate for the storage, $x_s^{flow,in}$ and $x_s^{flow,out}$ indicates the input and output flows, and $c_s^{eta_in}$ and $c_s^{eta_out}$ denotes the charging and discharging efficiencies of the storage.

The charging and discharging efficiencies are formulated from the roundtrip efficiency using $c_s^{eta} = \sqrt{c_s^{roundtrip_efficiency}}$. The input and output flows x_s^{flow} are constrained by the maximum power capacity $c_s^{capacity}$ as shown in (4.11). The energy level x_s^{level} is constrained by the maximum energy capacity $c_s^{storage_capacity}$ as shown in (4.12).

$$x_s^{flow}(t) \le c_s^{capacity} \quad \forall t \in T, \forall s \in S$$
(4.11)

$$x_s^{flow}(t) \le c_s^{storage_capacity} \quad \forall t \in T, \forall s \in S$$
(4.12)

4.2.7 Pumped Hydro Storage

The PHS are modeled as storage units with a constant inflow and possible spillage:

$$x_{phs}^{level}(t) = x_{phs}^{level}(t-1).\left(1 - c_{phs}^{loss_rate}\right) + x_{phs}^{profile}(t) - \frac{x_{phs}^{flow,out}(t)}{c_{phs}^{efficiency}} \quad \forall t \in T$$

$$(4.13)$$

where x_{phs}^{level} indicates the pumped hydro storage energy level, $c_{phs}^{loss_rate}$ marks the loss rate for the PHS, $x_{phs}^{profile}$ indicates the endogenous inflow profile, $x_{phs}^{flow,out}$ denotes the output flow from the PHS, and $c_{phs}^{efficiency}$ marks the efficiency of the PHS. The hydro inflow is constrained by an exogenous inflow profile:

$$0 \le x_{phs}^{profile}(t) \le c_{phs}^{profile}(t) \quad \forall t \in T$$
(4.14)

Therefore, if the inflow exceeds the maximum storage capacity, spillage is possible by setting $x_{phs}^{profile}$ to lower values. The spillage at time step *t* can therefore be defined by $c_{phs}^{profile}(t) - x_{phs}^{profile}(t)$.

4.2.8 Transmission Line

The electricity transmission between two energy systems is modeled using the transshipment approach, which facilitates simple electricity exchange (import-export) after considering a transmission loss factor. Therefore, transmission lines $m \in M$ are modeled according to the following mathematical formulation:

$$x_{m,from}^{flow}(t) = (1 - c_m^{loss}) \cdot x_{m,to}^{flow}(t) \quad \forall t \in T, \forall m \in M$$
(4.15)

where $x_{from,m}^{flow}$ indicates the flow from the supplying energy system, $x_{m,to}^{flow}$ indicates the flow to the receiving energy system, and c_m^{loss} indicates the loss on transmission line m.

4.2.9 Costs

The marginal costs $c_{v,chp,h,s}^{marginal_cost}$ are calculated based on the variable operation and maintenance (VOM) cost $c_{v,chp,h,s}^{VOM}$, carrier cost $c_{v,chp,h,s}^{carrier_cost}$, and the efficiency of the corresponding technology $\eta_{v,chp,h,s}$:

$$c_{\nu,chp,h,s}^{marginal_cost} = c_{\nu,chp,h,s}^{VOM} + \frac{c_{\nu,chp,h,s}^{carrier_cost}}{\eta_{\nu,chp,h,s}}$$
(4.16)

The capacity costs for volatile generators, CHP and heat pumps $c_{v,chp,h}^{capacity_cost}$ are calculated based on the fixed operation and maintenance (FOM) cost $c_{v,chp,h}^{FOM}$, and the annuity of the corresponding technology $c_{v,chp,h}^{annuity}$, as shown in (4.17). The annuity $c^{annuity}$ is calculated using (4.18), which consist of the initial capital expenditure c^{capex} , the weighted average cost of capital c^{WACC} , and the lifetime of the investment *n* for the respective technology.

$$c_{\nu,chp,h}^{capacity_cost} = c_{\nu,chp,h}^{FOM} + c_{\nu,chp,h}^{annuity}$$
(4.17)

$$c^{annuity} = c^{capex} \cdot \frac{(c^{WACC} \cdot (1 + c^{WACC})^n)}{((1 + c^{WACC})^n - 1)}$$
(4.18)

In case of storage, the capacity costs $c_s^{capacity_cost}$ and the storage capacity costs $c_s^{storage_capacity_cost}$ are calculated using (4.19)–(4.20):

$$c_s^{capacity_cost} = c_{s,power}^{annulty}$$
(4.19)

$$c_s^{storage_capacity_cost} = c_s^{FOM} + c_{s,energy}^{annuity}$$
(4.20)

where, $c_{s,power}^{annuity}$ is the annuity cost of storage power, and $c_{s,energy}^{annuity}$ is the annuity cost of storage energy. These two annuities are calculated using the formulation of (4.18). c_s^{FOM} is the fixed operation and maintenance cost (FOM) of energy storage.

In addition to these modeling equations, some costs are calculated and analyzed after a successful model run, based on the optimization results. The annual investment cost c^{AIV} is calculated multiplying the annuity $c^{annuity}$ and the optimized capacity $c^{optimized_capacity}$, as shown in (4.21). The total investment (overnight) investment cost c^{TIV} is calculated multiplying the capital expenditure c^{capex} , and the optimized capacity $c^{optimized_capacity}$, as shown in (4.21). The total investment (overnight) investment cost c^{TIV} is calculated multiplying the capital expenditure c^{capex} , and the optimized capacity $c^{optimized_capacity}$, as shown in (4.22). Furthermore, the Levelized Costs of Electricity c^{LCOE} is calculated from the ratio of the Net Present Value (NPV) of total costs of over lifetime (including fixed and variable operation and maintenance costs, fuel costs, and the discount rate), and the NPV of the electrical energy produced over the lifetime, as shown in (4.23).

$$c^{AIV} = c^{annuity} \cdot c^{optimized_capacity}$$
(4.21)

$$c^{TIV} = c^{capex} \cdot c^{optimized_capacity}$$

$$c^{LCOE} = \frac{\sum \frac{(I_n + M_n + F_n)}{(1+r)^n}}{\sum \frac{E_n}{(1+r)^n}}$$
(4.23)

(4.22)

where I_n indicates the initial cost of investment expenditures (same as c^{capex}), M_n indicates the sum of all operation and maintenance expenditures (sum of c^{VOM} and c^{FOM}), and F_n indicates the fuel expenditure (such as the carrier cost of biomass), E_n indicates the sum of all electrical energy generation, r indicates the discount rate (same as c^{WACC}), and n indicates the lifetime.

4.2.10 Objective Function

The objective function is created from all instantiated objects which use all operating costs and investment costs arguments:

$$(4.24)$$

$$min: \sum_{v,t} \overline{x_v^{flow}(t).c_v^{marginal_cost}} + \sum_v \overline{x_v^{capacity}.c_v^{capacity_cost}} + \sum_{v} \overline{x_v^{capacity_cost}} + \sum_{v} \overline{x_v^{capa$$

4.3 Model Architecture

The underlying concept of the OSeEM model uses the formulation of LP and MILP from a generic objectoriented structure of Oemof Solph [132, Krien et al. 2020]. Figure 4.2 shows a summary of the OSeEM model input and output.



Figure 4.2: Input and output of the OSeEM model

The input data used in the model are the capacities and potentials of renewable energy-based power plants (such as wind, PV), heat generation technologies (such as CHP, heat pump), electricity and heat demands, transshipment capacity, storage capacities, and their potential. Also, operating costs (i.e., marginal cost) and the investment costs (i.e., capacity cost) for all the considered technologies are provided as input. After solving the model using open model solvers, the results are post-processed using Oemof Tabular's post-processing scripts. The output of the model provides information on the generation mix, investment capacities according to the provided capacities and available potential, balance in each of the buses, import/export between energy systems, filling level of the storages and the shadow prices.

Python programming language is used for the model development as shown in Figure 4.3. After starting the necessary packages, input data and result directories are set up, and input data are read from external *.csv* files. Data preparation is an essential step of the model development process, where the data are normalized and scaled for use as inputs. Different scenarios are built with different datasets. The input datasets are pre-processed before importing them to the input *.csv* files. The energy system is created using Oemof Solph. Different components are added to the energy system using Oemof Tabular's *Facade* classes. Then the energy model is solved using Oemof Solph. After optimization, results are post-processed and written to several *.csv* files using the *Post-processing* tool, which are later illustrated using the *Plots* tool.



Figure 4.3: OSeEM model workflow

4.4 Summary

Chapter 4 describes the different elements of the OSeEM model, which includes onshore and offshore wind, solar PV, hydro ROR, CHP, ASHP, GSHP, PHS, Li-ion battery, Redox battery, H₂ storage, ACAES, and TES using hot water tanks. Then the Oemof-based mathematical equations for the elements and the objective function of the model are described. Two simple figures are used to describe the inputs and outputs (Figure 4.2), and the model workflow (Figure 4.3). The input data can be adjusted to create and investigate different scenarios. The model results are available in simple tabular form, which can be analyzed and visually presented using plots.

In the next two chapters, the OSeEM model is applied for two different case studies. Chapter 5 presents the case of Schleswig-Holstein, where OSeEM is validated for subnational energy systems. Later in Chapter 6, OSeEM will be used to analyze the case of Germany and answer critical current research questions.

Chapter 5 Modeling of a Subnational Energy System: Case Study of Schleswig-Holstein

5.1 Background

Schleswig-Holstein (SH), the northern-most federal state of Germany, is increasingly becoming an energy hub between Germany and the Scandinavian countries, due to its geographic location and the ongoing expansion of onshore wind energy [234,235]. In 2018, electricity generation from renewable energies in SH reached around 150%, which is almost four times Germany's national average of 38% [234, SH State Govt. Report 2020, p.54]. SH takes a leading position in the expansion of electricity generation from renewable energies. The share of renewable energies in SH was almost 15.8% in the heating sector, slightly above the Germany-wide share of 14.4% [234, SH State Govt. Report 2020, p.79]. When it comes to the percentage of renewable energies in gross final energy consumption, SH's 36.6% is well above the national average of 16.5% [234, SH State Govt. Report 2020, p.54]. SH aims to generate at least 37 terawatt-hours of electricity from renewable energies by the year 2025 [234, SH State Govt. Report 2020, p.13]. Figure 5.1 shows the individual energy sources' shares in the total final energy supply contribution (22.6 TWh) renewable energies 2018 [234, SH State Govt. Report 2020, p.79].



Figure 5.1: Shares of the renewable sources in the total renewable energy supply in Schleswig-Holstein in 2018. Source: [234, SH State Govt. Report 2020, p.10, p.79].

Due to its geographical conditions, SH is predestined for the use of wind energy. In SH, wind turbines with a nominal output of around 8.48 GW were installed by the end of 2018 [234, SH State Govt. Report 2020, p.10, p.39], which means that electricity from wind energy makes up the largest proportion of SH's electricity supply from renewable energies. SH considers the expansion of wind energy to increase to at least 25 GW by 2030¹⁰. Biomass represents one of the largest shares (32.5%) of renewable energies in SH's supply contribution [234, SH State Govt. Report 2020, p.55]. Wood, energy crops, straw, and biogas can sustainably generate a significant proportion of the energy requirement. SH is well-suited for solar systems, as the increased amount of wind between the seas provides natural cooling. Due to the lack of landscape conditions, water traditionally plays a subordinate role as an energy source in Schleswig-Holstein. However, the latest energy models to analyze the SH energy system should also consider the CAES and hydrogen as additional storage options.

The next sections discuss the OSeEM-SN model (SN indicates Subnational), where the case of Schleswig-Holstein is used to validate the OSeEM energy model. The energy system is similar to Figure 4.1 and uses the elements of Table 4.1.

5.2 Input Data

5.2.1 Hourly Renewable Profiles and Demand Data

The OSeEM-SN model is validated using historical data for a full year. According to [68, Brown 2018, p.721], data from 2011 are used for analyzing 2050 scenarios, except for hydro data, which uses 2016 data. Table 5.1 shows the hourly input data sources used for validating the OSeEM-SN model.

Data	Source	Remarks
Wind profiles	Renewables Ninja project [236]	Based on the MERRA-2 dataset.
Solar PV profiles		
Hydro ROR inflow	Dispa-SET project [114]	-
PHS scaled inflow		
Electricity demand	OPSD project [237]	Based on the ENTSO-e statistical database [238].
Space heat demand	OPSD project [237]	Based on the When2Heat dataset [239].

Table 5.1: Hourly input data sources for the OSeEM-SN model

The onshore wind profile is obtained from the MERRA-2, current fleet dataset for the NUTS-2 region (SH: DEF0) [236]. The offshore wind profile represents the offshore profile of Germany based on the MERRA-2 database [236]. The solar PV profile is also obtained for SH (NUTS2, DEF0) [236]. The hydro run-of-the-river (ROR) and PHS scaled inflows are obtained from Dispa-SET's 2016 data [114, Dispa-SET 2020]. The inflows are defined as the contribution of exogenous sources to the level (or state of charge) or the reservoir. Scaled inflows¹¹ are normalized values of the inflow concerning the nominal power of the storage unit. The PHS inflows are scaled down to match SH's inflow profile (in MWh). Germany's demand data (electricity, space heat, domestic hot water (DHW)) are downscaled based on population to represent SH's hourly

¹⁰ According to EEK.SH. Source: <u>https://www.eek-sh.de/de/wind.html</u>

¹¹ Scaling down the PHS inflow to match SH's inflow profile is done here for simplicity. However, there is no inflow into the upper basin in the PHS installation in Schleswig-Holstein (Geesthacht), and the river Elbe is used in the lower reservoir. Future SH models should consider this.

demand profiles. The wind, solar, and hydro normalized profiles do not change in the scenarios and can be visualized as shown in Figure 5.2.



Figure 5.2: Normalized input profiles of volatile generators of OSeEM-SN model, (a) offshore wind, (b) onshore wind, (c) solar photovoltaics (PV), and (d) hydro run-of-the-river (ROR)

Figure 5.3 shows the normalized demand profiles of SH in 2050. The total electricity demand for SH in 2050, based on the representative year, is 18.6 TWh_{el}. Total space heat demand is 18.6 TWh_{th}, and the DHW demand is 4 TWh_{th}. The amount of available biomass is calculated from the Hotmaps project [240, Hotmaps Project, D2.3 WP2 Report – Open Data Set for the EU28 2018]. The study assumes that the existing biomass and biogas power plants are converted to CHP plants by 2050. CHP's electrical and



thermal efficiencies are assumed to be 45%, and the condensing efficiency is assumed to be 50%. The COP of the ASHP and GSHP are assumed to be 2.3 and 3.9, respectively [241, ANGUS II 2020¹²].

