Modular Optimization for the Holistic Energy Management of Industrial Multi-Energy Systems

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Vienna, November 2023

Karl-Wihelm Schenzel

Abstract

The goal of establishing a sustainable and environmentally harmless energy supply and reducing energy-related emissions presents industrial companies with the challenge of adapting the volatility of renewable energy sources to the requirements of production processes. On the one hand, this requires technological transformations including the establishment of flexibilities; on the other hand, it increases both the requirements for energy management as well as associated opportunities. Additionally, considering the inherent existence of forecast uncertainties, this requires not only reliable, robust operational planning but also appropriate control for complying with desired schedules.

The applications of optimization in energy management and model predictive control (MPC) are already state of the art, but the implementation of respective tools into existing systems and organizational procedures is generally a very comprehensive and extensive task, often requiring specific professional expertise. Not least because of this, the development of easy-manageable methods for energy optimization as well as robust and adaptive MPC approaches are of great scientific interest, but a research gap can be identified in the combination of both features, especially for complex multi-component energy systems. Subsequently, also studies evaluating effective associated savings and operational performance improvements in close-to-real environments are very limited, which constitutes an essential barrier for companies to implement such tools.

Starting at this point, this work provides valuable contributions to overcome these gaps and tackles the topic from the integration of new technologies to a detailed evaluation of the performance and savings potentials in a close-to-real environment. On a methodical level, the development of a generic, modular framework for the simultaneous, online operational optimization and control of complex multi-energy systems, represents the central novelty. Establishing a fast, direct, and straightforward definition and implementation, the approach is characterized by a modular, component-based superstructure using a thermodynamic, energy carrier-related specification of the energy plants.

The added value of such an energy management and control system (EMCS) lies not only in the optimization of the internal energy use but also in the fact that decentralized energy systems can force and facilitate the grid-bound feed-in of renewable energy sources as plannable flexible consumers. Due to their modular structure, the advantages of the method increase in particular with the complexity of the systems. Therefore, it is essential to use a versatile and flexible energy system as a reference use-case, firstly for the development of the method, but most importantly to demonstrate the potential for improvement and savings.

The creation of this reference energy system (RES) therefore represents a major sub-goal of the work. The primary focus is on processes with heat demand at a temperature level below 170°C, which are particularly found in the food sector. For such processes, technologies for renewable generation as well as for storage and coupling of thermal and electrical energy exist. In particular, high-temperature heat pumps show promising flexibility and savings potentials, which makes the integration of this technology an important part of the energy system

under consideration. The general layout of this system is first derived empirically, based on analyses of real plants and literature research. Based on this, the integration of new technologies is done by using mathematical optimization for component design.

Subsequently, the EMCS is developed and tested on the RES. Since the real-time operating EMCS is in constant interaction with a real plant, for the development of the method is also necessary to create simulation models of all individual components in the RES, which can represent the behavior more accurately and in greater detail than the optimization models. These not only serve as counterparts to the optimization models but are also used for comparison with a conventional control strategy.

The central findings of this dissertation are oriented towards the challenge of adapting the energy demand of industrial processes to strongly fluctuating renewable generation and energy prices. Therefore, the step-wise approach which started with the design-optimization of the RES is complemented by a comprehensive functional performance evaluation of the EMCS. The qualitative and quantitative analysis is based on the comparison of different seasonal, methodological, configuration, and management scenarios and investigates potential economic, operational, and environmental improvement potentials.

From a methodological perspective, the accuracy of forward planning, the influence of forecasting as well as planning and modeling inaccuracies, and systemic adaptability are of essential interest. Focusing on operational, economic, and environmental perspectives, insights are provided in particular on the utilization of flexibilities to reduce energy-related emissions, substitution of energy sources, adaptation of grid-bound energy procurement as well as on the interrelation between design and operational aspects.

Kurzfassung

Das Ziel, energiebezogene Emissionen zu reduzieren, stellt Industriebetriebe vor die Herausforderung, die Volatilität erneuerbarer Energiequellen an den Energiebedarf der Produktionsprozesse anzupassen. Dies erfordert zum einen technologische Transformationen inklusive der Einrichtung von Flexibilitäten, zum anderen steigen dadurch sowohl die Anforderungen an das Energiemanagement, als auch damit verbundene Möglichkeiten. Unter Berücksichtigung von Prognoseschwankungen und Planungsunsicherheiten erfordert dies nicht nur eine zuverlässige, robuste Planung, sondern ebenso eine entsprechende Regelung zur Umsetzung der Fahrpläne.

Digitale, operative Energieoptimierung und adaptive, modelprädiktive Regelung (MPC) zählen zwar bereits zum Stand der Technik, allerdings ist die Erstellung entsprechender Werkzeuge im Allgemeinen eine sehr umfassende und umfangreiche Aufgabe, welche darüber hinaus große spezifische Expertise erfordert. Nicht zuletzt aufgrund dessen sind die Entwicklung anwenderfreundlicher Methoden zur Energieoptimierung, sowie adaptiver MPC-Ansätze von großem wissenschaftlichen Interesse, allerdings lässt sich eine Forschungslücke in der Kombination beider Instrumente, im Speziellen für komplexe Energiesysteme identifizieren.

Mit dem übergeordneten Ziel der Entwicklung einer generischen, modularen Methode zur simultanen, operativen online-Optimierung und Regelung von Energieanlagen setzt diese Doktorarbeit an dieser Stelle an. Der Mehrwert eines solchen Energy-Management and Control-Systems (EMCS) liegt dabei nicht nur in der Optimierung der innerbetrieblichen Energienutzung, sondern ebenso darin, dass dezentrale Energiesysteme als planbar flexible Konsumenten die netzgebundene Einspeisung erneuerbarer Energieträger forcieren und erleichtern können. Durch den modularen Aufbau steigen die Vorteile der Methode im Speziellen mit der Komplexität der Systeme an. Insbesondere daher ist es essentiell, dass für die Entwicklung der Methode ein entsprechend vielseitiges und flexibles Energiesystem als Referenz Use-Case herangezogen wird.

Die Erstellung dieses Referenzenergiesystems (RES) stellt deshalb ein wesentliches Teilziel der Arbeit dar. Der vorrangige Fokus gilt dabei Prozessen mit Wärmebedarf auf einem Temperaturniveau unter 170°C, wozu unter anderem der Lebensmittelsektor zählt. Für derartige Prozesse existieren bereits Technologien zur erneuerbaren Energiebereitstellung sowie auch zur Speicherung und Kopplung von thermischer und elektrischer Energie. Insbesondere weisen dabei Hochtemperaturwärmepumpen vielversprechende Flexibilitäts- und Einsparungspotentiale auf, was die Integration dieser Technologie zu einem wichtigen Bestandteil des betrachteten Energiesystems macht. Das allgemeine Layout dieses Systems wird zunächst empirisch, basierend auf Analysen realer Anlagen und Literaturrecherchen abgeleitet. Darauf aufbauend erfolgt die Integration neuer Technologien durch den Einsatz von mathematischer Optimierung zur Komponentenauslegung.

Auf Basis dieses Referenzenergiesystems wird im Anschluss das EMCS entwickelt und getestet. Zentraler Fokus gilt dabei der Entwicklung eines

generischen Modellierungsansatzes zur unmittelbaren, simultanen Erstellung hierarchisch agierender Optimierungsprobleme. Der Ansatz kennzeichnet sich durch eine modulare, komponentenbasiertes Konzept, welche sich an einer thermodynamischen, energieträgerbezogenen Spezifizierung der Energieanlagen orientiert. Dies soll eine rasche, direkte und unkomplizierte Definition der spezifischen Funktionen sowie die Interaktion der verschiedenen Optimierungsebenen im Sinne der Zusammensetzung von Kostenfunktion, Betriebs- und Randbedingungen ermöglichen.

Da das in Echtzeit arbeitende EMCS in ständiger Interaktion mit einer realen Anlage steht, ist es für die Entwicklung der Methode ebenso erforderlich, Simulationsmodelle aller Einzelkomponenten des RES zu erstellen, welche das Verhalten genauer und detaillierter abbilden können, als die Optimierungsmodelle. Diese dienen nicht nur als Gegenspieler zu den Optimierungsmodellen, sondern werden ebenso zum Vergleich mit einfachen konventionellen Regelstrategien beaufschlagt.

Die zentralen Erkenntnisse dieser Dissertation orientieren sich an der Herausforderung, den Energiebedarf industrieller Prozesse an stark schwankende erneuerbare Erzeugung und Energiepreise anzupassen. Dazu wird der schrittweise Ansatz, der mit der Design-Optimierung des RES begann, durch eine umfassende funktionale Leistungsbewertung des EMCS fortgeführt. Die qualitative und quantitative Analyse basiert auf dem Vergleich verschiedener saisonaler, methodischer, Konfigurations- und Managementszenarien und evaluiert mögliche wirtschaftliche, betriebliche und ökologische Verbesserungspotenziale.

Aus methodischer Sicht sind die vor allem die Genauigkeit der Vorausplanung, der Einfluss von Prognosen sowie Planungs- und Modellierungsungenauigkeiten und die systemische Anpassungsfähigkeit von wesentlichem Interesse. Aus betrieblicher, ökonomischer und ökologischer Sicht werden insbesondere Erkenntnisse über die Nutzung von Flexibilitäten zur Reduktion energiebedingter Emissionen, die Substitution von Energieträgern, die Anpassung der netzgebundenen Energiebeschaffung sowie die Wechselbeziehung zwischen technologischen und betrieblichen Aspekten dargelegt.

Acknowledgements

Pursuing my PhD has been a unique journey that has genuinely advanced my personal development and broadened my perspectives. This was only possible thanks to the support and understanding of various people around me, whom I would now like to include in my work with special thanks.

First of all, I express my sincere gratitude to my supervisor, Prof. René Hofmann, whose guidance has been invaluable and offered me unique opportunities. Especially, I am deeply grateful for the supervision of this dissertation and his support, confidence, and inspiration, which fundamentally contributed to my scientific advancements.

However, a very special tribute goes to a former colleague and dear friend who generously supported me in taking advantage of this unique opportunity. Especially because we had to accept with sadness that this person, Andreas Schwarz, passed away during the pandemic time we recently experienced, I would like to dedicate this work to him on behalf of all people who actively assist and encourage people to achieve their goals.

Moreover, I would like to thank my project colleagues for their professional, respectful, and supportive cooperation in achieving our common goals and advancements. It has been a pleasure to work with you. Next, I am deeply grateful to my dear colleagues at our research unit for sharing such a pleasant and creative atmosphere. Whether it was delightful conversations in the kitchen, skillful activities in the hallway, or assistance at the desk, I could always count on you.

However, my appreciation extends beyond academic circles to all my friends who provide the foundation that keeps me balanced and grounded while pursuing scientific ambitions. In particular, the shared adventurous explorations to the world's most unique places impinamize my sense of balance between the beauty of nature and technology. Above all, I express my heartfelt gratitude to my beloved Sophie, who accompanied me hand in hand on this exciting journey, while never holding back from experiencing the most beautiful natural venues.

Finally and most importantly, I really cannot get enough of thanking my family, who support me for every step I take and always provide me a very relaxing, attentive, and tasteful place to retreat.

If you think you know what you want,
you either know too much or you desire too little.

GEORGIJ MAKAZARIA

Preface

This dissertation was meticulously prepared in the course of my employment at TU Wien at the Institute of Energy Systems and Thermodynamics and compiled to attain the degree of Doctor Technicae. As a project assistant in the research unit of Industrial Energy Systems, I was granted the unique opportunity to contribute to scientific progress and technical advancements within the professional environment of several funded research projects, most importantly EDCSproof[1]. Industry4Redispatch[2].

The most essential and comprehensive scientific involvement, however, is attributable to the project EDCSproof (Energy Demand Control System–PROcess Optimization For industrial low-temperature systems), which is part of the Energy Model Region NEFI - New Energy for Industry and was funded by the Austrian Climate and Energy Fund [FFG, No.868837]. As part of the core project consortium, I present my individual contribution in this dissertation, which covers a substantial part of the project's research objectives that has not yet been published. These are:

- The generic superstructure-based modeling framework for the holistic optimization of multi-energy systems
- The Energy Management and Control System (EMCS) as a specific enhanced central application of the optimization superstructure. It constitutes the central novelty of the present work and also of the research project
- The Reference Energy System (RES) as a generalized use case representative for the subsector of industrial low-temperature energy systems, which is used for a comprehensive performance evaluation of the EMCS

Other adjacent works and publications emerging from this project therefore represent both essential inputs as well as complementary developments and accompanying contributions. Most notably, Fuhrmann et al.[1] proposed to hierarchically separate the essential tasks of long-term economic optimization and short-term control by using a two-level control architecture. I consequently adopted this conceptual architecture as a methodological basis for developing the EMCS framework. Moreover, in a cooperative activity of the central project consortium, we demonstrated and validated the functional capabilities of this control architecture in a real laboratory environment [2].

However, beyond demonstrating TRL 4 on a simple laboratory system, this dissertation tackles two essential aspects for transforming the methodical concept into an applicable and viable tool: The embedding into a concise, manageable modeling framework as well as the comprehensive performance demonstration on a complex, multi-energy system as typically

[1] https://www.nefi.at/de/projekt/edcsproof
[2] https://www.nefi.at/en/project/industry4redispatch

found at industrial sites. Since the EMCS is intended to operate as a real-time control system in continuous interaction with the plant, this is a particularly comprehensive task. It requires not only the implementation of the energy system in the optimization framework but also the creation of a comprehensive simulation model that is used to realistically evaluate control performance and potential savings on a holistic level. Therefore, mainly on account of the extensive modeling effort required to cover this issue adequately, the format of a monograph was chosen for this research contribution.

Due to its promising potential to facilitate the dispatching of industrial energy procurement, the EMCS represents an essential component within the follow-up project Industry4Redispatch. In addition to the identification and provision of flexibilities, it is also experimentally tested in three different real industrial environments. Furthermore, I could also contribute my experience to the project H2-DemoLAB, which aims to develop a decentralized hydrogen-based energy system powered by local renewables. The efficiency of this system may significantly benefit from the use of the developed EMCS, which combines sector coupling, load and storage management to optimize local energy use.

Since each project entails different objectives, stakeholders, perspectives, and scientific exchange, all contributed to the continuous process of expanding my methodological skills and substantive knowledge, which ultimately manifested in the present work.

Contents

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Nomenclature

Abbreviations & Acronyms

BAT	Best Available Technology
CAPEX	Capital Expenditures
CC	Conventional Control
CH	Chiller
CHP	Combined Heat and Power Plant
CO_2	Carbon Dioxide
COP	Coefficient of Performance
CRES	Conventional Reference Energy System
CRCC	Conventional Reference Control Concept
CS	Cold Side
CSP	Concentrated Solar Power
CT	Cooling Tower
DES	Decentralized Energy System
DH	District Heating
DO	Design Optimization
DOF	Degrees of Freedom
DP	Dynamic Programming
DT	Minimum Downtime
EH	Energy Hub
EMS	Energy Management System
EMCS	Energy Management and Control System
EU	European Union
GB	Gas Boiler
GHG	Greenhouse Gases
H2	Hydrogen
HC	Heat Consumer
HENS	Heat Exchanger Network Synthesis
HO	Hierarchical Optimization
HP	Heat Pump
HS	Hot-Side
HT	High-Temperature
HTHP	High-Temperature Heat Pump
HVAC	Heating, Ventilation and Air Conditioning
IPCC	Invergovernmental Panel on Climate Change
Irr	Irradiance
MES	Mult-Energy Systems
MIP	Mixed-Interger Programming

MILP	Mixed-Interger Linear Programming
MILNP	Mixed-Interger Non-Linear Programming
MPC	Model-Predictive Controller
MT	Medium Temperature
NLP	Non-linear Programming
NP	Non-deterministic Polynomial Time
RE	Renewable Energies
RES	Reference Energy System
OF	Objective Function
OO	Operational Optimization
OP	Operation Planner
OPEX	Operational Expenditures
OPP	Optimization Problem
O&M	Operational and Maintanace
PID	Proportional–Integral–Derivative Controller
LP	Linear Programming
LT	Low Temperature
LW	Liquid Water
PC	Power Consumer
PCM	Phase Change Material
PG	Power Grid
ppm	Parts Per Million
PV	Photovoltaics
RU, RD	Ramp-Up, Ramp-Down
SU,SD	Start-Up, Shut-Down
SOC	State Of Charge
St	Storage
ST	STeam
STES	Stratified Thermal Energy Storage
TAC	Total Annual Costs
TES	Thermal Energy Storage
UC	Unit Commitment
UT	Minimum Uptime
WHR	Waste Heat Recovery
TRL	Technology Readiness Level
36/45	Prediction Horizon of 36 hours in the OP and 45 minutes in the MPC
12/15	Prediction Horizon of 12 hours in the OP and 15 minutes in the MPC

Parameters & Variables

Ar	Area
a,b	Coefficients
an	Annual Investment Costs
B	Balance

CAP	Design Capacity
c	Costs
cp	Heat Capacity
e	Energy
f	Factor
fr	Frequency
h	Specific Enthalpy
ht	Height
H_u	Lower Heating Value
i	Electric Current
I	Investment Decsion
Irr	Irradiance
J	Objective
k	Thermal Conductivity
n	Networks
m	Mass
N	Number of
No	Normally Distributed Value
P	Power
p	Pressure
Q	Heat
r_{P2H}	Power to Heat Ratio
s	Stream
T	Temperature
U	Normalized Actuation Variable
u	Commitment Variable
V	Volume
Vo	Electric Voltage
v	Start-Up Variable
w	Shut-Down Variable
x	Generalized Variable

Variables are identified by bold characters

Indexes

bin	Binary
c	Continuous Value
ch	Charge
comb	Comustion
d	Discrete Value
dch	Discharge
el	Electricity
Err	Error
f,l+; f,l-	Upper face (l+); lower face (l-)

Frac	Fraction
fu	Fundamental
fuel	Fuel
hs	Heat Soucre
i	Unit/Component
in,out	In and Outlet Flows
int	Internal
inv	Investment
irr	Irreversible
j	Objective Criteria
l	Layer/Level
lb	Lower Bound
loss	Loss and Degradation
LW	Liquid Water
max	Maximum
meas	Measurement
min	Minimum
n	Networks
p	Port
r,l	Running Indices
slack	Slack Variable or Cost
SW	Saturated Water
t (superscript)	Time
t (subscript)	Total
th	Thermal
traj	Trajectory
ub	Upper Bound
v	Variables
w	Weighting
0 (superscript)	Normalized Value
α, β, γ, κ	Coefficients
η	Efficiency
λ	Fuel to Air Ratio
ρ	Density
δ	Inheretience Coefficient
ε_{def}	Properties

Sets

NW	Set of all Networks
Unit	Set of all Units
S	Set of all Streams

1 Introduction

1.1 Background and Motivation

The provision of commercially available, affordable and reliable energy is an essential foundation for human development, the prosperity of today's modern society, and subsequently, for viable complex economies. As a result, energy-intensive lifestyles have emerged whose per capita energy consumption exceeds more than 200 times the natural energy consumption of human metabolism of about 10,000 kJ, leading to the vast amount of 574 Exajoules of annual global human energy consumption. However, the developed global energy system, currently more than 80% based on fossil fuels, is associated with many problematic side effects concerning ecology, social imbalances, and geopolitical conflicts, that provoke systematic changes for establishing a sustainable global economy [3]. While in the past centuries, the scarcity of fossil energy stocks was of main concern, in the second half of the 20th century, the increasingly apparent environmental damage as well as social imbalances and geopolitical conflicts caused by the use of fossil energy sources came to the forefront of scientific, social and political discussions. Nowadays, the global warming caused by the greenhouse gas (GHG) effect and other associated environmental damage is recognized among the greatest challenges of mankind [4, 5]. As illustrated in Figure 1.1, the emission of GHG, of which approximately 73% can be attributed to the combustion of fossil fuels for energy production, is indisputably recognized as the main physical driver of global warming and subsequent climate risks by affecting the earth's radiative balance [6]. Among the GHG, with a share of 75%, CO_2 is the largest contributor of a total annual amount of 50 $GtCO_2$ equivalents increasingly imbalancing the global carbon cycle [7].

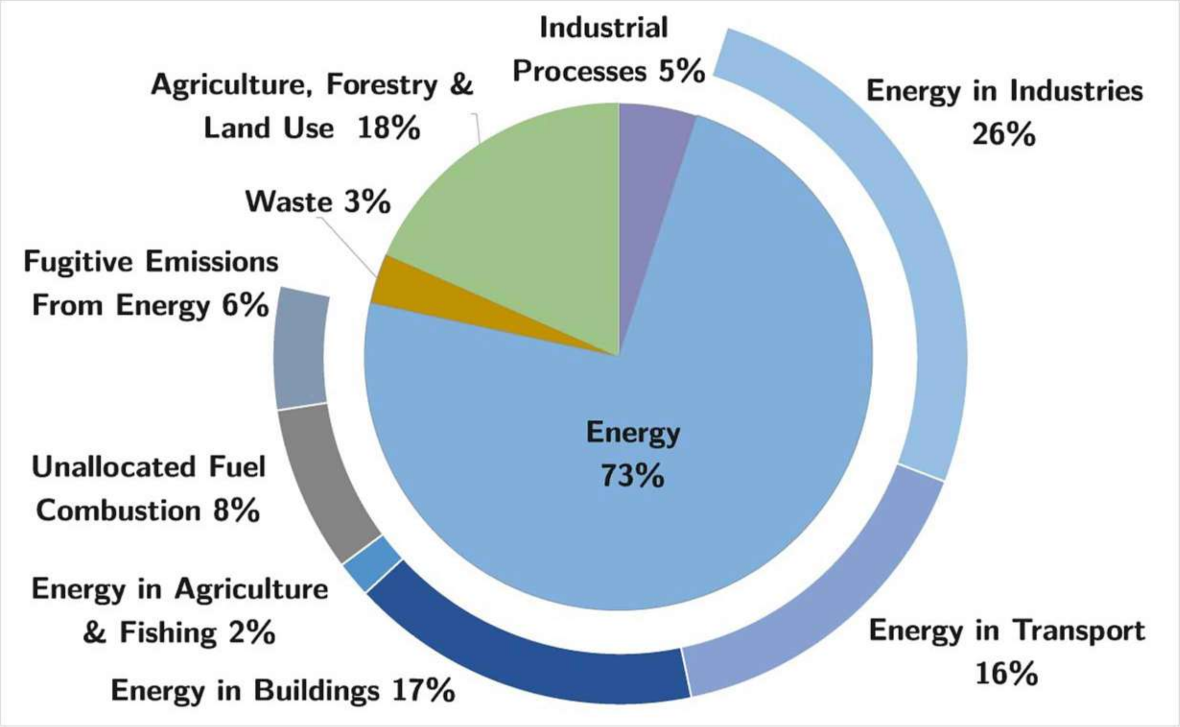


Figure 1.1 Global greenhouse gas emissions by end-use sectors, data source: [7]

Consequently, the atmospheric CO_2-concentration of currently 412 ppm (year 2020) compared to the pre-industrial time of 270 ppm in 1750, can be largely attributed to human activity and is reflected in an anthropogenic increase of global mean temperature of actually more than 1K. According to experts, it would continue to rise at an alarming state of more than 6K at business as usual behavior. Especially reflecting the increase of further related life-threatening natural hazards such as sea level rise, acidification, river floods, heatwaves, and droughts, leading to loss of biodiversity, extinction of species, and, above all, loss of human habitat, the urgency for human society to counteract and drastically change current behavioral patterns is highlighted [8]. Finally, in 2015, the seriousness of this problem was also acknowledged at global political levels to the extent that the Paris Agreement established an international legal commitment to address the limit for global warming at 1.5K above pre-industrial levels, which implies the reduction of GHG emissions to zero already by 2050 [9]. However, a further appeal to strengthen decarbonization targets was made by IPCC experts, asserting that the achievement of the 1.5°C goal requires an even more significant drop of GHG emissions of 45% already by 2030, and reaching zero net emissions in 2040 [10]. As these climate mitigation targets require more significant and comprehensive systemic changes, the EU-wide implementation of measures have been deeply integrated into the sustainable development framework of the European Green Deal, associated with a financial outlay of several thousand billion euros [11]. While the necessary mitigation of climate change represents the central reason for the switch from the non-sustainable use of fossil and nuclear fuels, the UN-SDGs[3] further propose, that future energy systems also need to meet social and ethical criteria, such as intergenerational distributive justice, security of supply, harmony with natural habitats, and harmlessness to public health.

The transition towards an energy system primarily reliant on sustainable, renewable energy sources (RE) holds the potential to concurrently satisfy multiple criteria, thereby presenting not solely a challenge but rather a compelling opportunity to address numerous challenges effectively. Obviously, the proposed mitigation and transition strategies comprise the use of RE and the reduction of energy consumption in a reasonable and equitable manner across all economic sectors. In addition, CO_2 removal processes could bring an assistive contribution, but the corresponding technologies and infrastructures are not yet sufficiently established for a substantial impact [10].

Focusing on energy provision patterns, fossil-based technologies can be installed at almost any location, at almost any capacity and allow for controllable power generation. Consequently, centralistic and unidirectional supply infrastructures have been established where energy can be supplied in a dispatchable manner to precisely meet consumption demands at any time. However, considering the characteristics of different renewable sources, only biofuels can be treated similarly to fossil sources, but above its often non-sustainable land-use management, it conflicts with other mostly more lucrative uses such as food production or as construction material [11]. Additionally, also geothermal and hydroelectric power plants potentially enable a controllable and dispatchable generation, comparable to conventional fossil-based technologies. Hydropower, however, currently, with 15% of the global power generation, the largest renewable source, only offers very limited expansion potential [13]. Geothermal energy can most suitably be used as a heat source but also for power generation. Still, the high temperatures required for both the generation of power and a large part of process heat are only economically exploitable at rare locations with geothermal

[3] United Nations Sustainable Development Goals https://sdgs.un.org/2030agenda

anomalies. In contrast, wind and photovoltaic (PV) sources exhibit substantial economic and technical potential for expansion, paired with broad, globally distributed coverage.

Unfortunately, both are subject to meteorological conditions and consequently related to temporal as well as geographical production fluctuations. Consequently, the management of these fluctuations will necessitate greater emphasis compared to the exclusive focus on consumption profiles [12]. Hence, the key challenge for large-scale RE integration can be conceived as establishing a secure and reliable power distribution by continuously balancing the temporal and geographic mismatch between generation and consumption. Since deregulation of the volatile producers is not a reasonable option due to the associated energy shortage, the task of balancing must be provided by a combination of cooperating measures across the entire energy system [12, 14], such as:

- Diversity in generation, both technologically and geographically, for statistical smoothing of feed-in due to the non-simultaneity of different distributed volatile sources
- Grid expansion to strengthen transmission capacities of geographically distant regions
- Selective use of controllable generation and storage units
- Utilization of Demand-side flexibilities
- Collaborative energy management based on a precise forecasts of volatile production

Accordingly, the transformation is projected to affect the entire energy system rather than just replacing primary energy sources. Furthermore, it becomes evident that not only the composition of large-scale energy systems will become more versatile, but also the requirements for appropriate operation and supply security will increase. Also, significant changes in energy markets are imperative due to the inherent volatility that poses considerable challenges in establishing precise delivery of long-term contracts, which currently account for roughly 80% of electricity trade in the EU. Considering these measures, it becomes clear that the transformation of energy systems design, operation, and energy markets is closely coupled [15, 16]. The expansion of grid- and large-scale storage capacities is a very complex and protracted decision process encompassing many stakeholders, diverse political issues, and, in addition, associated to high investment expenditures [17, 18]. In contrast, the establishment and utilization of demand-side flexibilities represent cost-and resource-efficient balancing measures, which become even more indispensable, with large shares of volatile feed-in.

However, making consumption more flexible is only one of several reasons why a focus on the demand side is essential. Initially, it is important to distinguish between two aspects of energy consumption. The consumer's individual demand patterns and the corresponding primary energy required to provide the specific final energy services. Apart from significant potential savings, the first part relates primarily to behavioral aspects of socioeconomic attitudes [19] and will thus not be explored further. The second, in contrast, more or less comprises the overall energy conversion efficiency of the various energy supply chains, where savings are attributed to technological solutions, investment decisions, and efficiency improvements. Considering the allocation of energy consumption, very different distributions and decarbonization strategies are observed among the individual sectors [19]. The transport sector, which constitutes nearly 30% of total global primary energy consumption, is currently about 95% based on fossil energy. In addition to a potential demand reduction of 30% due to transport prevention and increasing use of public means, decarbonization strategies propose transitioning to significantly more efficient alternative drive concepts based on electricity or hydrogen.

In the residential sector, large energy savings of more than 50% can be accomplished through more energy-efficient household devices and thermal insulation improvements. Moreover, due to moderate temperature requirements of space heating and cooling, these services can be established by sustainable technologies such as geothermal, solar thermal, and environmental heat by using heat pumps.

In the industrial sector, which already accounts for the largest share of about 40% of global final energy consumption and about 30% of global GHG emissions (see Figure 1.1 on Page 1), a promising efficiency savings potential of about 25% is reported through technological improvements. However, the sustainable supply of a large part of industrial heat is a very challenging task due to the high-temperature requirements. Currently, corresponding processes requiring temparatures exceeding 500°C, which account for more than 50% of the total industrial heat demand in the EU 28, are predominantly supplied by on-site fossil combustion. In addition to the use of biomass, the most promising sustainable alternatives for such processes are either based on electricity in a direct way or using hydrogen as a secondary energy carrier. Especially taking into account the significant conversion losses of hydrogen production, industrial power consumption is expected to increase as illustrated in Figure 1.2 [19, 20]. Additionally, Figure 1.3 indicates a significant rise in electrification that is expected to almost triple by 2050.

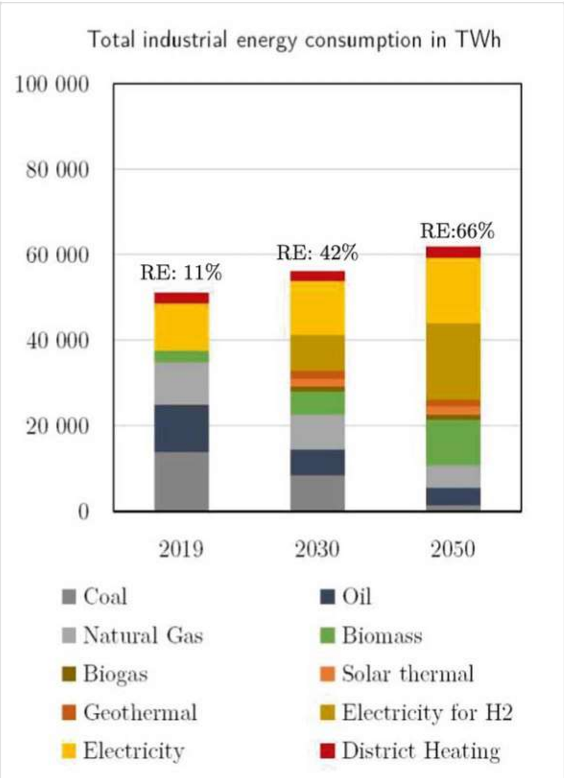


Figure 1.2 Projection of final energy consumption in industries, data source: [21]

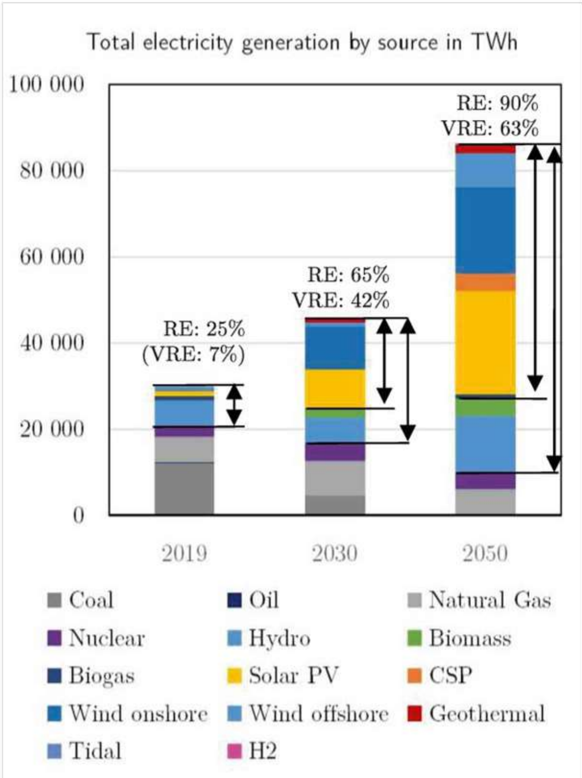


Figure 1.3: Projection of electricity generation, data source: [21]

To meet this demand, the capacity of intermittent wind and solar PV sources is projected to expand significantly, increasing the share of volatile RE from 7% in 2018 to a remarkable 63% in 2050, more than quadrupling total electricity generation capacity [19].

Accordingly, this highlights the critical importance of consumption flexibility for accomplishing energy transition, where the role of industry is of paramount importance for several reasons [21]. Reviewing both Figure 1.2 and Figure 1.3, industries will be the largest electricity consumption sector, accounting for about 43% of total electricity demand. In addition to the very expensive and difficult-to-realize undertakings of large-scale grid and storage expansion [17, 18], harnessing the flexibilities within the buildings and transportation sectors also presents its own set of challenges. The numerous small market participants at lower-level distribution power grids, each subjected to individual behavioral patterns, substantially complicates the coordination to provide flexibility and ensure consumption balancing at the large scale, making it almost impossible in practice [14, 22, 23].

In contrast, industrial facilities represent large consumption units at higher network levels that are, due to certain spatial limitations for renewable on-site production, even more reliant on large-scale power supply and consequently exposed to the adaption of supply fluctuations. This requires both technological adaptations including the introduction of flexibilities as well as the establishment of advanced operational concepts for managing corresponding dynamics in energy use. Above significant challenges, large synergies emerge between the sustainable supply of industrial processes and the balancing of large-scale fluctuating generation. Industrial plants acting as plannable, flexible players in power markets, not only open up the possibility to generate internal revenues but also represent a cost and resource-efficient way of balancing fluctuating supply on a macro-scale, thus significantly contributing to energy transition [14, 24, 25].

However, conventional energy management and control methods, as currently predominant in industrial plants, in combination with current energy market structures, only insufficiently meet the advanced operational requirements associated with more diverse and interconnected energy systems, especially considering highly fluctuating boundary conditions [26, 27]. Focusing on energy management and the predictable, flexible operation of industrial energy systems, this thesis investigates the impact and benefits of holistic planning, operation, and control through the utilization of a generically applicable mathematical optimization methodology.

1.2 Research Context and Problem Statement

Despite the urgent need for the adoption of decarbonization measures, the industrial sector still shows significant shortfalls in implementing appropriate sustainable energy solutions. Both in the integration of alternative, sustainable energy carriers and technologies but even more in implementing cutting-edge, state-of-the-art control and energy management systems (EMS) to meet the advanced operational requirements for harnessing efficiency improvements and managing fluctuating supply [28, 29]. In this relation, the precise consideration of future events on current decisions and vice versa is crucial for thoughtful operational decisions and strategies, which necessitates the use of advanced planning methods such as mathematical optimization. The development of respective tools and approaches to assist and improve the operation of energy systems has been of major research interest for decades ranging from novel control approaches to advances for plant-wide optimization as well as efficient methodical formulations and modular frameworks [30–33]. However, despite attracting interest due to potential operational improvements and associated competitive advantages, these concepts are only infrequently adopted by industrial enterprises, indicating to the persistent existence of implementation barriers and related operational and economic risks [34–35].

In general, potential obstacles to the widespread implementation of EMS can be attributed to uncertainties regarding the assessment of economic performance both in terms of expenses and benefits, as well as issues related to business processes and quality. In a comprehensive empirical investigation Brunke et al. [34] identified technical risks, limited access to capital, uncertainty about future economic conditions, insufficient top management support, uncertainties regarding hidden costs, lack of time, and other priorities as barriers for general energy efficiency measures. Furthermore, complicated integration of commercial tools, lack of expertise and experience within energy service companies, negligible improvements due to overly conservative operations, and lack of effort to change business processes are particularly valid with respect to non-technical operational improvements. Following a comprehensive review of energy management in manufacturing, May et al. [35] emphasized on the risk of adverse effects on production quality in case of significantly deviating planning. In this respect, Tombre et al. [27], showcased a decrease in production quality due to the violation of critical constraints affected by incorrect predictions. Additionally, information gaps in technical data and uncertainties of production parameters were detected as still prevalent in industries, resulting in difficulties in accurate modeling and prediction inputs [37]. Moreover in [38], potential foregone revenues due to conservative planning are indicated.

On a methodological level, performance deficiencies can be counteracted by enhancing and customizing EMS approaches to tackle specific effects, such as using a nonlinear multistage scenario tree approach [27], a robust adjustable optimization formulation [39], or a bi-level data-driven optimization [40]. However, these approaches show significant efforts in data processing, modeling, as well as deficiencies in reconfiguration and generic applicability (e.g. multivariate data analysis and extensive parameterization). The use of (meta-)heuristics as presented by Dengiz et al. [41] may reduce modeling complexity by simultaneously increasing robustness, however, such tailored approaches are of limited general applicability and adaptability. Consequently, besides certain performance improvements, such rather sophisticated approaches are affected by an intense modeling effort and high expertise in implementation and supervision.

In this regard, Isaksson et al. [42] highlighted the particular importance of efficient modeling and integration in order to avoid cost escalations in the implementation process. Especially considering that industrial plants tend to be historically grown structures and constantly changing facilities with different technological levels, also customization, adaptability, and adjustability of the systems represent decisive features [14, 43]. In this context, especially modularly structured modeling approaches are potentially advantageous. In particular, Mixed-Inter-Linear Programs (MILP), Unit-Commitment problems [33], and the energy hub concept [32] provide beneficial characteristics and are consequently recently of superior scientific popularity. For example, Halmschlager and Hofmann [44] adopted to the energy hub concept to present a modular optimization framework for industrial plants formulated as a MILP-based Unit-Commitment Problem. Moser et al. [45], presented a modular EMS approach for urban energy systems formulated as economic MPC. However, these approaches are presented only as single objective offline optimizations, without considering control tasks and respective interactions with the plant or dealing with uncertainties and inaccuracies. Thus, these are to be regarded exclusively as modeling approaches and concepts rather than deployable, real-time EMS. This research gap was especially highlighted in [46].

In terms of system architectures, the use of multiple interacting layers may exhibit functional advantages, especially when accomplishing heterogeneous tasks and objectives. Beykal et al., [40] use a two-layer EMS for scheduling and planning a chemical production under uncertainty, while alternative approaches [38, 47] employ real-time capable hierarchical strategies for storage management and control within HVAC systems. Above all, Fuhrmann et al. [1] introduced a two-layer model-predictive EMS combining economic optimization and real-time control using a lightweight MILP formulation. Despite its application to a rather simple energy system optimizing the heat supply of a thermal batch process, this concept exhibits prospective and promising features, therefore constituting an essential impact on this work.

1.2.1 Research Gaps

Conclusively, the following research gaps are identified and classified into methodological and application-specific aspects

Methodical

- Practical optimization approaches exclusively exist on a conceptual level, revealing significant deficiencies in terms of real-time capability and viability.
- Existing EMS tools typically require an elaborate, impractical, and resource-intensive implementation process.

Applicational

- Existing literature indicates substantial deficiencies in terms of comprehensive and insightful performance evaluations of EMS within authentic, realistic operational environments.
- Similarly, there is a pronounced associated deficiency in estimating performance divergences between theoretical case studies and actual real-world applications.

Rigorous modeling and data-acquisition processes, coupled with the requisite expertise for effective implementation and supervision, pose significant financial barriers and risks, impeding the adoption of EMS implementations. This indicates the importance of reducing implementation and operational effort. The multitude and variety of scientific works on EMS offer an extensive methodological set of useful approaches, concepts, and formulations, however, most of them represent concepts rather than viable reliable tools. The insights into the functional performance of these existing tools and approaches are largely restricted to overly abstracted or simplified application examples, thus failing to eliminate uncertainties about potential quality degradation or production constraints. Consequently, the operational risks and related costs may subjectively outweigh benefits, further hindering the broader penetration of EMS implementations within industrial enterprises.

These identified barriers and obstacles exhibit a strong interdependence, significantly influenced by new technological options for design improvements and operational efficiency efficiency measures. Hence, this thesis adopts an integrative approach that applies optimization across the entire thematical spectrum for establishing a sustainable and efficient industrial energy supply, ranging from energy systems design to real-time control applications.

1.3 Aim and Scope

Methodically, the central innovation aims at developing a generic, modular, and flexible optimization modeling framework for the holistic treatment of complex multi-energy systems. Subsequently, the applicational use cases comprise the optimal integration and dimensioning of new components in existing facilities and, above all, the holistic operational optimization and control of complex multi-energy systems. Consequently, the overall goal and culmination of the work is the incorporation of the modeling framework into a hierarchical optimization scheme denoted as energy management and control system (EMCS) that simultaneously accomplishes operational optimization and predictive online control. The added value of such an EMCS lies not only in the optimization of internal energy use but also in the fact that decentralized energy systems represent potentially cost- and resource-efficient means of facilitating large-scale grid-bound feed-in of renewable energy sources. Evidently, due to the generic and modular composition, the proposed EMCS method is intended to be especially advantageous with the increasing complexity of energy systems and problem statements. Therefore, it is essential to use a versatile and flexible energy system as a reference use case for the development of the method. In the derivation of this Reference Energy System (RES), the optimization approach is applied to a design task for the integration of new technologies into a persistent system to improve performance and reduce environmental impact. Conclusively, the research approach is specified by the following objectives and related research questions.

1.3.1 Research Objectives and Questions

Objective 1 - **Optimization Modeling**: Development of a practical, generic, modular, and adaptive optimization modeling framework for the holistic treatment of energy supply systems.

- Q1a: How is the method fundamentally structured and what basic optimization concepts are adopted and incorporated?

- Q1b: What are essential advantages compared to the state of the art and in which applications are they particularly effective?
- Q1c: How can a practical and flexible applicability be established?

Objective 2: **Derivation of the Reference Energy System as a Generalized Use Case** which is representative for the specific subsector of low-temperature industrial processes

- Q2a: Which components and technologies are representative for the specific subsector and how can they be suitably structured according to the present state of the art?
- Q2b: Which improvements can be achieved through the introduction of new sustainable technologies?
    - How much does the respective control concept affect the optimal design?
    - Which discrepancy can be identified between economic and environmental goals?

Objective 3: Development of a generic and adaptive method for the **holistic operative energy management and control of complex multi-energy systems** and the **evaluation of respective performance improvements.**

- Q3a: How can the presented modeling method be incorporated and extended to a viable real-time capable EMCS?
    - Which essential operative procedures are realized and which interaction between the plant and its operational environment is employed?
- Q3b: Which operational improvements can be achieved by applying the holistic EMCS to complex multi-energy systems?
    - How does the operation differ from conventional control concepts?
    - Which differences between the conventional and state-of-the-art design can be identified?
    - What is the influence of methodical parameters and prediction errors on the optimization performance?
    - Which prediction and planning accuracy can be expected?

1.3.2 Research Approach and Structure of this Work

Aligned with the division of the research gaps into a methodological and an applicational part, also the research objectives and the research approach can be classified in a comprehensible structured way according to Figure 1.4 (see Page 11). Initially, Chapter 2 provides an overview of the fundamental methods and concepts utilized in this work to outline the state of the art. Chapter 3 provides a thorough explanation of the modular optimization framework and the EMCS. The first use-case in Chapter 4 derives the RES and demonstrates the optimal integration of sustainable technologies into existing systems by applying the developed optimization superstructure. In the second use-case in Chapter 5, the designed system is taken up to execute a comprehensive performance demonstration of the developed EMCS in a dynamical simulation study.

1.4 Accompanying Academic Work

In addition to the central contents of this dissertation, further accompanying scientific contributions have been created and published.

First-Author Publications

- Paper A: "Optimal Integration of a Stratified Thermal Energy Storage into a Multi-Component Industrial Energy System"[48]
- Paper B: "Flexibility Identification of an Industrial Production" [49]

Contributions as Co-Author

- Paper C: "Simultaneous integration of heat pumps and different thermal energy storages into a tightened multi-period MILP HENS superstructure formulation for industrial applications" [50]
- Paper D: "Energy management for thermal batch processes with temporarily available energy sources– Laboratory experiments" [2]
- Paper E: "Multi-stage optimization for marketing industrial flexibility" [25]

Patent Application

Additionally, based on the novelty of the methodical developments and the promising potential for adoption in business environments, a patent application has been filed.

- „Verfahren zur Konfiguration und zum Betrieb eines Modellbasierten Optimal-Energiereglers innerhalb eins Prozessleitsystems"; Sumitted at the Austrian Patent association, 2022-04-29, Submission Nr: A 60058/2022, IPC: G06F [51]

The overview in Figure 1.4 illustrates the distribution of the individual research objectives across the Chapters of this dissertation specifically highlighting their further incorporations (blue arrows) and mutual influences (black dash-dotted arrows). The thick-bordered frames represent the core content of this dissertation. Additionally, the thin drawn fields indicate to accompanying research work published by me as the lead author while the thin dashed fields indicate the adjacent research work as co-authorship of published peer-reviewed work. Both of which are described below in Section 1.4. including an explanation of the contextual relations and influences on the topics of the work. Accordingly, the chronological interdependencies of the individual research contents become immediately evident. In particular, the thematic applications, each serving as a dedicated use case, have a fundamental impact on methodological advances.

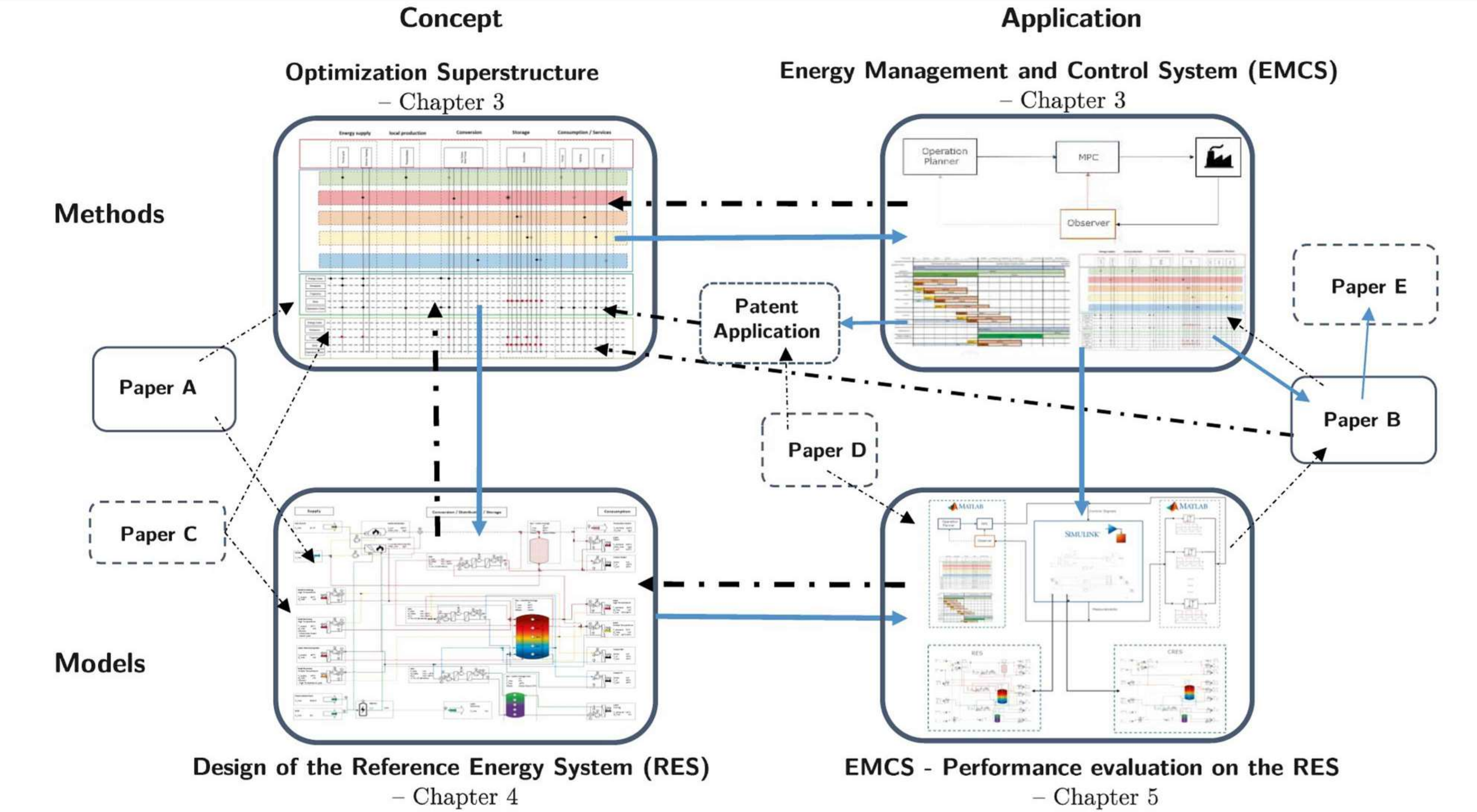


Figure 1.4: Illustration of the research approach and interrelation of comprised research contents

Contextual Relations and Influences to the Topics of this Dissertation Paper A and Paper C are to be classified thematically as well as chronologically before the content of the dissertation.

Paper A specifically examines the thermal management of a stratified storage tank, contrasting the benefits of economic optimal operation against quality degradation due to undesired temperature peaks. Since a multi-objective function is considered for switching operational priorities within an energy system with different energy services and cost sources it represents an essential basis for both the optimization superstructure and the reference energy system.

My contribution in Paper C comprises the basic modeling of heat pump characteristics to be modularly integrated into a HENS superstructure. Thus, experience was also gained for both, superstructure-based modeling as well as the integration of heat pumps into existing systems, a target objective for the RES, designed in Chapter 4.

Paper D, which presents the experimental laboratory test of the control concept, has already been discussed in the preface. Additionally to the model development, my contribution to the definition and interpretation of the experimental results brought vital experience for the simulation-based performance evaluations on the complex RES system. Successively, promising experimental as well as simulation-based improvement potentials led to the proposal of the patent, which fundamentally includes the contents of this dissertation.

Additionally, Paper B and Paper E already deal with content that builds on the findings and methods presented in this dissertation and has arisen thematically from the Industry4Redispatch project.

By adopting the developed superstructure, Paper B introduces a two-stage approach to identify and quantify potentially existing flexibilities based on variation of the optimization objective. Paper B therefore provided feedback on the modular configuration of the objective function in the superstructure.

In Paper E this approach was taken up by the lead author and further incorporated into a multi-stage approach to consider market price signals for trading the identified flexibilities.

Moreover, the development of the optimization superstructure was essentially influenced and methodically enhanced by the experience gained from the patent application. To address the identified application-related gaps, the focus was on introducing capabilities and features for easy and structured integration into typical process control system structures.

Complementary Academic Activities

Beyond the scope of this dissertation, my academic activities have extended further levels of dissemination. On the one hand, I had the privilege of presenting my research topic and discoveries to pertinent audiences at professional conferences, as well as in scientific reports. Furthermore, I was given the opportunity to share my acquired skills in the course of teaching and guidance of a master's thesis. For the respective list of activities please refer to the Appendix in Section A.

It's a learning curve.

MARC ODRON

2 Theoretical Background and State of the Art

Aim and Scope Initially, this chapter gives an introduction to the research topic and the employed methodologies and clarifies specific terms and concepts according to the perception of this work. The selection specifically aims to provide a fundamental overview of the state of the art on energy management and process control in industrial energy supply systems and the challenges in the respective industrial subsector of low-temperature heat processes. It is important to recognize, that specific terms discussed are often interrelated and may either overlap very strongly or are mutually dependent. In particular, the use of different terms to describe similar content, or vice versa, is also a notable observation in the existing literature. In order to create a clear picture, this chapter systematically provides precise definitions of each term and explains their interconnections within the broader context of energy systems management. The structure of this section follows a top-down approach, starting at the level of energy systems and gradually examining more specific topics.

2.1 Energy Systems

An energy system is understood as a comprehensive set of interacting technical facilities and processes related to energy production, conversion, storage, and distribution in order to provide final energy services to end users. Energy systems may range in scope, from a very micro scale such as electronic devices to a very macro scale such as the entire energy landscape of a country with arbitrarily definable boundaries. In this dissertation, emphasis is placed on decentral energy systems (DES), which include near-consumer energy generation and may comprise several different energy forms such as electricity, thermal energy for heating and cooling, as well as fossil fuel or synthetic energy carriers. Industrial energy supply systems, which constitute the central use case for the developed methodological set, are typical DES but also the energy systems of residential areas, isolated energy grids, or energy communities for which this dissertation also holds particular relevance. Especially due to the rather distributed renewable energy suppliers, such decentral multi-energy systems are currently of gaining importance as they are typically connected to medium- or low-voltage grids and thus may contribute to alleviating stress in transmission grids.

The developed methodology particularly aims to provide universal applicability without being restricted to specific processes or subsectors. However, according to the use cases of the research project *EDCSproof*, the main focus is on processes with a heat demand at a temperature level below 160°C. Particularly since technologies for renewable generation, energy storage and integration of thermal and electrical energy are already accessible, this sub-sector was focused, in order to conduct the intended laboratory tests using market-available components. Consequently, as this subsector represents the technological and application framework of this work, subsequently an overview of respective processes, energy use, and both conventional and sustainable technologies is provided.

2.1.1 Industrial Energy Systems for Low-Temperature Heat Processes

On a global level, the industrial sector accounts for about 37% of global final energy use [20, 52] and still more than 30% in the EU28 [53]. In Austria, a large share of 64 TWh (25%)

can be related to process heat while in Germany, this share comprises about 40% (532 TWh) and 53% in Switzerland (24 TWh) [54, 55]. Considering process heat consumption, the temperature level is a crucial characteristic as it restricts possible technologies and energy carriers that can comply with the specific requirements. In [20] a comprehensive macro-level investigation of temperature levels of industrial process heat demand is presented. The required heat supply temperatures range from very low levels of about 40°C up to 1400°C in very energy-intensive processes, such as the steel and materials industry. In the EU 28, about 50% of total heat demand is related to high-temperature processes that require more than 500°C. On the other hand, 30% of the final heat demand requires temperatures below 160°C. Respective industrial processes occur to a large extent in the industries of food, textile, pulp and paper, or chemicals.

Industrial Low-Temperature Heat Processes As can be observed from Table 2.1, which presents a selection of respective processes, these involve particularly washing and drying processes, evaporation as well as sterilization, pasteurization, and distillation which typically appear in the food, textile, chemical, and paper industries [56]. A comprehensive overview of processes is presented in the respective Best Available Techniques (BAT) Reference Documents for food industry, which is a central focus of this study [57], as well as for the pulp and paper [58] and textile industries [59] which exhibit similar temperature requirements and thus show significance in a broader context.

Table 2.1: temperature levels of thermal production processes, data source: [20]

sector	thermal processes	temperatures
food, drinks	pre-heating	20-60°C
	pasteurisation	70-120°C
	sterilization	70-120°C
	distillation	40-100°C
	drying	40-250°C
	reconcentrating	60-85°C
	baking	150-250°C
	cleaning	30-70°C
	evaporating	40-160°C
	thickening	125-130°C
textile	dyeing	50-130°C
	cleaning	30-70°C
	polishing	40-100°C
	bleaching	40-80°C
	varnishing	50-80°C
chemistry	pre-heating	40-60°C
	cooking	90-110°C
	distillation	110-300°C
	thermo-forming	120-150°C
	reconcentrating	60-75°C
	thickening	70-130°C
	cleaning	30-70°C
wood	drying	50-80°C
	shrinking	100-150°C
	varnishing	50-80°C
metall	galvanics	20-100°C
	pickling	30-60°C
	drying	60-90°C

Table 2.2: temperature levels of industrial waste heat sources, data source: [20]

waste heat source	temperatures
flue gas	50-400°C
cold water unit	20-45°C
air compressors	30-70°C
cleaning waste water	30-60°C
cooking processes	70-100°C
motors and drives	70-100°C
CHPs	80°C
injection moulding	30-80°C

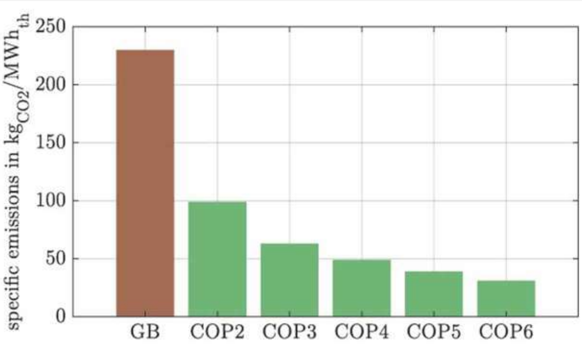


Figure 2.1: Specific CO_2 emissions of heat pumps as a function of COP compared to gas-fired heat generation based on the CO_2 content of the Austrian electricity mix, data source [56]

These processes and subsectors are of particular interest as their temperature demands are in the reasonable range of established renewable heat generation technologies such as solar-thermal, geothermal, and heat pumps. According to [55], the major final energy carriers in the austrian industrial energy supply are natural gas with more than 55%, and electrical energy with about 34%. Regarding heat consumption, 64% are used for process heat or thermal applications. With 23.8 TWh (39%), steam is the major energy carrier in final energy use, with over 90% of it generated from fossil fuels. With subject to heat demands below 160°C this share still accounts for more than 60%. Additionally, more than 10% of final industrial energy consumption can be attributed to the food, beverages, milk, and tobacco industries, in the EU28 [57]. In Austria, where this sector accounts for about 7.6 TWh (9% of final industrial energy consumption), a very large number of about 3,900 companies can be classified to this branch. Considering these numbers, it's obvious that 99% of the companies can be categorized as small or medium-size enterprises (<250 employees) [60].

The comprehensive analysis of the food, drink, and milk industries presented in [57] emphasizes a crucial issue: The wide variety of products and production steps is particularly characteristic for the food industries, leading to the challenge of very fluctuating consumption profiles for both process heat and electricity. The high variety of products and production steps in a factory results in volatile demand profiles of process heat and electricity. This requires, in particular, fast-responding heat generation units for which the efficiency is therefore of minor relevance. Also, many processes and production steps still need the support of human operators and workers, which is, among others, a reason forthe limited potential for scheduling and automation in the operation of the various production steps [61].

Energy Supply Systems in the Industrial Low-Temperature Heat Sector A general overview of common technologies and the state of the art of the supply of respective industrial processes is given in BAT reference documents for the food, drink, and milk Industries [57] as well as for the pulp and paper [58] and textile industries [59]. Additionally, a very comprehensive overview of energy facilities and technologies used in the respective industrial plants is provided in [31]. Collectively, electricity and heat account for the largest share of final energy services, followed by cooling and gas. When steam and electricity are required synchronously mostly on-site co-generation facilities are used. The main transport media for heat is steam, followed by hot water, thermal oil, refrigeration fluids, and air. According to the comprehensive study in [57] following high-level characteristics are summarized.

- Basic gas-fired boilers with an efficiency between 75-90% are still dominant in heat-only applications. This also includes direct heating of the product with natural gas or extra-light oil.
- Combined heat and power units (CHP) are the prevalent concept for on-site power generation: While high-pressure steam boilers with extraction turbines are primarily used at higher energy loads and temperatures, at lower scale and temperatures, gas- or diesel-fired engines (piston engines) with waste heat recovery for steam production, heating water or drying are employed. Typical overall efficiencies are in the range between 75%, and 95% when exhaust gas can be used for drying processes (direct contact)
- Common primary energy carriers are natural gas, light oil, and coal
- Thermal energy storage systems are commonly utilized in heat supply systems, whereas other forms, such as batteries or gas storage are infrequently present.

Energy Efficiency and Sustainable Technologies Addressing energy efficiency in industrial production, the study on industrial waste heat recovery in [62] indicates large unused waste heat potentials in a wide variety of production processes, pointing out that their economic benefits are often ignored. In conventional, unidirectional systems, waste heat is "disposed" at additional expense rather than being considered as a free avialable source used to generate energy. Unused waste heat potentials often occur due to low temperatures that are inadequate for direct reuse or existing temporal and spatial gaps between the waste heat source and the heat-demanding process. The additional technical equipment required for utilization constitutes a decisive barrier even under economic conditions [63]. However, considering the need for a sustainable heat source for heat pumps, waste heat becomes of high interest, as the thermal energy content mostly exceeds alternative environmental heat sources like ambient air or water. As previously stated, with the new technological developments in the field of high-temperature heat pumps and increasing CO_2 emission reduction potential can be exploited based on the source of waste heat [64]. In this respect, Table 2.2 on page 15 shows the process temperatures of industrial waste heat are sufficient for reuse as a source for industrial heat pumps to maintain reasonable COPs. In reference to [56], Figure 2.1, compares potential CO_2 emission savings achieved by switching from gas-fired heat generation to heat pumps for different COPs under the assumption of using a renewable heat source. Conclusively, waste heat recovery is an investment, but it is free of charge during operation. In addition, the operating costs for waste heat disposal, e.g. for the operation of fans in a recooling system, can also be saved.

As reported in [32], renewable generation was still of subordinate significance in industrial plants in 2017. However, in general, the scientific interest in the utilization of renewable thermal energy in industries became an essential measure in energy transition. Especially the impact and potential of heat pumps for the reduction of carbon emissions found extensive attention in research and is also a very popular subject concerning energy-related policy. In this respect, it is referred to [64], which outlines the general market overview, research status, and technology readiness, while application potentials, performance characteristics, and economic feasibilities are particularly addressed in [65]. Moreover, potential applications and concepts for increasing industrial waste heat utilization are given in [56]. Austria especially takes a leading role in this research field. E.g. the development of high-temperature heat pumps [66], the utilization of renewables [54], and also the use of solar-thermal collectors for process heat generation [42]. These contributions partly originated from the *EDCSproof* predecessor projects, namely *EnPro*[4] and *Renewables4industry*[5]. In the project *Renewables4industries*, technological decarbonization strategies were derived following a comprehensive process analysis and corresponding requirements. The project *EnPro* examined the integration of solar thermal collectors and heat pumps for process heat generation in various industry sectors and developed design guidelines for efficient systemic integration. Based on the use cases of a bakery and a brewery [67], the investigation identified integration potentials for heat requirements of up to 200°C. However, this investigation only considered the static perspective using a pinch point approach, thereby determining an economic potential for 7.7% of total process heat demand in Austria.

In addition to alternative sustainable generation, significant potential for enhancing efficiency can also be found in the integration of decentralized storage and improving the management

[4] https://www.klimafonds.gv.at/wp-content/uploads/sites/16/2017EnPro-ErneuerbareProzesswaerme.pdf

[5] https://energieforschung.at/projekt/abstimmung-des-energiebedarfs-von-industriellen-anlagen-und-der-energieversorgung-aus-fluktuierenden-erneuerbaren/

of currently available storage capacities. A comprehensive assessment of general energetic aspects and economics of thermal storage is presented in [68, 69], while practical examples for the integration of thermal storage are shown in [50, 70, 71]. In addition, the potential of optimization-based management of thermal and electrical storage is specifically shwocased in [27, 38, 48, 72].

Consequently, particularly for respective multi-energy systems, considerable performance improvements facilitating technical, economic, and environmental advantages, such as reducing fuel consumption, emissions, operating costs, and increasing system reliability are prospected. However, for the successful integration of these measures, it is crucial to deeply incorporate energy management within organizational procedures. Specifically, optimization-based EMS enable to use synergies in a beneficial manner, eliminating the isolation of individual challenges [26]. As highlighted in section 1.2, particularly with respect to flexible operation, the energy systems of the manufacturing industries, in general, do not yet meet these requirements, both in terms of design and operation [28, 29, 34].

2.1.2 Energy Management and Process Control in Industrial Plants

In the manufacturing industry, decision-making and operational procedures are typically distributed across different hierarchical organizational levels. Each of these levels typically relies on a range of digital tools to assist, automate, and streamline crucial procedures, enabling efficient workflows. The automation pyramid [73] serves as a well-established concept for classifying operations and assigning corresponding digital automation tools to each organizational level. Higher levels primarily utilize decision-support and planning tools, while lower levels focus on the automatic control of technical processes based on predefined rules. In between, monitoring and process control systems play a crucial role in maintaining operational supervision. The lowest field level includes sensors, actuators, and other devices that interact directly with the physical processes or machines. These also collect data and send signals to the higher layers in a mostly entirely automated workflow. Similarly, the control level is automated by using Distributed Control System (DCS), Programmable Logic Controllers (PLC), and Proportional-Integral-Derivative (PID)-controllers, while the supervisory level (SCADA) typically represents the interface to the human operators. The management and enterprise levels are responsible for production planning, resource allocation, and high-level, enterprise-wide long-term strategies. These long-term strategies are largely based on human decisions with the assistance of enterprise resource planning systems.

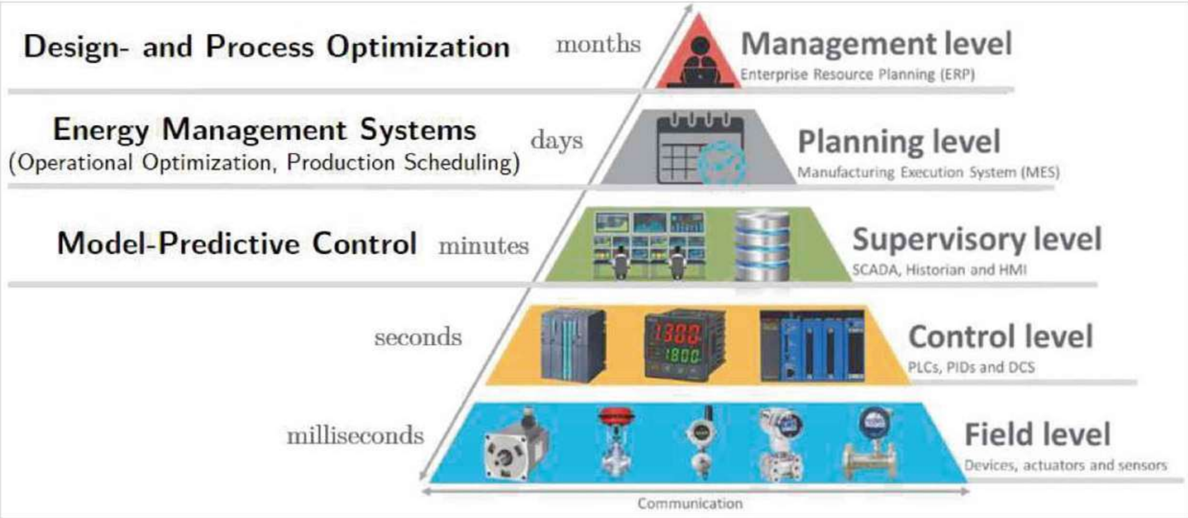


Figure 2.2: Categorization of optimization tasks according to the automation pyramid (extended from [73])

While energy management has traditionally held subordinate decision importance, rising energy prices, the urge to reduce emissions, evolving operative, economic, and regulatory conditions, and potential risks in supply security are among the essential drivers that call for an intensified systematic integration of energy-related decisions into the different levels. To assist organizations, and companies in effectively managing energy resources, the international standard ISO 50001 has been developed to facilitate the establishment of a systematic integration framework. As these activities encompass a broad spectrum, including design, planning, operation, and monitoring in a complex technical, organizational, and economic environment, the use of assistive tools becomes inevitable. As illustrated in Figure 2.2, mathematical optimization offers a sufficient spectrum of promising functions and applications, comprehensively introduced in Section 2.3, to be profitably applied at various levels. Notably, in this work, the interpretation of individual terms and applications adheres to the classification outlined in Figure 2.2 referring to both application level and time scales. Regarding MPC applications, these are often also employed on the control level. In this work, however, they are regarded as supervisory elements, specifying the setpoints for the subordinate control-level facilities. Concerning the terminology of energy management, occasionally terms such as "energy procurement", "energy controlling" and "energy monitoring" are associated. A precise delimitation is difficult in practice since on the one hand, there are different definitions of the terms and on the other hand, the terms are partly defined quite abstractly. Various definitions for energy management in literature are summarized by [28]. However, according to Figure 2.2, in this work, an energy management system (EMS) is understood as an integrated digital tool used to optimize, control, and improve the operational performance of energy systems and the related use of energy resources.

2.2 Mathematical Optimization

Mathematical optimization, often also denoted as mathematical programming constitutes an entire sub-discipline and research field within applied mathematics. Primarily, optimization aims to identify the most favorable states of systems within a typically constrained solution space of its decision variables, based on specific, definable evaluation criteria. The term optimization, for which several definitions, descriptions, and delimitations are present in literature, e.g.: [74, 75], is colloquially often adopted for improvements, however, without proving or referring to optimality in the mathematical sense. In contrast to the pure description or modeling of systems, the definition of a so-called optimization problem additionally comprises the specification of an objective function as characteristic element to evaluate and subsequently determine optimal solutions.