Figure 5.3: Normalized demand profiles of SH in 2050. Own illustration.

5.2.2 Capacity and Available Potential

The existing capacities and available potentials for the volatile generators and the storage investments are taken from different sources, namely the Hotmaps project [240, Hotmaps Project, D2.3 WP2 Report – Open Data Set for the EU28 2018], ANGUS II Project [241], Deutsche WindGuard [242], Agentur für Erneuerbare Energien (AEE) [243], and LIMES-EU project [244], as listed in Table 5.2. The available potentials are calculated from the maximum potentials and the existing capacities. The Li-ion, Redox, and H₂ potentials are assumed to be 5% of Germany's available potentials, as stated in the project databases. The ACAES potential is assumed to be 50% of Germany's total potential because of its availability in only Northern Germany.

Technology	Existing Capacity	Available Potential ¹³
Onshore Wind [GWel]	7 [242]	1.9 [243]
Offshore Wind [GWel]	1.7 [242]	25.2 ¹⁴ [244]
Solar PV [GW _{el}]	1.6 [243]	6.7 [243]

Table 3.2. Capacity and available potential for volatile generators and storage in Strin 200
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¹² The COP values can originally be referred to the PyPSA Project. Details are available in the CSES ANGUS II Project database. <u>https://github.com/ZNES-datapackages/angus-input-data/blob/master/technology/heat.csv</u>

¹³ The available potential is additional to the existing capacities.

¹⁴ The maximum offshore wind potential, according to the LIMES-EU project, is 83.6 GWel. The available potential of SH assumes the equal distribution of remaining capacities in the three northern states of Germany.

Hydro ROR [MW _{el}]	2 [243]	4 [243]
Biomass & Biogas	1 GWh [243]	21.8 PJ (6055.6 GWh) [240]
Li-ion [MW _{el}]	-	782.5 [241]
Redox [MW _{el}]	-	46.5 [241]
H ₂ [MW _{el}]	-	505 [241]
ACAES ¹⁵ [MW _{el}]	-	1715.5 [241]
PHS [MW _{el}]	120 [245]	-
TES [MWth]	-	1000 ¹⁶

5.2.3 Cost Data

Table 5.3 presents the cost data detailed in [246, Maruf 2021, p.20].

Technology	Onshore Wind	Offshore Wind	٩٧	ROR	Biomass	Li-ion	${\tt H}_2$	Redox	SHd	ASHP	GSHP	ACAES	TES
Capex (€/kW)	1075	2093	425	3000	1951	35	1000	600	2000	1050	1400	750	0
Lifetime (Years)	25	25	25	50	30	20	22.5	25	50	20	20	30	20
WACC	0.025	0.048	0.021	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05
VOM Cost (€/MWh)	0	0	0	0	11.3	1	1	1	0	0	0	1	0
FOM Cost (€/kWh)	35	80	25	60	100	10	10	10	20	36.75	49	10	0.38
Storage Capacity Cost (€/kWh)	-	-	-	-	-	187	0.2	70	-	-	-	40	38
Carrier Cost (€/MWh)	-	-	-	-	34.89	-	-	-	-	-	-	-	-

Table 5.3. Cost data for OSeEM-SN Model. Source: [246, Maruf 2021, p.20].

¹⁵ The ACAES energy capacity unit is MWh or GWh; however, the optimization model in this study considered the hourly power values, and thus the unit is expressed as MW.
¹⁶ Own assumption. The assumption in this study is minimum compared to the total heat demand. The author did not find any study

¹⁶ Own assumption. The assumption in this study is minimum compared to the total heat demand. The author did not find any study that predicts the thermal energy storage demand. However, the study by LUT and EWG can be followed in the future for a further accurate assumption which predicts TES as the most relevant heat storage technology in Europe with >2000 TWh_{th} in 2050 [193, Ram et al. 2018, p.3].

5.2.4 Other Data

The loss rate for TES is 1.4% [241, ANGUS II 2020¹⁷]. Hydro ROR efficiency is 90% [241, ANGUS II 2020¹⁸]. Other storage data used in the model are presented in Table 5.4.

Storage	Roundtrip Efficiency [%]	Maximum state of charge at full output capacity [Hrs]
Li-ion	92	6.5
Redox	80	3.3
H ₂	46	168
PHS	75	8
ACAES	73	7
TES	81	72

Table 5.4. Storage data for OSeEM-SN Model. Source: [241, ANGUS II 202	20 ¹⁹]
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Land limitation for onshore wind is 4 MW/km², and offshore wind is 6 MW/km² [244, LIMES-EU 2020²⁰]. The solar PV installations consider the protection of nature reserves and restricted zones.

5.3 Scenarios

The study assumes three scenarios for validating the OSeEM-SN model for Schleswig-Holstein: BM-25, BM-50, and BM-100. The scenarios represent 25%, 50%, and 100% of the total available biomass potentials, respectively. The study aims to investigate how the results change upon varying one parameter of the model. However, the model does not account for all the parametric variations for the input data; rather, it focuses on the model's usability to create different scenarios and examine different possible pathways.

5.4 Results

5.4.1 Supply-Demand Matching

The OSeEM-SN model reached feasible solutions for all three scenario assumptions. Figure 5.4 shows the supply-demand matching of electricity and heat demands for the three different scenarios over the year 2050.

¹⁷ The TES loss rate of 1.4% is taken from the PyPSA project. Further information is available in the ANGUS II project database. Source: https://github.com/ZNES-datapackages/angus-input-data/blob/master/technology/heat.csv ¹⁸ The PHS efficiency of 90% is taken from DIW. Further information is available in the ANGUS II project database. Source:

https://github.com/ZNES-datapackages/angus-input-data/blob/master/technology/technology.csv

¹⁹ The ANGUS II project database details the efficiency and maximum hour values for storage with references. Source: https://github.com/ZNES-datapackages/angus-input-data/blob/master/technology/technology.csv

²⁰ The land limitation was taken directly from the documentation of the LIMES-EU project. Source: Nahmmacher et al. 2014. Available at: https://www.pik-potsdam.de/en/institute/departments/transformation-pathways/models/limes/DocumentationLIMESEU_2014.pdf

However, the land limitation is not a direct input in the OSeEM model. Some of the recent studies assume that only a 20% fraction of the already restricted area is available for installation of wind generators due to competing land use and likely public acceptance issues. This argument was used in the PyPSA model for assuming a lower potential [68, Brown et al. 2018]. Also, Deutsche WindGuard GmbH commented in the BalticLINes project that the corrected capacity densities for European wind farms in the North Sea region is 6.0 MW/km², and in the Baltic Sea region is 5.5 MW/km² (Ref: https://maritime-spatial-planning.ec.europa.eu/practices/capacitydensities-european-offshore-wind-farms.)



— CHP (Heat) — GSHP •

_

ASHP

(b)

72



-CHP (Heat) -GSHP ASHP -Space Heat Demand ----- DHW Demand -.



Figure 5.4: Supply-demand matching for the three scenarios over the year 2050. (a) BM-25 electricity demand matching; (b) BM-25 heat demand matching; (c) BM-50 electricity demand matching; (d) BM-50 heat demand matching; (e) BM-100 electricity demand matching; (f) BM-100 heat demand matching

The energy generation from onshore wind in BM-25 is 26.6 TWh_{el}, which drops to 20.9 TWh_{el} in the BM-50 and BM-100 scenarios. Similarly, solar PV generation drops from 8.7 TWh_{el} in the BM-25 scenario to 6.8 TWh_{el} in the BM-50 scenario and 4.6 TWh_{el} in the BM-100 scenario. Offshore wind generation remains the same, 5.5 TWh_{el}, in all three scenarios. The CHP generation for electricity and heat increases with increasing biomass availability in the scenarios, from 1.5 TWh in the BM-25 to 3 TWh in the BM-50 scenario and 3.8 TWh in the BM-100 scenario. In contrast, heat pump (GSHP and ASHP) generation reduces from 21.5 TWh_{th} in BM-25 to 18.9 TWh_{th} in the BM-100 scenario. Therefore, it is obvious from the scenarios that, with increasing biomass penetration in the energy mix, the CHP plant capacities are expanded, increasing electricity and heat generation. This, in turn, reduces the expansion of other power plants and heat pumps to meet the demands.

5.4.2 Scenario Comparison

5.4.2.1 Capacity Expansion

According to the optimization from OSeEM-SN, the required investment of different technologies can be obtained. Table 5.5 compares the required investments on top of the existing capacities of Table 5.2 for the three scenarios.

Technology	Scenario-Wise Investments				
	BM-25	BM-50	BM-100		
Onshore Wind [GWeI]	1.9	0	0		
Offshore Wind [GWeI]	0	0	0		
Solar PV [GW _{el}]	6.7	4.9	2.7		
Hydro ROR [MW _{el}]	4	4	4		
CHP [GW]	1	1.6	1.9		
GSHP [GWth]	5	3.8	3		
ASHP [GWth]	1.3	2.1	3.1		
Li-ion [MW _{el}]	782.5	782.5	782.5		
Redox [MW _{el}]	46.5	46.5	46.5		
H ₂ [MW _{el}]	397	0	0		
ACAES [MWei]	357.1	357.1	357.1		
TES [MW _{th}]	1000	460.2	0		

Table 5.5: Comparison of capacity expansion for three scenarios

The results show no need for additional investment in offshore wind plants to meet SH's energy demand. As a result, the offshore capacities can be reserved for supplying other states' energy demand, especially those in Southern Germany. CHP investment rises because of the higher availability of biomass over the three scenarios and the high overall efficiency due to the combined production of electricity and heat. This impacts the investment in onshore wind and solar PV capacities and reduces investments in volatile generators. GSHP investment also decreases with increasing CHPs; however, ASHP investment increases to complement the heating demand. For storage, Li-ion, Redox, and ACAES are used to their maximum investment capacities for all three scenarios. Hydrogen storage is used only in the BM-25 scenario,

indicating its use only in low biomass availability cases. The need for TES storage decreases over the scenarios with more biomass availability. Therefore, with limited biomass, it is possible to meet the heat demand with a heat storage option.

5.4.2.2 Investment Cost

Figure 5.5 compares the volatile generators' investment cost, i.e., wind, solar PV, and hydro ROR plants. The total investment cost for the volatile generators in SH decreases by 76% (4.9 bn \in vs. 1.1 bn \in) over the scenarios. The annual investment cost decreases from 262.7 mn \in /yr to 61.5 mn \in /yr with the increasing biomass availability.



Investment Cost - Volatile Generators

Figure 5.5: Comparison of volatile generator investments in SH

Figure 5.6 compares the investment cost of CHP plants and heat pumps (GSHP and ASHP). Overall, the total investment cost increases by 7% (10.6 bn \in vs. 11.3 bn \in) over the scenarios. The annual investment cost increases from 819.2 mn \notin /yr in the BM-25 scenario to 853.7 mn \notin /yr in the BM-100 scenario.



Figure 5.6: Comparison of CHP and heat pump investments in SH

Figure 5.7 compares the storages' investment cost, i.e., Li-ion, Redox, H₂, ACAES, and TES. The total investment cost for the storages in SH decreases by 69% (4.5 bn \in vs. 1.3 bn \in) over the scenarios. The annual investment cost decreases from 357.6 mn \notin /yr in the BM-25 scenario to 105.1 mn \notin /yr in the BM-100 scenario.



The total investment in volatile generators, CHPs, and storages is 20.1 bn € in the BM-25 scenario. The investment decreases by 22% in the BM-50 scenario (15.6 bn €) and 30% in the BM-100 scenario (13.9 bn

€). The annual investment cost decreases accordingly, from 1.44 bn €/yr in the BM-25 scenario to 1.02 bn €/yr in the BM-100 scenario²¹. Figure 5.8 illustrates the total investments for different scenarios from OSeEM-SN optimization results.



Figure 5.8: Comparison of total investments (volatile generators, CHPs, and storages) in SH

5.4.2.3 Energy Mix

Figure 5.9 compares the energy mix results of the OSeEM-SN model. Figure 5.9 (a) compares the electricity generation from the combined (i.e., existing and new) capacities. The onshore wind generation dominates the energy mix because of high wind availability in SH. The onshore wind electricity generation varies between 20.9 TWh_{el} and 26.6 TWh_{el} for the three scenarios. The model does not suggest installing new offshore capacities, because of two reasons: (i) the cost of offshore is higher, and (ii) the demand is already met using other resources. However, this is only valid for SH's subnational case, where plenty of renewable resources are available. The scenario will be different for a larger case with a lack of adequate renewable resources. The offshore electricity generation from the existing capacities is the same for the three scenarios, 5.5 TWh_{el}. The hydro ROR electricity generation also remains the same, 0.016 TWh_{el} in the BM-100 scenario. Overall, the electricity generation decreases by 17% (42.4 TWh_{el} vs. 34.9 TWh_{el}) from the BM-25 scenario to the BM-100 scenario. Therefore, with high biomass-based CHPs in the energy mix, the curtailment of the generation from variable renewable energy plants can be decreased.

Figure 5.9 (b) compares the heat generation from the combined CHP capacities and new heat pump capacities. GSHPs dominate the heat mix; however, the installation of GSHP decreases as the biomass penetrates more into the energy mix. From the BM-25 to the BM-100 scenario, while the CHP-based heat generation increases by 154% (1.51 TWh_{th} vs. 3.84 TWh_{th}), the GSHP installation decreases by 28% (19.8 TWh_{th} vs. 14.1 TWh_{th}). However, the demand is also complemented by ASHPs, which increase from 1.69 TWh_{th} in the BM-25 scenario to 4.79 TWh_{th} in the BM-100 scenario.

²¹ The author recommends including the cost of biomass substrates in the model for more accurate calculations.



(b) Figure 5.9: Energy mix for different scenarios in SH (a) electricity mix and (b) heat mix

The analysis based on OSeEM-SN model results is summarized below:

- 1. SH has adequate renewable resources to meet its electricity and building heat demands.
- 2. The onshore wind dominates electricity generation.
- 3. Electric heat pumps, mainly GSHPs, dominate heat generation.
- 4. The batteries offer short-term storage solutions for electricity storage.
- 5. ACAES, H₂, and TES are promising storage solutions, especially when renewable energy availability is limited.
- 6. Power-to-heat devices, such as GSHP and ASHP, stand out as prominent heating options besides traditional CHPs.
- TES plays an important role in integrating the power and heat sectors in scenarios with low biomass shares.
- 8. Increasing biomass in the system impacts other technologies' investment costs and can reduce the overall system cost.
- 9. The optimization reached feasible solutions without utilizing the full potential of many resources. Therefore, the high amount of available potential, especially offshore wind resources, emerges as a promising alternative for powering up other parts of the country, especially Germany's high energy-consuming industrial southern states.