Consequently, optimization problems are not related to unambiguous solutions but are rather considered as undeterminate systems of equality and inequality constraints that specify and bounds the solution space of its variables. Hence, an optimization problem fundamentally consists of variables, constraints, and the objective function as optimality criteria. While all variable combinations that satisfy the constraints are considered admissible solutions, only the best possible solutions with respect to the objective function are denoted as optima. The solution method or algorithm for determining the optima is regarded as solver or optimizer and the whole process as optimization.

2.2.1 Classification and Distinction

Reflecting its manifold, multifaceted, and widespread fields of application, mathematical optimization can be classified on various levels and aspects. Most importantly, these regard the type of variables (continuous, discrete, binary), mathematical formulations (linear, non-linear, static or dynamic programs (DP)), dimension of the objective function (single-, multi-objective), or distinctions such as deterministic or stochastic problems (in the presence of uncertainty). Apart from the mathematical perspective, a practical classification differentiates between decision and approximation problems. While in decision tasks, variables primarily represent decisions or potential actions that can be manipulated, in approximation problems, the variables rather serve as parameters for optimal approximations of certain relationships, guided by a specific quality functional. The categorization of the problem is directly related to appropriate problem definition techniques, optimization procedures, and solving algorithms. These comprise linear programming (LP), nonlinear programming (NLP), mixed integer programming (MIP), mixed-integer linear (MILP), and nonlinear programming (MINLP) as well as evolutionary algorithms or reinforcement learning to explore the solution space and find the optimal solution that satisfies the constraints. Most algorithms iteratively evaluate and update the solution until an optimal or near-optimal solution is reached [74].

Optimization problems (OPP) are typically stated using a specific notation, which is stated in the equation sets in Eq. (2.1) in a general form as well as specifically for MILPs in Eq. (2.2). The essential elements of the problem are the variable quantities representing the solution and decision space, the constraints that describe the relations of the considered system, the objective function as criteria for the evaluation of solutions, as well as parameters and constant quantities of system behavior. Accordingly, solutions consist of two parts, the optimal values of the objective functions as well as the corresponding choice of variable combinations. OPP are often denoted by the term "program" which dates back to the beginning of Operations Research, where solutions were interpreted as programs in the sense of optimal procedures and schedules for operations, logistics, or allocations. In the case of a scalar objective function C, D, and F are column vectors, A and B are the coefficient matrixes for x_c and x_d. For an NLP or LP, x_d is an empty set.

$$\min_{x,y} f\ \boldsymbol{x_c}, \boldsymbol{x_d} \tag{2.1a}$$

$$s.t.\ \ h(\boldsymbol{x_c}, \boldsymbol{x_d}) = 0 \tag{2.1b}$$

$$g(\boldsymbol{x_c}, \boldsymbol{x_d}) \leq 0 \tag{2.1b}$$

$$\boldsymbol{x_c} \in X \subseteq \mathbb{R}^n\ \ \boldsymbol{x_d}\ \in Y \subseteq \mathbb{Z}^n \tag{2.1d}$$

$$\min_{x,y}\ C^T\boldsymbol{x_c} +\ D^T\boldsymbol{x_d} \tag{2.2a}$$

$$A\boldsymbol{x_c} +\ B\boldsymbol{x_d}\ \leq F \tag{2.2b}$$

$$\boldsymbol{x_c}\ \in X \subseteq \mathbb{R}^n \tag{2.2c}$$

$$\boldsymbol{x_d}\ \in Y \subseteq \mathbb{Z}^n \tag{2.2c}$$

Problem Complexity When it comes to the process of optimization, the complexity of the problem is crucial, where various aspects and perspectives need to be considered. Obviously, the number of variables, constraints, and objective criteria substantially affects the size and complexity of the fundamental problem. However, from a computational point of view, the most important aspect is the effort required to find appropriate optimal solutions. Thus, in addition, the problem type and respective optimizers come into focus. In mathematics, complexity theory classifies OPP according to their worst-case computational effort, where two fundamental classes are distinguished. The polynomial class P includes problems that can be solved in polynomial time, i.e., the computational time to solve a problem may be represented by a polynomial function (p is a finite positive number) of the number of variables n $O(n^p)$. Therefore, the formulation of problems that satisfy the class P is desirable, since in practice relatively short solution times can generally be expected.

On the contrary, for NP-complete problems (NP stands for "nondeterministic polynomial time"), no existing algorithm can provide a solution for the most difficult problem of the same type in polynomial time. Consequently, the computational time for optimizing NP-complete problems typically scales exponentially with the problem size $O(2^n)$. This represents an essential limiting criterion, often necessitating trade-offs in problem definition. Nonlinear problems are typically not efficiently solvable through gradient-based methods. Despite the increased use of heuristics or genetic evolutionary algorithms, this dissertation seeks to harness the benefits of linear programs.

Linear programs, in particular, are characterized by strict convexity, which means that every linear combination of different admissible solutions also represents an admissible solution. As a further consequence, this guarantees the existence of unique global optima. Consequently, LPs fundamentally belong to the polynomial class, which epitomizes its efficient application. Polynomial algorithms for linear programs include the ellipsoid and the interior-point method, which were already introduced in the 1970s and 1980s. However, the simplex algorithm, which dates back to the 1940s is the most widely applied and adopted method in linear optimization. The method is based on the fact that the optimal solution of an LP always occurs at a vertex. It initially determines a feasible solution and then systematically iterates through the edges of the solution polytope, constantly proceeding toward the optimal node. Despite its generally efficient and well-observable solution procedure, in theory, examples of exponential time are existent [74, 76].

2.2.2 Mixed Integer Linear Programming

While linear programs are characterized by their efficient handling and solution, they are subject to the crucial disadvantage that the scope of problems, processes, and systems they can adequately represent by such is limited. However, by creating a MILP through the additional introduction of discrete variables, an almost unlimited extension of the application range for real-world problems is achieved. Due to practical features and mathematical characteristics, MILP has experienced high scientific appeal and has produced significant achievements nowadays providing valuable benefits in a wide range of applications [75, 77]. Utilizing and adapting these beneficial characteristics, the developments and explorations in this dissertation also rely on the application of MILP.

MILP Optimizers and Algorithms The handling of the combinatorial character due to the existence of integer variables, which can be interpreted as decision trees, is the most challenging issue when solving MILP problems. Particularly, the great importance of the simplex algorithm mentioned above is also attributable to the fact that it is widely adopted and incorporated in the powerful commercial MILP solvers. Predominantly, the simplex algorithm is employed to determine the solutions of the LP-relaxations and its dual problems, representing the upper and lower bounds of each corresponding progression step. Additionally, branch&bound, cutting planes, or branch&cut (combination of both) methods are typically adopted to reduce the number of potential nodes by either discarding sub-optimal branches or introducing extra cuts to further tighten LP-relaxations within the decision tree. While the computational effort for solving MILP generally scales exponentially with the number of integer variables n_d with $O(2^{n_d})$, however, they are still more efficient to solve than general NLP [75]. Presently, very powerful and efficient solvers for MILP problems are commercially available, such as the Gurobi optimizer, the IBM ILOG CPLEX optimizer as well as Mosek or the FICO Xpress Solver. In this work, the Gurobi optimizer [78] served as the primary computational solver (Version 9.12 and 10.01). The process of model formulation and the development of associated methods were executed within the MATLAB [129] environment, leveraging the capabilities of the YALMIP optimization toolbox [79].

Compactness, Convex Hull, and Tightness Despite their importance, the computational effort in solving optimization problems not only depends on the solution algorithms but also on the fundamental problem definition. Specifically, the attributes compactness, convex hull, and tightness are decisive when describing the solution space of OPP. Compactness denotes the size or complexity of the problem formulation with respect to the number of variables and constraints. A problem is considered more compact and typically easier to solve when it involves fewer variables and constraints. Moreover, the convex hull represents the smallest convex polytope that contains all feasible solutions of the problem. In this context, tightness assesses how close the linear relaxation of the MILP approximates the convex hull of all admissible integer points, and thus also refers to the precision of the relaxation. Although both compactness and tightness are critical for efficient problem formulations, there is typically a trade-off. For instance, achieving tightness might require additional constraints, which may negatively impact compactness [75].

2.2.3 Objective Functions

Considering optimization as a decision-making tool, the importance of the decision criteria comes to prominence. Representing the instrument to evaluate and compare different admissible but also inadmissible variable combinations with respect to optimality, objective functions must be regarded as decisive elements in optimization problems. Fundamentally, decisions and corresponding solutions can be evaluated from different perspectives or subject to different aspects and categories that generally tend to be mutually contradicting or represent non-substitutable quantities. Typically, objective criteria may represent monetary, environmental, temporal, or geometrical aspects as well as safety, resource use, well-being, or physical parameters such as temperatures, or mechanical stresses in design tasks. Moreover, for instance, in game theory, different agents may be following different subjective preferences and consequently may have seperated OF, respectively. Also, the existence of uncertainty can be considered and treated sufficiently by incorporation in objective criteria. Most common trade-offs in Energy Systems arise between economic and environmental aspects, however in conceptual design often trade-offs arise between efficiency vs. maximum power [80, 81].

Methodically, an essential distinction can be made whether the objective is expressed by a scalar or vector-valued function, which significantly affects the procedure for the identification of optima. While the optimum of a scalar or single-objective function is unambiguously linked to the optimization of the problem, the simultaneous existence or consideration of several different criteria potentially introduces optimization conflicts and consequently decision complexity. (Apart from the possibility that there exists one solution, which simultaneously appears to be the optimum of all criteria. Though theoretically possible, this practically rare case holds no further significance in this respect). According to the principle of Pareto optimality, a possibly infinite number of different, non-dominated solutions may exist [80]. Moreover, exclusively in the case of the existence of mutually subjective preferences, a multi-objective problem may be transformed to a single objective. Thus multi-criteria decision-making is strongly dependent on the preferences of mostly human decision-makers. Due to the subjective nature of preferences, the mathematical treatment is not an unambiguous and straightforward process and there are different solutions types and methods.

Most conveniently, different criteria are incorporated into a single scalar function that can be optimized. For this scalarization process, there are various methods and procedures, which show different suitability depending on the type of problem and the information basis. Decisive factors are whether these are known a priori, as well as the establishment of an equitable basis for evaluation and comparison. According to the theory of welfare economics, there exists a utility function that describes the total utility of all criteria and consequently defines optimality [82]. However, in practice, the determination of such a function accurately incorporating all criteria and preferences is, especially a priori, a rather invaluably extensive task and can only rarely be applied. For practical and convenient application, a variety of viable mathematical methods exist, which however may abstract and also distort the original problem to a certain extent.

Fundamentally, two types of approaches can be distinguished, either defining the preferences in advance (a priori) or choosing the preferred solution during or after the optimization process (a posteriori). A posteriori methods typically represent the original mutlicriterial problem as a set of Pareto optimal solutions (Pareto Frontier) to provide a profound basis for a posterior decsion on the optimal solution. However, this typically requires a more elaborate optimization process, which is why a priori approaches are often more attractive when a quick solution is needed (e.g., in operational optimization or MPC).

A Priori Specification The most common approaches combine individual objectives by means of mathematical or statistical weighting methods. Most commonly, the construction of scalar functions uses the linear normalized weighted sum approach Eq. (2.3), which is especially very convenient for linear problems.

$$J = \sum_{j=1}^{nj} \alpha_j \, (\boldsymbol{j}_j) \tag{2.3}$$

In Eq. (2.3), α_j denote the respective weightings for the individual contributions $\boldsymbol{j}_j$. Since the individual target functions can be of entirely different magnitude, special emphasis must be placed on an appropriate normalization for equitable and consistent treatment. Ideally, each criterion in the weighting function only takes values between 0 and 1 in a dimensionless manner. As shown in Eq. (2.4) this normalization maps the criterion independently of its original range.

$$J^0 = \frac{\mathrm{J}\,(\mathbf{x}) - \mathrm{a1}}{\mathrm{a2} - \mathrm{a3}} \tag{2.4}$$

The values α_1 and α_3 are to be understood as certain lower bounds and α_3 as an upper bound. The more precise these values are, the better the normalization performance. In [83], a variety of approaches for estimating these bounds, also known as utopia points are presented. However, it may potentially require extensive effort to determine respective values, consequently, more simple estimable approximations are often used by accepting little normalization drawbacks. The arithmetically weighted sum approach has been extensively applied and also adapted. However, due to certain inabilities, especially in nonlinear problems, alternative, more sophisticated mathematical harmonizing and weighting methods were investigated such as the weighted product method, general weighted exponential sum, or exponentially weighted criteria. In addition to approaches based on mathematical averaging, several advanced alternative approaches were presented, such as the ε-constraint or bounded objective function method, which focuses on the hierarchically most important objective and presents the others as constraints, or the weighted Chebyshev method with a min-max formulation. Moreover, in the goal-programming method, certain partial targets are specified for each objective in order to minimize the total deviation from the target vector (subjected to a certain norm) to obtain the optimal, multi-criteria solution. Additionally, also sequential methods are based on a classification of objectives according to importance, such as the lexicographic or hierarchical method have proven suitable applicability. In general, scalarization allows a simple treatment, but also abstracts and may also distort the original problem, as individual weightings are to a certain extent subjective [80-83].

2.3 Optimization in Energy Systems Engineering

In energy systems engineering, especially two central types of optimization problems emerged of major importance as the most valuable, beneficial, and significant applications: Design and operational optimization. Both are extensively adopted within the scientific community, which has developed a wide variety of customized solution approaches and corresponding problem definition concepts. This is mainly due to the high implementation effort or high costs of corresponding commercial software packages. Similarly, the use of several different software packages is a barrier to an integrated, automated operation and process. The tool of optimization has demonstrated great versatility in many instances, particularly in intricate decision-making processes. Nevertheless, long setup and solution durations have impeded a more widespread adoption.

2.3.1 Operational Optimization

In general, operational optimization aims to maximize performance and resource efficiency in systems or processes over a specified time horizon within fixed system design, configuration, and production capacities. In the industrial context, typical applications range from the planning of production, scheduling of processes, logistics as well as the utilization of energy generation capacities and process control. The execution can be both selective at a point in time for finite periods or continuously performing a receding horizon scheme (see Figure 2.3). While in continuous applications, like MPC, operational decisions rather focus on real-time or near real-time actions, selective applications tend to optimize for a specific period, such as determining the economical energy dispatch for the next day. Consequently, observation periods may vary significantly, ranging from minutes, such as in the control of dynamic processes, to up to one week, e.g., in the operation of a cement production [24, 36]. Within the scope of energy systems operation, MPC and the Unit Commitment Problem (UC) are of particular interest and gained overriding scientific interest [26].

Traditionally, the operation of technical systems and facilities was ensured by conventional rule-based or more advanced PID controllers, in which the corresponding setpoints of the significant process quantities were specified by the higher-level operational strategy or human supervisors. While these concepts work properly for systems with limited variables and dynamics, significant deficiencies in the control of complex, multivariable dynamics, such as those existing in chemical industries, emerged to adopt model-based approaches. These enable a more accurate consideration of intertemporal effects and limitations and can methodically act in the sense of optimality. However, the procedure is only reasonable and expedient if sufficient reliable information about future events is available, particularly regarding system boundaries and disturbances.

The origin of MPC dates back to the late 1960s when plant models were already formulated as dynamic optimization problems to obtain the optimal course of manipulated variables. Methodically, the associated receding horizon concept, depicted in Figure 2.3, not only became an essential characteristic of MPC but also for a variety of operational optimization applications [84].

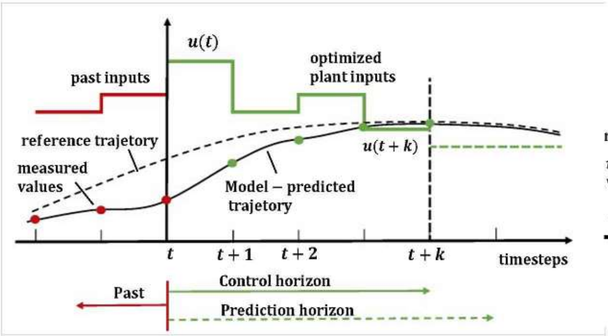


Figure 2.3: Simple illustration of a receding horizon scheme

The central objective is to determine the optimal sequence for the control input in order to efficiently follow the reference trajectory as desired operational progression. For determining the control input, the optimization algorithm predicts the system's future states for the entire prediction horizon, and by using real-time feedback, the MPC continuously adapts to disturbances and model inaccuracies. Hence, due to the consecutive execution, only the control signals of the immediate upcoming timesteps are actually proceeded to the plant. By shifting the prediction horizon and using the actual measured states as initial conditions for the next time step, this procedure is continuously repeated for each successive time step. Since operations must be ensured on a continuous basis, decisions and actions must be accomplished in reasonably short periods of time. Thus, solution times must also be kept sufficiently short, placing special emphasis on the reduction of model complexity. Besides using efficient formulations, this especially concerns the length of the prediction horizons. In this trade-off, two practical aspects are of essential importance. On the one hand, the temporal expression of the fundamental system dynamics must be sufficiently capured. On the other hand, reliable planning is only meaningful to the extent of sufficiently accurate predictions.

2.3.2 Unit Commitment Problem

Optimization has also established as an essentially valuable method in the operation of large-scale energy systems. In order to establish a secure energy supply it is essential to continuously fulfill the demand or supply contracts precisely through the available generation and storage units. However, for the efficient supply (either to increase revenues or improving competitiveness by minimizing production costs), the cost- and resource-efficient utilization of the different units, what is also referred to as economic dispatch, is a central operational objective. Addressing the issue of determining this economic dispatch, which can be very complex due to a potentially large number of units with heterogeneous characteristics and costs, the so-called unit-commitment (UC) problem originated already in the 1940s [85]. Due to the related valuable applicational potential, the UC has continuously attracted research interests already for decades [86] and consequently emerged to a fundamental class of optimization problems in energy systems engineering [26]. From a mathematical perspective, on account of the discrete decisions the UC is of combinatorial nature and therefore generally nonlinear and complex to solve [55, 71]. Therefore extensive and widespread scientific participation has developed a variety of different solution procedures, which are comprehesively discussed in already existing survey and review papers [33, 86, 87]. In particular, significant advances in the development of solvers and optimization algorithms for MILP problems were achieved (e.g.: Gurobi [78]), which, together with the increased resources in computing capacities, further contributed to the attractiveness of MILP [77]. Most popular applications range from single plant unit operations [88, 89], scheduling of thermal units [47], or multi-energy hubs [44] up to nationwide large-scale power management [90].

Considering the operating principles and technical processes in individual units, these often only work properly in certain operating or partial load ranges. Similarly, due to technical limitations, individual load conditions may not be changed in arbitrarily high gradients. Moreover, in order to bring the corresponding operating principles of technical processes into operation or to switch them off, certain auxiliary processes may be required that differ significantly from the nominal behavior and are subject to certain time limits as well as standstill periods. Since the exact representation of such operational procedures requires a very high level of detail, which potentially over-extends the optimization problem, the simplified and efficient modeling of such typical operational restrictions gained particular scientific interest [32].

Unit Commitment Formulations From a modeling perspective, it is more efficient to constrain the feasible region of the units' representative state variables rather than describing such special events and restrictive processes in detail. Thus, the superior importance for reduction of computational effort is emphasized on the development of MILP-based UC-formulations for the efficient modeling of typical system dynamics [91, 92]. Due to the large number of respective publications, the development of efficient MILP formulations can also be regarded as an own discipline. Already in 1962, Garver initially presented a MIP formulation [88] using three commitment statuses on/off, start-up and shut-down, represented by binary variables. Especially in the last two decades the use of characteristic MILP-based UC-formulations has gained very intense scientific activity and engagement for improving computational efficiency, an extension of scope or incorporation into generic models. While Carrion and Arroyo presented a more compact singel-binary (1bin) MILP formulation [91], also a 2bin-approach was developed by Yang et al. [92] showcasing improved performance. The 2bin approach is more compact than the 3bin formulation and exhibits a tighter formulation than the 1bin approach. Furthermore, a crucial contribution to the current state of the art was presented by Morales-Espagna et al., specifically tailored for thermal applications [93]. Additionally, the tightening of the feasible operational range of generation units [94] as well as the convex hull description of thermal units [95] constitute significant contributions marking the respective state of the art. In [77], Knueven et al., provide an overview of a variety of recently published specific UC-formulations particularly evaluating their compactness, tightness, and overall computational effort based on real-world data experimental tests.

However, despite mathematical superiorities, advanced more compact, and tight formulations can be more elaborate to model may be less practical for generic implementations. Moreover, modern commercial solvers incorporate advanced preprocessing techniques that automatically tighten original formulations. In addition, supportive modeling tools and parsers are accessible (e.g. YALMIP), which transform the original problems into more efficient and compact representations. Consequently, widely used standard formulations are often preferred due to their more convenient implementation, especially as their disadvantages may also be compensated by assistive tools and solvers.

Subsequently, from Eq. (2.5) to Eq. (2.15) the respective UC-constraints are stated according to their formulations used in this work. As established in scientific publications $\boldsymbol{u}_i^t$ denotes the operation state (on/off), $\boldsymbol{v}_i^t$ refers to the event of a start-up and $\boldsymbol{w}_i^t$ of a shutdown of a specific unit i or an operating process within a unit that is represented by a continuous decision variable $\boldsymbol{x}^t$ in time-step t, respectively. In this application, these variables can only assume the discrete values 1 and 0.

$$0 \leq \boldsymbol{u}^t \leq 1 \quad , \forall\, t \in [1, N_t] \tag{2.5}$$

$$0 \leq \boldsymbol{v}^t \leq 1 \quad , \forall\, t \in [1, N_t] \tag{2.6}$$

$$0 \leq \boldsymbol{w}^t \leq 1 \quad , \forall\, t \in [1, N_t] \tag{2.7}$$

The minimum and maximum generation limit of $\boldsymbol{x}^t$ is only active if the process is in operation.

$$\boldsymbol{u}^t x_{min} \leq \boldsymbol{x}^t \leq \boldsymbol{u}^t x_{max} \quad , \forall\, t \in [1, N_t] \tag{2.8}$$

Eq. (2.9) and Eq. (2.10) are employed to account for the limitations on maximum ramp-up, ramp-down, as well as start-up and shutdown, denoted by the parameters RU,RD and SU,SD respectively.

$$\boldsymbol{x}^t - \boldsymbol{x}^{t-1} \leq RU\boldsymbol{u}_{i-1} + SU\boldsymbol{v}_i \quad , \forall\, t \in [1, N_t] \tag{2.9}$$

$$\boldsymbol{x}^{t-1} - \boldsymbol{x}^t \leq RD\boldsymbol{u}_i + SD\boldsymbol{w}_i \quad , \forall\, t \in [1, N_t] \tag{2.10}$$

The event variables for start up and shutdown can be defined as by a state change of u between consecutive time steps. An additional formulation is necessary to ensure that a start-up and shut-down cannot occur simultaneously

$$\boldsymbol{v}^t - \boldsymbol{w}^t = \boldsymbol{u}^t - \boldsymbol{u}^{t-1} \quad , \forall\, t \in [2, N_t] \tag{2.11}$$

$$\boldsymbol{v}^t + \boldsymbol{w}^t \leq 2 - \boldsymbol{u}^t - \boldsymbol{u}^{t-1} \quad , \forall\, t \in [2, N_t] \tag{2.12}$$

$$\boldsymbol{v}^t + \boldsymbol{w}^t \leq 1 \quad , \forall\, t \in [1, N_t] \tag{2.13}$$

The consideration of a Minimum Uptime UT / Downtime DT is implemented by

$$\sum_{t=t-UT+1}^{t} \boldsymbol{v}^t \leq \boldsymbol{u}^t \quad , \forall\, t \in [UT, N_t] \tag{2.14}$$

$$\sum_{t=t-DT+1}^{t} \boldsymbol{w}^t \leq 1 - \boldsymbol{u}^t \quad , \forall\, t \in [DT, N_t] \tag{2.15}$$

2.3.3 Design Optimization

Performance capabilities of single technological processes, whole industrial facilities but also large-scale energy systems are strongly related to the corresponding technical design and implementation [18, 30]. Considering a potentially large number of possible choices together with potentially complex relations of significant design variables and a wide range of influencing factors, the use of optimization for the identification of best possible investment decisions is nearly inevitable [71]. From a mathematical point of view, the simultaneous existence of binary, integer as well as real-valued variables, representing either discrete decisions or continuous process and energy flows, are typical for design problems. Consequently, these fundamentally correspond to the MINLP [96]. Since it is of particular importance to consider all possible configurations regarding supply and conversion, technological options, consumption processes as well as corresponding transmission systems in a generic manner, so-called synthesis problems are typically formulated using superstructures [26]. Particular relevance for industrial processes and thermal energy systems can be attributed to the concept of heat exchanger network synthesis (HENS), which has its origins already in the 1940s and emerged as an extensively studied concept as indicated by the overviews of [97, 98]. In numerous subsequent scientific contributions, the stage-wise superstructure, originally formulated as MILNP by Yee and Grossman [99], was adopted to be extended and adapted for wider applicability and improvement of computational performance. For example, considering multi-period problems [100], simplifications for obtaining tight and compact MILP formulations [50, 101], technological and sectoral extensions as well as investigating meta-heuristic solvers such as particle swarm optimization [102], sequential approaches[103] or genetical algorithms [70].

Besides efficiency, other typical applications address the synthesis of process intensification [104], supply chain networks [105], or holistic energy supply networks [106]. With subject to single industrial plants or process-specific heat integration, design tasks are of manageable complexity [71]. However, the growing diversity of technologies and increasing dynamics of systemic boundaries, such as the volatility of renewable sources and energy prices as well as discontinuous batch processes, require an increasing consideration of operational aspects. Although extensions of the HENS concept for multi-period applications have already been investigated, [107–109], its basic structure is rather suitable to optimize for single design points than considering dynamical events. In contrast, the UC approach, which is well established for representing operational issues, can be extended to include decisions for integration and dimensioning of single units. However, this method is more suitable for the integration of individual technologies at specific points, rather than providing a generic method for the optimal “green field” design of an overall process-specific heat integration system. If certain restrictions are accepted, design optimization tasks can be performed based UC approach even using a MILP formulation [71].

2.3.4 Hierarchical Optimization and Control

Hierarchical optimization (HO) offers a structured approach to handle optimization problems decomposed into a set of smaller, more manageable subproblems. This strategy is particularly suitable in large, complex optimization problems when decisions or tasks can be divided into different levels according to priority or sequence, or where the tasks are elementary subjected to hierarchies [110]. This concept proved to be particularly suitable for technical applications such as the planning of transportation routes [111], robotics, or, most importantly for this work, in industrial process control [73] as well as in the planning and operation of energy systems [38, 112]. In this context, it is referred to Section 2.1.2, where the specific optimization applications employed in this work are categorized into the hierarchical levels of the automation pyramid. For a comprehensive review, Scattaloni [113] presented a variety of different HO architectures for distributed and hierarchical MPC indicating their close connection. On the other hand, the suitability of HO for the optimal operation of large-scale power systems is emphasized. However, the approaches of Shin et al. [114] or Gholinejad et al. [115] indicated that these complex issues require a more advanced conceptual embedding.

On the methodological level, the communication and coordination between the levels are fundamental to the functionality of the concept. The higher levels communicate strategies and objectives to the lower levels through targets and constraints, and the lower levels report back observations and their status. Accordingly, there are various possible solutions for cooperation between the hierarchical levels. Faísca et al. [110] propose a versatile approach that enables both decentralized and hierarchical structures using multi-level parametric programming. However, depending on the application, hierarchical structures can also be implemented in a more simple way. For instance, especially when the hierarchical ranking is unambiguously defined, the very convenient, soft constrained approach shown in Eq. (2.16) can be applied. This formulation minimizes the deviation of the time course of a variable $\boldsymbol{x}^t$ from its targeted the hierarchical defined trajectory x^t_{traj} .

$$J_{traj} = \min_{x} \sum_{t=1}^{N_t} \left| \boldsymbol{x}^t - x^t_{traj} \right| \tag{2.16}$$

Due to its simplicity, this robust approach constitutes an established practice in hierarchical optimization [74] and proved its capabilities in a variety of applications such as for temperature control in a single stirred tank [116], in energy management for thermal batch-processes [1], or the identification of industrial flexibilities [49].

2.3.5 Approaches and Concepts for Modularization

Following the previous introductions to the fundamental topics and the central methodologies and tools, particular relevant methods and subsequent concepts are highlighted more comprehensively. Especially the contributions subjected energy management systems, MPC and Energy Hubs are most frequently related to operational optimization. With regard to this work, special attention is paid to the modularity and decomposability of individual energy system modeling methods for the flexible creation and definition of optimization problems. In this context, the term modularity is also interpreted in different ways. On the one hand, at the level of technical elements, technologies and functions, and on the other hand, at the pure methodical level.

Energy Hub The term energy hub originally arose in 2005 reffering to the conversion and storage of energy carriers in an integrated unit. Mohammadi et al. [32] presented a comprehensive overview of this term, indicating an evolving concept as it has been frequently adopted to further develop different structural representations, model formulations, and applications to various different issues. As illustrated in Figure 2.4 a variety of different technologies, energy carriers, and grid-based energy sources have been addressed, most of which have been incorporated into optimization tasks such as optimal planning, control, scheduling, demand-side management, and investment decisions under uncertainty.

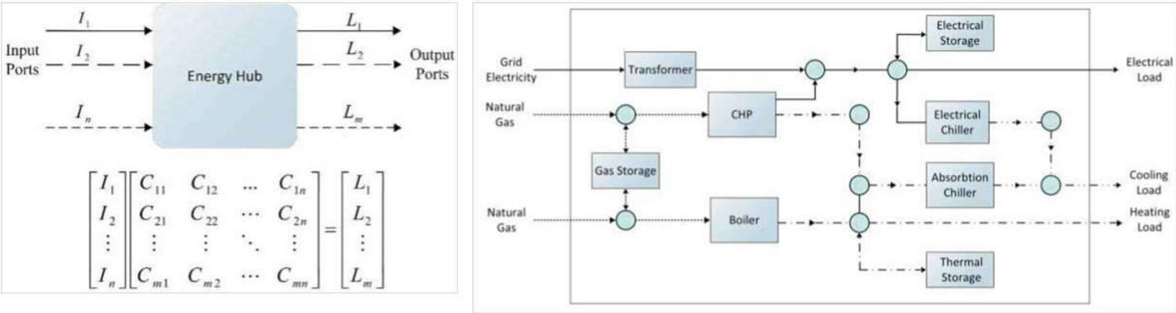


Figure 2.4: Illustration of the energy hub concept, taken with permission from [32]

On a methodical level, above all, the practical treatment of energy systems divided into inputs, outputs, conversion, and storage of multiple energy carriers has established a foundation for the incorporation into modular modeling approaches. Moreover, as proposed by Ramirez-Elizondo et al. [117], this classification proved particular suitability for unit-commitment problems of multi-energy systems. However, most applications of energy hub concepts are strongly related to energy management issues and a strong overlap between these two terms can be observed in scientific contributions. Hence, in addition to numerous contributions that directly refer to this concept, there are even more that contain the conceptual criteria of energy hubs, however, without mentioning the term. In this respect, also the terms of Energy Management Systems and MPC also often appear jointly. For instance, Moser et al. [45] distinguish between technical components (prosumers) and connections that link two prosumers via ports. Complete systems are assembled according to the modular principle to express an MPC formulation using MILP. The contributions of Halmschlager et al. [44, 118] propose a framework approach for a modular definition of MILP-based unit-commitment problems enabling a more flexible and structured modeling process. Panuschka et al. [119] introduce different modeling schemes depending on the number of continuous and binary decision variables for individual models with different degrees of freedom to formulate a MILP-UC. The generic superstructure-based method presented by Chen et al. [120] allows a straightforward modeling of large-scale multi-unit systems, however, as it only considers proportional conversion processes it exhibits significant limitations.

Superstructures A superstructure uses clearly (pre-)defined elements of certain functions and properties to express a mostly simplified and abstract model representation of arbitrary systems of specific types in order to handle certain potentially complex problems or analysis tasks in a systematic, generic, and convenient way. For their formulation, it is essential that all systemic alternatives, opportunities, attributes, and issues can be considered. Especially in the case of optimization, mostly the problem definition and type of the solution are already set by the superstructure formulation. They act as the basis of comprehensive analysis, assembling, or modeling. Thus they are especially widely used in Energy Optimization. Especially conveniently manageable generic modeling approaches rely on the practicability of the underlying superstructure. Particularly when modeling more complex multi-energy structures, it is important to be able to systematically handle all possible energy flows, conversion, and reference options, characteristics that favor the application of superstructure-based approaches [26].

Especially in design optimization of so-called synthesis problems, superstructures have proven to be extremely practical and represent a scientifically very extensively studied area. Very prominent is the design of heat integration systems, which can be traced back to a HENS superstructure originally presented by Yee and Grossman [99]. The central elements of this approach are streams, so-called utilities, and the units for which originally only heat exchangers were considered, but numerous extensions have been introduced that also include various other components such as heat pumps, storage tanks, or CHPs. Moreover, superstructures are also applied for the generic treatment of problems which less focuses on the design but more on operations and energy management in a dynamic perspective [120–123]. These use different superstructures elements such as generators, converters, storage, external sources and sinks, and energy flows as pure connection elements. i.e. Chen et al. [120] use an abstract superstructure using exclusively power components to obtain a linear model on a dispatch problem. The superstructure used in [123] is built in a similar manner however considering different forms of energy applied to a design problem of an urban energy system formulated as a MILP. Li et al. [121] proposed a superstructure for optimizing the operation strategy for a multiple complementary energy supply chain using a MILP formulation. In the energy hub overview paper [32], a conceptual model is presented of energy systems which shows a systematic representation of energy systems. A main distinction, especially in terms of mathematical formulation, can be identified between flow and balance-based superstructures. Thus, in HENS as well as in for instance in the approach of Li et al. [121] energy flows are represented with a fixed flow direction and a fixed flow sequence. In contrast, the approaches [120, 123] use energy balances between components instead of simple flow, thus representing a more generic and less abstract concept. With subject to design tasks, the flow-based approaches may have advantages for holistic design optimization for certain sequential steps in an energy flow pathway. However, the additional generic consideration .]of energy balances representing mixing or splitting points, which would provide to design of energy systems with significantly more operational flexibility, would increase the complexity of the problem severely.

If one does not know to which port one is sailing,
no wind is favorable.

LUCIUS ANNAEUS SENECA

3 Methodology

Aim and Scope This chapter describes the development and derivation of the central methodical innovations including the adoption of basic concepts that constitute the central foundation of this thesis. These include:

- The generic superstructure-based modeling method for the holistic optimization of multi-energy systems. This mainly tackles the research gap of establishing an efficient, adaptive, and universally applicable modeling as a central basis for cost-effective implementation.
- The Energy Management and Control System (EMCS) represents the second and more enhanced application. By incorporating the modeling superstructure into a hierarchical optimization architecture, the research gap of an easily implementable and PCS-compatible EMS is addressed.

3.1 Optimization Superstructure

As outlined in Section 2.3.5, the modular modeling of systems and processes has established as useful and beneficial practice in the field of energy systems engineering. Accordingly, the development of modular approaches and especially the incorporation in more comprehensive optimization frameworks has recently attracted substantial scientific engagement, especially with respect to unit-commitment problems (e.g.: [32, 45, 118]). However, as previously emphasized, these rather theoretical approaches still have notable shortcomings when it comes to integration into actual physical facilities. Consequently, they possess deficient real-time capabilities in terms of plant interaction and the effective execution of control tasks. Addressing these functional gaps, the forthcoming approach is particularly desired to ensure a practical and efficient implementation alongside robust and time-efficient solvability. The component modeling approach, described in section 3.3, is based on the energy hub concept [32] and systematically incorporates generic elements to ensure efficient modeling. As presented in the following section, the superstructure derives from practical, mathematical, and logical considerations and adopts particular features of the approaches discussed in section 2.4.

3.1.1 Basic Concept

The methodical concept combines the use of a higher-level system assembling superstructure and a modular component modeling approach to create a plant-wide Unit-Commitment problem in a holistic manner based on a generic MILP formulation. The intention is to streamline the modeling of large, multi-component energy systems with a variety of energy carriers while still offering the possibility of modeling detailed effects within components. Initially, the principal conceptual considerations and logic for the classification of energy systems are explained. Moreover, the corresponding purpose, functions, and definitions of the different modeling objects are introduced in order to derive mathematical formulations. Since the implementation of the framework is strongly connected to the use of computational and programming tools, the description not only addresses the mathematical aspects but also considers its integration with digital methods and objects.

Energy System Classification The conceptual idea is based on a classification of energy systems into energy networks and units, which may further be grouped into functional categories such as supply, local production, conversion, storage, and consumption. Thus, a clear and concise two-dimensionally organized, abstract representation of energy systems is obtained, which serves as the starting point for modeling. Thereby the internal distribution networks of the various energy sources are arranged vertically, each extending across all horizontally arranged functional categories. The individual components are integrated allocated to their category and interconnected with their corresponding energy networks. This approach is demonstrated using the simple exemplary energy system shown in Figure 3.1. While this representation is similar to a piping and instrumentation diagram (P&ID) commonly used in industrial companies, the classified two-dimensional system model is depicted in Figure 3.2.

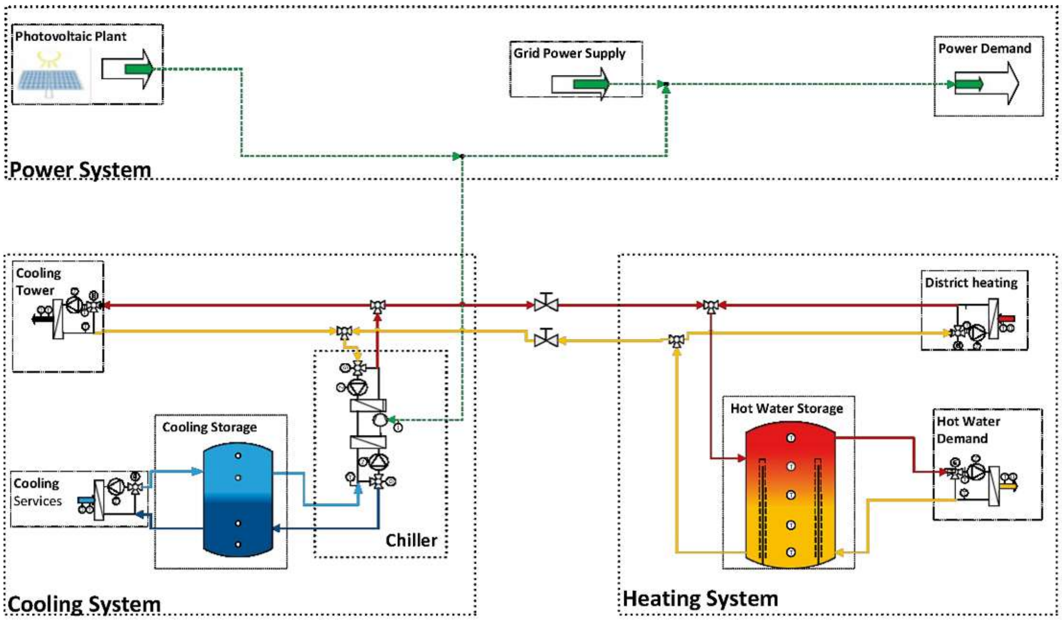


Figure 3.1: R&I illustration of an exemplary energy system

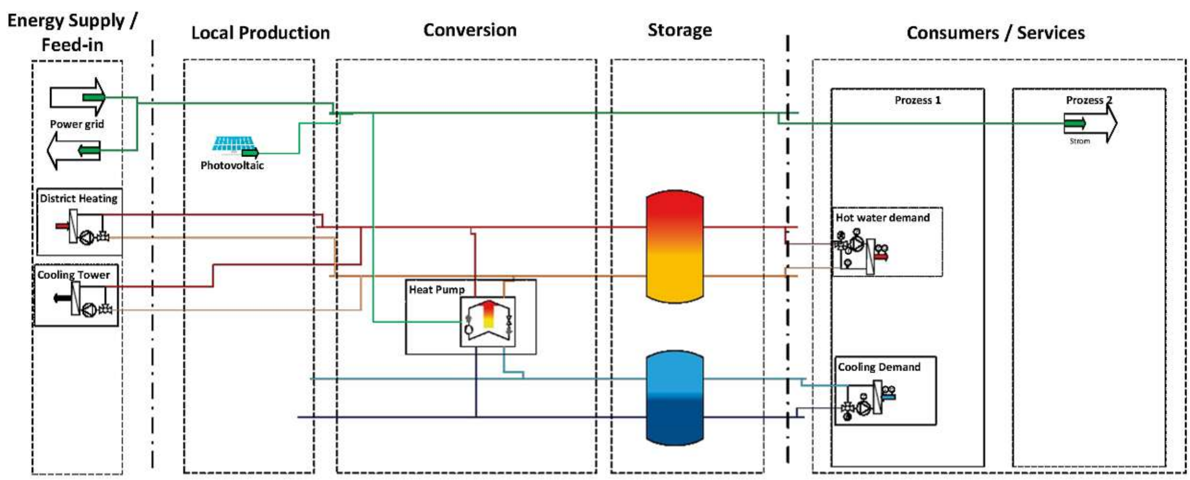


Figure 3.2: Structured classification of the exemplary plant

Thereby, Figure 3.1 intentionally refers to a widespread pattern often encountered in industrial companies: For each energy service, distinct process or P&ID schemas are adopted, indicating the typical practice of treating different energy services in a delineated manner. In contrast, the representation in Figure 3.2 serves as a convenient basis for a more comprehensive and systemic understanding of components and operational functions within the overall energy system. Based on these fundamental considerations, the modeling approach is described starting from the specific features, attributes, and functions of the individual modeling objects.

3.1.2 Modeling Objects

Modularity is established by the systematic assembling of distinct modeling objects to form the corresponding optimization problem. These are units, networks, and energy carriers. Among these, the following fundamental assumptions, definitions, and delimitations apply.

Units Energy supply, generation, conversion, storage, and consumption are considered to only occur within unit objects. As subordinate objects, ports are assigned, which represent the interfaces for the exchange of energy and mass between the global structure and the individual model. The global part exclusively includes the definition of ports by specifying corresponding energy carrier types. In contrast, the individual part includes the actual modeling of the behavior and thermodynamic processes occurring inside the component.

Network Objects Within industrial plants, energy distribution is usually accomplished using collectors and distributors which corresponds to the primary task of network objects. For modeling purposes, however, the aim of using networks is the streamlining of the system assembly process. In this context, it is assumed that the exchange of energy or mass between components takes place at constant intensive state quantities and material properties. This assumption is a fundamental characteristic for establishing a linear modeling structure.

Energy Carriers Within this conceptual framework, particular emphasis is placed on achieving consistency of energy carriers and process media properties between network objects and connected components ports. This is achieved by predefining standardized types of energy carriers, such as thermal, electrical, or fuels, with prescriptions of the respective media properties as shown in Table 3.1. There, also the "general" type is recognized which is intended to be used for streams where the energy content is insignificant such as by-products of processes.

Consequently, the introduction of a network object entails the selection of its type and the specification of the respective properties. Additionally, in order to establish compatibility, the linkage of a port to a network is only feasible when both are of the same type. If this condition is met, the port will adopt the attributes of the network object.

Table 3.1: Definition and comparison of energy carrier types

type	Parameters: properties	Parameters: specific energy content	Variables: primary	Variables: secondary
thermal	$p, T, medium$	$h(p,T,medium)$	$\boldsymbol{m}$	$\boldsymbol{q} = \dot{\boldsymbol{m}}\, h$
fuel	$p, T, medium$	$H_u(p,T,medium)$	$\mathbf{m}$	$\boldsymbol{e} = \dot{\boldsymbol{m}}\, H_u$
electrical	Vo, fr, φ	$\widehat{Vo}$[6]	$\boldsymbol{P}$	$\boldsymbol{i} = \boldsymbol{P}/\widehat{Vo}$
general	$\Delta e, medium$	Δe	$\boldsymbol{s}$	$\boldsymbol{e} = \mathbf{s}\,\Delta e$

In Figure 3.3, the inheritance of properties using the example of connecting a heat pump with two different network objects is shown. The port $\boldsymbol{Sink_{in}}$ is of the same type, which is why a connection is established and the properties of the thermal network are adopted. In contrast, a connection of the electrical port $\boldsymbol{Power_{in}}$ to the thermal network is not permitted. The component representation also highlights the division of a component model by emphasizing the global part and only diffusely depicting the individual model.

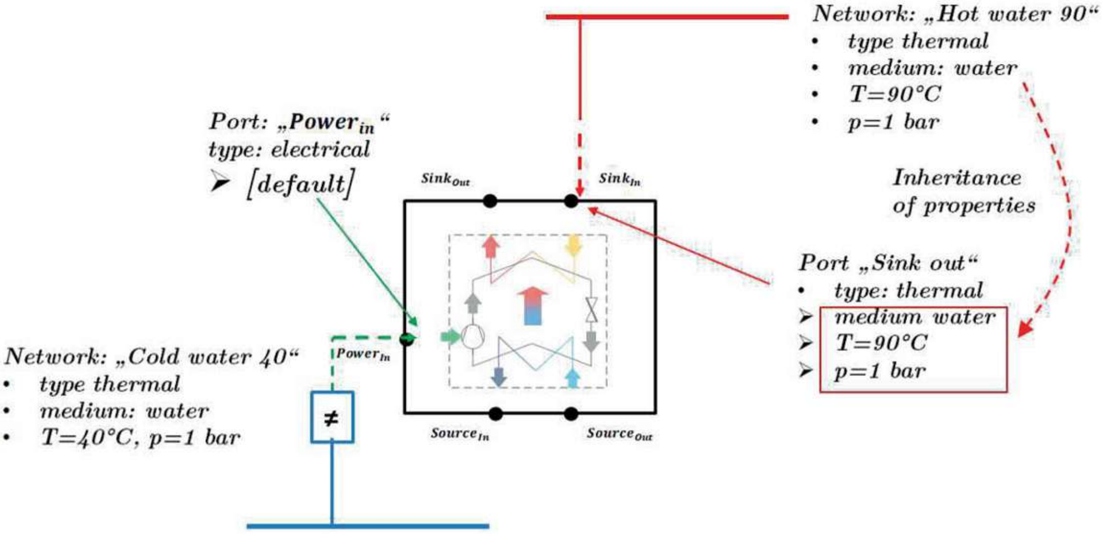


Figure 3.3: Interconnection of a component model

Discrete Quality Approach Reflecting these definitions, it is essentially repeated that intensive state properties are considered as constant parameters, whereas extensive properties, and thus also their transport streams, are represented by variables. This assumption fundamentally serves to establish linear relations between the transport streams of the respective process media and the absolute energy flows, denoted as primary and secondary variables in Table 3.1. Since their intensive state variables are considered constant, the process streams can only occur at discrete levels, which, in an abstract way, can also be regarded as energy carrier qualities. Consequently, this assumption essentially underpins model linearity and establishes the simultaneous balancing of both energy and mass quantities.

[6] $\widehat{Vo} = Vo \cos\varphi$

3.2 Mathematical Formulation

Proceeding from the preliminary introduction of modeling objects and their attributes, subsequently, the composition of the mathematical statement is explained particularly emphasizing the systematic and distributed problem formulation. In compliance with MILP paradigms, the problem is expressed according to the general notation stated in Eq. (3.1).

$$
\begin{gathered}
\min J\ \boldsymbol{x_c}, \boldsymbol{x_d} \\
s.t \\
g\ \boldsymbol{x_c}, \boldsymbol{x_d}\ \geq 0 \\
\boldsymbol{x_c} \in \boldsymbol{X} \subseteq\ \mathbb{R}^{N_c} \\
\boldsymbol{x_d}\ \in Y \subseteq \mathbb{Z}^{N_d}
\end{gathered}
\tag{3.1}
$$

In this respect $\boldsymbol{x}_c$ and $\boldsymbol{x}_d$ denote N_c continuous and N_d integer variables. The optimization objective $\boldsymbol{J}\ \boldsymbol{x}_c, \boldsymbol{x}_b$ generally incorporates a multi-criteria formulation with arbitrarily definable criteria and functions. As will be shown subsequently in Section 3.2.2, a weighted sum approach based on the use of generic functions can conveniently be embedded in the modular structure to establish an efficient definition process. In reference to the central modeling objects previously introduced, according to Eq. (3.2), the set of constraints is composed by stringing together component-specific contributions in conjunction with those emerging due to system assembling and the energy carrier definitions.

$$
[\boldsymbol{g}\ (\boldsymbol{x}_c, \boldsymbol{x}_d\ ) \geq 0]_{tot} = \begin{bmatrix} [\boldsymbol{g}\ (\boldsymbol{x}_c) \geq 0]_{\mathrm{N_p}} & \} & \mathit{Ports/Streams} \\ [\boldsymbol{g}\ (\boldsymbol{x}_c) \geq 0]_{\mathrm{N}_n} & \} & \mathit{Networks} \\ [\boldsymbol{g}\ (\boldsymbol{x}_c, \boldsymbol{x}_d\ ) \geq 0]_{\mathrm{N}_n} & \} & \mathit{Individual\ components} \end{bmatrix}
\tag{3.2}
$$

Initially, the mathematical formulations created through the system assembling are introduced by simultaneously indicating the principles of the superstructure. The energy- or process streams $\boldsymbol{e}$ and $\boldsymbol{s}$ exchanged between components and networks are represented by continuous, time-variant variables, which are introduced with the definition of its associated ports as indicated by Figure 3.3 and described in the previous section 3.1.2. Thus, for each component a time-varying vector comprising all port streams is present.

3.2.1 Creation of Networks Constraints - Composition of Systems

Network Balances Considering network objects, the mass- and energy balances can be represented according to the laws of conservation and the first law of thermodynamics. The negligence of geometrical expansions and inertial effects of energy transport as well as transmission losses is a foundation for keeping linearity and allows a consideration as zero-dimensional nodes according to Eq. (3.3) and Eq. (3.4).

$$\frac{d\boldsymbol{m}^t}{dt} = \sum_{r \in in} \boldsymbol{m}_r^t - \sum_{l \in out} \boldsymbol{m}_l^t \quad \forall\, t \in \mathrm{N}_t \tag{3.3}$$

$$\frac{d\boldsymbol{e}^t}{dt} = \sum_{r \in in} \boldsymbol{e}_r^t - \sum_{l \in out} \boldsymbol{e}_l^t \quad \forall\, t \in \mathrm{N}_t \tag{3.4}$$

By neglecting transient behaviour and effects, the time derivatives de/dt and dm/dt are zero and steady-state balance equations are obtained. Referring to Table 3.1, Eq. (3.5) states the general linear relation between the process media stream $\boldsymbol{s}$ and their energy flows $\boldsymbol{e}$ through the specific energy content Δe.

$$\boldsymbol{e} = \boldsymbol{s}\,\Delta e \tag{3.5}$$

Consequently, it is sufficient to only balance either in terms of energy or mass and the resulting network balances $\boldsymbol{B}$ are expressed by Eq. (3.6).

$$\boldsymbol{B_n} = \sum_{l \in L_n} \boldsymbol{s}_l^t - \sum_{r \in R_n} \boldsymbol{s}_r^t = 0 \quad \forall\, \boldsymbol{n} \in \boldsymbol{NW}, \quad \forall\, t \in \mathrm{N}_t \tag{3.6}$$
$$L_n = \{\boldsymbol{s}_l \in \boldsymbol{S} \mid \boldsymbol{s}_l \; withdraws\; from\; network\; n\}$$
$$R_n = \{\boldsymbol{s}_r \in \boldsymbol{S} \mid \boldsymbol{s}_r \; feeds\; into\; network\; n\}$$

Connection Matrices The connection, either input or output, of port p of unit i to the network balance of $\boldsymbol{B_n}$, can be expressed by using connection coefficients $\alpha_{p,i,n}$, which are -1 if the port-stream is considered to consume/withdraw from the network n, +1 in the case of a feed-in and zero if there is no connection.

$$\boldsymbol{B_{p,i,n}} = \boldsymbol{s_p}\,\alpha_{p,i,n} \tag{3.7}$$

$$\alpha_{p,i,n} = \begin{cases} 1 & \forall p,i,n \in \{p,i,n \mid \; port\; p\; feeds\; into\; network\; n\} \\ -1 & \forall p,i,n \in \{p,i,n \mid \; port\; p\; withdraws\; from\; network\; n\} \\ 0 & otherwise \end{cases} \tag{3.8}$$

The connection coefficients of a specific port to all networks can be sorted to a column vector $\alpha_{p,i}$ which length equals the number of network objects and its Euclidean norm is limited to a maximum length of 1 (A port can be connected to a maximum of one network).

$$\alpha_{p,i} = \left(\alpha_{p,i,1}, \;\; \alpha_{p,i,2}, \dots, \alpha_{p,i,\boldsymbol{n_n}}\right)^T \tag{3.9}$$
$$0 \le \left\|\alpha_{p,i}\right\| \le 1$$

In a similar way, connection matrices for the individual units α_i can be assembled as shown in Eq. (3.10), where the subsequent conditions in Eq. (3.11) has to be ensured.

$$\alpha_i = \left(\alpha_{1,i}\,,\quad \alpha_{2,i}\,,\qquad .... \quad \alpha_{np,i}\right) \tag{3.10}$$

$$0 \leq \sum_{p}^{N_p} \left\|\alpha_{P,i}\right\| \leq N_p \tag{3.11}$$

Creation of Networks Constraints By using the introduced unit connection matrices α_i, the contribution of one unit to all network balances can be obtained according to Eq. (3.12), where $\boldsymbol{s_i}$ represents the vector of port streams of unit i.

$$\boldsymbol{B_i} = \alpha_i\ \boldsymbol{s_i} = \boldsymbol{0} \tag{3.12}$$

Consequently, based on the presented deliberations, the overall system assembling is expressed by the set of balance constraints of the respective network objects, which are composed using the overall connection matrix α and the combined column vector of all ports streams $\boldsymbol{s}$ as stated by Eq. (3.13).

$$\begin{gathered} \boldsymbol{B} = \alpha\ \boldsymbol{s} = \boldsymbol{0} \\ \alpha = \left(\alpha_1\,, \alpha_2\,, \qquad ... \quad \alpha_{\mathrm{N}_i}\ \right) \\ \boldsymbol{s} = \left(\boldsymbol{s}_{\ 1}\,;\quad \boldsymbol{s}_{\ 2}\,;\ \ ...\ \ \boldsymbol{s}_{\mathrm{N}_s}\ \right)^T \end{gathered} \tag{3.13}$$

It needs to be emphasized, that the specification of the connection coefficients $\alpha_{\mathrm{p,i,n}}$ is the only required methodical input for interconnecting the individual components to the energy system. Consequently, special diligence must be practiced in order to ensure a correct interconnection. To clarify the process of coefficient determination, Box 1 shows the specification of the coefficients for the exemplary interconnection of a heat pump to five different networks according to Figure 3.4. The connection matrix α is assembled according to Eq. (3.9).

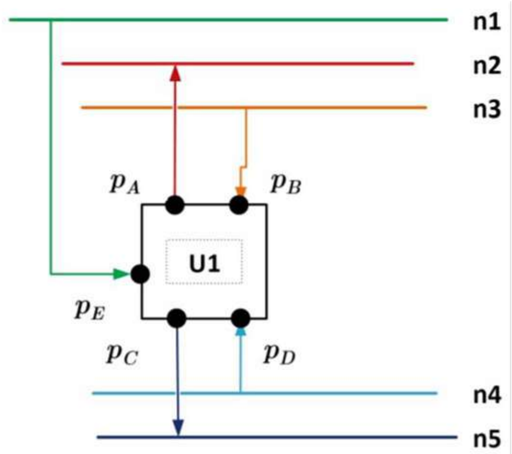


Figure 3.4: Exemplary connection of a component

Box 1

$$\begin{array}{c c} & \begin{matrix} \alpha_A & \alpha_B & \alpha_C & \alpha_D & \alpha_E \end{matrix} \\ \begin{matrix} n1 \\ n2 \\ n3 \\ n4 \\ n5 \end{matrix} & \begin{pmatrix} 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

$$\alpha = (\alpha_A\,,\quad \alpha_B\,,\quad \alpha_C,\quad \alpha_D\,,\quad \alpha_E\,)$$

Inheritance and Assignment of Properties By aggregating the specific stream properties in a vector ε, the previously described inheritance of properties can be expressed similarly using the derived connection coefficients $\alpha_{p,i,n}$. The corresponding expressions are stated in Eq. (3.14) and Eq. (3.15), where δ represents the inheritence and ε_{def} stands for the default properties.

$$\varepsilon_{p,i} = \varepsilon_n \left|\alpha_{p,i,n}\right| \delta_{p,i,n} + \varepsilon_{def}\,(1 - \delta_{p,i,n}) \tag{3.14}$$

$$\delta_{p,i,n} = \begin{cases} 1 & n \text{ and } p \text{ have the same type} \\ 0 & \text{otherwise} \end{cases} \tag{3.15}$$

Superstructure Representation The stated formulations provide a generic approach to model the interactions and constraints imposed by the plant configuration by only specifying the connection matrices. Concerning the exemplary plant, the respective connection matrixes are listed in Table 3.2 for all comprised components. Accordingly, as shown in Figure 3.5, the modeled system can be systematically arranged in an abstract form clearly indicating the modular nature of superstructure. The constraints for representing the behavior of the specific units originate from the individual component models. The respective component modeling approach is comprehensively described in Section 3.3.

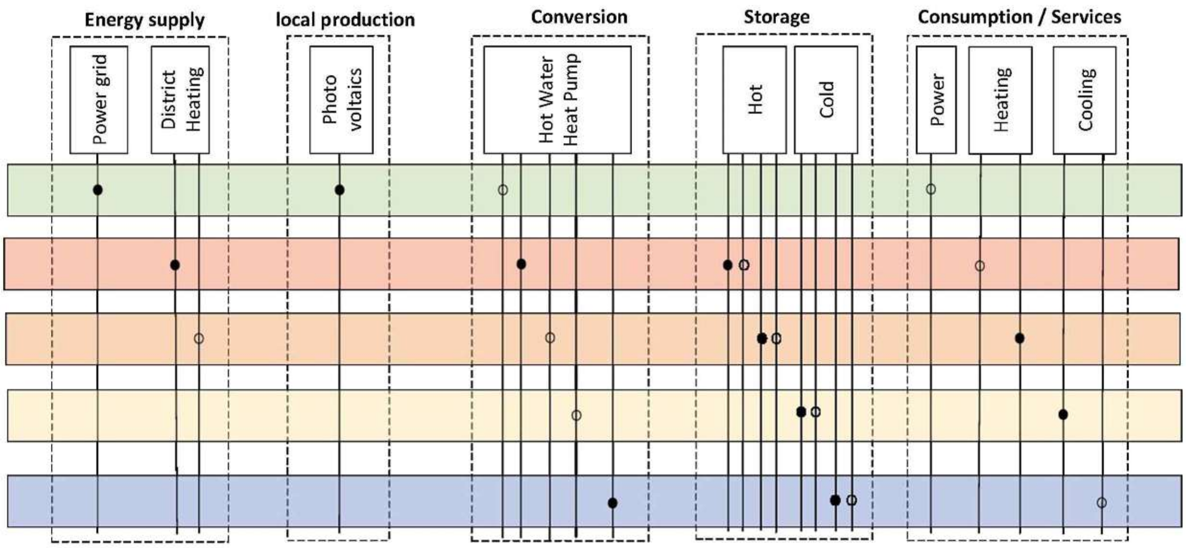


Figure 3.5: Superstructure representation of the exemplary plant form Figure 3.1

Table 3.2: Component connection matrices of the examplary plant

Component	Vector of port variables	Connection matrixes
Power grid	$s_{PG} = (P_{PG})$	$\alpha_{PG}{}^{T} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \end{pmatrix}$
District Heating	$s_{DH} = \begin{pmatrix} m_{DH,Hot} \\ m_{DH,Cold} \end{pmatrix}$	$\alpha_{DH}{}^{T} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \end{pmatrix}$
Photovoltaic	$s_{PV} = (P_{PV})$	$\alpha_{PV}{}^{T} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \end{pmatrix}$
Heat Pump	$s_{HP} = \begin{pmatrix} P_{HP} \\ m_{SiH,HP} \\ m_{SiC,HP} \\ m_{So,C,HP} \\ m_{So,C,HP} \end{pmatrix}$	$\alpha_{HP}{}^{T} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
Storage Hot	$s_{STH} = \begin{pmatrix} M_{in,T1} \\ M_{out,T1} \\ M_{in,T2} \\ M_{out,T2} \end{pmatrix}$	$\alpha_{STH}{}^{T} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \end{pmatrix}$
Storage Cold	$s_{STC} = \begin{pmatrix} M_{in,T3} \\ M_{out,T3} \\ M_{in,T4} \\ M_{out,T4} \end{pmatrix}$	$\alpha_{STC}{}^{T} = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}$
Power Consumer	$s_{PC} = (P_{PC})$	$\alpha_{PC}{}^{T} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \end{pmatrix}$
Heat Consumer	$s_{HC} = \begin{pmatrix} m_{HC,Hot} \\ m_{HC,Cold} \end{pmatrix}$	$\alpha_{HC}{}^{T} = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}$
Cooling Consumer	$s_{CC} = \begin{pmatrix} m_{CC,Hot} \\ m_{CC,Cold} \end{pmatrix}$	$\alpha_{CC}{}^{T} = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$

Remarks on the Superstructure In Section 2.3.5, an introduction of the application of superstructures was presented specifically examining selected commonly employed and recently proposed methodologies. Although the described development process is not specifically customized to any particular approaches, certain similarities can still be recognized. The approach of Chen et al., 2019 [120] integrates conversion and storage models which are, in line with the energy hub model paradigms, integrated into a flow-based abstract matrix structure. Nevertheless, the incorporation of conversion characteristics within the matrices imposes significant limitations as it restricts the consideration solely to linear relationships. This inherent limitation considerably restricts the functionality and applicability of the approach. Chen, et al. [123] as well as Li et al. [121] use a similar classification into the superior categories "generation", "conversion", "storage" and "demand", which underpins the viability and practicability of this categorization. Unfortunately, these approaches are purely flow-based and lack the ability to consider distribution networks within the energy systems.

However, in the approach of Chen et al. [123], which mainly targets urban energy systems, the interconnection to regional grids is considered. As pointed out in section 3.1.2, internal distribution networks are especially persistent in more comprehensive, multi-component energy systems, such as industrial plants, where the application of these methods is consequently restricted or significantly more complicated. Mohammadi et al., 2017 [32] presented a central contribution reviewing the energy hub concept, especially in terms of applications and conceptual advancements. By summarizing all contents and components recorded within the comprehensive literature research, a conceptual illustration was presented, systematically assigning several encountered technical components to networks of certain energy carriers. Therefore, this depiction inherently aligns with the characteristics of a superstructure. Particularly with regard to the basic structure, the introduction and utilization of networks and the classification of technologies, there are noteworthy parallels to the approach derived and presented in this chapter. However, it should be noted, that it primarily served as a conceptual model, orientated on future-thinking considerations rather than a viable and applicable modeling method.

3.2.2 Objective Function - Composition and Integration

An introduction to the role and functional significance of objective functions as well as an overview of different types, approaches, and formulations was given in the previous chapter 2. Referring to the central methodological paradigm of ensuring an efficient and adaptive modeling process within a wide range of different energy-management issues, the approach aims to handle and define objectives in a generic and modular way similar to the energy systems assembling. However, in optimization, both the problem statements themselves as well as the formulation of the corresponding objectives may be very diverse and elaborate. For example, the mathematical formulation of the objective function varies considerably depending on whether the objective is to minimize production costs, maximize consumption flexibilities, or achieve certain load changes within a minimum time. Consequently, simple assignment matrices are not sufficient to formulate appropriate objectives. However, a similar modular component-based composition is achieved by using generically applicable functions, in which arbitrary advanced mathematical expressions can be embedded. In this context, reference is given to Section 3.2.3 below, where typical formulations for objective criteria frequently used in MILP-UC problem were stated. Systematically integrated into the superstructure, a parametric single objective is formulated based on a normalized weighted sum approach.

Generic Functions For a more profound understanding, the approach of using generic functions is first illustrated by an accompanying example in order to derive the general formulation in a comprehensible way. In the example, the operation of a heat pump is evaluated based on two different criteria. On the one hand, the energy costs of power consumption are to be minimized, which is expressed by Eq. (3.16).

$$\boldsymbol{j_{Pc}} = \sum_{t=1}^{N_t} \boldsymbol{P^t}\, c_{el}^t \;=\; f_{cost}(\boldsymbol{P}, c_{el}) \tag{3.16}$$

In addition, the heat generation at the hot side $\boldsymbol{Q_{hs}}$ is intended to pursue a desired given course (trajectory) which is denoted as $Q_{hs,traj}$ in Eq. (3.17).

$$\boldsymbol{j_{traj}} = \sum_{t=1}^{N_t} \left(abs\left(Q_{hs,traj}^t - \boldsymbol{Q_{hs}^t} \right) \right) = f_{traj}(\boldsymbol{Q_{hs}}, Q_{hs,traj}) \tag{3.17}$$

As indicated in Eq. (3.16) and Eq. (3.17) the corresponding summations are equivalent to the exemplary functions f_{cost} and f_{traj} when applied to the respecitve variables $\boldsymbol{P_{el}}$ and $\boldsymbol{Q_{hs}}$ with c_{el} and $Q_{hs,traj}$ representing constant or time-variant function parameters. Methodically, all respective formulations and contributions used for defining the objective function may solely be created in this way.

Allocation to High-Level Criteria Considering the two objective terms on a functional level, it becomes apparent that these are to be assigned to different global goals that are potentially contradictory (if the desired trajectory is not in line with minimum power prices). In principle, any function can be applied to any variable and assigned to any respective higher-level criterion. Methodically this is accomplished in a practical way by allocating the respective generic construction functions (specified with their parameters) to a vector according to the associated higher-level criteria. For clarification, the previous example is taken up and extended by additionally considering the criterion of CO_2 emissions and the arbitrary cost function f_a (with the exemplary parameters a1 and a2), both affected solely by power consumption. The resulting vector-valued construction functions $J_P(\boldsymbol{P})$ and $J_Q(\boldsymbol{Q_{hs}})$ are stated in (3.18) and (3.19). Similarly, for any variable, these vector-valued construction functions can be employed to define their respective contributions to the various criteria.

$$J_P(\boldsymbol{P}) = \begin{pmatrix} f_{cost}(\boldsymbol{P}, c_{el}) + f_a(\boldsymbol{P}, a1, a2) \\ 0 \\ f_{cost}(\boldsymbol{P}, c_{Co2}) \end{pmatrix} \tag{3.18}$$

$$J_Q(\boldsymbol{Q_{hs}}) = \begin{pmatrix} 0 \\ f_{traj}(\boldsymbol{Q_{hs}}, Q_{hs,traj}) \\ 0 \end{pmatrix} \tag{3.19}$$

In a further step, the entire objective function can be assembled as shown in Figure 3.6. In reference, the dashed boxes represent the high-level criteria while the individual single functions are represented by the horizontal lines. The use of such vector-valued construction functions aims at the efficient definition of the objective function as well as facilitating adaptability and reconfigurability. It needs to be emphasized, that the formulation of contributions is not solely restricted to the use and embedding of generic functions. Alternatively, specific formulations can be directly embedded, which, however, necessitates direct interventions and modifications of models and thus relates to an increased effort.