5.5 Summary

The increasing penetration of the energy system with predominantly volatile generation units leads to a farreaching techno-economic and social transformation process. The advancement of the energy transition leads to the fact that power generation plants, instead of being located in the consumer centers' immediate vicinity, are increasingly located in places with the best site conditions for the respective plants. With the increasing feed-in of supply-dependent renewable energy, consumption and generation are falling apart in time, placing new demands on the system. Due to its special location, Schleswig-Holstein already represents a system that can be considered exemplary for future energy systems, with shares of 100% renewable energies. Analyses of future energy systems with a very high share of renewable energies, in which consumption and generation must be coordinated, can already be carried out today using Schleswig-Holstein as an example. Schleswig-Holstein can thus already act as a blueprint for future renewable energy systems.

Model-based analyses play a central role in the analysis of such increasingly complex energy systems. In addition to purely technical modeling, open science approaches for the reproducibility of scientific results have become increasingly important in recent years. Therefore, models must address the diverse issues in the field of energy system analysis and, at the same time, meet high scientific standards in the sense of open science. To accompany the energy transition's progress and transfer it to the heating sector, an energy model is needed to map the complex interdependencies between the individual sectors. It makes sense to make the model and its databases freely accessible to enable scientists, political decision-makers, entrepreneurs, and citizens, alike, to use and further develop it.

Highly renewable-based energy systems at the subregional level are becoming popular in energy transition studies. Such studies include investigation of 100% renewable energy systems in Hvar (Croatia) [247], Samsø (Denmark) [248], the Åland Islands (Finland) [249], Orkney (Scotland) [248], the Canary Islands (Spain) [250], California (USA) [251], and New York State (USA) [252]. It is more common to analyze electricity systems than integrated energy systems.

Chapter 5 aims to apply the OSeEM model in the context of the Schleswig-Holstein system. The OSeEM-SN model, consisting of scripts and tabular database concepts, was developed to achieve the outlined requirements. The basic concept serves the general description of sector-coupled energy systems. It is based on a graph-theoretical approach, which provides a generic basis for different simulation and optimization models. This concept was implemented within the Oemof framework, using the optimization library Oemof Solph. Comprehensive similar applications using Oemof are *renpass* [134], *openMod.sh* [135], and *reegis^{hp}* [136]. However, their usability is limited. For instance, *renpass* is an electricity market model, *openMod.sh* focuses on one region, and *reegis^{hp}* evaluates district heating and CHP [120]. In contrast, the scope and upgradability of OSeEM-SN are broader and simpler. The model's openness allows other users to actively develop the tool and modification for specific purposes to answer research questions within a subregional framework. The tool is also useful for investigating island energy systems using only renewables. Therefore, the OSeEM-SN model is unique for analyzing power and heat sector-coupled energy systems at the regional level. With the gradual integration of more sectors and upgradation of the model, the tool can be useful for researchers and policymakers to answer energy transition-related questions using a straightforward approach. The development of the OSeEM-SN model confirms the findings by [120, Hilpert et al. 2018], i.e., the flexibility in a new tool development using Oemof allows adjustments and changing research objectives, avoiding lock-in effects.

For simplicity and Oemof Tabular model limitations, the study did not consider geothermal calculations. In the future, the geothermal heat for district heating in SH should be taken into consideration.

Chapter 6 will extend the OSeEM model to analyze the national energy system of Germany. The German sector-coupled model, OSeEM-DE, will be used to investigate capacity expansion and flexibility relevant research questions.

Chapter 6 Modeling of a National Energy System: Case Study of Germany

6.1 Background

The expansion of renewable energies in Germany will increase the need for grid expansion, particularly in local distribution grids for solar PV and onshore wind plants, and in transmission grids for offshore wind power. The current power system of Germany has many fossil fuel-based and nuclear-based power plants in Southern Germany. A gradual exit from fossil fuel and nuclear power will require shifting to renewables from offshore wind plants in Northern Germany. Therefore, there will be a need for transmission grid expansion from North to South at the same time. The transmission grid operators and the federal government of Germany have accelerated the development of Grids from Northern to Southern Germany, with 4,650 kilometers to be constructed by 2025 [253]. Figure 6.1 shows the status of grid expansion in Germany in which the expansion plan from north to south and other grids in the planning and development stages is illustrated [254].



Figure 6.1: Current status of electricity transmission network planning and development in Germany. The orange, red, and yellow lines show that many North-South grid extension projects are in the planning and development phase. Source: Federal Network Agency of Germany (Bundesnetzagentur) 2020 [254].

In the last two decades, both 'sector coupling' and '100% renewable energy systems' have been subjects of interest for energy researchers globally. Several pieces of research investigated 100% or near-100% renewable energy systems from national perspectives. Such investigations include energy system analysis of Australia, Barbados, Belgium, Brazil, Canada, China, Colombia, Costa Rica, Croatia, Denmark, Finland, France, Germany, Great Britain, Iceland, India and the SAARC region, Iran, Ireland, Italy, Japan, Macedonia, New Zealand, Nicaragua, Nigeria, Norway, Pakistan, Paraguay, Portugal, Saudi Arabia, Sevchelles, Tokelau, Turkey, Ukraine, the United Kingdom, the United States, and Uruguay [25,32,34,35,37-39,45,46,52,55,63,255-289]. Other than these national studies, there are many other 100% renewable system studies larger than national energy systems covering the World, North-East Asia, the ASEAN region, Europe and its neighbors, Europe, South-East Europe, and the Americas [44,61,288,290–305]. Similarly, there are also a number of regional-level studies on 100% system including Hvar (Croatia), Samsø (Denmark), the Åland Islands (Finland), Mecklenburg-Vorpommern (Germany), Schleswig-Holstein (Germany), Orkney (Scotland), the Canary Islands (Spain), California (USA), and New York State (USA) [247-252,306]. Most of these studies focus on 100% renewable-based electricity systems, and only a few consider energy transition pathways for reaching the target, including all relevant energy sectors [307]. Among the 100% renewable energy system studies that include all energy sectors, there are two main technologically and economically feasible concepts. The first concept is 'Smart Energy Systems,' which has been studied and analyzed in many research articles. The concept takes an integrated and holistic focus to include electricity, heating, cooling, industry, building, and transportation sectors and discusses the potential benefits of sectoral and infrastructure integration in the energy system. The second concept is 'wind-water-solar (WWS) for all purposes', which has been discussed in many research articles. The WWS concept presents roadmaps from local to global levels to electrify all energy sectors (i.e., transportation, heating, cooling, industry, agriculture, forestry, and fishing) using only wind, water, and solar power. The WWS roadmaps present the benefits of the energy transition in terms of energy access, mitigation of global warming and avoidance of air pollution deaths, creation of jobs, and costs such as energy, health, climate, and social costs.

In German energy system analyses, several studies focus on individual energy sectors such as the heating market, transportation, future electricity market. For achieving the energy transition towards climateneutrality, Schmid et al. identified and characterized actors who can put the energy transition into practice, but they focused on the power sector only [308]. In a similar publication, Lehmann and Nowakowski analyzed three scenarios for Germany's future electricity system [309]. Robinius et al. reviewed sector coupling scenarios for Germany linking electricity and transport sectors [66,67]. Gullberg et al. described how Norway and Germany's interconnection could ensure a low-carbon energy future [310]. Scholz et al. identified the bottlenecks of using only renewables for the energy transition [311]. Schroeder et al. compared different scenarios to investigate the need for grid expansions in Germany [312].

Although there are various models and analyses on the German energy transition towards climate neutrality, most of them focus either on specific aspects of an individual energy sector or the markets and actors linked with the energy system. A few studies outline a detailed techno-economic analysis using 100% renewables, including multiple energy sectors. Henning and Palzer showed that a 100% renewable energy system for power and heat is technically possible, and the overall annual cost for the system will be comparable to today's price [38,39]. However, their analysis assumes that heat requirement is reduced by 60% in the building sector in the future compared to today's demand, and their analyzing tool REMod-D is not an open-source model. In another recent publication, Hansen et al. concluded that the full energy system transition towards 100% renewables by 2050 in Germany is technically and economically possible, but resource potentials such as biomass is a big challenge for this transition [268]. Hansen et al. used EnergyPLAN for their analysis, a popular free-to-use simulation tool for modeling 100% systems for all energy sectors. However, it is not possible to analyze the capacity expansion mechanism and reach an

optimum solution using EnergyPLAN [313]. The literature review in Chapter 2 showed a clear research gap in applying cross-sectoral holistic approaches using comprehensive open modeling techniques for analyzing 100% renewable and sector-coupled energy systems in Germany and the other countries in the NS region. Therefore, based on the scope, the following research question is formulated for the German case study:

How feasible is it to transform towards a 100% renewable energy system for both power and building heat in Germany by 2050?

Answering the research question raises additional questions on the overall energy mix, investment cost and capacities, the issue of grid expansion within Germany, and different flexibility aspects of the system; which formulates the following sub-research questions:

- 1. In which capacities could such a system be implemented?
- 2. What are the estimated investment costs for the different system components?
- 3. What are the flexibility aspects of grid expansion, storage, and dispatchable loads in such a system?

Chapter 6's main objective is to apply the OSeEM-DE model to the German power-heat coupled energy system and investigate the above-mentioned research questions. The model analyzes different scenarios to investigate moderate to extreme conditions to determine the plausible energy mix and required investment in component-wise capacities and costs. The model considers dividing the German energy system into two subnational regions to analyze the grid expansion from Northern to Southern Germany. It also helps to understand the underlying energy flow mechanism and different energy components' roles from national and subnational perspectives. The heating sector analysis in this model is limited to the use of building heat, including space heating and domestic hot water demands. This study does not consider the industrial process heating demands. The industrial process heating is planned to be included in the upgraded version of the model.

6.2 The OSeEM-DE Model

OSeEM-DE follows a hybrid approach where the current technology capacities are exogenously defined, and the future investment capacities are endogenously determined. System boundaries, according to technology potentials, are set to avoid any unrealistic solution based on overestimation.



Figure 6.2: The German national energy system with two sub-national nodes, NDE (shown using blue color) and SDE (shown using green color). Map source: Wikimedia Commons [314].

As shown in Figure 6.2, the two German sub-national energy system nodes are Northern Germany (NDE) and Southern Germany (SDE). NDE consists of Schleswig-Holstein, Lower Saxony, Bremen, Hamburg, and Mecklenburg-Vorpommern, and SDE consists of the remaining eleven states of Germany. The power exchange between NDE and SDE is possible using the transshipment approach via NDE-SDE Link.

Figure 6.3 illustrates the Oemof-based OSeEM-DE energy system model. Two identical systems are connected using the NDE-SDE Link. The Offshore wind and ACAES components are only available in NDE. The transmission capacity between NDE and SDE is limited exogenously. The model follows the formulation described in Chapter 4.



Figure 6.3: Simplified block diagram of the OSeEM-DE model for Germany showing NDE and SDE nodes

6.3 Input Data

The model optimizes investment and operation for a full year of historical hourly data, with 2011 chosen as the primary representative year because of its average wind conditions, high solar irradiation (representing the expected warm condition in 2050 due to climate change), slightly lower overall heating demand, and duration of maximum heating demand during the winter days [68, Brown 2018, p.721].

6.3.1 Electricity and Heat Load

The hourly electricity load data based on the ENTSO-e statistical database are obtained from the OPSD project [237,238]. Hourly normalized time series are obtained from the electricity load data for both NDE and SDE energy systems based on population-based clustering. The total electricity demand for Germany in 2050, based on the representative year, is 532.77 TWh_{el}, of which NDE accounts for 96.6 TWh_{el}, and SDE accounts for 436.16 TWh_{el}.

The hourly heat load data based on the When2Heat project are obtained from the OPSD project [209,237,239]. Heat demand time series for space heat and hot water for Germany are obtained separately from the When2Heat profiles and are clustered and normalized for use as inputs of the model. The total heat demand for Germany in 2050, based on the representative year, is 648.53 TWh_{th}. Total space heating demand accounts for 533.6 TWh_{th}, of which NDE accounts for 96.75 TWh_{th}, and SDE accounts for 436.85 TWh_{th}. Total hot water demand accounts for 114.92 TWh_{th}, of which NDE accounts for 20.83 TWh_{th}, and SDE accounts for 94.08 TWh_{th}.

6.3.2 Volatile Generator

Normalized onshore wind profiles based on MERRA-2 datasets are obtained separately for NDE and SDE energy systems from the Renewables Ninja project [236]. Normalized offshore wind profiles based on MERRA-2 datasets are also obtained from the Renewables Ninja project [236]. Similarly, normalized solar PV profiles based on MERRA-2 datasets are obtained separately for NDE and SDE energy systems from the Renewables Ninja project [236]. Hydro inflow data for the ROR plants are obtained and normalized from the Dispa-SET project [114, Dispa-SET 2020]. The current capacity and potential data are obtained or calculated from the Deutsche WindGuard [242], Agency for Renewable Energies [243], LIMES-EU project [244], CSES (ZNES) [315], PyPSA [125,126,316,317], and ANGUS II Project databases [241]. Table 6.1 shows the capacity and available potential data for the volatile generators in 2050.

Energy System		Onshore Wind [GW _{el}]	Offshore Wind [GWel]	Solar PV [GW _{el}]	Hydro ROR [GW₀I]	
NDE	Capacity	22.12	6.66	7.56	0.09	
	Available Potential	49.88	76.94 ²²	55.77	0.06	
SDE	Capacity	31.79	-	37.66	4.2	
	Available Potential	118.81	-	188.07	1.1	
Germany	Total Capacity	53.91	6.66	45.23	4.29	
	Total Available Potential	168.69	76.94	243.84	1.16	

Table 6.1: Capacity and potential for volatile generators in the German energy system in 2050

The placement of volatile generators considers certain land limitations to account for competing land uses and minimum-distance regulations. For onshore wind, the maximum capacity density on the available area is 4 MW/km², as described in the LIMES-EU project [244]. The share of suitable areas available for RES is 30% and 5% for agricultural and forest areas, respectively. Public acceptance and nature reserves limit the share of the available onshore wind installation. For offshore wind, a maximum depth of 50 m is considered, and other factors such as 55 km maximum distance to shore, placement within the exclusive economic zone [244]²³. Besides, only 50% of the resultant area is considered with a maximum capacity density of 6 MW/km² to prevent turbine installations close to the mainland and allow a shipping corridor²⁴. For solar PV, the limitations include protecting nature reserves and restricted areas listed in the Natura2000 Database, and land use types according to the CORINE Land Cover Database, as described by Hörsch et al. [126]. The efficiency of the hydro ROR plant is 90% [241].

https://www.pik-potsdam.de/en/institute/departments/transformation-pathways/models/limes/DocumentationLIMESEU_2014.pdf).