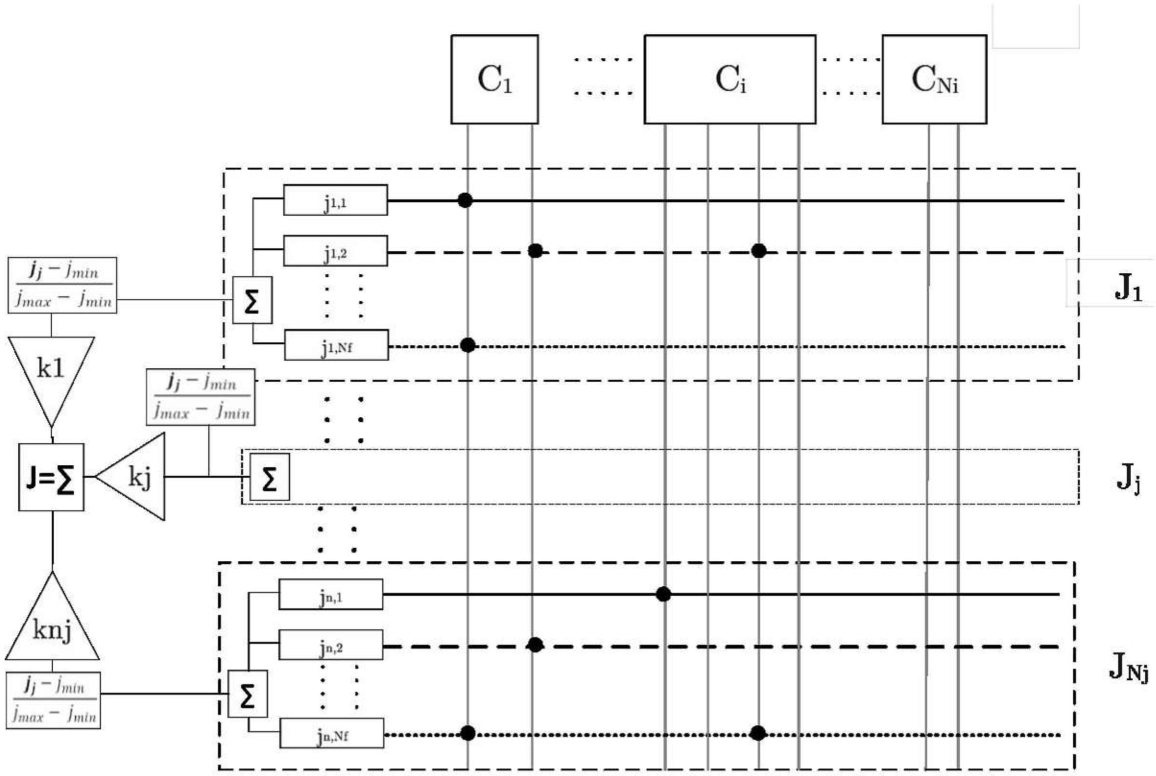


Figure 3.6: Illustration of the modular composition of the objective function

In Figure 3.6, the dashed boxes represent the high-level criteria J_j while the individual single contributions $j_{j,f}$ are represented by the horizontal lines. The vertical lines symbolize the variables that are associated to their corresponding components C_i. Consequently, the marked intersection points serve to indicate the relationships between components and their contribution to specific targets through the utilization of the respective functions. The high-level criteria J_j are each normalized according to Eq. (3.21) and may be individually weighted by the factors k_j.

Linear Normalized Weighted-Sum Aggregation The existence of multiple criteria and corresponding assignments have already been discussed. For resolving them to an overall problem statement, special emphasis needs to be placed on normalization and weighting. The scaling factors cover the possible ranges for normalization, while the weighting factors assign relative significance or priorities among the individual objectives. Precise calibration of these factors is crucial for accurate methodical performance and their manipulation may significantly influence the final outcomes, which becomes particularly demonstrated in the course of the case study in Chapter 5. The general form of a linear weighted sum is given by Eq.
(3.20) where the j_j^0 represent different equitable or normalized criteria which ideally take values between 0 and 1 in a non-**dimensional manner for guaranteeing a fair evaluation.**

$$\mathrm{j} = \sum_{j=1}^{N_j} f_j\, j_j^0 \tag{3.20}$$

In this respect, a general arithmetical normalization transforming the original objective j to be non-dimensional and independently of the original range is stated in Eq. (3.21) using j_{min} as lower bound and j_{max} as upper bound.

$$j^0 = \frac{j - j_{min}}{j_{max} - j_{min}} \tag{3.21}$$

Obviously, the effectiveness of this normalization is strongly linked to the quality of these bounds. However, it is important to note, that depending on the circumstances and formulations, certain bounds may also be omitted or show minor relevance. Moreover, their determination is not always trivial and can be related to high effort, which, additionally, may not always be expedient. Depending on the relationships and functions, weighting and normalization may be necessary at various levels. With respect to this method, an inclusion within the generic functions is most suitable at the lowest level. Referring to the previous example, normalization is typically necessary when given trajectories are to be pursued. In this way, the maximum heat generation $Q_{hs,max}$ is introduced to Eq. (3.17) for normalization as well as the weighting factor k_{traj} as represented by Eq. (3.21).

$$j_{Traj} = k_{traj} \sum_{t=1}^{N_t} \left(\frac{abs\left(Q^t_{hs,traj} - \boldsymbol{Q}^t_{hs}\right)}{Q_{hs,max}} \right) = f_{traj}(k_{traj}, \boldsymbol{Q_{hs}}, Q_{hs,traj}, Q_{hs,max}) \tag{3.22}$$

As high-level counterpart to Eq. (3.22), Figure 3.6 illustrates the aggregate plant-wide normalization and weighting in a general manner, which aligns with the mathematical formulation stated in Eq. (3.23). Here $J_j(\boldsymbol{x_v})$ denote the vector-valued construction functions of applicable to eventually all system variables $\boldsymbol{x_v}$.

$$\sum_{j}^{N_j} \left(\left(\frac{k_j}{j_{max,j} - j_{min,j}} \right)_j \sum_{v=1}^{N_v} J_{j,v}(\boldsymbol{x_v}) - j_{min,j} \right) \tag{3.23}$$

In remark to the normalization, it is not advisable to normalize costs or emissions at the lower level. However, it becomes crucial for a meaningful evaluation to normalize them when comparing the at global level.

3.2.3 Typical Objective Function Formulations

In the preceding explanations, the employment of generic functions was emphasized as characteristic feature for establishing modularity and reconfigurability. While their fundamental principle and integration were previously introduced through the accompanying example, a more comprehensive compilation and explanation of typical, commonly used formulations specifically relevant for MILP-UC problems is provided in the following. As indicated these formulations can be seamlessly incorporated into construction functions, facilitating a practical and efficient implementation.

Weighting of Variables

$$j_w(\boldsymbol{x}, c) = \sum_{t=1}^{N_t} \boldsymbol{x}^t c^t \tag{3.24}$$

The objective function is directly influenced by the decision variable in a proportional manner. In many cases the weights are not constant but exhibit profiles, which is the central distinction to a simple global weighting. This type of objective function can also effectively represent discrete decisions, such as investments. The essential parameters for this function are the weighting profiles. This approach finds particular relevance in scenarios such as energy costs, revenues, or environmental impacts, where varying weights over time or other factors are involved.

Minimize the Variation of a Variable

$$j_{varmin}(\boldsymbol{x}, x_{max}, x_{min}\ k) = k \sum_{t=1}^{N_t-1} \frac{|\boldsymbol{x}^{t+1} - \boldsymbol{x}^t|}{x_{max} - x_{min}} \tag{3.25}$$

The value of the objective function is influenced proportionally to (temporal) changes and variations in the variables. This property is particularly relevant for ensuring control stability, favoring smooth temporal progressions and avoid large oscillations, which potentially appear due to numerical reasons. As evident from the mathematical formulation, this type of objective function involves resolving an absolute term according to Eq. (3.26) ([124]), what underpins the usability of a functional incorporation. Additionally, weighting and normalization are crucial when applying this principle.

$$|\boldsymbol{x}| = \boldsymbol{x}_{abs} \Leftrightarrow \begin{cases} \boldsymbol{x} & \leq \boldsymbol{x}_{abs} \\ -\boldsymbol{x} & \geq \boldsymbol{x}_{abs} \end{cases} \tag{3.26}$$

Soft Constraints

$$\begin{gathered} g\,(\boldsymbol{x}_c, \boldsymbol{x}_d) \geq 0 \rightarrow g(\boldsymbol{x}_c, \boldsymbol{x}_d) + \boldsymbol{x}_{slack} \geq 0 \\ j_{sc}(\boldsymbol{x}_{slack}, c) = j_w(\boldsymbol{x}_{slack}, c) \end{gathered} \tag{3.27}$$

Soft constraints are employed to handle constraint violations effectively. Instead of generating an infeasible solution, the objective function is significantly influenced to account for these violations. Soft constraints can be seen as practical numerical tools that enhance the robustness and reduce susceptibility to incorrect input or initial values in optimization problems, which is particularly important in control tasks. While a generic implementation may be less convenient due to the fact that any arbitrary constraint can be handled in this manner, the introduction of a slack variable $\boldsymbol{x}_{slack}$ enables the treatment of soft constraints either as weighted variables or by incorporating trajectory progression.

Trajectory Progression

$$j_{traj}\left(\boldsymbol{x}, x_{traj}, x_{min}\ x_{max}, x_{min}\ k\right) = k \sum_{t=1}^{N_t} \frac{|\boldsymbol{x} - x_{traj}|}{x_{max} - x_{min}} \tag{3.28}$$

The objective function is influenced by the disparity between the variable and a predefined desired trajectory. This type of objective function is commonly employed when compliance with specific schedules or timetables is required. Deviations are methodically allowed and do not necessarily have to be strictly avoided but are associated with significant costs. Compared to an exact specification as a hard constraint, this approach is a more robust alternative and consequently holds significant importance in hierarchical optimization. Particularly for the hierarchical optimization procedure performed by the EMCS outlined below, these method plays a crucial functional role.

3.2.4 Graphical Representation of Holistic Optimization Problems

Figure 3.7 depicts the implementation of the example system from Figure 3.1 comprehensibly according to the presented optimization superstructure. Apparently, the clear and structured organization of the method provides to illustrate the complete optimization problem, comprising the composition of the energy system as well as the objective function in a solitary graphic. The vertical lines represent the contributions of the various components to the network balances and the individual objectives. Here, it must be recognized, that in contrast to Figure 3.5, all ports of a component have been combined into one line for the sake of clarity. Furthermore, reference is made to the different weighting factors, which are indicated in exemplary magnitudes by different color rings.

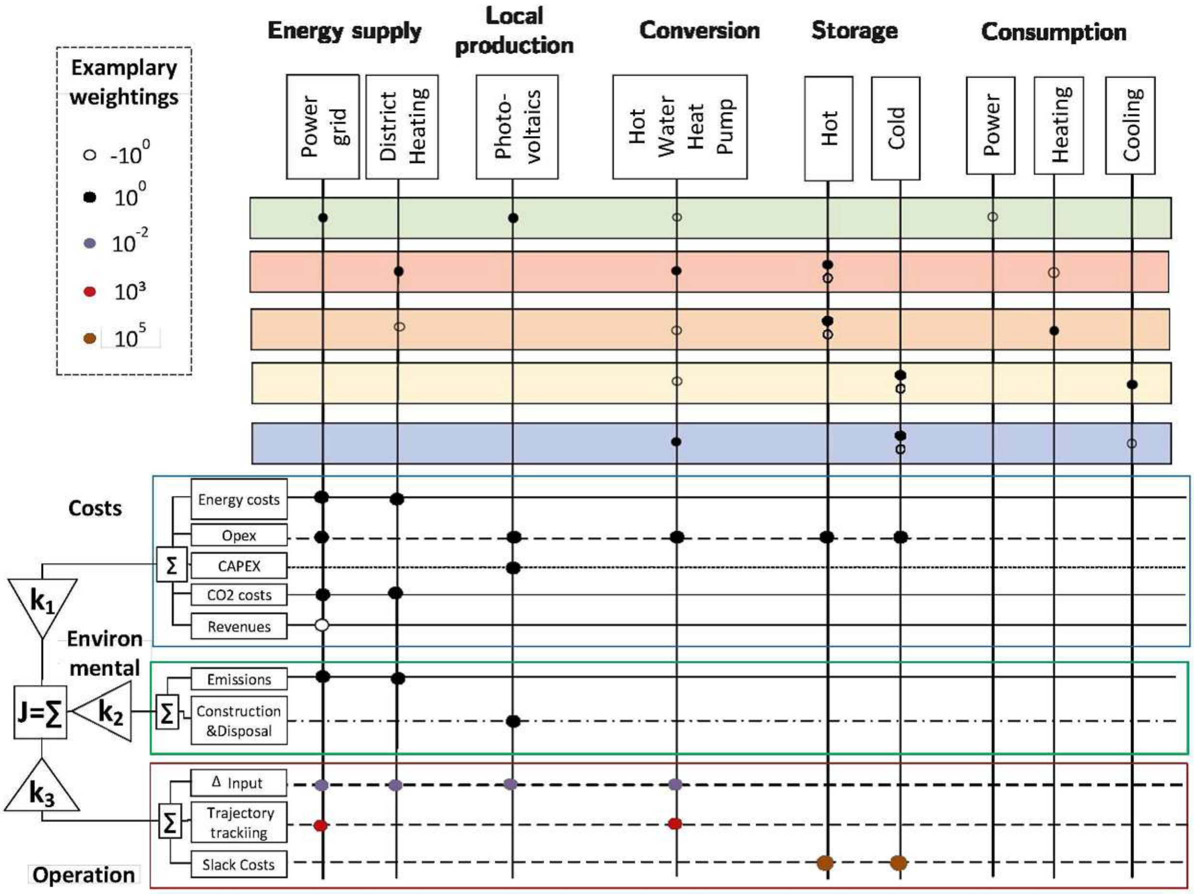


Figure 3.7: Superstructure representation of an examplary multi-objective optimization problem of the plant shown in Figure 3.1

3.3 Component Modeling

In the previous section, emphasis was placed on facilitating the treatment of multi-component energy systems from a holistic, plant-level perspective. There, the component models were exclusively considered on the basis of their ports, the interfaces between the global superstructure, and individual component models. As indicated by Figure 3.8, representing the counterpart to Figure 3.3, in this section the attention is extended to the inside of the interfaces, focusing on respective modeling issues, characteristics, and behavior of associated technical processes. While the formulation of the behavior of the processes occurring inside this boundary envelope through equality and inequality constraints was already indicated, the following section provides a more comprehensive insight and additionally addresses particularly relevant aspects. To emphasize the generic nature and flexible applicability, at this point, the description is intentionally kept rather on a general perspective followed by a specific example.

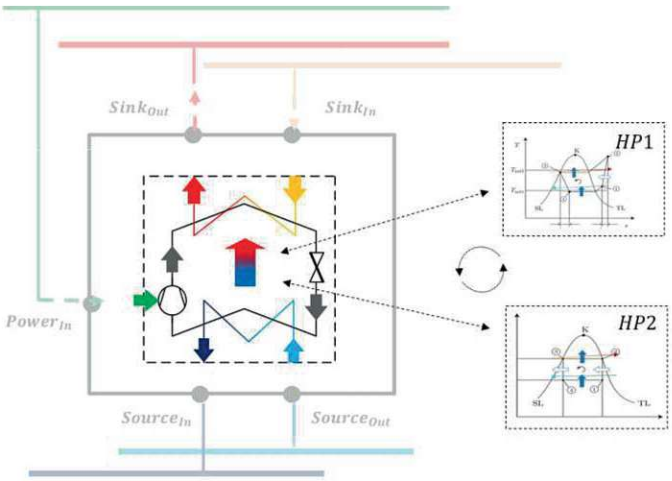


Figure 3.8: Modeling the behaviour inside the envelope

Basic concept In principle, the modeling of components adopts to basic paradigms as emphasized by Halmschlager et al. [43], however, the representation of internal processes is essentially not limited to pure conversion but enables to consider arbitrary dynamic behavior and introduces respective state variables. Additionally, specific modeling elements such as commitment formulations and objective functions are applicable in a generic manner individually to any system variable, without being restricted to input or output streams. To facilitate a consistent and seamless integration into the overall superstructure, the standardized stream types, as introduced in Table 3.1, need to be established at the ports. Hence, it becomes advantageous to modularly separate the modeling into two parts. The global part exclusively comprises the ports for ensuring superstructure consistency, in order to flexibly and interchangeably use various representations for the internal component model (see Figure 3.8). On a mathematical level, potential formulations may include any arbitrary number of additional variables and constraints and need to satisfy the requirements of MILP according to the generalized statement in Eq. (3.27).

$$g(x_c, x_d) = Ax_{i,c} + Bx_{i,d} + c \geq 0 \tag{3.27}$$

For the sake of generalization, the inequality operator ≥ was used in Eq. (3.27). According to Eq. (3.28) the set of variables of a respective unit $\boldsymbol{x_i}$ generally comprises both global port variables, summarized in the vector $\boldsymbol{s}$, and individual internal variables, denoted by $\boldsymbol{x_{i,int}}$.

$$\boldsymbol{x_i} = (\boldsymbol{s_i}, \boldsymbol{x_{i,int}}) \tag{3.28}$$

At this point, it is referred to the modeling and consideration of nonlinear effects, where linear representations fall short of adequately capturing the behavior. MILP offers the possibility to adopt piecewise linear formulations of which different techniques are described in detail in [75]. Using a straightforward approach, a nonlinear relationship $\boldsymbol{f}$ of r variables $\boldsymbol{x_r}$ can be approximated by l linear subsegments $\boldsymbol{f_l}$ with each exhibiting different constant parameters d_l and the vector of linear coefficients $c_{l,r}$ according to Eq. (3.29). Utilizing binary switching variables $\mathbf{b}_\mathrm{l}$, Eq. (3.30) ensures that only one particular linear segment is active.

$$\boldsymbol{f}(\boldsymbol{x_r}) = \sum_{\mathrm{l}} \boldsymbol{f_l}(\boldsymbol{x_{r,l}}) = \sum_{\mathrm{l}} \mathbf{b}_\mathrm{l}\, a_l + c_{l,r}\, \boldsymbol{x_{r,l}} \tag{3.29}$$

$$\sum_{\mathrm{l}} \mathbf{b}_\mathrm{l} = \mathbf{1} \tag{3.30}$$

The introduction of range constraints according to Eq. (3.31) subdivides the individual segments by constraining the respective vector of variables $\boldsymbol{x_{r,l}}$ with their lower and upper sgement bounds $x_{r,l,min}$ and $x_{r,l,max}$. Finally, the Big-M formulations stated by Eq. (3.32) and Eq. (3.33), establish the specific activation of individual segments.

$$\mathrm{x_{r,l,min}}\, \mathbf{b}_\mathrm{l} \leq \boldsymbol{x_{r,l}} \leq x_{r,l,max}\, \mathbf{b}_\mathrm{l} \tag{3.31}$$

$$A_{l,min}\, \boldsymbol{x_{r,l}} - d_{l,min} \geq -\mathrm{M}\,(1 - \boldsymbol{b_l}) \tag{3.32}$$

$$A_{l,max}\, \boldsymbol{x_{r,l}} - d_{l,max} \leq +\mathrm{M}\,(1 - \boldsymbol{b_l}) \tag{3.33}$$

Similarly, the same applies to the activation and deactivation of single linear relationships. Before the application example is presented, specific modeling-related properties and attributes, are discussed and highlighted.

Commitment Formulations Methodically, the formulations as stated in the expressions from Eq. (2.5) – Eq. (2.15) including the associated binary auxiliary variables are created generically by applying construction functions Γ to certain system variables. The function $\Gamma_l(\boldsymbol{x}, x_{min}, x_{max})$, where the parameters x_{min}, x_{max} denote the respective upper and lower bounds, creates the constraints stated in Eq. (2.8) and introduces the respective binary auxiliary variable u_x representing the on/off status of $\boldsymbol{x}$. In the same way $\Gamma_R(\boldsymbol{x}, RU, RD, SU, SD)$ additionally adds the binary auxiliary variables $\boldsymbol{v_x}$ and $\boldsymbol{w_x}$ and creates the constraints in Eq. (2.9) - Eq. (2.13) to introduce corresponding ramping as well as start-up/shut-down limits. Further, with Γ_T $\boldsymbol{x}, UT, DT$ the constraints of Eq. (2.14) and Eq. (2.15) are added to consider a minimum active or inactive time of $\boldsymbol{x}$.

While these constraints can be methodically applied to any system variable, practically, it is reasonable to apply them only to selected characteristic variables that are essentially related to the original real-world limitations. For computational efficiency, the aim is to use limit as few variables as possible to keep the optimization problem lean. As demonstrated in the RES Use-Case, constraining only one characteristic variable per component typically proves to be sufficient, however, it specifically depends to the prevailing number of system states and degrees of freedom. The component models used in the RES are described in detail in the appendix, including an assignment of the generic functions applied to the respective variables.

System States and Degrees of Freedom In a systemic context, dynamical processes, and systems can be characterized on the basis of their states and degrees of freedom (DOF). Both refer to related properties providing different insights into systems configuration, behavior and potential capabilities for modification and manipulation. Emphasizing the crucial importance of both terms with respect to operational optimization and control, which constitute desired main applications of the method, this section briefly outlines the relationships and distinctions between the two related terms. According to control theory, state variables represent a comprehensive set of quantities completely describing the overall condition and configuration of a system at any point in time. In the context of dynamic systems, these may also be interpreted as concentrated energy storages. DOFs, on the other hand, refer to mutually independent interventions, actions or decisions to modify or manipulate the systems configuration. These rather reflect the potential variability and flexibility of systems in reference to external interventions and internal connections. In essence, it is emphasized that the number of system states may differ from the number of DOFs. Conclusively, especially with respect to plant control, DOFs can be regarded as potential options for intervention to be manipulated through respective input signals in order to realize desired plant operations represented by system states.

First-Principle Modeling Fundamentally, processes and systems can be modeled either theoretically on the basis of their fundamental physical principles or, on the other hand, by analyzing data and deriving specific mathematical relationships. Each methodology possesses distinct advantages and particularly suitable applications. However, the preceding considerations evidently propose theoretical approaches to establish the equivalent presence of characteristic states and manipulatable variables of real systems in the respective models. Consequently, this work predominantly adheres to theoretical modeling.

3.3.1 Component Modeling Example

Based on the general descriptions and considerations, the component modeling approach is demonstrated in the specific example of a compression heat pump, depicted in Figure 3.9 performing a Clausius-Rankine cycle according to Figure 3.10. Focusing on the global part the physical connections comprise four thermal ports and one electric port for which the specific properties are to be considered as externally specified by connected networks. For the sake of completeness, Table 3.3 lists the properties in relation to the illustration of Figure 3.9. Regarding the individual model, the compressor is assumed to work at a constant isentropic efficiency η_{comp} and is restricted to operate at a certain minimum and maximum capacity. Furthermore, the cycle process is subject to a certain minimum switch-on and switch-off time as well as ramp-up and ramp-down limitations.

Model Derivation In the following the essential model relations are first derived and comprehensively explained.

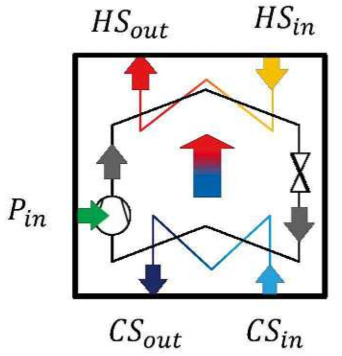


Figure 3.9: Ports of the heat pump model

Table 3.3: Port properties of a heat pump unit

Port	type	Properties	
		Variable	Parameters
HS_{in}	thermal	$\dot{m}, \dot{Q}$	$p, T, medium$
HS_{out}	thermal	$\dot{m}, \dot{Q}$	$p, T, medium$
CS_{in}	thermal	$\dot{m}, \dot{Q}$	$p, T, medium)$
CS_{out}	thermal	$\dot{m}, \dot{Q}$	$p, T, medium$
P_{in}	electrical	P	V, f

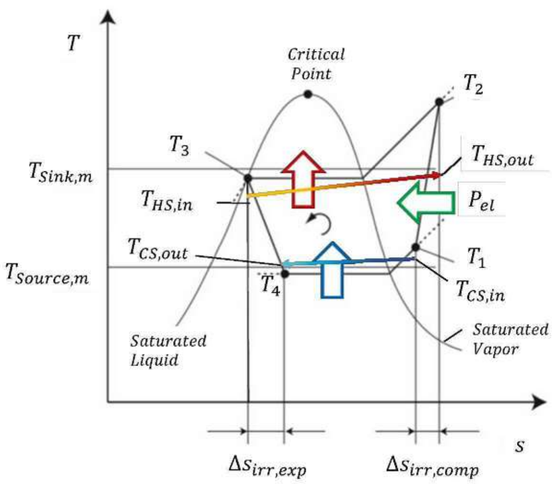


Figure 3.10: T-s diagram of the Clausius Rankine Process in a compression heat pump

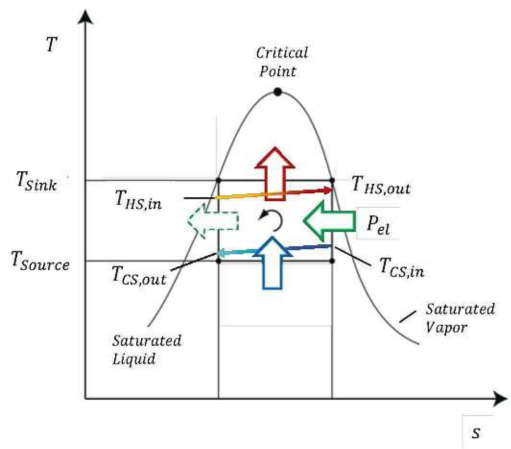


Figure 3.11: T-s diagram of the carnot reference process as the basis of the simplified abstract model

Figure 3.10 shows the T-s diagramm of a Clausius-Rankine cycle, and Figure 3.11 the corresponding simplified Carnot process implemented in the model. The properties of the thermal ports determine the inlet and outlet temperatures of the heat transfer media at the source and sink. In both heat exchangers, fixed temperature differences are considered, linking the upper and lower temperatures T_{Source} and T_{Sink} of the left-handed carnot process with the respective outlet temperatures of the source and sink as stated in Eq. (3.34) and Eq. (3.35).

$$T_{HS,out} + \Delta T_{HS} = T_{Sink} \tag{3.34}$$

$$T_{CS,out} - \Delta T_{CS} = T_{Source} \tag{3.35}$$

The simplification of considering a carnot process allows expressing the coefficient of performance by the reciprocal of the Carnot efficiency. Consequently, the expression in (3.36) is obtained, which describes the COP as an essential parameter regarding the energy conversion of the component.

$$COP = \frac{T_{HS,out} + \Delta T_{HS}}{T_{HS,out} + \Delta T_{HS} - T_{CS,out} + \Delta T_{CS}} \eta_{comp} \tag{3.36}$$

By the use of the COP as a derived model parameter, linear correlations are persistent between the electrical power input $\boldsymbol{P}$ and transferred heat at the sink $\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{HS}}$, and source $\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{CS}}$. In contrast to the electrical power input, which is predefined as a global port variable, the transferred heat at the sink and source represent additional internal variables.

$$\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{HS}} = \boldsymbol{P}\ COP \tag{3.37}$$

$$\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{CS}} = \Delta\dot{\boldsymbol{Q}}_{\boldsymbol{HS}} - \boldsymbol{P} = \boldsymbol{P}\ (COP - 1) \tag{3.38}$$

In addition, the relations presented in Eq. (3.39) and express the heat transfer at the source and sink.

$$\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{HS}} = \dot{\boldsymbol{m}}_{\boldsymbol{HS}}\ \left(h(p,T,medium)_{HS.in} - h(p,T,medium)_{HS,out}\right) \tag{3.39}$$

$$\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{CS}} = \dot{\boldsymbol{m}}_{\boldsymbol{CS}}\ \left(h(p,T,medium)_{CS,in} - h(p,T,medium)_{CS,out}\right) \tag{3.40}$$

Additionally, the normalized actuating variable $\boldsymbol{U}$ is introduced, which in this case refers to the ht output at the sink.heat $\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{CS}}$.

$$\boldsymbol{U} = \frac{\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{CS}}}{\Delta\dot{Q}_{max}} \tag{3.41}$$

Apparently, the different variables are all correlated with each other and consequently, this model only features 1 DOF but introduces 7 variables. In addition to the global variables represented by the vector $\boldsymbol{s}_{HP}$, the vector $\boldsymbol{x}_{\boldsymbol{HP,int}}$ comprises the additional internal variables.

$$\boldsymbol{x}_{HP} = \Big(\overbrace{\dot{\boldsymbol{m}}_{HS_{in}}\quad \dot{\boldsymbol{m}}_{HS_{out}}\quad \dot{\boldsymbol{m}}_{CS_{in}}\quad \dot{\boldsymbol{m}}_{CS_{out}}\quad \boldsymbol{P}}^{s_{HP}}\quad \overbrace{\Delta\dot{\boldsymbol{Q}}_{\boldsymbol{HS}}\quad \Delta\dot{\boldsymbol{Q}}_{\boldsymbol{CS}}\quad \boldsymbol{U}}^{x_{HP,int}}\Big)^T \tag{3.42}$$

3.4 Distributed Modeling Process

So far, the modular superstructure-based modeling approach has been explained regarding its conceptual methodology and associated mathematical formulations. Conclusively, focusing on the practical implementation, the holistic model definition of entire multi-component systems is subsequently illustrated and clarified. Utilizing the different modeling objects and auxiliary functions, a distributed problem definition is achieved. The modular integration also serves as the foundation for presenting the complete model in a coherent structure that emphasizes the division into global, individual, and generic elements. In Table 3.4, the distributed model definition is illustrated based on the accompanying heat pump example. The blue areas indicate the global defined objects, the individual specifications are highlighted in green, and the generic constructors in orange.

At the global level, plant-wide data including the different types of energy carriers with their characteristic properties, networks and connection matrices as well as the system boundaries and the composition of the global objective are specified. Consequently, as illustrated in Figure 3.12, the definition of the optimization problem is classified into five categories and three types of steps. Based on the global definitions, the modeling and mapping of the processes and procedures within the components is implemented individually as well as the definition of individual objectives. For efficient modeling, this process is facilitated by generically created formulations.

Table 3.4: Modular distributed definition of a component model

		global					individual		
Ports		CS_{in}	CS_{out}	HS_{in}	HS_{out}	P_{in}	$Q_{HS,min}, Q_{HS,max}\ Q_{HS,RURD}$		
Type/Parameters		*thermal*	*thermal*	*thermal*	*thermal*	*electrical*	$\eta_{Comp}, \Delta T_{HS}, \Delta T_{CS}$		
Variables		m	m	m	m	P	Q_{CS}	Q_{HS}	U
Objectives	**Costs**					j_w		j_{SUSD},	
								j_{traj}, j_{var}	
	Emissions					j_w			
UC Constraints								$\Gamma_L, \Gamma_R, \Gamma_S, \Gamma_T$	
Auxiliary Variables								u, v, w	
Connection		$\begin{pmatrix}-1\\0\\0\\0\\0\end{pmatrix}$	$\begin{pmatrix}0\\1\\0\\0\\0\end{pmatrix}$	$\begin{pmatrix}0\\0\\-1\\0\\0\end{pmatrix}$	$\begin{pmatrix}0\\0\\0\\1\\0\end{pmatrix}$	$\begin{pmatrix}0\\0\\0\\0\\-1\end{pmatrix}$			
Internal Model		$T_{HS,out} + \Delta T_{HS} = T_{Sink}, \quad T_{CS,out} + \Delta T_{CS} = T_{Source}$ $COP = \frac{T_{HS,out} + \Delta T_{HS}}{T_{HS,out} + \Delta T_{HS} - T_{CS,out} + \Delta T_{CS}} \eta_{comp}$ $\Delta\dot{Q}_{HS} - P = \Delta\dot{Q}_{CS} \quad COP = \frac{\Delta\dot{Q}_{HS}}{P}$ $\Delta\dot{Q}_{CS} = \dot{m}_{CS}\ (h(p,T,medium)_{CS,in} - h(p,T,medium)_{CS,out})$ $\Delta\dot{Q}_{HS} = \dot{m}_{HS}\ (h(p,T,medium)_{HS,in} - h(p,T,medium)_{HS,out})$							

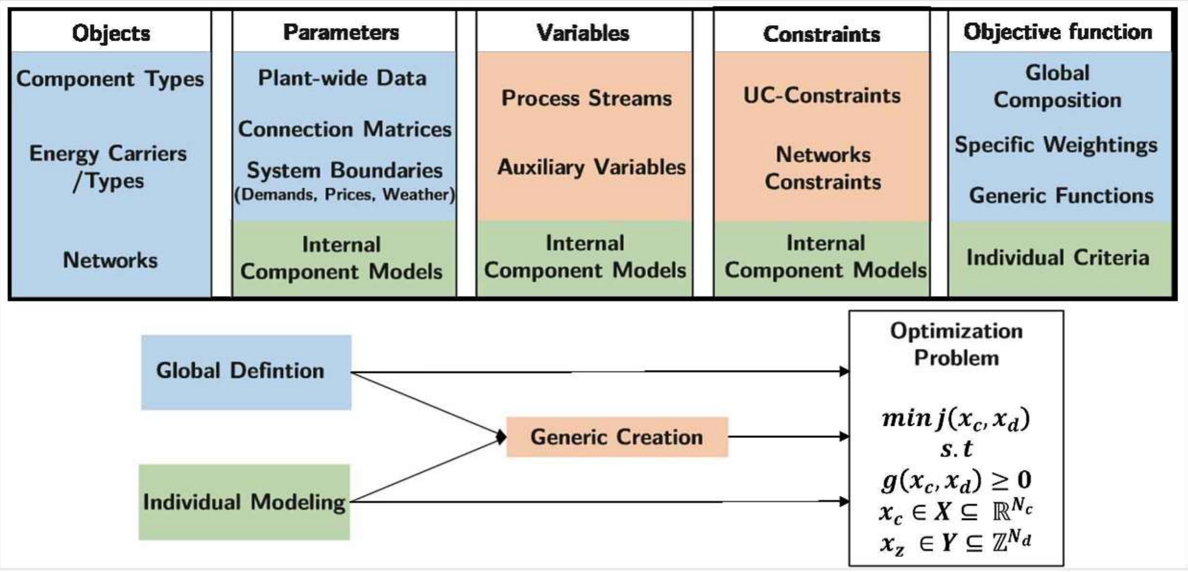


Figure 3.12 Illustration of the distributed problem definition

The specification of the models including formulations and basic equations can be done individually, however, a library of generic formulations supports an efficient modeling process. Thereby the correct connection and use of the port properties and variables within the individual formulations is crucial. As depicted in Figure 3.12, the generic part comprises the creation of operational constraints (Unit Commitment formulations), associated auxilliary variables as well as the balancing of process streams within the networks constraints. In principle, the flexible modeling approach makes it possible to apply commitment constraints to any variable. However, it is important to remember that it is not practical to apply them to more variables than there are degrees of freedom within a component.

3.5 Concluding Remarks

The presented optimization framework advances existing state-of-the-art approaches by combining a generic and modular superstructure for the holistic treatment of complex multi-energy systems with an intuitive, streamlined, and user-friendly modeling and implementation. The use of standardized modeling objects such as components, distribution networks, and streams enables a distributed modeling approach that emphasizes model adaptability and efficient reconfiguration. This applies not only to the modeling of the physical units, but also to the specification of objective functions through the use of generic elements serving the basis for a similar component-based composition. To facilitate an efficient real-world integration, primarly first-principle models are used to a enable an uncomplicated parameterization based on characteristic technical data. In addition, instances of component models and respective interfaces are organized according to typical process control systems to enable simple a implementation and integration process. Moreover, the identified parallels with the extensively derived conceptual model presented in [32] indicate for the generic and broad applicability of the fundamental superstructure. Consequently, the approach strives for a holsitic treatment, which is particularly advantegeous for complex multi-energy systems.

3.5.1 Maintaining Linearity

The establishment and maintenance of linear models are crucial for robust modeling and efficient solvability. The following list highlights the essential assumptions, approaches, and simplifications applied in the present method to obtain linear relations for the model formulation.

- In distribution networks, constant discrete intensive state properties are assumed, such as temperature and pressure, (also denoted as discrete quality approach). Additionally, dynamic behavior, inertial effects, and spatial dimensions are neglected.
- Quasi-static state changes are assumed. This allows the efficient representation of dynamic limitations and operational constraints using the typical UC-formulations according to Eq. (2.5) - Eq. (2.15) described in Section 2.3.2.
- Energy conversion and storage only occur within components. The representation of transient system dynamics is employed by using discrete, time-variant state variables. For representing higher-order dynamics, if necessary, state variables of several time steps are to be represented in single constraints. For instance, in a very simplified form, this is applied for considering minimum up-downtime as expressed in Eq. (2.14) and Eq. (2.15). In the applied models, however, predominately two consecutive time steps appear in the constraints, reflecting first-order derivatives.

3.5.2 Application of the Optimization Superstructure

The developed method has already been applied in different use cases which are briefly listed here:

- The Design Optimization for the integration of new technologies in existing conventionally designed systems, presented in Chapter 4.
- The Two-level hierarchical optimization concept for the holistic energy management and real-time control of industrial plants will be described in Section 3.6 and demonstrated in Chapter 5 on the plant design obtained in Chapter 4.
- The mulii-stage optimization procedure for the "Flexibility Identification of an Industrial Production" [49] is based on a use case within the paper and pulp industry. This investigation, whose connection to this work is described in more detail in Section 1.4, comprises an interconnected energy system of two production sites, which are connected to the medium-voltage grid via a common transformer.

3.6 Energy Management and Control System

When developing the presented optimization modeling superstructure, special emphasis was placed not only on efficient modeling but also on the establishment of features and capabilities for viable incorporation into real-time operating environments. This Section presents the respective further enhancement to a holistic energy management and control concept, representing the ultimate novelty of this work. In this context, the modular superstructure offers notable advantages by facilitating an immediate and simultaneous formulation of multiple hierarchically interacting optimization problems, especially for complex multi-energy systems.

3.6.1 Basic Architecture

As already mentioned in the preface, the two-level control scheme proposed by Fuhrmann et al. [1], developed in the collaborative research project EDCSproof, was adopted and forms a fundamental conceptual basis regarding system architecture and operational principles. The respective extended approach used in this work is shown in Figure 3.13, which in particular incorporates the two-layer optimization procedure comprehensively into the operational environment of the energy system. The fundamental characteristic lies in the division of core functional responsibilities related to plant operation. The higher level is mainly responsible for determining the optimal medium-term energy management strategy. These decisions are essentially influenced by the predicted trajectories of system boundaries and the technical constraints of the components. Conversely, the lower level primarily focuses on operational safety and control, operating on a shorter time scale and acting in the sense of a typical MPC. Methodically, the separation into different temporal scales allows for a more effective and distributed decision-making process and avoids potential conflicts: Long-term energy management decisions can be determined without the immediate influence of short-term control implications. On the other hand, short-term control can be focused on the necessary immediate actions where energy management aspects are of subordinate importance.

3.6.2 Operational Mechanism

To establish a viable functioning and ensure a harmonious coexistence, the optimization procedure needs to be neatly integrated into the operational environment of the controlled plant, as indicated by Figure 3.13. Determining optimal operation schedules requires sufficient knowledge of external system boundaries and, most importantly, the energy requirements of the processes. The predictions and planned sequences are therefore the essential inputs for determining the optimal energy management. At this point, it is important to note, that scheduling of consumption processes is not considered within this thesis, i.e. the energy demands are to be accepted as a given and cannot be manipulated. On the other hand, the measured data and the monitored operation are essential inputs to be able to realize the optimal schedules efficiently in terms of control. The control signals for operating and activating individual units represent the central outputs of the EMCS.

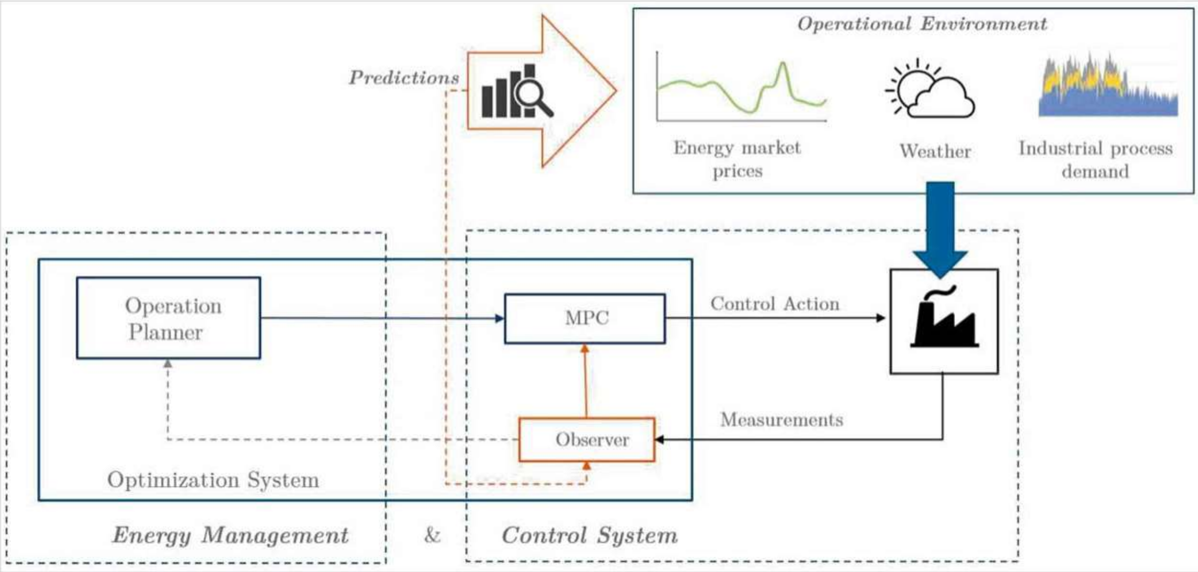


Figure 3.13: Architecture of the Energy Management and Control System

3.6.3 Model Implementation

So far, the specific working principles, characteristics, and functions of the energy management system have been illustrated, thus defining the foundations and requirements for the model implementation. According to the illustration in Figure 3.14, the composition of the hierarchical optimization problem within the EMCS can effectively be accomplished as a special advanced application of the developed modeling superstructure. Especially refering to the holistic incorporation into the plant's operational environment, the modular modeling is particularly advantageous as it enables a flexible setting of system boundaries to units by utilizing generic functions.

It is emphasized, that the optimization problems of the two levels are intended to be nearly identical with respect to the plant and component models, while the objective functions are expected to differ significantly. Using different individual models for specific units is an option as long as the global properties, including port types, energy carriers, and most importantly, the characteristic state variables remain consistent. In addition, it is also feasible to consider (slightly) different plant compositions within the two levels. For example, especially in the lower layer, individual subsystems can be treated separately, neglecting certain physical connections which can have both positive as well as negative effects in terms of performance, as demonstrated by the case study in Chapter 5.

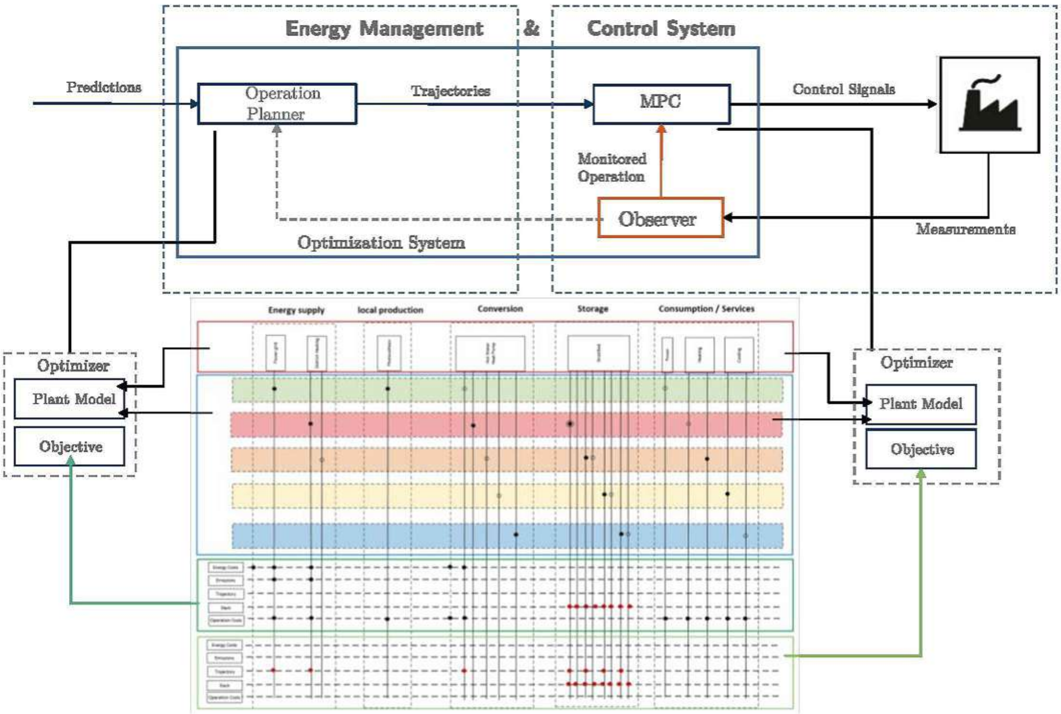


Figure 3.14: Realization of the hierarchical optimization system as application of the modeling superstructure

3.6.4 Hierarchical Coupling

The hierarchical coupling of the two optimization levels is facilitated by tracking desired set-point and state trajectories, dictated by the higher level to be followed by the subordinate controller. Due to the prevailing unambiguous hierarchies between the two levels, the approach presented in Eq. (2.16) is employed. Thus, the objective function of the MPC constitutes the key instrument for linking the two optimization levels. According to Eq. (3.43), the total contribution of trajectory tracking $\boldsymbol{J}_{\mathbf{traj}}$ is a weighted sum of all units.

$$\boldsymbol{J}_{\mathbf{traj}} = \sum_{x_r \in X_x} \mathrm{f_w} \sum_{\mathbf{t=1}}^{\mathbf{N_t}} \left| \boldsymbol{x}_{\mathbf{r}}^{\mathbf{t}} - x_{r,traj}^{t} \right| \tag{3.43}$$

$$X_x = \{\boldsymbol{x}_r \in \boldsymbol{X} \mid \boldsymbol{x}_r \ \ follows\ a\ trajectory\} \tag{3.43b}$$

Methodically, this formulation is created component based on generic functions and incorporated to the objective function according to Eq. (3.28). In Figure 3.15, the hierarchical connection is illustrated based on the simple subsystem. The black vertical lines represent port variables and the green lines specify internal variables of the units. While port variables connect different units within one layer, the trajectory tracking is reasonably applied to characteristic internal state variables.

In this illustration, the thick green lines symbolize that a connection between OP, MPC, and plant is established via this variable. The black arrows shown at the EMCS structure on the left indicate that any measured values and derived quantities (e.g.: SOC) are provided by the observer to the higher levels, while the higher levels only communicate the respective selective variables (illustrated as green dashed arrows) to the lower level via trajectories.

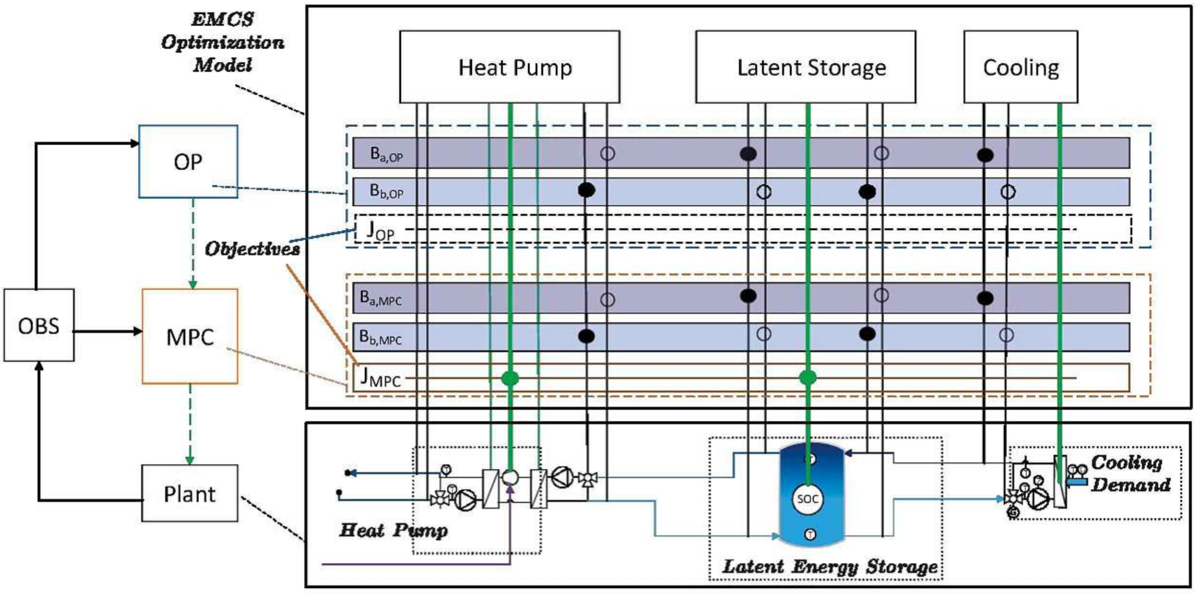


Figure 3.15: Hierarchical linking through trajectory tracking of certain variables in the MPC

While potentially all variables between both levels could be linked, the following aspects need to be considered in this context: Contrary to the notion that extensive linkage ensures enhanced performance, computational as well as modeling effort rather suggest the opposite. Moreover, considering the existence of imperfect prediction and inaccuracies of the optimization models, the tracking of particularly dependent variables may introduce conflicting criteria in the subordinate levels' objective function. This is an essential methodical aspect that will be comprehensively discussed and showcased in a respective case study.

3.6.1 Operative Procedure

In Figure 3.16, the temporal procedure of the two-level receding horizon optimization is illustrated. Both axes are chronologically subdivided into consecutive time steps and periods. The horizontal axis corresponds to the time steps that are considered in the different actions and procedures. The vertical axis indicates the respective time steps at which the individual procedures and actions are performed or carried out. The calculation for a certain time period is always carried out at preceding time periods to be completed before the actual operational time. Since the calculations are of a certain duration, it is necessary to start them sufficiently in advance in order to be completed before execution. As characteristic of a receding horizon procedure, the optimization is only executed until a more recent calculation is available for the corresponding time steps. The observation focuses centrally on the time step τ and considers the actions around this time. While the MPC has a sampling time of one time step, the comparatively much longer sampling time of the OP is denoted by Δts_{OP}. The MPC can be regarded as an online optimizer since it performs a new calculation at every time step and continuously considers the most recent measurements. In contrast, the OP is to be regarded as an offline optimizer, since it periodically performs a new calculation only at certain time intervals. Also, its calculation is based entirely on predictions since obviously, no measurements are available for the respective upcoming timestep. The two-layer receding horizon optimization is realized according to the execution flow principle shown in Figure 3.17.

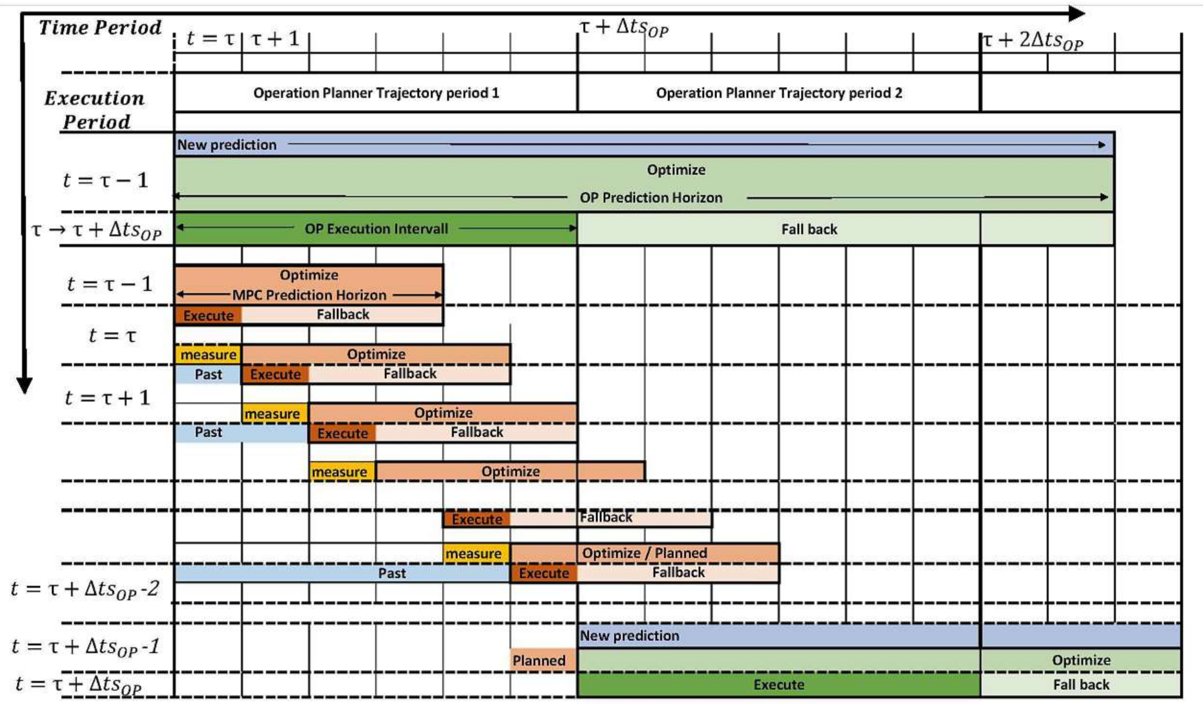


Figure 3.16: Two level optimization receding horizon procedure

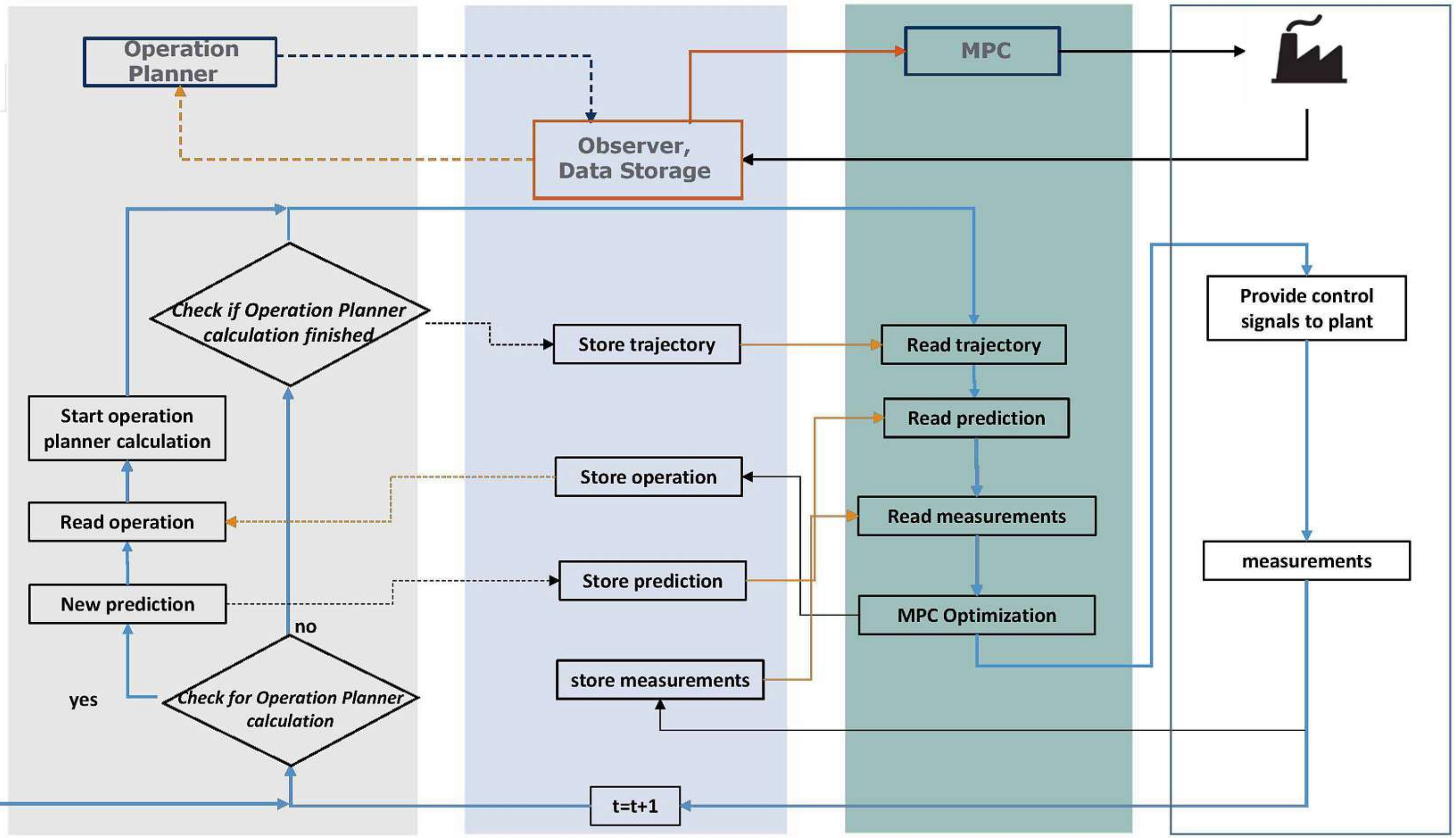


Figure 3.17: Operative execution flow diagram

3.6.2 Functional Demonstration Example

To enhance the understanding of the hierarchical optimization procedure, the simple subsystem shown in Figure 3.18 is considered, which consists of a thermal storage tank and a heat pump that uses this storage as a reservoir on the cold side.

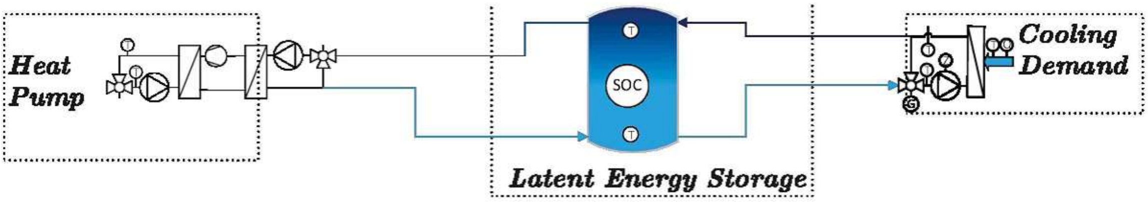


Figure 3.18: Configuration of the examplary subsystem

For the storage, the SOC is used as the characteristic quantity to observe and evaluate its operational state. For the heat pump, the heat output at the hot side is used. In the provided charts from Figure 3.19 to Figure 3.23, a black solid line represents the actual operation as observed ("measured") from the simulation model. The green dashed lines display the long-term optimal operation determined by the OP which may account timespans of up to several days and is adjusted periodically every few hours to maintain accuracy with the measured states. The respective sections until the next periodic adaption are to be considered as active parts and are highlighted in blue. The orange lines indicate the short-term predictions of the MPC, from which the actuating signals are derived that are finally applied to the controllable components in each time step. Moreover, the current time is indicated by a vertical dotted line. When examining the determination of a long-term trajectory, it is important to consider that the corresponding optimization process requires a certain amount of time. Consequently, it is less appropriate to use the units' current states as initial conditions for the calculation. Instead, it is more sufficient to predict the value of the states at the time the optimization process is completed. Reasonably, this prediction time aligns with the maximum permissible calculation time for the optimization. Considering potential deviations between the intended operational paths and the actual measured states, the most recent MPC prediction for this upcoming time is accessed as initial condition. In Figure 3.19, the discussed calculation time gap is highlighted by the short green line, which indicates the starting time for the new long-term optimal course, originating from the respective value of the MPC prediction. This trajectory then represents the desired operation to be pursued until the succeeding periodic calculation may adjust this desired optimal course. As described, this procedure is repeated periodically for each respective time period. In Figure 3.20, which shows the status after one period has elapsed, a noticeable deviation between the targeted trajectory (depicted in blue) and measured course (shown in black) is recognized at the storage on the right. Such deviations are mainly attributable to model or forecast inaccuracies. Instead, at the heat pump, the measured states in black match the desired course very well as the blue color is completely covered. The following Figure 3.21 reveals the situation one calculation period later, where a delay of the SOC progression from its intended course can immediately be recognized. Consequently, when observing the operation of the heat pump on the left side of the chart, also a short time shift of the start-up can be recognized as an associated adjustment of the optimal operation. In Figure 3.22, which displays the status after two further periods, however, shows a more reliable operational progression in this subsequent period.

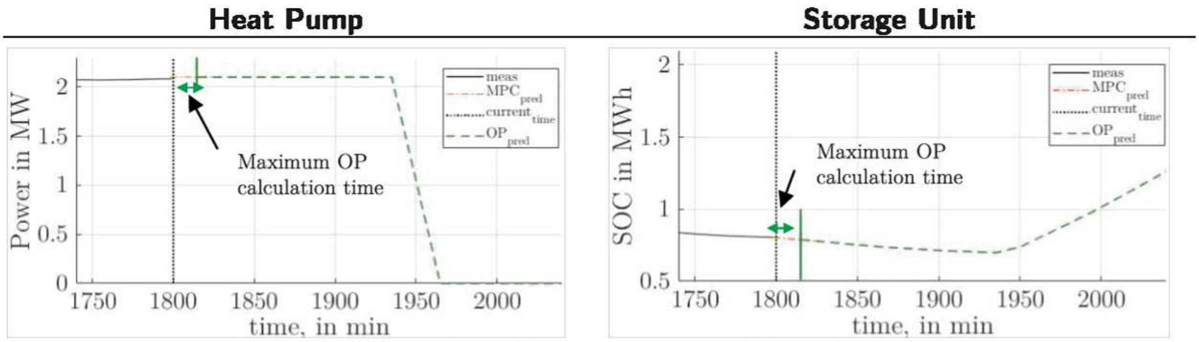


Figure 3.19: Beginning of the determination of the optimal course

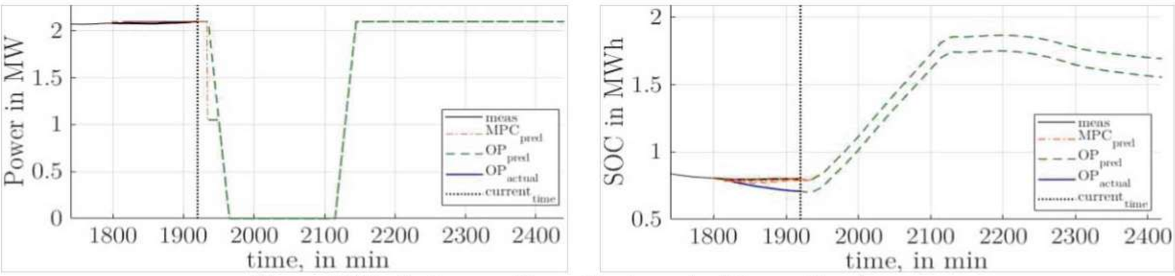


Figure 3.20: first suceeding adjustment of the optimal course

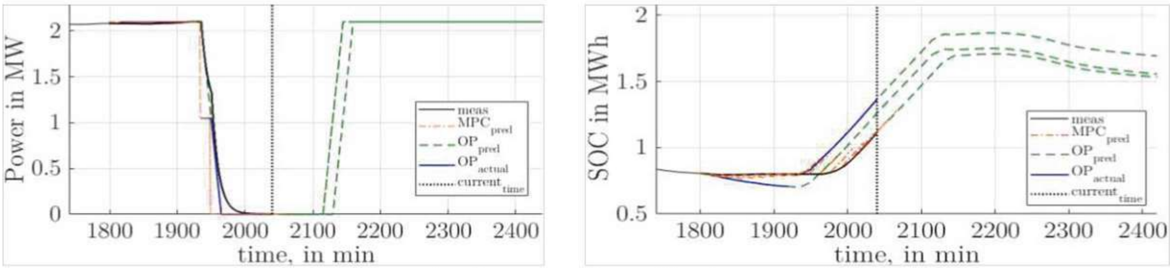


Figure 3.21: next subsequent the optimal course calculation

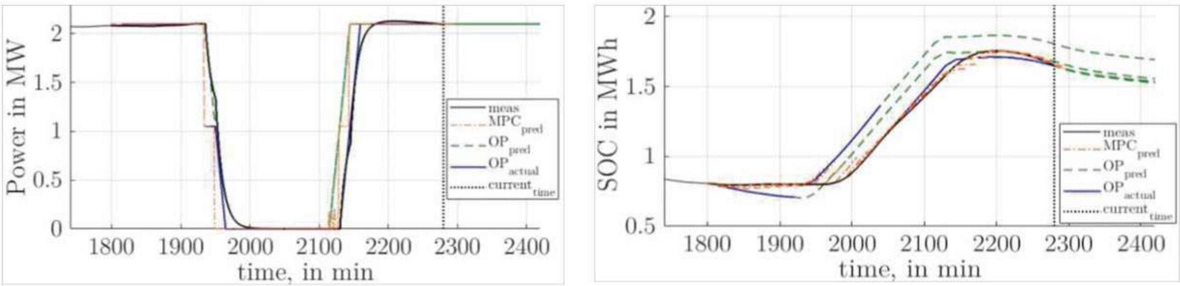


Figure 3.22: progression of periodic optimal course adaptions

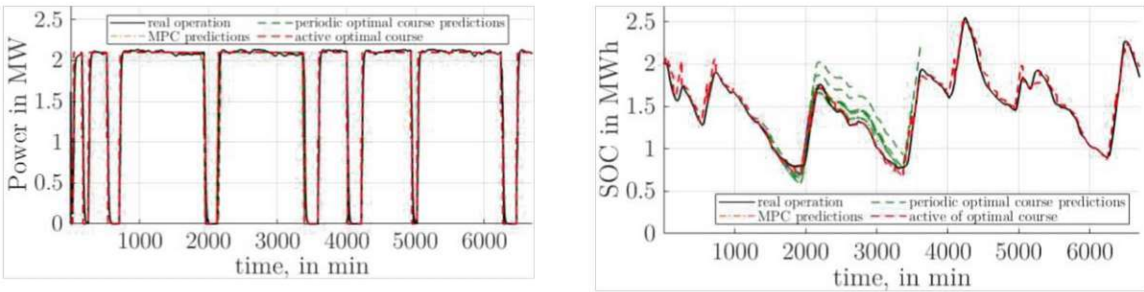


Figure 3.23: Comparison between the active optimal trajectories and the realized operation

The last illustrations in Figure 3.23 show the entire operational progress of the two components over the period of five days. The red dashed line shows the optimal operation path, which is formed by linking the active segments from each of the successive repeated long-term optimizations. Additionally, the temporary trajectories from the respective time sections examined in more detail are adopted and equally represented as green dashed lines. While the storage exhibits more significant deviations, at the heat pump, a notable alignment between the desired optimal trajectories and the measured operations can be observed. Nevertheless, it can be recognized, that the interim optimal predictions show a sufficient level of compliance with the qualitative trend of the realized operation. By this example, it becomes evident how the outlined two-layer receding horizon optimization procedure enables to handle and compensate model and forecast errors and consequently proves robust, precise planning and control capabilities.

Remarks on Model Accuracy and Weighting In the higher optimization level, certain overarching, mostly physically quantifiable objectives, such as costs, emissions, or production quality are pursued. Consequently, also a simultaneous multi-criteria consideration of various different criteria needs to be accomplished at the higher level. However, typically there is only one superordinate criterion, mostly costs, to which superior importance is attached. In this case, despite the inclusion of methodological terms like soft constraints or for smoothening operations, the introduction of specific weightings or normalization measures is generally less appropriate at this level. For a suitable performance, soft constraints typically require significantly higher magnitudes than the sensible "physical" objective ($>10^3$), while the minimization of control input variations (see Eq. (3.25)) typically works properly already when significantly lower magnitudes are specified.

In contrast, at the lower level, both normalization and weighting are of crucial significance and essential for a proper functioning of the operative mechanism [125]. In the example above, for the heat pump, less deviations and a more accurate alignment to the predicted optimal trajectory can be observed compared to the storage. This indicates a higher compliance between the optimization and the simulation model. Consequently, it is reasonable to prioritize the progression of the heat pump trajectory compared to the storage. For demonstration, the illustrations from Figure 3.24 to Figure 3.28 show the same example case with the same operational conditions, but prioritizing the trajectory tracking a the storage unit within the objective function of the MPC. Comparing both progressions, a quite similar qualitative trend is observed for the storage, however at a higher average SOC. By the time the detailed observation starts, the SOC is already 0.8 MWh higher. Conversely, the heat pump shows a completely different course, characterized by significant state fluctuations, which become especially evident when observing the entire period shown in Figure 3.28. The main reason for these deviations can be attributed to the more simplified model of the storage as previously mentioned. In the detailed observation above, especially at condition changes, delays of the measured SOC compared to its operational planning by the optimization model were observed (see Figure 3.21). The imperfect optimization model used for prediction determines a trajectory that cannot be accomplished by the real component (or the simulation model). Due to the high weighting, the MPC receding horizon optimization nevertheless tries to realize the desired states and thereby causes a suboptimal operation of the connected heat pump. On the one hand, this comparison indicates that the capabilities and potentials of the method strongly depend on the models in combination with methodological parameters. On the other hand, it also proves that significant improvements can be achieved even when using simple or less accurate models.