²² The reference value of 77 GW_{el} offshore wind (Table 6.1) is adapted based on the ZNES database (ANGUS). (See ZNES Datapackages: <u>https://github.com/ZNES-datapackages/technology-potential/blob/master/data/renewable.csv</u>). The available potential was calculated by subtracting the existing capacity of 6.6 GW from the total potential of 83.6 GW.

²³ The reference value of 55 km maximum distance to shore is not a direct input to the OseEM model. The value is taken from the documentation of the LIMES-EU project, (See Nahmmacher et al. 2014:

The maximum distance to shore can be much higher as depicted by the Federal Maritime and Hydrographic Agency of Germany (BSH) Maps. For example, they mentioned in their site development plan that for the exclusive economic zone (EEZ) of the North Sea route lengths of more than 100 km are to be expected in the future. (Source: Site Development Plan 2020 for the German North Sea and Baltic Sea:

https://www.bsh.de/EN/TOPICS/Offshore/Sectoral_planning/Site_development_plan/_Anlagen/Downloads/FEP_2020/Site_Development_Plan_2020.pdf)

²⁴ The Federal Maritime and Hydrographic Agency of Germany (BSH) considers a higher value of power density in the range of 9-10 MW/km² Plan (See Site Development 2019 for the German North Sea and Baltic Sea: https://www.bsh.de/DE/PUBLIKATIONEN/_Anlagen/Downloads/Offshore/FEP/EN-Flaechenentwicklungsplan2019.pdf)

6.3.3 CHP and Heat Pump

The amount of available biomass is calculated from the Hotmaps project [240, Hotmaps Project, D2.3 WP2 Report – Open Data Set for the EU28 2018]. For a full year, the biomass potential for Germany is 634.33 PJ. For the current capacities, it is assumed that the existing biomass and biogas power plants are converted to CHP plants by 2050. Therefore, 4.74 GW CHP in NDE and 8.86 GW CHP in SDE energy systems are assumed to be installed and fully operational by 2050. It is also assumed that the CHP's electrical and thermal efficiencies are 45%, and the condensing efficiency is 50%. The current heat pump capacities are considered zero, and their investment potentials are not constrained²⁵. However, since heat pumps are P2H devices, their investment capacities depend upon limited available power from the potentially constrained volatile generators. The COP for ASHP and GSHP are 2.3 and 3.9, respectively [241, ANGUS II 2020¹²].

6.3.4 Storage

The capacity and maximum potential data for storage investments are described in Table 6.2.

Energy System		Li-ion [GWel]	Redox [GW _{el}]	H₂ [GWel]	ACAES [GWel]	PHS [GWel]	TES ¹⁶ [GWth]
NDE	Capacity	0	0	0	0.29	0.34	0
	Available Potential	2.82	0.17	1.82	3.43	-	1.8
SDE	Capacity	0	0	0	-	0.82	0
	Available Potential	12.83	0.76	8.28	-	-	8.2
Germany	Capacity	0	0	0	0.29	8.57	0
	Available Potential	15.65	0.93	10.1	3.43	-	10

Table 6.2: Capacity and maximum potential for storage investments

Data for Li-ion and Redox flow batteries, H₂ storages, and ACAES are obtained from the ANGUS II project scenarios for Germany in 2050 [241, ANGUS II 2020]. PHS data are obtained from the Dispa-SET project²⁶ [114, Dispa-SET 2020]. For batteries, H₂ storage, and TES, it is assumed that 18% of the total potential is available for NDE, and the rest is available for SDE. The energy storage potentials for the batteries, H₂ storage, and ACAES investment are subject to optimization. The storage potential for the existing ACAES plant in Huntorf is 0.58 GWh_{el} [318, IRENA 2017, p.58]. PHS's inflow data are derived from the Dispa-SET project's scaled inflow dataset and Germany's current PHS capacity [114, Dispa-SET 2020]. PHS's storage capacities are taken from the Dispa-SET project, which is 1.7 GWh_{el} for NDE, and 717 GWh_{el} for SDE [114, Dispa-SET 2020]. PHS investment is excluded because of the limited expansion capacity. For TES, the considered loss rate is 1.4% for TES [125,241]. The loss rate indicates the relative loss of the storage content per time unit. The roundtrip efficiencies and the maximum state of charge capacity in terms of hours at full output capacities are obtained from Table 5.4 (See Section 5.2.4).

²⁵ The green field scenario here is assumed for the sake of optimization only. In reality, more than 1.3 million heat pumps are in operation in Germany (See more at Statista 2022: <u>https://www.statista.com/statistics/740451/heat-pumps-in-operation-germany</u>)
²⁶ The detailed hydro datasets are available at: <u>https://github.com/energy-modelling-toolkit/Dispa-SET/tree/master/Database/HydroData</u>
6.3.5 Transmission Line

The transmission lines in between NDE and SDE energy systems (NDE-SDE Link) are modeled as transshipment capacities. The total transmission capacity is set and varied exogenously for different scenarios. According to the IEA data for Germany, a transmission and distribution line loss of 4% is considered [319].

6.3.6 Cost Data

The investment capacity costs are based on annuity and fixed operation and maintenance (O&M) costs, and the marginal costs are based on variable O&M costs, the carrier costs, and the efficiencies. The carbon costs are not considered in the marginal costs since the system is 100% renewable. The required data for calculating the costs, such as capital expenditure, lifetime, the Weighted Average Cost of Capital (WACC), storage capacity cost, carrier cost, fixed and variable O&M costs, are taken from ANGUS II Project [241]. The OSeEM-DE model uses the cost data from the OSeEM-SN Model, as described in Table 5.3.

6.4 Scenarios

Three scenarios, namely Base, Conservative, and Progressive, are developed and analyzed to answer the research questions in different conditions. The volatile generator inputs remain the same in all scenarios. The existing PHS and ACAES capacities also stay the same. The variation of the other parameters for different scenarios is shown in Table 6.3.

Scenario	Electricity Demand [TWh _{el}]	Total Heat Demand [TWhel]	Total Grid Capacity ²⁷ [GW₀l]	Biomass Potential [PJ]	Electricity Storage Potential [GW _{el}]	Heat Storage Potential ¹⁶ [GW _{th}]
Base	532.77	648.53	35	634.33	Li-ion: 15.65	7.5
					Redox: 0.93	
					ACAES: 1.71	
Conservative	586.04	648.53	32	697.76	Li-ion: 15.65	5
Progressive	479.49	583.68	38	570.89	Li-ion: 15.65	10
					Redox: 0.93	
					ACAES: 3.43	
					H ₂ : 10.1	

Table 6.3: Parametric variation for different scenarios

Regarding weather data and demands in 2050, the model considers 2011 as the representative weather year in the base scenario, according to [68, Brown 2018, p.721]. The model also investigates the change in future electricity and heat demands considering that the demand will go high if there is a higher population or low if due to increased use of efficient, innovative, and demand-responsive technologies.

²⁷ In reality, the two nodes of the OseEM model (NDE and SDE) are fictional. To assume the power transfer these two nodes, the grid loads 31 GW (Ampirion), 16 GW (50 hertz), TransnetBW (10 GW) and Tennet (25 GW) are referred (Electricity Grid Planning in Germany 2018: <u>https://www.renac.de/fileadmin/renac/media/Projects/Energy Dialogue/2018 June/02 BMWi Genz web.pdf</u>). Based on this information, the base capacity of the OseEM model is assumed at 35 GW, and it is varied in the conservative and progressive scenarios.

6.4.1 Base Scenario

The base scenario assumes that electricity and heating demands remain the same as the representative year (2011) in 2050. For storage, Li-ion batteries, PHS, and ACAES (NDE) are considered. The full biomass potential from forest residues, livestock effluents, and agricultural residues in Germany is used as CHP input. For the electrical storage, Li-ion and Redox batteries up to their maximum potential are used. Besides, half of the total ACAES potential is considered for investment.

6.4.2 Conservative Scenario

The conservative scenario assumes that the electricity demand will increase by 10% than the base scenario in 2050. The heating demand is kept the same. For the grid transmission from NDE to SDE, a reduced capacity is considered. An additional 10% of biomass import is considered on top of Germany's full potential. For storage, ACAES and Redox investment possibilities are omitted, and only Li-ion battery investment is considered.

6.4.3 Progressive Scenario

The progressive scenario assumes that both the electricity and heat demand will reduce by 10% than in the base scenario in 2050. For the grid transmission from NDE to SDE, increased maximum capacity is considered. The maximum usage of biomass is reduced by 10%. All electrical and heat storage are optimized for investment up to their full potentials.

6.5 Results

6.5.1 Sufficiency of the Energy System

The model runs reached feasible solutions for all three scenarios. Figure 6.4 shows examples of hourly energy supply-demand variation after cost-optimization in Germany's electricity and heat buses for the base scenario. Figure 6.4 (a) shows the electricity supply using the volatile generators, CHP, and electrical storages to satisfy the electricity demand in NDE during a week in June 2050. Figure 6.4 (b) shows the heat supply using heat pumps, CHP, and TES to satisfy the space heat and domestic hot water demands in SDE during a week in December 2050. Detailed scenario-wise and percentage-wise optimization results for NDE and SDE are available in Appendix E.





Figure 6.4: Exemplary optimization results of the OSeEM-DE model for the electricity and heat buses in the base scenario in 2050 (a) hourly supply-demand variation of the electric bus for a week in June 2050 in NDE (b) hourly supply-demand variation of the heat bus for a week in December 2050 in SDE

Table 6.4 summarizes the results for the three scenarios in terms of energy generation.

Scenario		Onshore Wind [TWh ₆]	Offshore Wind [TWh _{el}]	Solar PV [TWh _{el}]	CHP (Electricity) [TWh _{el}]	Hydro ROR [TWh _{el}]	GSHP [TWh _{th}]	ASHP [TWh _{th}]	CHP (Heat) [TWh _{th}]	NDE to SDE [TWh _{el}]	SDE to NDE [TWh _{el}]
Base	NDE	155.19	188.43	17.4	39.19	0.4	66.86	16.11	39.19	122.22	3.3
	SDE	197.98	-	269.38	61.71	14.56	460.7	13.47	61.1		
Conservative	NDE	155.19	257.98	67.97	43.11	0.4	65.04	18.5	43.11	143.16	0.04
	SDE	197.98	-	269.38	67.83	14.56	457.73	8.2	67.7		
Progressive	NDE	155.19	101.17	8.11	35.27	0.4	58.74	13.2	35.27	94.56	6.26
	SDE	197.98	-	250.22	55.92	14.56	409.28	22.53	51.6		

Table 6.4: Energy generation for different scenarios from the OSeEM-DE Model

Onshore wind and hydro ROR remain the same in all three scenarios. The change from the base scenario for the other generation technologies is summarized in Table 6.5.

Generation Technologies	Change from the Base Scenario [%]				
	Conservative Scenario	Progressive Scenario			
Onshore Wind	0%	0%			
Offshore Wind	+36%	-46%			
Solar PV	+17%	-10%			
CHP (Electricity)	+10%	-10%			
Hydro ROR	0%	0%			
Heat Pumps (GSHP, ASHP)	-1%	-10%			
CHP (Heat)	+10%	-13%			

Table 6.5: Change in energy generation with reference to the base scenario

Therefore, the model results show that Germany's renewable resources are sufficient to meet its electricity and building heat demands. The model suggests maximum usage of onshore wind and hydro ROR, and the rest of the demands are met using offshore wind, solar PV, CHP, and heat pumps. The decrease of 46% in the progressive scenario indicates that reducing electricity and heating demands can heavily affect Germany's offshore wind investment. An increase in electricity export from NDE to SDE is observed in the conservative scenario, indicating the matching of SDE demand using NDE's resources. The increase in biomass usage in the conservative scenario indicates the necessity of biomass import from other countries if the electricity demand is higher. The opposite situation can be observed in the progressive scenario when the electricity and heat demands are lower than the base scenario. Also, almost all the storages, except Hydrogen, are used to their maximum capacities in the progressive scenario. Two critical observations from the model run are:

- Without the biomass-based CHPs, there was no feasible solution for a power-building heat coupled system. That being the case, it is evident that Germany needs to use other alternative heating technologies besides heat pumps, combined with various heat storage options, to reduce its dependency on only biomass for meeting the heat demand.
- 2. While the model prefers ACAES and batteries, it does not choose Hydrogen for these three scenarios. The results may change for a system with industrial process heating demand and inexpensive Hydrogen.

6.5.2 Capacities and Investments

6.5.2.1 Volatile Generator

6.5.2.1.1 Volatile Generator Capacity and Investment

Figure 6.5 compares the existing capacities and required investments of the volatile generators. For onshore wind plants illustrated by Figure 6.5 (a), in addition to the existing 53.91 GW_{el}, investment in 168.69 GW_{el} is necessary for all three scenarios for Germany, of which 49.88 GW_{el} is in the NDE, and 118.81 GW_{el} is in the SDE energy system. Therefore, the model suggests maximum utilization of the available potential of all onshore wind energy in Germany. In the case of offshore wind plants shown by Figure 6.5 (b), on top of the existing 6.66 GW_{el}, the base scenario suggests installing 54.4 GW_{el}, the conservative scenario recommends installing 76.94 GW_{el} and the progressive scenario suggests installing 26.13 GW_{el} capacities.





Figure 6.5: Scenario-wise comparison of installed capacity and required investments for volatile generators in Germany (a) onshore wind (b) offshore wind (c) PV (d) hydro ROR plants

For solar PV, as shown in Fig. 6.5 (c), in addition to the existing 45.23 GW_{el} capacity, the base and conservative scenarios suggest installing 188.07 GW_{el} in the SDE energy system. Contrarily, the progressive scenario in SDE suggests a reduced solar PV installation of 172 GW_{el}. In Northern Germany, the model suggests installing 8.65 GW_{el} in the base scenario and 55.77 GW_{el} in the conservative scenario. Interestingly, the progressive scenario suggests that no additional solar PV installation is necessary for NDE. In the case of Hydro ROR plants shown in Fig. 6.5 (d), both the NDE and SDE systems suggest capacity increment to the maximum available potentials, i.e., 0.06 GW_{el} in NDE and 1.1 GW_{el} in SDE, on top of the existing 4.29 GW_{el} in Germany.