Heat Pump **Storage Unit**

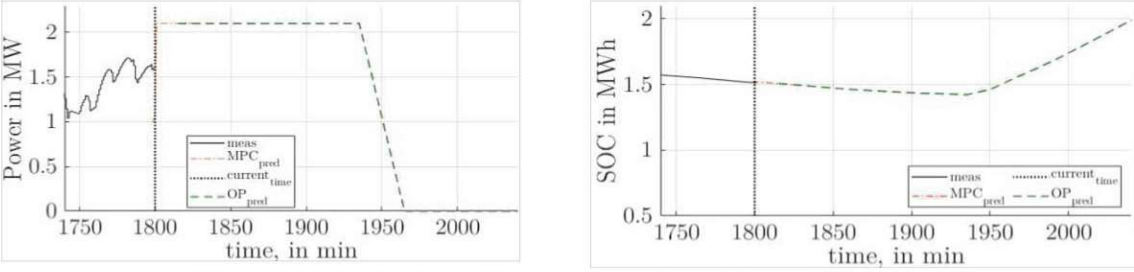


Figure 3.24: Beginning of the determination of the optimal course

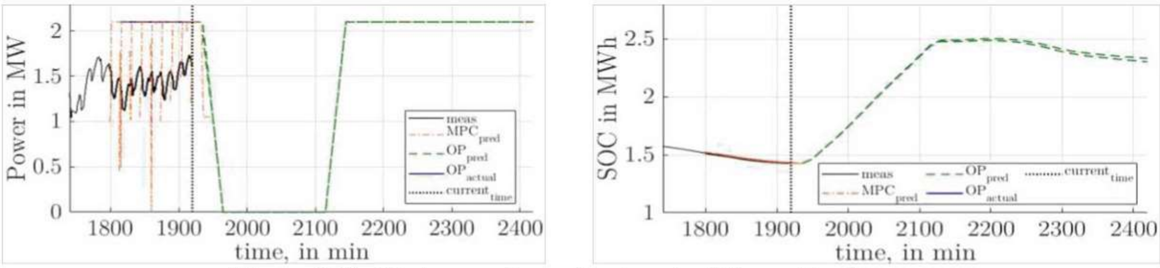


Figure 3.25: First suceeding adjustment of the optimal course

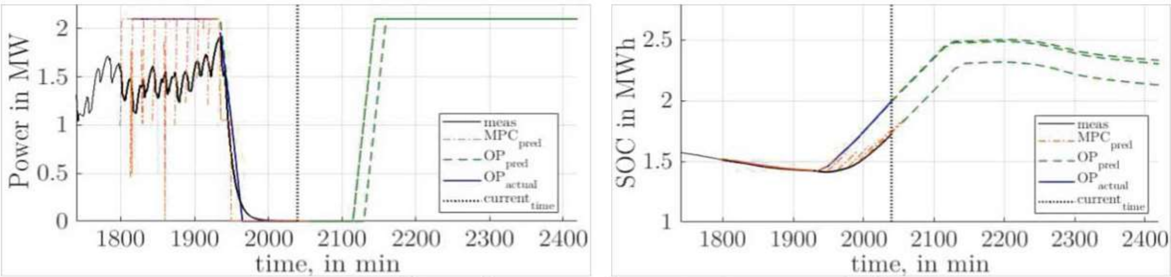


Figure 3.26: Next subsequent the optimal course calculation

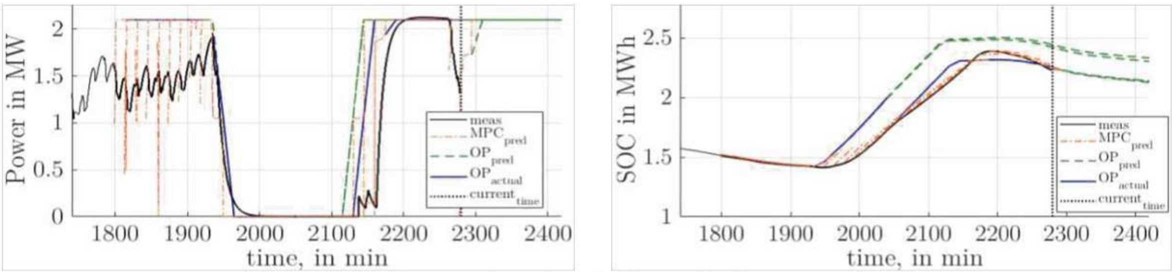


Figure 3.27: Progression of periodic optimal course adaptions

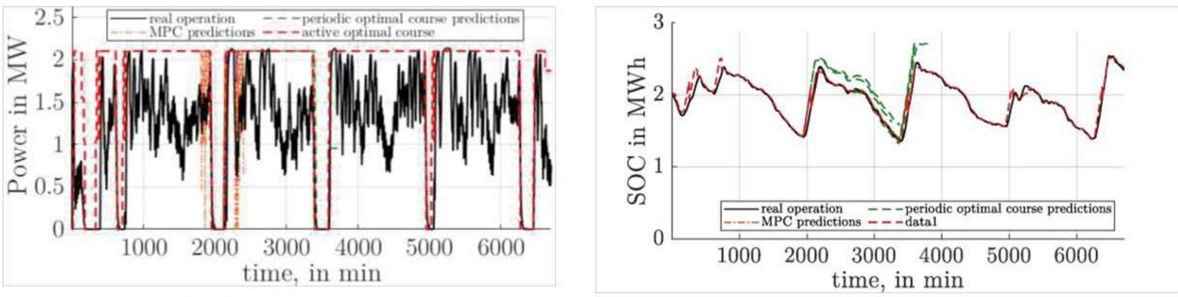


Figure 3.28: Comparison between the active optimal trajectories and the realized operation

3.7 Simulation Modeling

Simulation models are desired to emulate the behavior of real systems by accurately reproducing their physical relations, corresponding systems states, and outputs in a causal way. Simulation models are most frequently used for prediction, analysis, and assessment of process performance to provide a profound understanding of complex system behavior. Unlike descriptive optimization models, simulation models are predominantly of a causal nature (cause-effect models) and typically formulated in a procedural manner. In this way, a dynamic and transient system behavior can replicated by the time-dependent specification of model inputs.

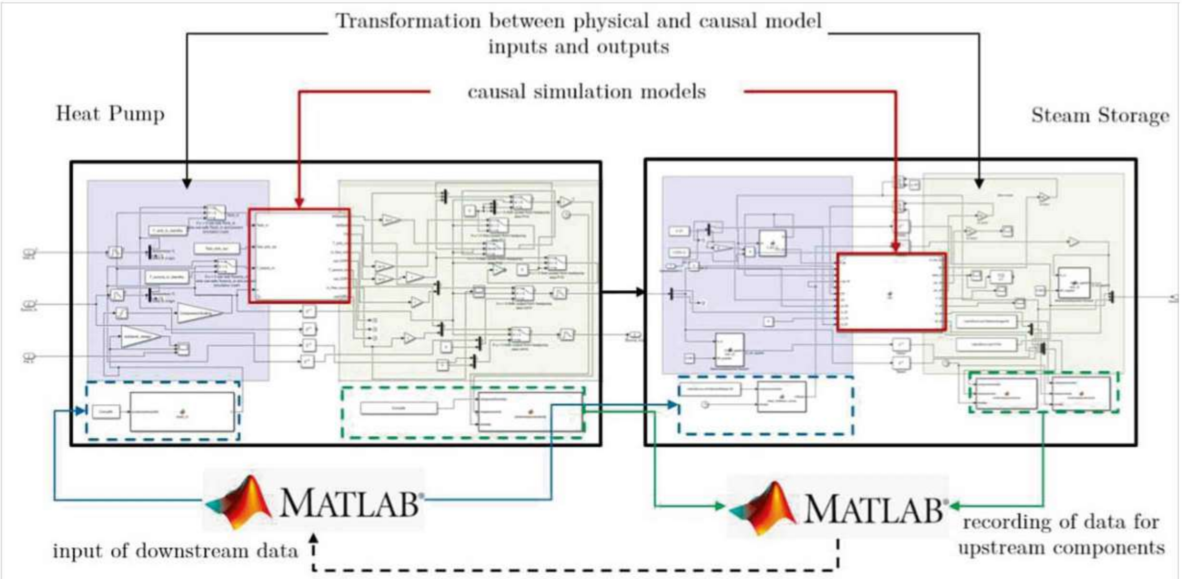


Figure 3.29: Transformation of causal relations to physical structure

From a systemic perspective, a notable disparity between the physical structure of a system and its underlying causal mechanisms is to be emphasized. The causal input and output variables of the models' equation systems differ in comparison to the inputs and outputs at physical system boundaries. Properties of output streams on the physical level may be model inputs on the causal level and vice versa. In the context of this work, these circumstances assume particular significance due to the utilization of SIMULINK, a graphical simulation environment integrated in MATLAB, which is characterized by a unidirectional, causal signal and data flow structure. In general, the determination of causal relations and dependencies in dynamical systems cannot immediately be derived solely by examining the physical system boundaries, and with rising complexity, the causality of systems becomes increasingly cumbersome. Consequently, while causal-oriented model formulations are suitable for studying the behavior of single processes, components, or simple systems with a limited number of states, they become highly impractical when dealing with complex systems comprising multiple interacting components, each possessing distinct characteristics. As a remedy, organizing and modeling energy systems based on their physical configuration offers a more practical, synoptic, and efficient approach. This is accomplished by incorporating the causal relations and procedures in containers, reflecting the physical interfaces (serving as a practical workaround to enable straightforward and efficient assembly of energy systems based on distinct component models).

The ability to concisely compose complete models of energy systems in a modular way by assembling single component models is a central feature of this approach. Nonetheless, the utilization of Simulink imposes a noteworthy limitation related to its unidirectional signal processing, allowing causal effects to be only taken into account downstream, disregarding the existence of upstream relations. For example, the pressure or SOC of a thermal storage imposes a causal influence on the performance of an upstream utility. Tackling this restriction, MATLAB is employed as a data-processing interface for ensuring the upstream consideration of system properties, consequently creating pseudo-bidirectional causal modeling. However, it is necessary to additionally specify the respective connected components. Specifically of importance for the later case study, this approach offers the important advantage that optimization and simulation models both have identical system boundaries and interface properties.

Figure 3.29 illustrates the described procedure by providing an insight into the containers based on the example of a connected heat pump and thermal storage. The actual models, reproducing the dynamic behavior of the corresponding processes in the components, are represented by the red frames. The signal transformation to the model inputs and from the outputs are indicated by the blue and green areas. The dashed frames indicate the interfaces to MATLAB data processing, which establishes the pseudo-bidirectionality of the signal flows. In addition, it should be noted that the simulation is performed at fixed, constant discrete time steps using the ode45[7] solver. Thus, the input variables remain constant for the entire time step and there is a delay of one time step between the variables on the input and output side. The actual model relations are either implemented as MATLAB functions or using Simulink library blocks as well as using Functional Mockup units. The employed models used for the various considered components and technologies are listed and described in more detail in the Appendix.

[7]The ode45 solver is a function in MATLAB and refers to a one-step integration method for Ordinary Differential Equations The method uses 4th order method to move forward in each step, but it uses a 5th order method to estimate the error and decide on the appropriate step size for next step.

Never globalize a problem if it can possibly be dealt with locally.

GARRETT HARDIN

4 Design of a Reference Energy System

Aim and Scope of this Chapter To effectively demonstrate and validate the applicability and functionality of the methods presented in Chapter 3, it is imperative to use a suitable comprehensive, close-to-real energy system as a reference use case. In this context, it is particularly refered to the research gaps highlighted in Chapter 1. As a result, the creation of the reference energy system (RES) emerges as a crucial sub-goal to adequately tackle the core substance of this thesis. The primary emphasis is placed on industrial processes with a heat demand below 160°C, with particular focus on the food sector, driven by the presence of promising technologies that can facilitate significant decarbonization for these consumption requirements. However, despite of large improvement potentials, these technologies have not become standard in current technological portfolios of industrial energy supply facilities. Therefore, as a reference for comparison, a conventional configuration (CRES) excluding these modern, more sustainable components is additionally introduced. This initial conventional layout of this system is derived empirically by analyzing real plants from EDCSproof[8] project partners (see Preface) in addition to a respective literature research. Subsequently, the integration of new technologies is achieved through mathematical design optimization. This approach allows for a targeted and optimal integration of these technologies, showcasing how existing systems can be upgraded to meet state-of-the-art standards and assess the resulting economic and ecological impacts. To provide broader, more comprehensive, and sector-specific insights and conclusions, the RES is designed as a generalized state-of-the art use-case, serving as a representative model for the subsector rather than an individual plant configuration. As emphasized in Chapter 1, plant design and the corresponding control and energy management strategies are closely linked, which is also particularly addressed in the design optimization based of the respective scenarios.

4.1 Basic Concept

The basic idea is depicted by the simplified example in Figure 4.1. Conventional energy supply structures (shown in grey), typically exhibit a relatively straightforward and unidirectional structures. Heat is generated in certain temperatures and then transported to the consumption processes. However, in these systems, energy conversion or transfer between different energy carriers is often lacking or inefficient. Although thermal storages are present in almost every energy supply system, they predominately tend to be operated as hydraulic switches rather than fully exploiting possible storage utilization. However, in the transition to renewable and carbon-free alternatives, the need for flexibility becomes crucial, especially considering the inherent volatile and less planable energy generation. To address this challenge, additional measures must be taken, such as incorporating energy storages for establishing a more diverse portfolio of supply options, and implementing effective energy management strategies. In particular, high-temperature heat pumps show promising CO_2 reduction potential, especially in combination with thermal energy storages for improving both efficiency and flexibility [56].

[8] https://www.nefi.at/de/projekt/edcsproof

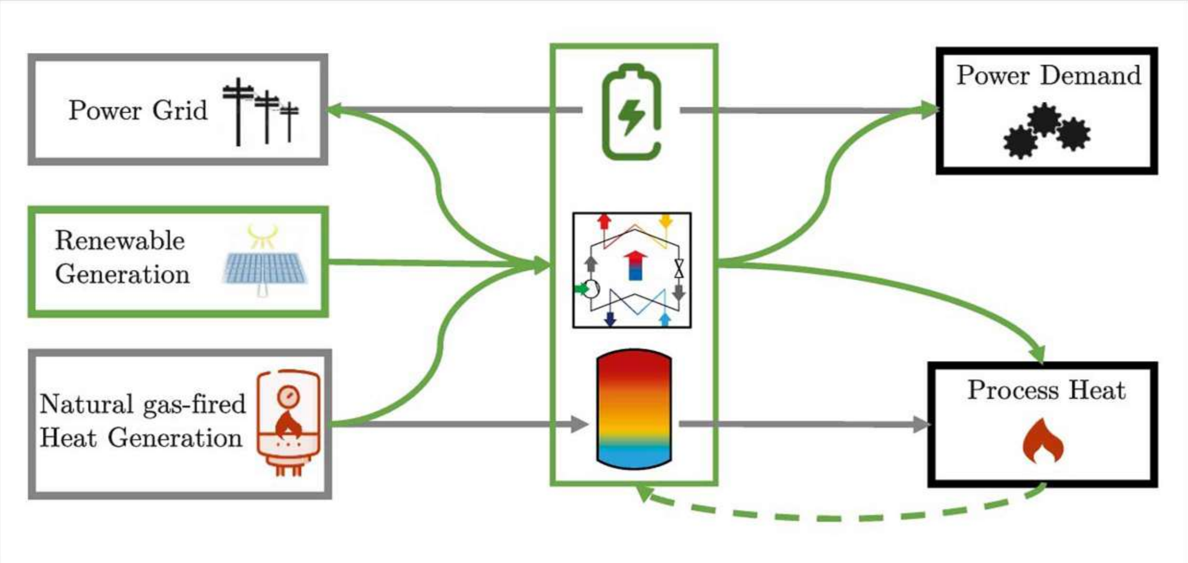


Figure 4.1: Establishing flexibility by the targeted integrating of sustainable technologies (green) into conventional unidirectional energy supply structures (grey)

Figure 4.1 illustrates the strategic integration of sustainable technologies (indicated by green frames) into conventional unidirectional structures (shown in grey) to establish flexibility for a reliable and secure transition from fossil-based generation to intermittent renewable energy suppliers.

4.1.1 Materials, Methods and Design Approach

As shown in Figure 4.2, the reference energy system is derived and configurated by merging the essential components from three industrial plants of the project partners in combination with the findings of the literature research and predecessor research projects. Initially, a fundamental knowledge basis on respective process characteristics, technologies, and energy sources is gained through literature research, which is comprehensively described in Section. However, little information was available on the structural designs of complete energy supply systems, more specifically on the arrangement and interconnection of internal distribution systems as well as conversion and storage units. To gain a more comprehensive insight and a better understanding of internal structural configurations in typical industrial energy systems, the project partners' plants were consulted and examined. Through comprehensive data acquisition and processing, the systems of the three use cases were thoroughly analyzed both quantitatively and qualitatively to identify the essential components and assess their operational characteristics. Subsequently, these components were systematically grouped into subsystems and categorized into the overarching categories of supply, conversion, distribution, storage, and consumption.

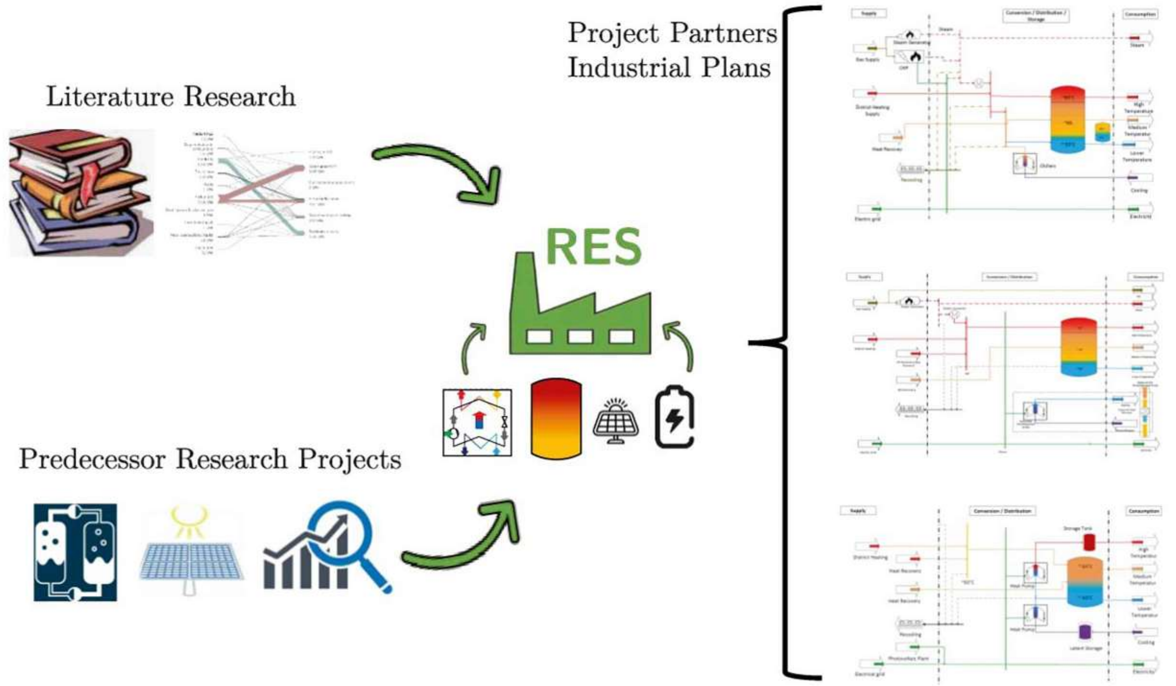


Figure 4.2: Data and Information Sources of the RES

Based on this preceding structuring, the three use cases could be merged and combined with the findings of the literature research to derive the CRES layout. In a final step, starting from the CRES, potential integration possibilities of new components and technologies were explored. For determining the integration and dimensions of the new components, a design optimization was executed for the following components: Photovoltaic System (PV), Electrical Energy Storage (EES), Hot-Water Heat Pump(HWHP), High Temperatur Heat Pump (HTHP) and Steam Storage (StST). Additionally, the utilization of local renewable sources, specifically photovoltaics and solar thermal energy (PV, ST) as well as electrical and latent cooling storage is evaluated. The derivation of a reasonable design was continuously and iteratively consulted in coordination meetings within the team of the research project EDCSproof. The aim was to assess whether the various technologies are representative or eligible from a functional and quantitative perspective. It was also desired to create a wide range of options for subsequent assessments while ensuring a high degree of flexibility and maintaining a clear and intuitive structure for the system.

4.1.2 Literature Research Summary

For the derivation of the RES design, the essential findings of the literature review discussed in Section 2.1.1., are summarized below.

Industrial State of the Art

- The food industry is characterized by a wide variety of products and production steps, leading to very fluctuating consumption profiles for both process heat and electricity.

- For the supply of these highly fluctuating demand patterns, controllable generation units with rapid load changes are of central importance, where lower conversion efficiencies are therefore accepted.
- Gas- or diesel-fired combined power engines with waste heat recovery are the main source for on-site power generation.
- The major final energy carriers are natural gas with more than 55% and electrical energy with about 34%. For temperatures up to 160°C, more than 60% of the energy for steam production comes from fossil fuels.

Identified Improvement Potentials

- Waste heat potentials are often not utilized due to low temperatures or existing temporal and spatial gaps between the waste heat source and the heat demand.
- In particular, high-temperature heat pumps show promising CO2-reduction potential, especially in combination with thermal energy storages to improve both efficiency and flexibility. Depending on the COP, heat pumps show promising CO_2 savings potential between 70% (COP=3) and over 80% (COP=6).
- Solar heat is mainly suitable for temperatures below 100°C, which accounts for 7.7% of process heat in the EU28.
- Thermal storage units are present in almost any industrial supply system. However, they are primarily operated as hydraulic switches and show unused flexible potential.

4.1.3 Characteristics of the Industrial Plants within the Project EDCSproof

In the following, an overview of the energy supply systems of three project partners' plants is given. For the examination of the specific characteristics, similarities, and differences, simplified schemes are illustrated first followed by a description of components, energy carriers, and processes.

Plant A In this plant, a gas-fired CHP unit with a total capacity of about 1,1 MW generates power, steam, and hot water due to engine cooling. Additionally, a gas-fired Steam generator, with a maximum generation capacity of 4,5 MW is also used for steam production. A district heating supply as well as a heat recovery system, and a recooling tower are also present. Heat is supplied using distribution grids of steam at a temperature of 160°C, as well as at 90°C and 65°C by hot water. Cooling services are provided at about -15°C and -30°C where waste heat from the cooling supply is partially recovered for the heat supply. A Stratified storage is used as a hydraulic swith to decouple supply and demand for the 90°C and 65°C levels. The residual electrical demand beyond self-generation is covered by the grid.

Plant B In contrast to the other plants steam is not used as an energy carrier in plant B. Heat is supplied using hot water distribution grids at temperatures 90°C, 60°C, and 40°C. Cooling services are provided at about -15°C where waste heat is partially recovered for the heat supply. Also, a stratified thermal storage is used as a hydraulic switch to decouple thermal supply and demand. In a separate subsystem, two cascaded heat pumps are simultaneously providing heating and cooling of batch processes at the assistance of two water storage tanks. The residual electricity demand beyond self-generation is covered by the grid.

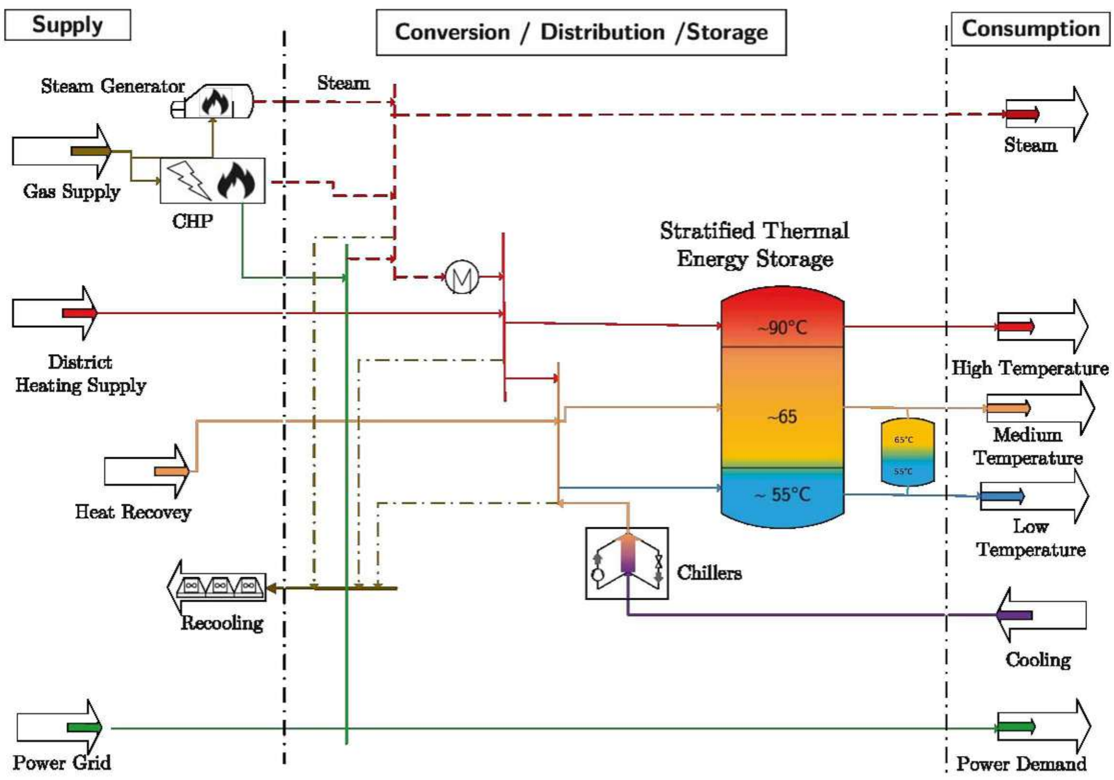


Figure 4.3: Simplified scheme of industrial plant A

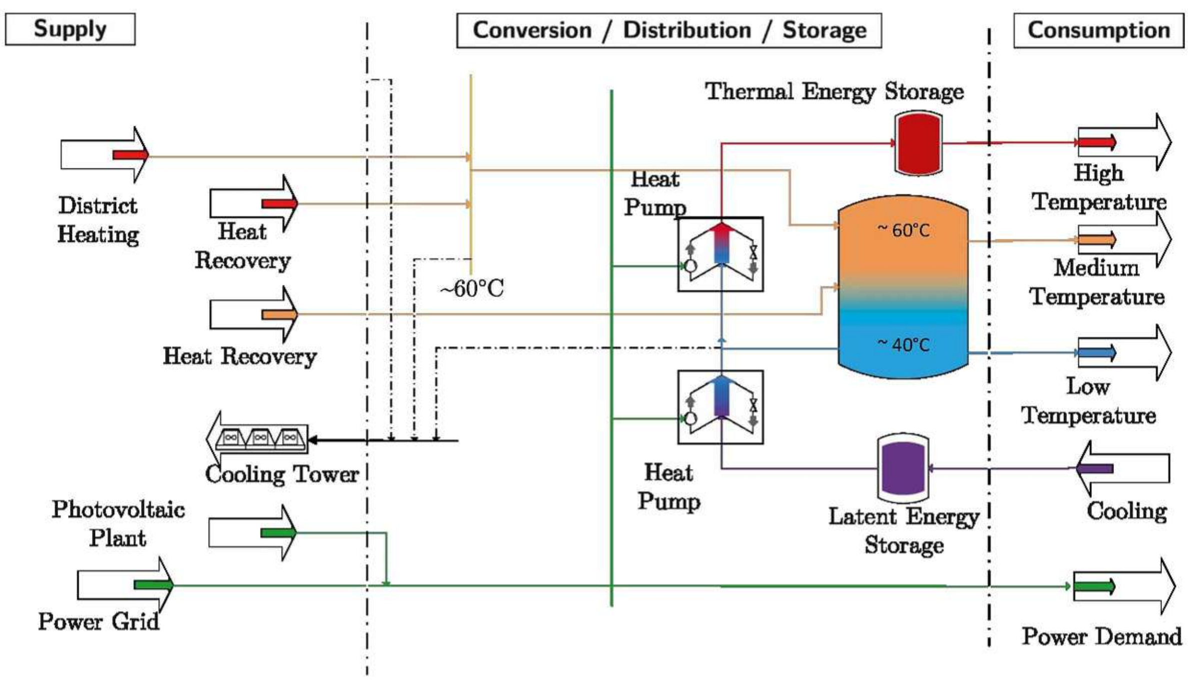


Figure 4.4: Simplified scheme of industrial plant B

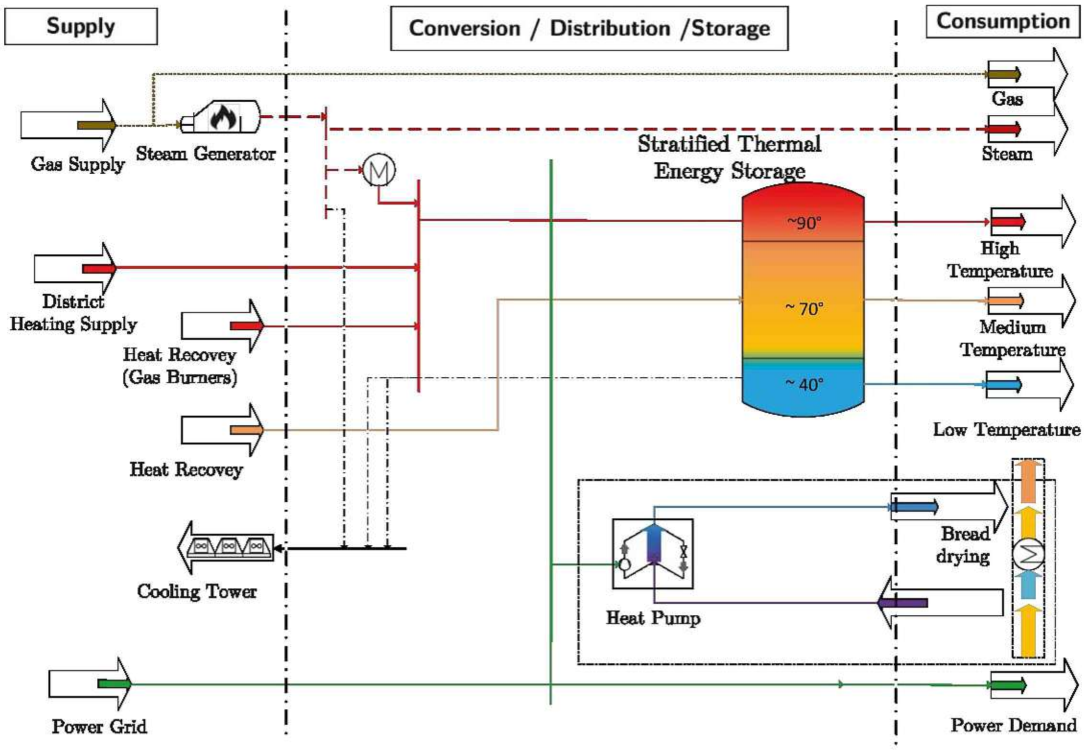


Figure 4.5: Simplified scheme of industrial plant C

Plant C In this plant, a gas-fired unit is used for steam production. Also, natural gas is directly used for providing process heat and a district heating supply as well as two heat recovery units are present. Heat is supplied using distribution grids of steam at a temperature of 160°C, as well as at 90°C, 70°C and 40°C by hot water. Cooling services are provided at about -20°C and a heat pump is used to recover waste heat from a drying process. Similar to the other plants, a stratified storage is present acting as a central hot-water hub. The electricity demand is covered by the grid.

Conclusively, natural gas, district heating, and electricity were identified as the main energy sources on the supply side. Gas is used at plants A, and C for steam generation and as fuel for the CHP. District heating is used at plants A, B and C. The power supply of all systems is mainly provided with electricity from the grid. On the consumption side, the following categories of consumers can be found: Steam is required for the production processes at plant A and C. In all three use cases, heat is distributed at (at least) three different temperature levels, where water is used as a heat transfer medium. Furthermore, cooling at temperatures below 0 °C is present among all three use cases. Regarding the energy conversion and distribution systems, heat storages (latent and sensible) are already part of each of the three systems. Heat pumps can be found at Plant B and C. Below the various specific production processes are listed and classified according to their final energy service type

- Electricity
    - Cutting, slicing, chopping, mincing, pulping, pressing mixing, blending, homogenization, conching, grinding, milling, crushing
    - Forming, moulding, extruding, lightning, compressed-air generation

- Heat
  - Baking, roasting, frying, tempering, pasteurization, sterilization
  - Evaporation (liquid to vapor), drying (liquid to solid), dehydration (solid to solid)
  - Cleaning and disinfection
- Cooling
  - Cooling, chilling, cold stabilization, freezing, freeze-drying, lyophilization refrigeration, vacuum generation

4.2 Composition of the Reference Energy System

The configuration shown in Figure 4.6 and Figure 4.7 was developed as Conventional Reference Energy System (CRES). While this system does not fully represent any of the individual use cases in total, it is a reasonable, and extensive overlap so that the findings of the research are valid to be scaled and related to the individual plants. Also, by setting different limits, parameters and switching of non-essential components, all significant subsystems of the use cases can be recreated.