6.5.2.1.2 Volatile Generator Investment Cost

Figure 6.6 shows the investment costs of the volatile generators. Figure 6.6 (a) shows that the annual investment cost remains the same for onshore wind (9.84 bn \in /yr) and hydro ROR plants (0.19 bn \in /yr). The annual investment is 7.92 bn \in /yr for offshore wind, which increases in the conservative scenario (11.2 bn \in /yr) and decreases in the progressive scenario (3.8 bn \in /yr). For solar PV, the base scenario investment of 4.33 bn \in /yr goes high in the conservative scenario (5.37 bn \in /yr) and goes low in the progressive scenario (3.79 bn \in /yr). Figure 6.6 (b) compares the total investment cost for all volatile generators. The annual investment cost for all the volatile generators is 22.28 bn \in /yr, which increases by 19% in the conservative scenario (26.6 bn \in /yr) and decreases by 21% in the progressive scenario (17.62 bn \in /yr).





Figure 6.6: Scenario-wise comparison of investment costs for volatile generators in Germany (a) technology-wise comparison (b) total investment cost for all volatile generators. The primary vertical axis (left) shows the total investment cost for the whole time-horizon in billion euros (shown as stacked columns), and the secondary vertical axis (right) shows the annual investment cost in billion euros/year (shown in markers).

6.5.2.2 CHP and Heat Pump

6.5.2.2.1 CHP and Heat Pump Capacity and Investment

Figure 6.7 compares the existing capacities and required investments for the heat generators. For CHP shown by Figure 6.7 (a), in addition to the existing 13.6 GW, investment in 68.61 GW, 73.62 GW, and 58.26 GW, additional capacities are necessary for the base, conservative, and progressive scenarios, respectively. Figure 6.7 (b) shows a similar pattern for heat pumps (GSHP and ASHP) in Figure 6.7 (b), where the base scenario requires 173.41 GW_{th} investment, the conservative scenario requires an increased 181.86 GW_{th} investment, and the progressive scenario requires a decreased 154.93 GW_{th} investment in Germany.



Figure 6.7: Scenario-wise comparison of installed capacity and required investments for CHP and Heat Pump in Germany (a) CHP (b) Heat Pump (GSHP and ASHP)

Although the heat demand did not change in the conservative scenario, heat generator installations increases because of the following reasons:

- 1. Since volatile generators are already installed up to their maximum potential, increased CHP installations are required to meet the additional electricity demand.
- Reduced grid transfer capacity minimizes the power exchange scope between the grids and hence lessens the scope of P2H conversion with power from the other energy system. This circumstance enforces the model to install additional local heat pumps in individual energy systems.
- Heat generation in this energy system depends on both electrical (because of P2H) and heat storage. Since electrical and heat storages are reduced in the conservative scenario, supplydemand balancing requires additional heat generators.

This additional heat generator in the conservative scenario also results in surplus heat in both energy systems at different hours over the year. Nevertheless, this additional heat investment problem is minimized in the progressive scenario where we have reduced electricity and heat demands, increased grid transfer capacity, and increased electrical and heat storage.

6.5.2.2.2 CHP and Heat Pump Investment Cost

Figure 6.8 shows the technology-wise investment costs of the CHPs and heat pumps for NDE and SDE and the total costs. As shown in Figure 6.8 (a), the annual investment cost for CHPs in the base scenario is 8.71 bn \notin /yr, which increases to 9.34 bn \notin /yr in the conservative and decreases to 7.39 bn \notin /yr in the progressive scenario. Similarly, for heat pumps, the base scenario investment of 18.47 bn \notin /yr increases to 19.44 bn \notin /yr in the conservative scenario and decreases to 16.28 bn \notin /yr in the progressive scenario.





Figure 6.8: Scenario-wise comparison of investment costs for CHP and heat pump in Germany (a) technology-wise comparison (b) total investment cost for all heat generators (CHPs & heat pumps)

Figure 6.8 (b) compares the total investment cost for all CHPs and heat pumps. The annual investment cost for all the heat generators is 27.18 bn \in /yr, which increases by 5% in the conservative scenario (28.78 bn \in /yr), and decreases by 13% in the progressive scenario (23.67 bn \in /yr).

6.5.2.3 Storage

6.5.2.3.1 Storage Capacity and Investment

Figure 6.9 compares the investment for all types of storage. The model does not suggest any investment in H₂ storage because of the high cost. Figure 6.9 (a) and Figure 6.9 (b) show the required investment capacities of Li-ion and Redox batteries. Both batteries are used up to their maximum given potential whenever used as an input. According to Figure 6.9 (a), for a total of 15.65 GW_{el} Li-ion batteries, the total optimized energy capacity is 102 GWh_{el} (NDE=18.32 GWh_{el}, SDE=83.42 GWh_{el}). As shown in Figure 6.9 (b), for 0.93 GW_{el} Redox batteries in Germany, the total optimized energy capacity is 3 GWh_{el} (NDE= 0.56 GWh_{el}, SDE=2.52 GWh_{el}).







(d) Figure 6.9: Scenario-wise comparison of required power and energy storage investments for electrical and heat storages in Germany (a) Li-ion (b) Redox (c) ACAES (d) TES. The primary vertical axis (left) shows the power capacity in GW_{el}/GW_{th} (shown as stacked columns), and the secondary vertical axis (right) shows the energy storage capacity GW_{hel}/GW_{ht} (shown in markers).

However, the ACAES are used partially with an optimized power of 0.15 GW_{el} and optimized energy storage of 2.5 GWh_{el} in the base scenario, and an increased optimized capacity of 0.51 GW_{el} and optimized energy storage of 5 GWh_{el} in the progressive scenario, as shown in Figure 6.9 (c). Figure 6.9 (d) shows the usage of TES capacities up to their maximum exogenous potential, with the total optimized energy storage capacity varying in between 360 GWh_{th} (conservative) and 720 GWh_{th} (progressive).

6.5.2.3.2 Storage Investment Cost

Figure 6.10 shows the investment costs of the electrical and heat storage and the total costs. As shown in Figure 6.10 (a), Li-ion batteries' annual investment cost is 1.57 bn \notin /yr. For Redox batteries, the base scenario's annual investment cost and the progressive scenario are 0.05 bn \notin /yr. In the case of ACAES, the annual investment cost is 0.01 bn \notin /yr in the base scenario and 0.03 bn \notin /yr in the progressive scenario. The annual investment cost of heat storage depends mainly upon the volume of the storage capacity, which is 1.66 bn \notin /yr in the base scenario for 540 GWhth. As the storage capacity goes down to 360 GWhth in the conservative scenario, the yearly investment reduces to 1.1 bn \notin /yr. In the progressive scenario, the annual investment again increases to 2.21 bn \notin /yr since the total storage capacity increases to 720 GWhth.

Figure 6.10 (b) shows the total investment costs for all storages. The annual investment for all storages is 3.29 bn \notin /yr in the base scenario, which decreases by 18% to 2.67 bn \notin /yr in the conservative scenario with reduced storage provisions and increases by 17% to 3.86 bn \notin /yr in the progressive scenario with high storage provisions.





Figure 6.10: Scenario-wise comparison of investment costs for electrical and heat storages in Germany (a) technology-wise comparison (b) total investment cost for all storages

6.5.3 Energy Mix and Flexibility Aspects

6.5.3.1 Energy Mix

Figure 6.11 compares the energy mix results. Figure 6.11 (a) shows the composition of the electricity generation mix. The total electricity generation in the base scenario is 944 TWhel, increasing to 1074 TWhel in the conservative scenario with excess demand, less storage, reduced grid capacity; and decreased to 818 TWhel in the progressive scenario with reduced demand, more storage, and increased grid capacity. The energy mix also shows that, while all three scenarios need maximum offshore wind and hydro ROR, additional solar PV, offshore wind, and CHP can supply the rest of the demand. The base scenario mix comprises 37% onshore wind, 19% offshore wind, 30% solar PV, 10% CHP, and 0.01% hydro ROR plants. The progressive scenario shows similar results: 43% onshore wind, 12% offshore wind, 31% solar PV, 11% CHP, and 0.01% hydro ROR. These results are compared and cross-validated with a study from Fraunhofer Institute for Solar Energy System (ISE) [320, Henning and Palzer 2015, p.54], which showed that an 85% renewable-based system in Germany producing 800 TWhel electricity comprises 47% onshore wind, 16% offshore wind, and 22% solar PV. According to the OSeEM-DE results, CHPs can replace the remaining 15% fossil-fuel-based generation using Germany's available biomass potential. Such a system also needs high electrification of the heating sector. Figure 6.11 (b) shows that with less demand, more heat storage capacity, and more grid transfer capacity, the progressive scenario yields a reduced heat generation of 590 TWh_{th}.



Figure 6.11: Scenario-wise comparison for energy generation (a) electricity generation (b) heat generation

The heat generation results also show that heat pumps dominate the heat generation (around 80%), and biomass-CHPs cover the rest of the demand. In heat pumps, the comparatively more efficient but expensive GSHPs are preferable over less efficient and cheaper ASHPs. Though the model considers only CHPs and heat pumps, other renewable applications such as electric boiler, solar heating, biofuel heating, Hydrogen heating, and geothermal heating should be investigated to produce heat, primarily process heating in industries.

Excess generation from renewables is a challenge that needs to be solved using a combination of plausible solutions. The OSeEM-DE results show that the least amount of excess generation occurs in the progressive scenario, indicating the apparent solution of using more storage. Also, the developed model is currently an island model with no interconnection between neighboring countries. A German energy system and its neighboring countries can reduce the curtailment problem with reduced optimized generation and storage capacities. Furthermore, demand response activities and the transport sector's inclusion with electric vehicles are also needed to reduce the curtailment or utilize the excess generation. The Levelized Cost of Electricity (LCOE) is calculated from the optimization results according to Equation (4.23) (See Section 4.2.9). The LCOE values from the OSeEM-DE model are compared to a study from Fraunhofer ISE, which illustrates the 2018 LCOE values, and the learning curve-based predicted LCOE values (2035) in Germany [321, Kost et al. 2018, p.14]. We can see from Table 6.6 that the LCOE results from the OSeEM-DE model for onshore and offshore wind and solar PV technologies are very close to the lower range of LCOE values in 2035 as forecasted in the Fraunhofer ISE study. While the Fraunhofer ISE study considers biogas for electricity generation, the OSeEM-DE considers biomass for electricity and heat generation, resulting in higher LCOE values.

Tashnalagu	Levelized Cost of Electricity [€ cent/kWh]						
rechnology	Fraunhofer ISE	Fraunhofer ISE Study (2035) [321]	OSeEM-DE Model (2050)				
	[321]		Base	Conservative	Progressive		
Onshore Wind	3.99 - 8.23	3.49 - 7.09	4.99	4.99	4.99		
Offshore Wind	7.49 – 13.79	5.67 - 10.07	6.79	6.93	6.34		
Solar PV	3.71 – 11.54	2.41 - 4.70	3.61	3.73	3.56		
Biogas/Biomass	10.14 - 14.74	10.14 - 14.74	20.26	19.76	19.47		

Table 6.6: LCOE comparison of Fraunhofer ISE study [321, Kost et al. 2018, p.14] and OSeEM-DE model results

The total LCOE for the OSeEM-DE model ranges between 6.34 – 7.92 € cent/kWh.

6.5.3.2 Flexibility Aspects

6.5.3.2.1 Grid Expansion

This study's primary assumption is the growth of grid connection in 2050, resulting in a significant increase of power exchange between northern and southern Germany. The results suggest a large amount of grid exchange from NDE to SDE. For example, 28% of the SDE electrical demand comes from NDE (122.22 TWh_{el} vs. 436.16 TWh_{el}) in the base scenario. Similarly, in the conservative scenario, around 29% of the SDE electrical demand comes from NDE (143.17 TWh_{el} vs. 479.78 TWh_{el}), and in the progressive scenario, around 24% of the SDE demand comes from NDE (94.57 TWh_{el} vs. 392.55 TWh_{el}). A sensitivity analysis is conducted to inspect the effect of grid expansion. For this analysis, the base scenario is modified where all

the storage capacities are optimized to their maximum potentials, and the grid capacity varies between 25 GW_{el} and 40 GW_{el} .

Figure 6.12 (a) shows that with the grid expansion from 25 GW_{el} to 40 GW_{el}, the offshore wind investment reduces by 15% from 59.75 GW_{el} to 50.68 GW_{el}. Solar PV investment reduces by 22% from 241.22 GW_{el} to 188.07 GW_{el}. The onshore wind and hydro ROR investments remain the same. Heat pump investment decreases by 5% (171.37 GW_{th} vs. 171.21 GW_{th}). While grid expansion decreases offshore wind plant capacities, relatively less expensive biomass-based CHPs replace a share of the curtailed offshore generation. Therefore, CHP installation increases by 2% (66.97 GW vs. 68.30 GW) with the grid expansion from 25 GW_{el} to 40 GW_{el}. Figure 6.12 (b) shows the increase in the total electricity transfer between NDE and SDE for increasing grid capacities. For the grid expansion from 25 GW_{el} to 40 GW_{el}, an increase of 2.5% (119.64 TWh_{el} vs. 122.72 TWh_{el}) from NDE to SDE is observed. On the other hand, from SDE to NDE, though the transfer amount is much less compared with NDE to SDE, a sharp increment rate can be observed (0.21 TWh_{el} vs. 6 TWh_{el}) when grid capacity expands.







(b)

Figure 6.12: Effect of grid capacity expansion between Northern and Southern Germany (a) investment in electricity and heat generators. The varying values of offshore wind, solar PV, CHP, and heat pumps are shown using lines, and the steady onshore wind and hydro ROR capacities are shown using columns (b) total annual electrical energy transfer between NDE and SDE. Two different vertical axes are used for showing the exchange, the primary vertical one (left) for NDE to SDE, and the secondary vertical one (right) for SDE to NDE.

The results for power and energy capacities for all the storage remained constant for all grid capacities, which indicated the maximum usage of the exogenously provided potentials. Therefore, the impact on the storage capacity for the grid expansion could not be measured using this sensitivity analysis. However, the grid expansion facilitates a smoother balance between the two systems, resulting in increased electricity exchange, thus requiring less investment in offshore wind, solar PV, and heat pump installations. Therefore, the expansion of the electrical grid between Northern and Southern Germany should be considered as a promising option for supporting a 100% renewable-based sector-coupled system for Germany. However, the cost of grid expansion vs. investment in generation facilities, which has not been conducted in this research, must be investigated to reach an optimum solution and draw a conclusion.

6.5.3.2.2 Storage and Dispatchable Load

Electrical storages and dispatchable loads (i.e., heat pumps) with heat storage tend towards flexibility and interdependence in all the scenarios. The existing hydro ROR plants and PHS help the system to balance both the short-term and long-term. Also, the biomass-fed CHPs are used as dispatchable generation resources that serve as a backup to counter the volatile generation's variability from solar PV and wind. Both Li-ion and Redox batteries act as critical storage technologies to be utilized for shorter periods. On the other hand, ACAES shows promising prospects to aid the PHS. The large-scale investment of heat pumps confirm the findings of Hedegaard and Münster, i.e., the individual heat pumps can have a positive contribution towards large scale wind power investments to reduce the system cost and pressure on the limited biomass potential [322]. The dispatchable heat pumps can use surplus power from the variable renewable generation, which supplements other heat generation sources and offers flexible operations. A sensitivity analysis is conducted to inspect the effect of storage expansion. For this analysis, the grid capacity is fixed at 20 GW_{el}, and the batteries (Li-ion and Redox), H₂ storage, and TES are gradually doubled from their current maximum exogenous potential. The ACAES and PHS capacities are not expanded since spatial constraints limit their maximum potentials.





Figure 6.13: Effect of storage expansion from current capacity (0%) to double capacity (100%) (a) investment in electricity and heat generators. The varying values of offshore wind, CHP and heat pumps are shown using lines, and the steady onshore wind, solar PV and hydro ROR capacities are shown using columns (b) total annual electrical energy transfer between NDE and SDE.

As shown in Figure 6.13 (a), the onshore wind, solar PV, and hydro ROR capacities do not change with the increase in storage capacities, but the offshore investment drops by 47% (55.53 GW_{el} vs. 29.1 GW_{el}) when the storages are doubled. Similarly, both CHP and heat pump investment decreased by 13% (62.5 GW vs. 54.32 GW) and 6% (189.87 GW_{th} vs. 177.39 GW_{th}), respectively. Hence, increased storage options offer additional flexibility to curtail peak/reserve capacities for the energy system.

On the other hand, electricity exchange decreases from NDE to SDE by more than 9% (113.88 GW_{el} vs. 102.77 GW_{el}) when the storage capacity is doubled, as shown in Figure 6.13 (b). Contrarily, the electricity transmission from SDE to NDE is almost a straight line, with a much lower value. The decrease of investment in offshore wind, CHP, and heat pumps and the reduced energy transfer from NDE to SDE indicate that storage expansion in local energy systems can be another viable flexibility option for reducing investment in generation capacities and grid expansion.

Considering the limited reserve capacity of cobalt, expanding the battery capacities is a matter of further investigation [232, Hilpert 2020, p.13]. The sensitivity analysis for storage expansion also reveals the usage of H₂ storages in three instances (0%, 20%, and 40%) when the grid capacity was comparatively low (20 GW_{el}), and the other storage options were not sufficient. This result indicates the possibility of H₂ storage as another plausible alternative, especially for local energy systems, when other resources for batteries are not adequate and when the grid expansion is limited. In addition to H₂ storage, Norwegian large hydro capacities are another promising storage option for the future German energy system. This requires additional investment in interconnection capacities between Norway and Germany and is subject to policy discussions.

6.6 Summary

The analysis shows that a 100% renewable energy system for both power and building heat sectors are feasible for moderate to extreme scenario considerations. For onshore wind and hydro ROR investments, maximum potentials should be utilized to meet the demand. In contrast, in the case of PV and offshore wind turbines, the investment capacities depend upon variation in electricity and heat demand, transmission grid expansion, available biomass potential, and storage provisions. The energy mix of such a system is composed of all the possible volatile generator resources, biomass resources, and the already existing renewable capacities. The model chooses PHS, ACAES, and batteries over relatively expensive H_2 . The results may be different when the industrial heating sector is coupled, and large-scale electrolyzers produce H_2 .

In volatile generator investments, the scenario analysis shows that a fixed investment of 168.69 GWel onshore wind and 1.16 GWel hydro ROR plants are necessary, along with varying investments of 26.13 – 76.94 GW_{el} offshore wind and 172 – 243.84 GW_{el} solar PV capacities for the three developed scenarios. Onshore wind plants require an annual investment of 9.84 bn \notin /yr, and hydro ROR plants require a yearly investment of 0.19 bn \notin /yr. Offshore wind and solar PV requires varying investments in different scenarios, 3.8 – 11.2 bn \notin /yr for offshore wind and 3.79 – 5.37 bn \notin /yr for solar PV. The total cost for the volatile generators in Germany varies between 17.62 bn \notin /yr and 26.6 bn \notin /yr, which sums up to 312 – 450 bn \notin over the lifetime.

Heat generator capacities vary for CHPs between 58.26 GW_{th} and 73.62 GW_{th}, while the heat pump acts as a more preferred alternative heating option for buildings, requiring 154.93 – 181.86 GW_{th} installations for Germany. The cost varies accordingly, for CHPs in between 7.39 bn €/yr and 9.34 bn €/yr, and the heat pumps in between 16.28 bn €/yr and 19.44 bn €/yr. Therefore, the total cost for the heat generators in Germany varies between 23.67 bn €/yr and 28.78 bn €/yr, which sums up to 316 – 385 bn € over the lifetime.

For storages, while partial investment is suggested for ACAES varying from 0.15 GW_{el} to 0.51 GW_{el}, batteries are preferred over hydrogen storages for all three scenarios. Existing PHS and ACAES capacities are used throughout the year, and the TES are utilized to their maximum exogenous capacities. The total cost of power and storage shows that maximum investment is required for Li-ion batteries (1.57 bn €/yr) and TES storage capacities (1.1 – 2.21 bn €/yr). With minimum storage provision in the conservative scenario and maximum storage provision in the progressive scenario, the total cost for electrical and heat storages in Germany varies between 2.67 bn €/yr (conservative) and 3.86 bn €/yr (progressive), which sums up to around 33 – 48 bn € over the full lifetime.

The energy mix comparison with Fraunhofer ISE's studies suggests that a transformation towards 100%system according to the OSeEM-DE model results is feasible by 2050, where the energy mix consists of onshore wind, solar PV, offshore wind, CHP, and hydro ROR plants. The biomass-CHP is a promising option to replace the 15% fossil-fuel-based generation of the 85% system of Fraunhofer ISE's study, and the optimized results from the OSeEM-DE model shows that the German potential is sufficient to meet this requirement. The LCOE values have been compared with another Fraunhofer ISE study, which cross-validates the model results. The LCOE for onshore wind is $4.99 \in \text{cent/kWh}$, offshore wind ranges between $6.34 - 6.93 \in \text{cent/kWh}$, solar PV ranges between $3.56 - 3.73 \in \text{cent/kWh}$, and Biomass ranges between $19.47 - 20.26 \in \text{cent/kWh}$. The total LCOE for the OSeEM-DE model ranges between $6.34 - 7.92 \in \text{cent/kWh}$.

The flexibility of the system was examined via sensitivity analysis of the grid and storage capacities. It is observed that with grid expansion, the cost of offshore wind, solar PV, and heat pump decreases, but the CHP investment increases slightly. On the other hand, with the gradual expansion of storage, offshore wind, CHP, heat pump investment, and energy transfer from NDE to SDE decreases. Therefore, maximum utilization of the storage usage and optimum grid expansion can provide additional flexibility to the system and decrease the overall investment cost. The cost of grid expansion vs. investment in generation and storage facilities must be investigated to reach the optimum solution. The limited capacity of battery materials should also be taken into consideration. A possible alternative storage solution is Norwegian hydro storages with the interconnection between Norway and Germany, subject to further investigation.

Chapter 7 Conclusion

7.1 Summary of the Main Findings

Sector coupling is one of the emerging topics in recent energy and climate change policy discussions. It can play a significant role in creating the pathway of a renewable-based energy system in the European energy sector. The NSR is likely to play a critical role in transitioning to a sustainable energy system. Although different energy modeling approaches allow a versatile use, they lead to an unclear understanding of specific aspects of sector coupling and the relevance of existing tools and techniques to model and analyze such a system. The study presents a clear perception of the concept of sector coupling. The review concludes that sector coupling can be advantageous from the viewpoints of decarbonization, flexibility, network optimization, and system efficiency. To solve the coupling barriers, diversified techno-socio-economic circumstances should be taken into account through the use of model collaboration. The study demonstrates how a list of appropriate tools for model collaboration can be picked up methodologically from an available wide range of models. The study uses Oemof as an advanced tool to design a sector-coupled and renewable-based energy system in the NSR.

Most of the P2H and TES technologies are mature and already impact the European energy transition. However, detailed models of these technologies are usually very complex, making it challenging to implement them in large-scale energy models, where simplicity, e.g., linearity and appropriate accuracy, are desirable due to computational limitations. Previous studies have not clearly identified and characterized the main P2H and TES technologies across all sectors. Their potential roles have not been fully discussed from the European perspective, and their mathematical modeling equations have not been presented in a compiled form. The study contributes to the research gap in three main parts. First, it identifies and classifies the major P2H and TES technologies that are climate-neutral, efficient, and technologically matured to supplement or substitute the current fossil fuel-based heating. The second part presents the technology readiness levels of the identified technologies and discusses their potential role in a sustainable European energy system. The third part presents the mathematical modeling equations for the technologies in large-scale optimization energy models. The study identifies electric heat pumps, electric boilers, electric resistance heaters, and hybrid heating systems as the most promising P2H options. Then the study groups the most promising TES technologies under four major categories. Low-temperature electric heat pumps, electric boilers, electric resistance heaters, and sensible and latent heat storages show high technology readiness levels to facilitate a large share of the heat demand. Finally, the mathematical formulations capture the main effects of the identified technologies. However, the modeling of TES is very generic, and more appropriate for hot water storage without stratification effects. The equations should only be used for large-scale optimization models.

The study developed a unique hourly optimization tool using a hybrid approach. The Open Sector-coupled Energy Model (OSeEM) is created using Oemof. Different elements of the OSeEM model includes onshore and offshore wind, solar PV, hydro ROR, CHP, ASHP, GSHP, PHS, Li-ion battery, Redox battery, H₂ storage, ACAES, and TES using hot water tanks. Mathematical equations for the elements and the objective function of the model are described.

The model validation is performed using two case studies. First, the model OSeEM-SN is validated using the case study of Schleswig-Holstein. OSeEM-SN reaches feasible solutions without additional offshore wind investment, indicating that it can be reserved for supplying other states' energy demand. The annual investment cost varies between 1.02 and 1.44 bn €/year for the three scenarios. The electricity generation decreases by 17%, indicating that, with high biomass-based combined heat and power plants, the curtailment from other renewable plants can be decreased. GSHPs dominate the heat mix; however, their

installation decreases by 28% as the biomass penetrates fully into the energy mix. The validation confirms OSeEM-SN as a beneficial tool to examine different scenarios for subnational energy systems.

Then the model OSeEM-DE is validated using the case study of Germany. As one of the EU's leading industrialized countries, Germany has adopted several climate-action plans for the realistic implementation and maximum utilization of renewable energies in its energy system. The model results show that a 100% renewable-based and sector-coupled system for electricity and building heat is feasible in Germany. The investment capacities and component costs depend on the parametric variations of the developed scenarios. The annual investment costs vary between 17.6 - 26.6 bn \notin /yr for volatile generators and between 23.7 - 28.8 bn \notin /yr for heat generators. The model suggests an investment of a minimum of 2.7 - 3.9 bn \notin /yr for electricity and heat storage. Comparison of OSeEM-DE results with recent studies validates the percentage-wise energy mix composition and the calculated LCOE values from the model. Sensitivity analyses indicate that storage and grid expansion maximize the system's flexibility and decrease the investment cost.

7.2 Research Limitations

This study's modeling approach has five main aspects that could alter the results:

- 1. Detailed transmission modeling and consideration of transmission costs;
- 2. Inclusion of industrial heating demand;
- 3. Inclusion of other renewable and heating technologies;
- 4. Inclusion of other storage options; and
- 5. Interconnection with neighboring countries.

Regarding the transmission modeling, the transmission lines between two nodes (e.g., Northern and Southern Germany) were modeled as transshipment capacities between two nodes. The internal transmission constraints are not considered, and the grid expansion's investment costs are not calculated. Therefore, the benefits of grid expansion in a sector coupled network in terms of net system cost, including the cost of transmission, could not be determined. Schlachtberger et al. showed that there could be a 'compromise grid' in-between 'today's grid' and the 'optimal grid', in a highly renewable European electricity network [317]. While optimal grid expansion can be infeasible due to social acceptance issues, the compromise grid offers the maximum benefit at an adequate amount of transmission. A similar scenario is expected in the German electricity system, which should be investigated with detailed transmission grid modeling and consider facts such as meshed networks and power handling capabilities [323].

Second, the heating sector does not include industrial heating demand (i.e., process heat). There are two main reasons: (1) model complexity of high-temperature heating applications, and (2) the availability of hourly industrial heating time series data. The industrial heating demand can be satisfied using several renewable-based approaches, including P2H technologies such as high-temperature heat pumps and electrode boilers, green Hydrogen for cement, iron, and steel production [324], and biogas-based heating. An alternative solution should be figured out in the next phase of the research to translate aggregated industrial heating demand data to hourly time series data. With the inclusion of industrial process heating demand, the feasibility of a 100% power-heat coupled system for Germany needs to be re-investigated. In future research, it is recommended to analyze the industrial heat data, which can be translated from aggregated to hourly time series, as most high temperature heat processes run continuously.

Third, the current model only considers solar PV, wind, hydro, and biomass and does not include other options such as plants. The heating is therefore highly dependent upon the use of biomass, which is limited

in potential. A model run without biomass resources as heating, using only electricity-based heat pumps, resulted in an infeasible optimization solution. The inclusion of geothermal plants and other heating technologies such as electric and electrode boilers and green Hydrogen-based heating may reduce the need for biomass-based CHPs, which should be investigated in future research works.

Fourth, only hot water-based TES was considered as a heat storage option in the model. Other storage options, such as long-term (seasonal) underground TES in boreholes or water pits, were not considered in the model. The main reason for excluding these options is the complex modeling characteristics of these types of storage. The model also simplifies the hot water storage based on simplified assumptions, such as the water inside the tank is thoroughly mixed and has a uniform temperature. Such a simplified model can offer simple and computationally feasible solutions for aggregated power systems. Nevertheless, in the case of a comprehensive analysis of energy systems, it is essential to include all the possible heat storage options with detailed modeling.

Finally, the import and export of electricity between countries, an essential part of the combined energy transition towards the EU's climate-neutrality, were not considered in the model. The inclusion of electricity trade with neighboring countries will affect the calculated investment capacities and costs. The gradual inclusion of all the EU countries is currently considered a future development step of the model.

In addition, inclusion of transport demand into the sector-coupled model will alter the results. The model results will also alter if it considers different factors such as higher work/energy ratio of electricity over combustion, elimination of upstream emissions, and policy-driven increases in end-use energy efficiency, as described by Jacobson et al. [296]. The least-cost options for a 100% renewable energy system are not limited to the current OSeEM model components. While this study shows one of the possible pathways for achieving decarbonization in power and building heat sectors, the result will differ when other energy sectors are coupled. There can be a different set of solutions with cheaper Hydrogen or a system with vehicle-to-grid (V2G) and demand-side management (DSM). The benefits of highly renewable and sectorcoupled systems can only be realized with a combination of different solutions. For example, the concept of 'Smart Energy Systems' includes solid, gas, and liquid fuel storage, heat pumps with TES, battery electric vehicles, smart thermal grids (district heating and cooling), ICT-based smart electricity grids, smart gas grids, and other fuel infrastructures. The concept of 'WWS' includes wave, tidal, geothermal, and CSP plants with the other renewable options for providing 100% energy. Besides, 'WWS' studies also focus on issues such as social costs and job creation. The PyPSA based studies focus on the benefits of sectorcoupling and transmission expansion in a highly interconnected and renewable-based European network. The author refers to all the relevant '100% system' and 'Sector Coupling' studies since there is not a single pathway for the energy transition, but many possible pathways, with different advantages and disadvantages. The OSeEM model should be seen as a tool, which can be adjusted for different scale energy systems for the EU to investigate different energy-related research questions.

The author wants to clarify that the mentioned limitations do not affect the current model's architecture. Only the results will alter with the inclusion of new technologies (e.g., transmission line, geothermal, electrode boiler, H₂-heating), new costs (e.g., transmission expansion cost), new demand data (e.g., industrial heating, transport), and interconnections (e.g., between Germany and Norway). The methodology, including mathematical formulations, and the development of the architecture, will not change in further development. Nevertheless, the model upgrade plans will allow the user to investigate more scenarios. For example, considering the inclusion of detailed transmission line modeling, the second version of the model will enable a user to investigate the case of grid expansion against sector-coupling, and the results will be different from this study. However, the previous architecture remains the same, and

the only change, in this case, will be the addition of transmission model components and respective system costs to the first version of the model.

7.3 Research Contributions

OSeEM is a comprehensive energy system *model* constructed using the toolbox from the *framework* Oemof, which includes the *model generator* Oemof Solph. The *models* represent the real-world energy systems with a specific regional focus and temporal resolution concretely and may consist of linked submodels to answer straightforward research questions. *Model generators* employ specific analytical and mathematical approaches by using predefined sets of equations. A *framework* is a structured toolbox that includes sub-frameworks, model generators, and specific models. Besides, an *application* can be developed using one or more *framework* libraries depending on scope and purpose. The Oemof libraries can be used to build different energy system models, which can be referred to as *applications*. The model is novel and unique for the following responses-

- 1. A unique feature of the OSeEM model is that it allows a user to modify the model at two different levels. At the basic level, the user can use the model with simple tabular data and scripts. Therefore, the basic level user can visualize the scenario beforehand, prepare the scenario by changing input data in *.csv* data files to develop the scenarios, use the given Python scripts and modify them to reflect his developed scenario. On the other hand, the advanced level users can access the underlying structures, including the *model generator* Oemof Solph and the *class* Oemof Tabular *Facades* to enhance the analytical and mathematical formulations. The unique feature allows energy system analysis ranging from aggregated analysis (e.g., basic level analysis with low resolution) to comprehensive analysis (e.g., advanced level analysis of energy systems with high resolution).
- 2. The model follows a hybrid approach where the users can define current capacities exogenously, and the future investments are determined endogenously, with a limit of the maximum potential of different technologies. The unique feature allows to create different scenarios ranging from brownfield to greenfield approaches and evaluate a more holistic view of the energy system investments.
- 3. The use of heat pumps with storage as dispatchable loads is another unique feature of the model. OSeEM uses heat pump technologies (ASHP and GSHP) combined with hot water-based heat storage (TES), which allows flexible operation of heat pumps in 100% renewable energy systems and reduces the need for electricity storage units.
- 4. While a previous model (REMod-D) [38,39] represented 60% of the building heat demand, OSeEM presents 100% of the demand to decarbonize the building heat sector of Germany fully. Besides, OSeEM is an open-source model in contrast to other models doing similar investigations.
- 5. The model offers extended storage provisions. The model considers Redox, H₂, and ACAES as storage options in addition to traditional Li-ion and PHS options. The use of ACAES is unique because it is not very common to include the technology in energy models. The availability of salt caverns in Northern Germany allows a considerable potential for decentralized renewable energy storage, which is considered an essential input of the OSeEM model.
- 6. The model considers biomass potential from forest residues, livestock effluents, and agricultural residues to use them as CHP fuels. In contrast to energy models, which rely heavily on P2H for heat decarbonization, the OSeEM model uses biomass-CHPs with realistic biomass availability data from the *Hotmaps* project [240, Hotmaps Project, D2.3 WP2 Report Open Data Set for the EU28 2018]. Using a combination of P2H and traditional CHPs based on renewable resources is unique and new and paves the pathway for similar future analysis.

One of the objectives for developing the model is to use simple scripts and tabular data sources to construct complex energy systems. While the internal architecture of Oemof Solph is comparatively complex and intended for the expert developers, the OSeEM model is intended for the users who can use existing Oemof Tabular *Facades*, tabular *.csv* data files, and simple Python scripts to build the energy system. The current *Facades* include dispatchable generation (to allow modeling of fossil-fuel-based generation), volatile generation, storage, reservoir (for pumped hydro storage), backpressure and extraction turbines (for CHP), commodity (for limiting the amount of available fuel), conversion (for modeling transformers or heat pumps), load, link (for transshipment-based transmission), and excess (for handling the excess generation from the renewable sources in the optimization model). These classes can also be mixed with the Oemof Solph is transparent, and the equations and logics behind the component development are also available in the documentation of Oemof Solph [132, Krien et al. 2020].

To use the OSeEM model for different energy system contexts, the user needs to add or delete the relevant components, buses and substitute the input data. The simple scripting method also allows splitting up countries into several regions, which allows for comprehensive subregional analysis. For example, suppose a user wants to investigate the impacts of connecting the Norwegian pumped hydro storage to the German energy system. In that case, he can develop the OSeEM-DENO model adding the Norwegian energy system using similar scripts but different input data. In any generation that differs from the German system, the user can use the relevant *Facade* class to create the component and add it to the model. If there is a nuclear generation in the system, the user can write a simple script for adding the 'dispatchable' *Facade* class with relevant nuclear input data in the tabular file. Similarly, the model can scale up to a highly interconnected European energy system (e.g., OSeEM-EU), where each country is represented by one or several nodes. The availability of the source code and input data of the model increases transparency and reduces the user's effort to build up a different energy system for investigation.

7.4 Future Research Outlook

The open modeling tool OSeEM paves the pathway towards modeling and analyzing plausible sectorcoupled scenarios for 100% renewable-based national and sub-national energy systems. At the same time, this study shows how different energy mix options and their component-wise investment capacities and costs can be investigated using the model; hence, Schleswig-Holstein and Germany's cases can be followed for other similar regions to conduct the feasibility analysis of 100% renewable-based sectorcoupled systems. The study also reveals that sensitivity analyses can help identify the system's flexibility aspects in future energy infrastructure. The following modeling plans are outlined for further development:

- 1. Detailed transmission grid and high voltage direct current (HVDC) transmission line;
- 2. High-temperature industrial process heating and district heating network components;
- 3. Renewable technology components such as CSP, geothermal plants, and solar thermal collectors;
- 4. Storage components such as latent heat and chemical heat storages;
- 5. Transport components such as battery and fuel cell electric vehicles with the provision of V2G; and
- 6. DSM components.

The model results can be compared and cross-validated with similar modeling tools. The model can be regularly updated in GitHub, with source code and input data, so that other energy researchers can use the model for investigating different research questions for the renewable and sector-coupled energy systems in the EU context. The author proposes the following research questions for the future researchers:

- 1. Feasibility of a 100% renewable power-heat-transport coupled energy system for Germany;
- Impact of Nordic hydro expansion on electricity cost and supply mix for the European energy system in 2050;

3. Investigation on Nordic countries' profitability as flexibility providers for the highly interconnected continental Europe using their green batteries.

The background of the proposed research questions on the Nordic hydro expansion is further discussed in Section 7.3.2. In this study, the maximum capacity density on the available area is considered to be 4 MW/km² for onshore wind and 6 MW/km² for offshore wind plants, according to the LIMES-EU project [244]. Similar strategies to consider land limitations were also considered in studies by Brown et al. [125], Schlachtberger et al. [316,317], and Hörsch et al. [126]. A recent study from Enevoldsen and Jacobson estimates that the maximum output power densities are much higher for Europe,19.8 MW/km² for onshore wind farms, and 7.2 MW/km² for offshore wind farms [325, Enevoldsen and Jacobson 2021, p.40]. The updated values in output power densities directly impact the large-scale development of onshore wind power plants since significantly fewer land areas will be needed for new wind project developments. The study by Enevoldsen and Jacobson also implies that the electrical infrastructure and the land acquisition costs will be lowered [325, Enevoldsen and Jacobson 2021, p.40]. Therefore, with the updated capacity density values into consideration, OSeEM will have a higher value of maximum available potential as the optimization model inputs. This is particularly important for future investigations of OSeEM, with industrial heat and transport demands in the model. The increased maximum potential will allow the installation of more wind turbines, with reduced investment costs, to satisfy the industrial heat and transport loads, providing additional flexibility to decarbonize the industrial heat and transport sectors.

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Data

Data, source codes, and results of the model is available in the following Github repositories:

- 1. https://github.com/znes/OSeEM-SN
- 2. https://github.com/znes/OSeEM-DE

Appendices

Appendix A: Providing Flexibility to the European Electricity System using the 'Green Battery'

The idea of using Norwegian hydropower resources to provide flexibility to the European electricity system is widely regarded as the 'green battery' function. While the European actors imply the enormous pumped hydro storage potential in Norway as the green battery, the Norwegian actors look at it as Norway's opportunity to provide balancing power for Europe using hydropower, not necessarily using only pumped hydro storage [1]. Norway has a total installed capacity of 32 GW for hydropower, which contributes to 24% of Europe's total annual hydroelectricity production [2,3]. The reservoir capacity in Norway accounts for half of Europe's hydro reservoir storage. Currently, the hydropower in Norway enables more than 20% VRE integration in the Nordic electricity system, mainly for wind power in Denmark [4]. Using hydropower in Norway to balance the continental European electricity system's variation has raised interest from academia and industry. Maaz et al. showed that Norwegian hydropower might reduce the European electricity system's variable cost [5]. Several other studies found that utilizing the hydropower in Norway may reduce the average electricity price and the price variation for the future European electricity system with a large VRE share [4,6–9]. Apart from Norway, Sweden also has rich hydropower resources with a capacity of 16 GW producing nearly 60 TWh electricity annually [3]. Although most of the studies focused only on Norwegian hydropower, hydropower in Sweden can also provide flexibility to the European electricity system [10,11].

Transmission expansion is critical in utilizing hydropower's flexibility in the Nordic countries, as the transmission bottleneck directly constrains the maximum amount of instantaneously shared flexibility. Several studies assessed the benefits of cross-border transmission expansion between the Nordic region and continental Europe. Jaehnert et al. and Grabaak et al. found that an extension of transmission grids in Northern Europe may reduce the electricity price and price volatility [7,9]. Similarly, Zakeri et al. showed that interconnecting the UK electricity system to the Nordic electricity system could lower the UK's electricity price [12]. Farahmand et al. estimated that expanding transmission grids between the Norwegian and European electricity systems reduces the system operation cost [6]. Apart from the studies on the NSR, many other studies addressed transmission expansion of the European electricity system and found that expanding cross-border transmission capacity reduces electricity system cost [13–17].

As for sector coupling, some studies have analyzed its impact on the electricity system. Göransson et al. estimated that the integration of electricity, residential heat, transport, and steel industry could lead to an 8% cost reduction for the North European energy system [18]. Pavičević et al. showed that sector coupling might increase the penetration level of wind and solar by 5% and 15%, respectively, and reduce 30% more CO₂ emission than an energy system without sector coupling [19]. Sector coupling may strongly influence Nordic hydropower's 'green battery' function for the continental European electricity system. The reason is two-fold. First, electricity demand may increase substantially due to sector coupling. It is unclear whether the hydropower will be utilized more locally as bulk electricity supply for the Nordic countries or provide more flexibility to the European continent. Second, with more flexibility from other sectors locally, less transmission expansion and traded flexibility might be needed. Brown et al. analyzed the benefits of cross-border transmission expansion under different sector coupling levels for a highly renewable European electricity system. They found that with more sector coupling, the benefit of transmission expansion in reducing system cost is weakened [20]. Thus, it remains unknown whether the emerging sector coupling would enhance or impede Nordic hydropower's 'green battery' function.

In summary, it is clear that the Nordic hydropower benefits the continental low-carbon electricity system for Europe and these benefits might be further enhanced if there is an expansion of cross-border transmission

connection. However, it is unclear how the emerging sector coupling in the NSR would affect the Nordic hydropower's flexibility to the continental energy system. In future research it will be interesting to make a comprehensive analysis of the above question and investigate the integrated electricity, heat, and transport system for the NSR.

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Appendix B

Table B.1: Open Energy Models. Based on [108,110].

SI.	ΤοοΙ	Geographical Scope	SI.	Tool	Geographical Scope
1	BALMOREL (Bottom-up partial equilibrium energy system optimisation model)	Global	31	JMM (Joint Market Model)	Multi-regional
2	Calliope	User-defined	32	LEAP	National
3	COMPETES (Comprehensive Market Power in Electricity Transmission and Energy Simulator)	National, Continental	33	LUSYM	National, Continental
4	COMPOSE (Compare Options for Sustainable Energy)	Single System	34	MEDEAS	National, Continental, Global
5	DER-CAM (Distributed Energy Resources Customer Adoption Model)	Single System, Local, Regional	35	MOCES (Modeling of Complex Energy Systems)	User-defined
6	DESSTINEE	National, Continental (Europe)	36	NEMO (National Electricity Market Optimiser)	National
7	DIETER (Dispatch and Investment Evaluation Tool with Endogenous Renewables)	Germany	37	Oemof	User-defined
8	Dispa-SET	NUTS 1 (EU)	38	OnSSET (Open Source Spatial Electrification Tool)	Sub-Saharan Africa, developing Asia, Latin America
9	DynPP (Dynamic Power Plant Model)	Single System	39	OpenDSS (Open Distribution System Simulator)	Distribution Networks
10	EA-PSM (Energy Advice Power System Modelling)Electric Arc Flash	National, Continental, Global	40	OSeMOSYS	Community, Continental
11	EA-PSM Electric Short Circuit	National, Continental, Global	41	PLEXOS Open EU (PLEXOS Integrated Energy Model)	Northwest Europe
12	ELMOD	National, Continental	42	PowerGAMA	Regional, National
13	EMLab-Generation (Energy Modelling Laboratory - Generation)	Central Western Europe	43	PowerMatcher	Distribution Networks
14	EMMA (The European Electricity Market Model)	North-western Europe	44	PyPSA	National, Continental
15	EMPIRE (European Model for Power system Investment with Renewable Energy)	Continental (Europe)	45	RAPSim (Renewable Alternative Powersystems Simulation)	Local
16	Energy Numbers-Balancing	National	46	Region4FLEX	Germany
17	EnergyPlan	Local, National	47	renpass (Renewable Energy Pathways Simulation System)	Regional, National
18	EnergyRt (Energy systems modeling R-toolbox)	Multi-regional	48	RETScreen	All
19	ESO-X ESO refers to Electricity Systems Optimisation (ESO) framework	Single-node	49	SAM (System Advisor Model)	Single System
20	ETM (1) (EUROfusion Times Model)	Global (17 Regions)	50	SciGRID (Open Source Model of European Energy Networks)	Europe and Germany (any other EU country also possible)
21	ETM (2) (Energy Transition Model)	Community— International	51	SimSES (Simulation of stationary energy storage systems)	Global
22	ETSAP-TIAM (The TIMES Integrated Assessment Model)	Global (15 Regions)	52	SIREN	Regional, National

23	ficus	Local, National	53	SNOW (Statistics Norway's World Model)	National, Global
24	GAMAMOD (The Gas Market Model)	Europe	54	stELMOD	National, Continental
25	GCAM (Global Change Assessment Model)	Global	55	SWITCH	Regional, National
26	GENESYS (Genetic Optimization of a European Energy Supply System)	EU-MENA (21 Regions)	56	TIMES Évora (TIMES refers to The Integrated MARKAL- EFOM System)	Évora (Portugal)
27	GridCal	Transmission Networks	57	TIMES-PT	Portugal
28	GridLAB-D	Local, National	58	Temoa (Tools for Energy Model Optimization and Analysis)	US
29	iHOGA (Improved Hybrid Optimization by Genetic Algorithms)	Local	59	urbs	Local, Regional, National
30	IRiE (Integrated Regulating power market in Europe)	26 Areas of Northern Europe			

Table B.2: Detailed Comparison of Selected Tools. Based on [108,110].

SI.	Tool	Investment & Decision Support	Top-Down & Bottom-Up Approach	All Storage Inclusion	Net Transfer Capacity	Commodity (Electricity & Heat)	Inelastic Demand	Supply - Demand Modeling	CO ₂ Cost	CO ₂ Emission
1	Calliope	\checkmark	-	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
2	DESSTinEE	\checkmark	-	-	\checkmark	-	\checkmark	-	\checkmark	\checkmark
3	Dispa-SET	\checkmark	-	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
4	ELMOD	\checkmark	-	\checkmark	-	\checkmark	-	\checkmark	\checkmark	\checkmark
5	ficus	\checkmark	-	\checkmark	-	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
6	LEAP	-	\checkmark	\checkmark	-	\checkmark	-	\checkmark	\checkmark	\checkmark
7	LUSYM	-	-	\checkmark	-	-	\checkmark	\checkmark	\checkmark	\checkmark
8	MEDEAS	-	-	-	-	\checkmark	-	-	\checkmark	\checkmark
9	OSeMOSYS	\checkmark	-	\checkmark	-	-	\checkmark	\checkmark	\checkmark	\checkmark
10	PowerGAMA	\checkmark	-	\checkmark	-	-	\checkmark	\checkmark	-	-
11	PyPSA	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
12	RETScreen	\checkmark	\checkmark	-	-	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
13	SIREN	-	-	\checkmark	\checkmark	-	\checkmark	\checkmark	-	\checkmark
14	SWITCH	\checkmark	-	\checkmark	\checkmark	-	\checkmark	\checkmark	-	\checkmark
15	urbs	\checkmark	-	\checkmark	\checkmark	\checkmark	\checkmark	-	\checkmark	\checkmark
16	Oemof	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark

Appendix C

Technology	Study	Primary Focus	Reference
Heat Pump	Hers et al.	Potential (National)	1
	Bloess et al.	Modeling and flexibility (General)	2
	Yilmaz et al.	Potential (Europe)	3
	Yilmaz et al.	Flexibility (Europe)	4
	Leitner et al.	System analysis/Sector coupling (Local)	5
	Kirkerud et al.	Flexibility (Nordic)	6
	Kuprat et al.	Flexibility (National)	7
	Schuewer et al.	Industrial application (National)	8
	Den Ouden et al.	Industrial application (National)	9
	Garcia et al.	Market potential (Europe)	10
	Heinen et al.	Research trend (Europe)	11
	Heinen et al.	Investment modeling (Local)	12
	Sandberg et al.	Framework conditions (Nordic)	13
	Strbac et al.	Decarbonization pathways (National)	14
	Hast et al.	System analysis/Sector coupling (Local)	15
	Levihn et al.	System analysis/Sector coupling (Local)	16
	Meibom et al.	Economic analysis (North Europe)	17
	Kavvadias et al.	Sector coupling/Decarbonization (EU)	18
	Ünlü	Sector coupling/Flexibility (General)	19
	Brown et al.	Sector coupling (Europe)	20
Electric Boiler	Hers et al.	Potential (National)	1
	Bloess et al.	Modeling and flexibility (General)	2
	Yilmaz et al.	Potential (Europe)	3
	Yilmaz et al.	Flexibility (Europe)	4
	Kirkerud et al.	Flexibility (Nordic)	6
	Kuprat et al.	Flexibility (National)	7
	Schuewer et al.	Industrial application (National)	8
	Den Ouden et al.	Industrial application (National)	9
	Garcia et al.	Market potential (Europe)	10
	Heinen et al.	Research trend (Europe)	11
	Heinen et al.	Investment modeling (Local)	12
	Sandberg et al.	Framework conditions (Nordic)	13
	Strbac et al.	Decarbonization pathways (National)	14
	Meibom et al.	Economic analysis (North Europe)	17
	Ünlü	Sector coupling/Flexibility (General)	19
	Brown et al.	Sector coupling (Europe)	20
	Schweiger et al.	Potential (National)	21
	Böttger et al.	Potential (National)	22
	De Wolff et al.	Industrial application (National)	23
	Wang et al.	Flexibility/Optimization modeling (Local)	24
Electric	Bloess et al.	Modeling and flexibility (General)	2
Resistance	Yilmaz et al.	Potential (Europe)	3
Heater	Yilmaz et al.	Flexibility (Europe)	4
	Leitner et al.	System analysis/Sector coupling (Local)	5
	Schuewer et al.	Industrial application (National)	8
	Den Ouden et al.	Industrial application (National)	9
	Heinen et al.	Research trend (Europe)	11

Table C.1: Studies presenting prominent P2H and TES technologies

	Heinen et al.	Investment modeling (Local)	12
	Sandberg et al.	Framework conditions (Nordic)	13
	Strbac et al.	Decarbonization pathways (National)	14
	Kavvadias et al.	Sector coupling/Decarbonization (EU)	18
	Ünlü	Sector coupling/Flexibility (General)	19
	Brown et al.	Sector coupling (Europe)	20
CHP	Hers et al.	Potential (National)	1
	Bloess et al.	Modeling and flexibility (General)	2
	Yilmaz et al.	Potential (Europe)	3
	Yilmaz et al.	Flexibility (Europe)	4
	Kirkerud et al.	Flexibility (Nordic)	6
	Schuewer et al.	Industrial application (National)	8
	Den Ouden et al.	Industrial application (National)	9
	Böttger et al.	Potential (National)	22
	Garcia et al.	Market potential (Europe)	10
	Heinen et al.	Research trend (Europe)	11
	Heinen et al.	Investment modeling (Local)	12
	Strbac et al.	Decarbonization pathways (National)	14
	Hast et al.	System analysis/Sector coupling (Local)	15
	Levihn et al.	System analysis/Sector coupling (Local)	16
	Meibom et al.	Economic analysis (North Europe)	17
	Kavvadias et al.	Sector coupling/Decarbonization (EU)	18
	Ünlü	Sector coupling/Flexibility (General)	19
	Brown et al.	Sector coupling (Europe)	20
	Wang et al.	Flexibility/Optimization modeling (Local)	24
Thermal Energy	Sarbu et al.	Review of technologies	25
Storage	Pfleger et al.	Sensible and latent heat storage	26
	Hailu et al.	Seasonal solar thermal storage	27
	Socaciu et al.	Seasonal thermal storage	28
	Monde et al.	Solar thermal storage	29
	IRENA	Innovation outlook	30

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SI.	Technology	Merits	Demerits	Reference
1	Heat Pump	 High efficiency Low energy cost Less maintenance Easy installation (most cases) Better safety standard 	 High upfront cost Issues in cold weather Some heat pump installations are complex 	1,2,3
2	Electric Boiler	 High efficiency Low initial cost Simple maintenance Robust and compact design Quiet operation 	High heating output is complex	4,5,6

Table C.2: Merits and demerits of the P2H technologies

3	Electric Resistance Heater Hybrid Heating System	 Requires less space Faster startup Less investment cost Increased system reliability Reduced dependency Energy efficient 	 Lower lifespan* Lower efficiency* Higher carbon footprint* High installation cost Complex maintenance 	7,8,9
5	СНР	 Operations are automatic (most cases) Increased fuel efficiency Increased reliability Reduced energy wastage Reduced energy costs 	 Heating and electricity demand must remain consistent Capital intensive 	13,14,15

*Compared to other P2H technologies

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SI.	Technology	Merits	Demerits	Reference
1	Sensible Heat	Low cost	 Significant heat loss over 	1,2,3,4,5,6
	Storage (SHS)	Reliable	time (depending on level of	
		Simple application with	insulation)	
		available materials	Large volume needed	
		Long lifetime		
		Commercially available		

Table C.3: Merits and demerits of the TES technologies

2	Latent Heat Storage (LHS)	 Medium storage density Small volumes Short distance transport possibility Commercially available 	 Low heat conductivity Corrosivity of materials Significant heat losses (depending on level of insulation) Limited lifetime due to storage material cycling 	
3	Thermo- chemical Heat Storage (THS)	 High storage density Low heat losses (storage at ambient temperatures) Long storage period Long distance transport possibility Highly compact energy storage 	 High capital costs Technically complex Lifetime depends on reactant degradation and side reactions Generally, not available, but undergoing research and pilot project tests 	
4	Thermo- mechanical Energy Storage (TMS)	 ACAES Capable of storing huge amounts of energy High efficiency (~ 70%) percent) Fast response time Inexpensive LAES Relatively high energy density Does not require any scarce or toxic materials Does not produce toxic waste Components used are technologically mature and long lasting 	 ACAES Highly complex Requires sealed storage caverns Not yet fully developed LAES Low round trip efficiency Not practical for small scale energy storage Safety issues 	7,8,9,10

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Appendix D

TRL	Description	Status
1	Basic principles observed and reported	Theory
2	Technology concept and/or application formulated	
3	Analytical and experimental critical function and/or characteristic proof of concept	Laboratory
4	Component and/or breadboard validation in laboratory environment	
5	Component and/or breadboard validation in relevant environment	
6	System/subsystem model or prototype demonstration in relevant environment	Prototype
7	System prototype demonstration in operational environment	
8	Actual system completed and qualified through test and demonstration	
9	Actual system proven through successful mission operations	Established

Table D.1: Technology Readiness Level. Based on [160].



Base Scenario



(a)



(b)



Figure E.1: Optimization results of the electricity buses in the base scenario in 2050 (a) supply-demand variation for NDE (b) %wise use of electricity generators for NDE (c) supply-demand variation for SDE (d) %-wise use of electricity generators for SDE





(d) Figure E.2: Optimization results of the heat buses in the base scenario in 2050 (a) supply-demand variation for NDE (b) %-wise use of heat generators for NDE (c) supply-demand variation for SDE (d) %-wise use of heat generators for SDE



Conservative Scenario

Onshore NDE, 29.58%



(b)

Offshore NDE, 49.17%



Figure E.4: Optimization results of the electricity buses in the conservative scenario in 2050 (a) supply-demand variation for NDE (b) %-wise use of electricity generators for NDE (c) supply-demand variation for SDE (d) %-wise use of electricity generators for SDE





(d) Figure E.5: Optimization results of the heat buses in the conservative scenario in 2050 (a) supply-demand variation for NDE (b) %-wise use of heat generators for NDE (c) supply-demand variation for SDE (d) %-wise use of heat generators for SDE



(a)

(b)





(a)



(b)



Figure E.7: Optimization results of the electricity buses in the progressive scenario in 2050 (a) supply-demand variation for NDE (b) %-wise use of electricity generators for NDE (c) supply-demand variation for SDE (d) %-wise use of electricity generators for SDE





(d) Figure E.8: Optimization results of the heat buses in the progressive scenario in 2050 (a) supply-demand variation for NDE (b) %wise use of heat generators for NDE (c) supply-demand variation for SDE (d) %-wise use of heat generators for SDE



List of Publications

SI.	Title	Journal	Type/ Impact Factor 2023	Status	Position/ Authors
1	M.N.I. Maruf, Sector Coupling in the North Sea Region—A Review on the Energy System Modelling Perspective, Energies. 12 (2019) 4298. <u>https://doi.org/10.3390/en12224298</u> .	Energies (MDPI)	Peer-reviewed 3.252	Published	1/1
2	M.N.I. Maruf, A Novel Method for Analyzing Highly Renewable and Sector-Coupled Subnational Energy Systems—Case Study of Schleswig-Holstein, Sustainability. 13 (2021) 3852. <u>https://doi.org/10.3390/su13073852</u> .	Sustainability (MDPI)	Peer-reviewed 3.889	Published	1/1
3	M.N.I. Maruf, Open model-based analysis of a 100% renewable and sector-coupled energy system–The case of Germany in 2050, Appl. Energy. 288 (2021) 116618. https://doi.org/10.1016/j.apenergy.2021.116618.	Applied Energy (Elsevier)	Peer-reviewed	Published	1/1
4	M.N.I. Maruf, G. Morales-Espana, J. Sijm, N. Helisto, J. Kiviluoma, Classification, potential role, and modeling of power-to-heat and thermal energy storage in energy systems: A review, Sustainable Energy Technologies and Assessments, 53, (2022) p.102553. https://doi.org/10.1016/j.seta.2022.102553.	Sustainable Energy Technologies and Assessments (Elsevier)	Peer-reviewed 7.632	Published	1/5