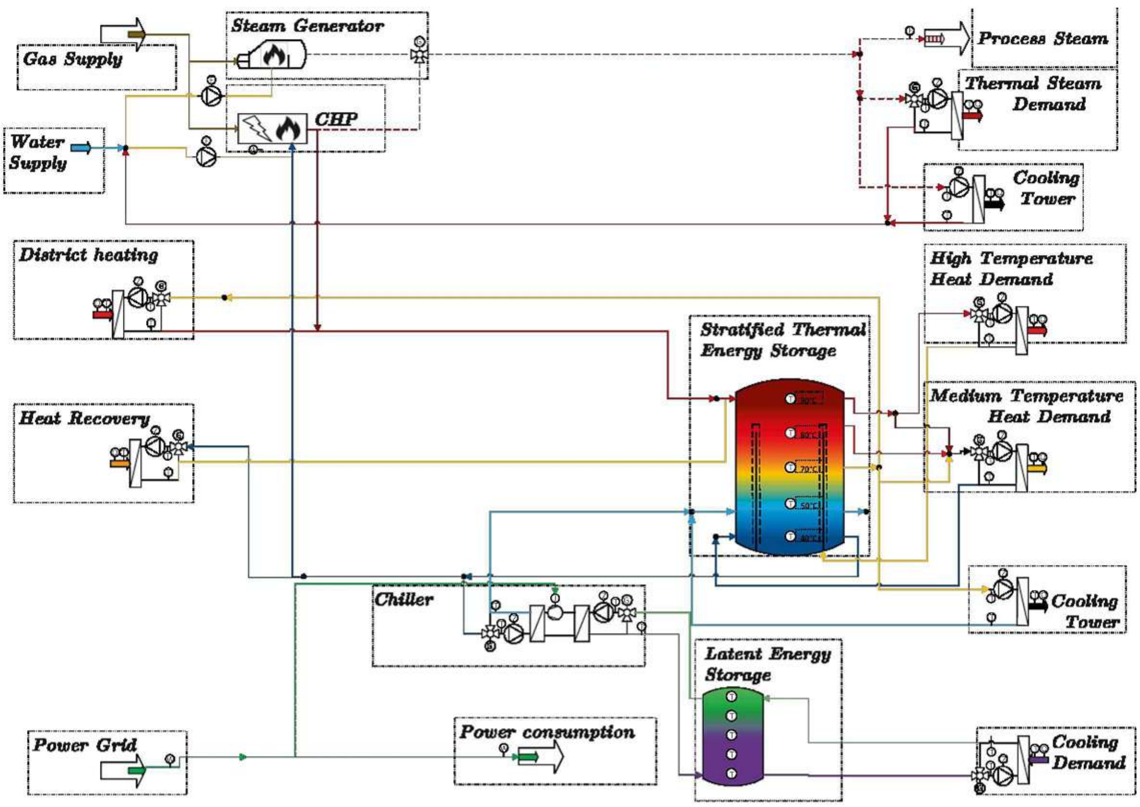


Figure 4.6: Scheme of the CRES

In addition, the RES also considers alternative technological design extensions (heat pumps, heat storages, renewable suppliers) to be able to carry out and analyze process and efficiency improvements. Figure 4.7 shows the RES in an extensive, very detailed illustration according to its ultimate design which was created as a guideline for the purpose of a model-based implementation. As indicated by the large number of connections, in the RES great emphasis was placed on providing a wide range of possible options for energy distribution to maximize flexibility. A further design characteristic to be emphasized is the staggered placement of the heat pumps and storage as central components decoupling consumers from supply. On the one hand to level the supply in case of batch processes, on the other hand, to minimize consumption-related limitations for the times of cost-effective power supply. The direct connection of heat pumps and storage tanks as well as their dimensioning can also be related to the design optimization presented in Section 4.5. Finally, however, it needs to be noted that it is not a real existing physical system.

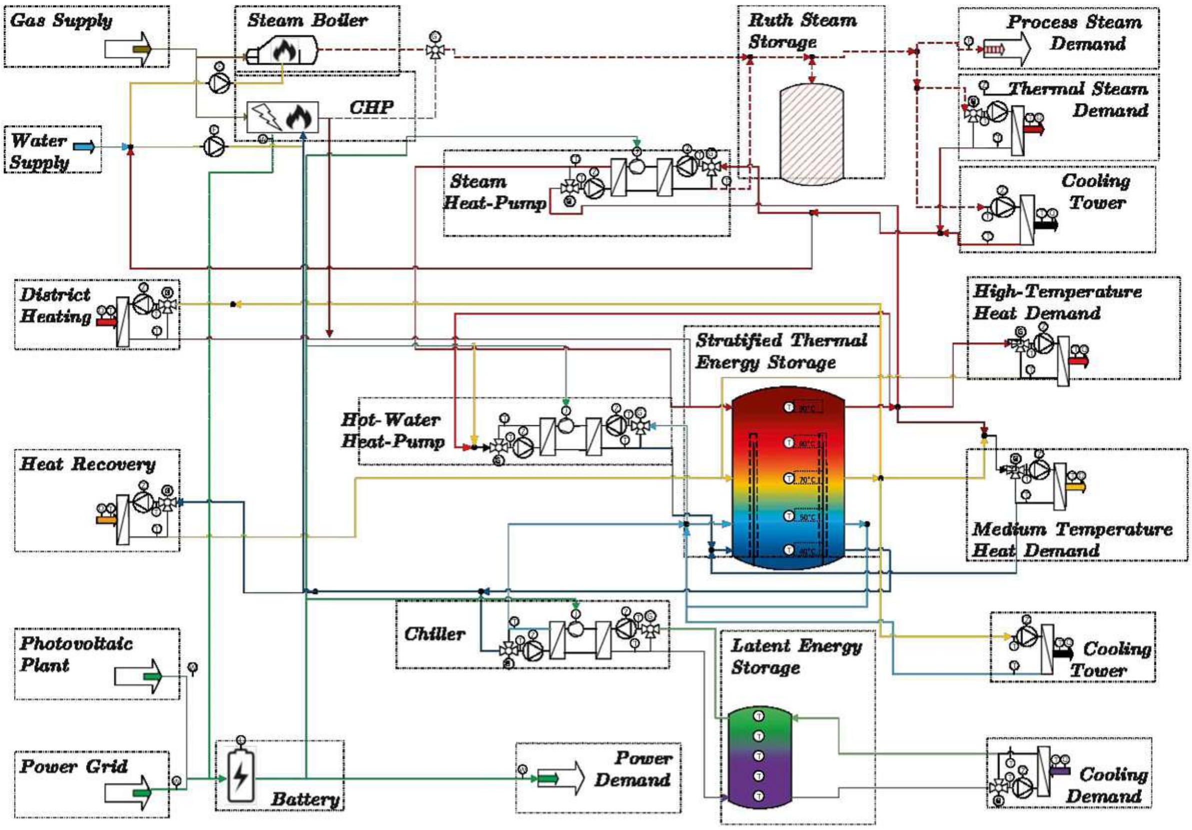


Figure 4.7: Scheme of RES

4.3 Components in the RES

In the following section, the individual components are discussed with regard to purpose, functions, and origin as well as overall technical description and specification.

4.3.1 Energy Supply and Conversion

Gas-fired Steam Generator More than 55% of the final energy in the Austrian food sector is provided by natural gas and 80% of this gas is used for steam generation. This is also evident in two of three use cases, where gas boilers are used for steam generation solely. The Gas boiler consumes natural gas as fuel and converts the chemical energy to thermal energy at a certain efficiency (75-90%). The thermal energy is transferred to the boiler to evaporate water. This component has inlets for natural gas, air, and fresh water and outlets for hot steam and exhaust gas.

CHPThe combined heat and power generation is most commonly found in industrial production sites. While for industries with higher power and process temperature requirements back-pressure turbines are more suitable, piston engines are more frequently used for lower temperature requirements and power demands. Such so-called CHPs are also stated in Bref for the food industries. CHPs are supplied by an external fuel, mostly natural gas or biomass, and are modular systems that convert the chemical energy of the fuel in both thermal and electrical energy. The thermal expansion of the hot gas generates mechanical energy, which drives an electric generator. Simultaneously, waste heat is released at high temperature through the hot exhaust gas. Also, heat at low temperatures occur due to the cooling of engines. The CHP has an inlet flow of fuel and outlet flows of electrical power as well as inlet and outlet flows of the process fluid (here water/steam) and also inlet and outlet flows for the cooling fluids (water). The high fuel utilization rate (high total efficiency) and the high load flexibility (from a few seconds to full load) make CHP units a central bridging technology.

The gas boiler and the CHP represent conventional fossil fuel-based BAT and BREF energy supply technologies in industrial energy systems. They are part of the RES to be able to analyze how their utilization can be improved or alternatively be replaced by alternative renewable-based energy supply technologies, such as HTHPs in combination with PV, Solar thermal energy or waste heat.

District Heating Although the research on energy sources in the Austrian food sector only assigns a minor role to district heating, which accounts for less than 10% of the final supply, it is part of the systems in two use cases. At the district heating transfer point, heat is extracted from the centrally powered thermal supply grid via a heat exchanger. In the RES it represents a grid-based thermal energy source or in the case of a district heating feed-in. Thermal energy is transferred by heat transfer to the process fluid, which inlet and outlet needs to be allocated to two temperature levels.

Heat Pumps transfer heat from a lower temperature source to a higher temperature sink using electrical power. Especially when supplied with renewable power and using waste heat, they represent a highly promising sustainable alternative to fossil-based heat generation. The evaluation of this technology with respect to its contribution for decarbonization is one of the central research questions in the edcsproof project. Thus heat pumps are part of the RES in different positions (Steam-generation, hot-water generation, and cooling), each closely connected to a storage to enhance the range of utilization through bridging the temporal gaps between generation and consumption.

Solar Thermal System Solar thermal energy is already a well-established technology for generating renewable heat and currently, mainly applied at low temperatures in HVAC systems. While yet not very common in industrial applications and also not part in any of the use cases, the predecessor project EnPro [126] focused on the integration of solar thermal collectors for process heat generation. It was found that more than half of the processes investigated require less than 100°C. Furthermore, integration possibilities for higher temperature applications were identified, including in combination with heat pumps thus integration options and potentials is considered.

Photovoltaic System Along with wind energy, photovoltaic systems are among the most promising technology for decarbonizing electricity production. Their field of application is constantly expanding, both on a large scale and for decentralized generation. At plant A and B, PV systems have already been installed. Especially in combination with heat pumps and storage, renewable PV electricity offers significant potential to decarbonize industrial energy production. A photovoltaic system converts solar irradiation to electrical power.

Cooling Towers and Recooling units Recooling units dissipate heat to the environment, i.e. the heat is withdrawn from the system. They are part of (almost) every energy system as they are also needed for security reasons to avoid superheating. For better cooling characteristics in summer and better operational flexibility, they are often equipped with a ventilator that consumes electrical energy. Again, thermal energy is transferred by heat transfer to the process fluid, which inlet and outlet needs to be allocated to two temperature level.

4.3.2 Energy storages

Stratified Thermal Energy Storage are already part of almost any low-temperature energy supply system both in the building sector as well as in industrial applications. These can also be found several times in the use cases. In conventionally designed systems these are mainly used as hydraulic switches, neglecting possible alternative functions and applications. Characteristic for this concept is the natural stratification: At the very top there is the warmest layer and below there are successively colder layers.

This results in a great advantage that, depending on the available feed-in temperature and current temperature stratification, it is always possible to feed into the correspondingly warm storage layer. The same applies to discharge. Thus exegetically inefficient mixing of the storage temperature can be avoided. In particular, this is very beneficial in the case of a large number of feeders with many different feed-in temperatures and temperature fluctuations. Especially with this concept appropriate predictive storage management opens up great potential for increasing energy efficiency and integrating renewables into the energy mix. Stratified storages can have an arbitrary number of connections (inlets and outlets). Each layer can have inlets and outlets.

Steam Storage Although steam storage units are yet neither standard in industrial energy systems nor present in any of the use cases, they offer promising potential for increasing system flexibility and decarbonization of industrial energy systems. Especially when considering that steam accounts for more than 40% of final energy consumption and in combination with innovative Power-to-Heat technologies (e.g. high-temperature heat pumps). From a technological point of view, both high-temperature latent storages and Ruth steam storages are promising concepts. Steam storages have an inlet and outlet for steam and condensed hot water each. In general, there is also an additional external heat source for the supply of the thermal energy. This is especially necessary to prevent condensation in case of heat loss.

Latent Energy Storage are characterized by a high heat storage density through the heat capacity of the phase change. As already established in industrial applications also at plant B, a latent heat storage is used as buffer storage on the cooling system. In general, they are connected to two different temperature levels which each have one inlet and one outlet.

Electrical Energy Storage Also known as batteries, these systems have only been of marginal importance in industrial energy systems in the past. However, they take on an important role in future-oriented flexible energy systems, as they can store electrical energy with high efficiency and are rapidly accessible. Especially in combination with photovoltaic systems, renewable energy can be provided in accordance with production requirements. The main technical data of these components are presented in Table 4.1.

4.4 Reference Scenarios

In the following, reference scenarios are defined for the energy demand as well as environemtal, and economic boundary conditions. The energy demand and energy prices are derived from measurement data of the industrial partners' plants including reasonable assumptions where data were not accessible in suitable quality. To account for differences in the annual cycle, three different consumption periods are considered: Summer, transition, and winter. For each of these periods, the reference demand for one week was determined. Besides the electrical energy demand, there are four different temperature levels of thermal energy demand:

- Steam (150°C)
- HT (90°C)
- MT (70°C)
- Cooling (-15°C)

Since the respective demand curves originated from different facilities and sources, a scaling process was performed to establish equitable and harmonized load profiles. The aim was to achieve more comparable consumption levels across the different energy consumers, enabling more balanced and generalized comparison. Thus, each consumption curve was normalized to an average value of 1 MW over the three entire reference weeks (7 days). Similarly, also the state-of-the-art components, present in the CRES, were scaled in accordance to their associated consumption profiles to maintain a coherent overall layout.

Steam Demand

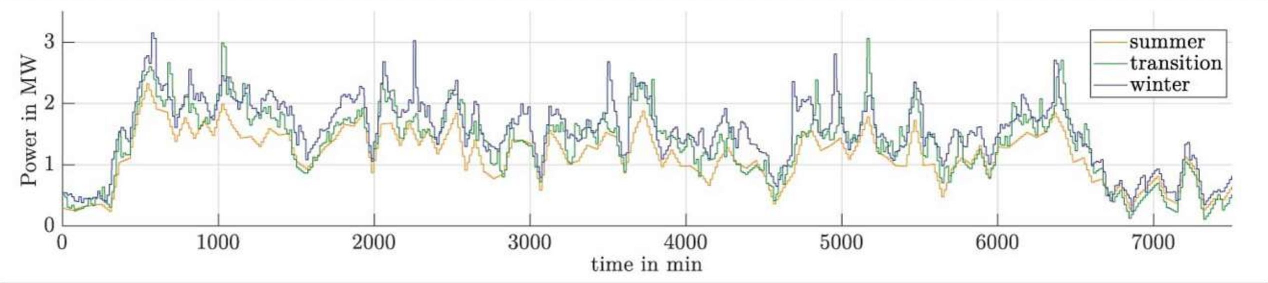


Figure 4.8: Steam demand

In Figure 4.8 the steam demand for the three scenario weeks is shown. The data is derived from hourly measurement data from Plant A. Looking at the individual seasonal scenarios, demand is highest in winter and lowest in summer. The fluctuations are also unevenly pronounced, however, in the weekly trends, similarities are observed. It can be clearly seen, that there is a deviating operation on workdays and weekends.

HT Heat Demand

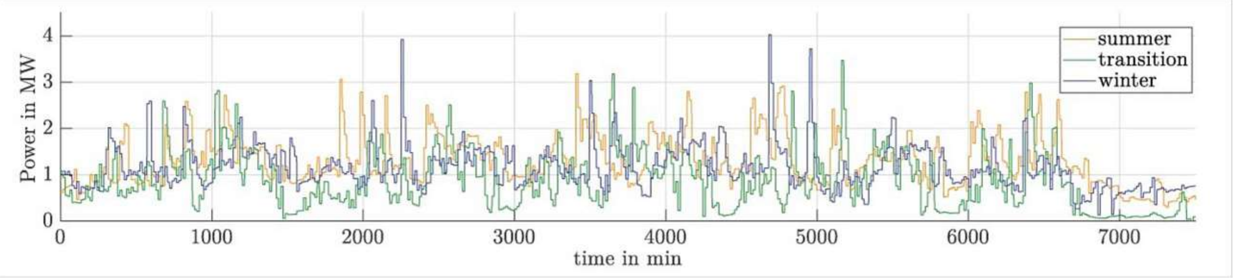


Figure 4.9: HT heat demand

In Figure 4.9 the HT demand for the three scenario weeks is shown. The data is derived from measurement data from Plant B. The original data was transformed to a 15-minute resolution from a 1-minute resolution by using the respective mean values. The spikes result from the underlying sous-vide processes in a plant subsystem, which requires high heating power for a short duration. This heat demand actually consists of two data series, one for the sous-vide processes and the other one from a different consumer with slightly lower temperature requirement. Looking at the individual seasonal scenarios, also unevenly pronounced fluctuations are observed.

MT Heat Demand

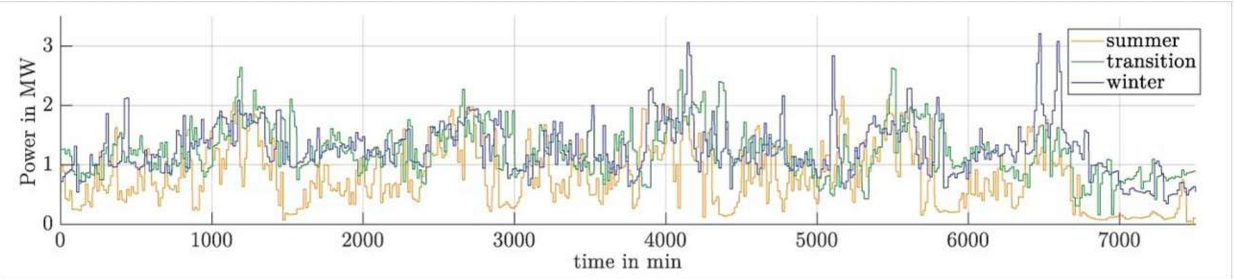


Figure 4.10: MT demand

In Figure 4.10 the MT heat demand for the three scenarios is shown. The data are derived from measurement data from Plant B. The original data was transformed to a 15-minute resolution from a 1-minute resolution via mean value. It can be clearly seen, that there is a deviating operation on workdays and weekends.

Cooling Demand

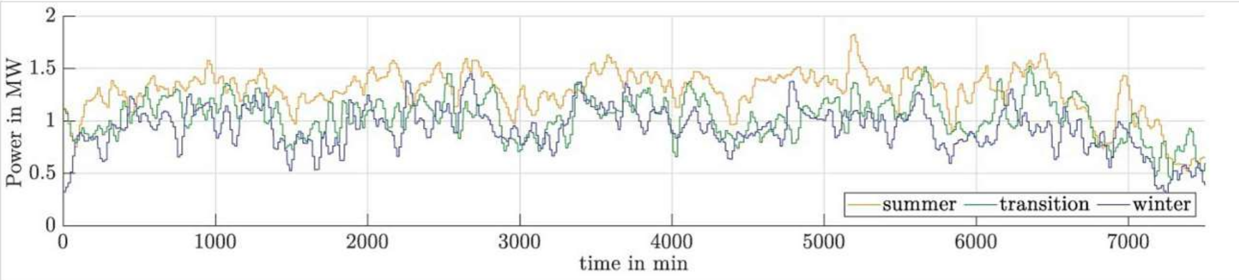


Figure 4.11: Cooling demand

In Figure 4.11 the Cooling demand for the three scenario weeks is shown. The data is derived from measurement data of the electrical consumption of the cooling units multiplied by the COP from Plant B. The original data was transformed to a 15-minute resolution from a 1-minute resolution via mean value. Again, that there is a deviating operation on workdays and weekends.

Electrical Energy Demand

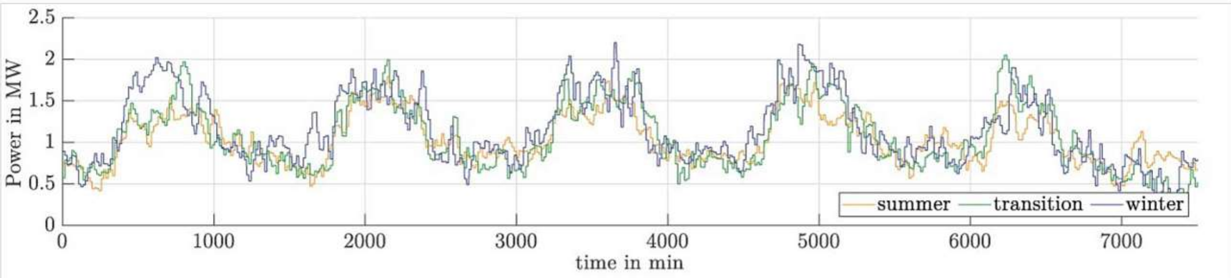


Figure 4.12: Electrical energy demand

In Figure 4.12 the electric energy demand for the three scenario weeks is shown. The data is taken from consumption data at plant A.

Solar Irradiation

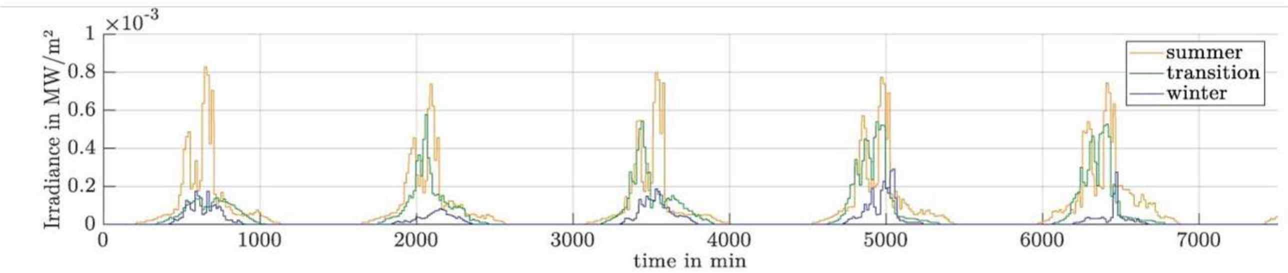


Figure 4.13: Solar irradiation

The solar radiation data for the three scenario weeks shown in Figure 4.13 were acquired at plant B.

Ambient Temperatures

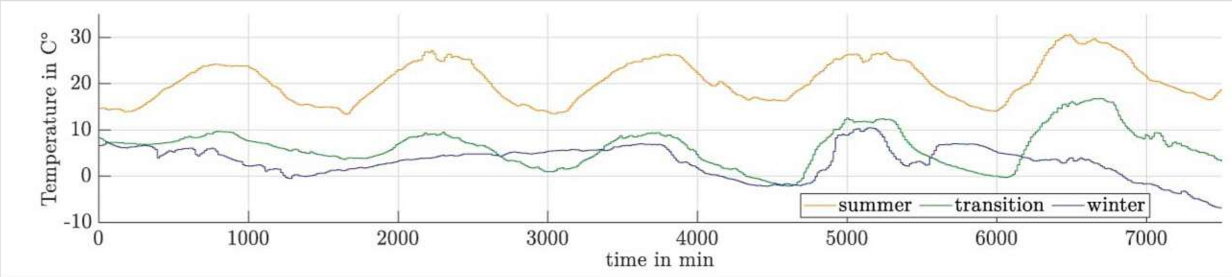


Figure 4.14: Ambient temperatures

In Figure 4.14 the ambient temperatures for the three scenario weeks are shown. The original data were measured at plant B in 1-minute resolution, which was transformed to a 15-minute resolution with mean values.

Electricity Prices

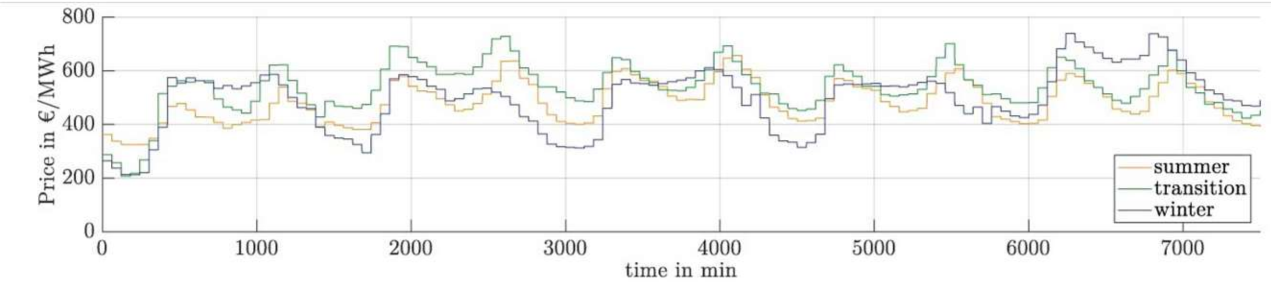


Figure 4.15: Electricity prices

The electricity prices shown in Figure 4.15 are market data from the austrian energy exchange[9] for the respective seasonal reference weeks from 2020, which have been adjusted to 10/2022 in line with the austrian electricity price index[10][11].

[9] https://www.exaa.at/en/
[10] https://www.energyagency.at/fakten/strompreisindex
[11] The market data from 2020 were provided free of charge at the time, but this service became fee-based, hence the electricity price index was used for price adjustments

4.5 Design and Dimensioning

4.5.1 Properties of Conventional Components

While the configuration and arrangement of the units as well as the boundaries regarding energy demands, prices, and ambient conditions have been defined, the dimensions and parameters of the new components are to be determined. As mentioned above, the state-of-the-art components present in the CRES were also reasonably scaled according to their respective energy consumers demand profiles. Whereas the complete description of the models can be found in the Appendix, the key parameters are listed below in Table 4.1. Since there are no comparative units in the real plants for the new components that are added to complete the extended RES, an optimization-based dimensioning needs to be conducted to determine the sizes of the new units.

Table 4.1 Technical and Operational Parameters of present supply and storage units

Unit	Maximum Capacity	Min Part Load	Energy Conversion	Max Ramp Up/Down	Min Time Up/Down
CHP	El. power: 2 MW Steam: 1 MW HT: 1 MW	40%	η_{tot}= 0.75	100% / 15min	30 min
GB	Steam: 2 MW	40%	η_{th}= 0.80	50% / 15min	30 min
CH	MT: 1.5 MW	50%	COP: 3.2	50% / 15min	1h
DH	HT: 3 MW	20%	1	100% / 15min	15min
CT	Cooling: 3 MW	20%	1	100% / 15min	15min
PG	El. power +/-4 MW	0%	1	100% / 15min	15min
STES	100 m³	Vmin=10%	$\eta_{ch,dch}$=0.99 η_{sdch}=0.99	100% / 15min	
STcl	1.3 MWh	Vmin=10%	$\eta_{ch,dch}$=0.99 η_{sdch}=0.99	100% / 15min	

4.5.2 Problem description

As for the corresponding task both the plant layout and locations of units as well as the energy demand including the consumer's characteristics were already defined, a process-orientated heat integration is less expedient. Above all, the aim is to determine the optimal size of energy components in a multi-component multi-energy system. From the perspective of the plant operator, this means the optimal investment decisions. In accordance with the advantages outlined above, the method of mathematical gradient-based optimization using mixed integer linear formulations (MILP) is applied. Apart from the convenient usability, the main advantages are on the one hand the feature that the global optimum can be determined unambiguously and on the other hand the availability of efficient solvers. The central optimization problem is formulated as a UC-problem and optimizes the design of the specific components in combination with the correpsonding optimal operation of all components (economic dispatch). For those units where the optimal size is designed, instead of being a model parameter, the maximum capacity of this unit appears as an additional time-independent decision variable. In this case the sizing variable $\boldsymbol{CAP_i}$ is constrained with an upper an lower bound $CAP_{i,min}$, $CAP_{i,max}$ and as shown in Eq. (4.1). $\boldsymbol{I}$ represents a binary decision variable, specifying whether the unit is installed or not.

$$\boldsymbol{I}\, CAP_{i,min} \leq \boldsymbol{CAP_i} \leq \boldsymbol{I}\, \mathrm{CAP}_{\mathrm{i,max}} \tag{4.1}$$

The sizing variable limits the respective time-variant decision variable $\boldsymbol{x}$ which can either represent the generation of a specific resource in a conversion process or the state of charge in a storage.

$$\boldsymbol{0} \leq \boldsymbol{x} \leq \boldsymbol{CAP_i} \tag{4.2}$$

Considering mathematical formulations from a general perspective, the transformation of a model parameter to a decision variable can produce nonlinear formulations, which are to be avoided as they complicate the problem significantly and may require different solution methods. The linearization of energy conversion processes in design problems will not be addressed from a general perspective, however linear formulations for the minimum operation as well as maximum ramp-ups and ramp-downs are considered as they are of significant importance for considering dynamical, time-invariant operations in the design optimization. Since the maximum capacity is a decision variable in the optimization problem, it is not expedient to specify partial load capacity exactly in advance, instead a relative part load capacity α_{min} is applied producing the adapted part load constraint.

$$\alpha_{min,i}\, \boldsymbol{CAP_i} - (1-\boldsymbol{u_i})\alpha_{min.i}\, \boldsymbol{CAP_{i,max}} \leq \boldsymbol{x_i} \leq \boldsymbol{u_i}\, \boldsymbol{CAP_{i,max}} \tag{4.3}$$

Similarly, adapted formulations for maximum ramps, start-ups, and shutdowns are imposed. To avoid that the component size parameter occurs as a product with the commitment variable u (on/off) the relative maximum ramps are related to the respective upper bonds and lower of the design variables, represented as β and κ.

$$-\overbrace{\boldsymbol{w_i^t}\, \kappa\, CAP_{i,max}}^{SD} - \overbrace{\beta\, CAP_{i,max}\ \boldsymbol{u_i^t}}^{RD} \leq \boldsymbol{x_i^t} - \boldsymbol{x_i^{t-1}} \leq \overbrace{\beta\, CAP_{i,max}\ \boldsymbol{u_i^t}}^{RU} + \boldsymbol{v_i^t}\overbrace{\kappa\ CAP_{i,max}}^{SU} \tag{4.4}$$

Figure 4.16 depicts the abstract model-based illustration of the original system from Figure 4.7. The black dashed boxes indicate those components for which a dimensioning task will be carried out in the optimization. The determination of the weighting factors for the objective function is carried out both superordinately as well as in the definition of component models. The detailed discription and mathematical formulations of the component models is documented in the next section.

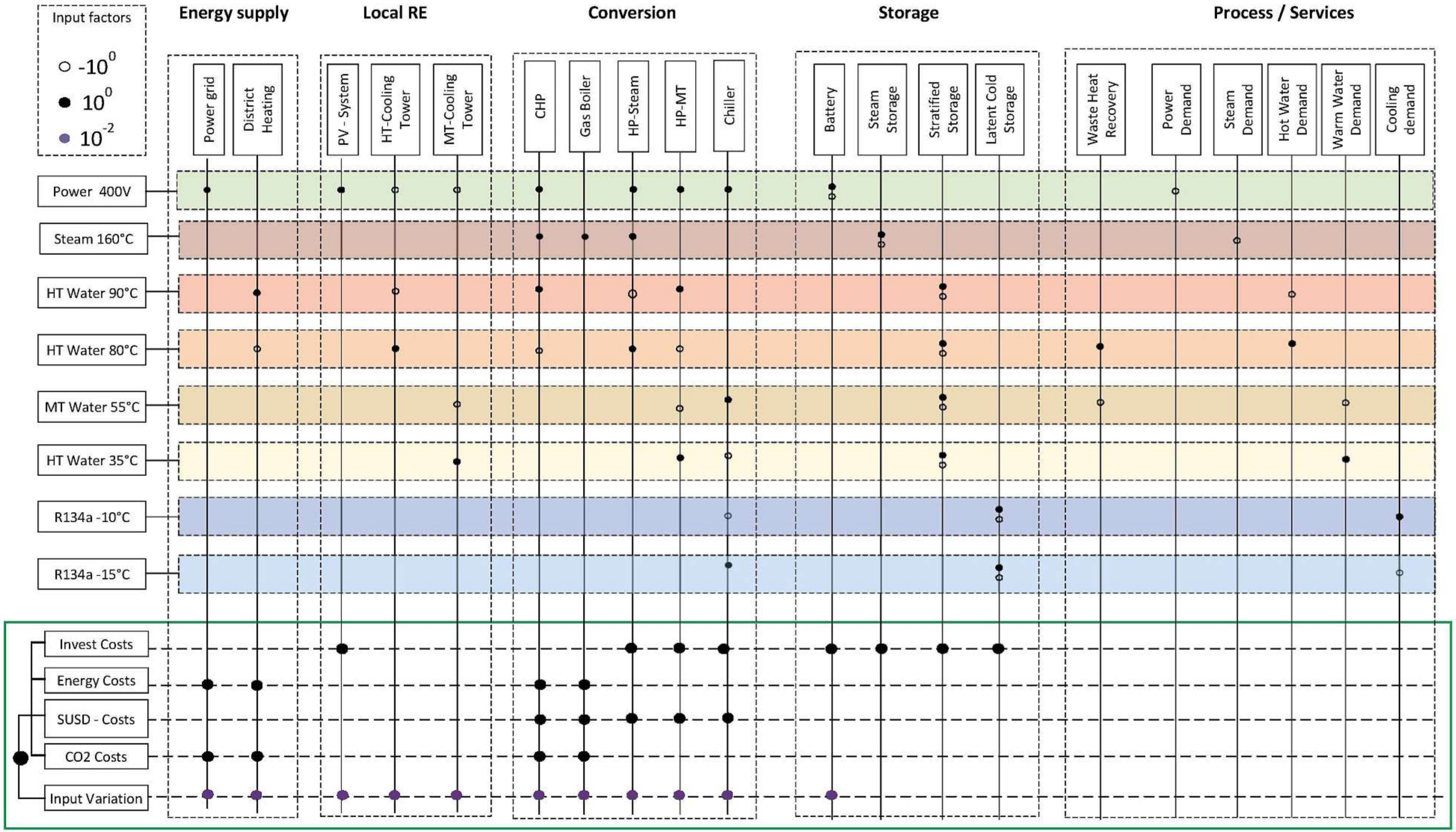


Figure 4.16: Superstructure representation of the RES

Objective Function The various contributions of individual units to the objective function and its overall compositing can be gathered from Figure 4.20. Additionally, the following explanations are provided to emphasize on certain further aspects. According to Eq. (4.5), the objective function is composed of investment costs and operation costs. Thereby an_{inv} represent the specific annualized investment taking into account an annual interest rate of 2% and including operation and maintenance costs of the different units in consideration of the respective depreciation periods. The corresponding data are listed in Table 4.1.

$$TAC = \sum_{i} f_{CO2,i}\, an_{inv,i}\, \boldsymbol{CAP_i} + 52 \sum_{t}^{Nr_t} \sum_{i} f_{CO2,i}\, c_{ec,i}^{t}\, \boldsymbol{P_{ec,i}^{t}} + \boldsymbol{C_{SUSD,i}^{t}} + \boldsymbol{C_{\Delta U,i}^{t}} \tag{4.5}$$

The factor f_{CO2i} is introduced for the transformation of the objective function for an environmental consideration. Hence, this factor equals one for economic considerations and adopts the specific emission factors of energy sources[12] [127] as well as production-related [128] emissions at the design of components. For considering the different seasonal scenarios, the consideration of three complete weeks would exceed the calculation effort. As a remedy, a reference week is compiled by using 2 respective production days of each of the 3 seasons. This reference week then consists of 6 production days with a 15-minute time-step resolution and one day on which it is assumed that the plant is not operated. Using the superstructure modeling comprehensively explained in Section 3.1, the constraints and objective functions are formulated component-based in a generic form and assembled as depicted in Figure 4.16. The modeling process is implemented in MATLAB [129] using the optimization modeling language Yalmip [79] and the GUROBI solver [78].

4.5.3 Operational Aspects in Design

When considering the optimization of plant design or dimensioning of individual components, there is a strong connection to operational aspects. Considering dynamic behavior including operational performance and security, an optimal design is strongly connected to the available control method and strategy. A design optimization based on a unit commitment formulation targeting the economic dispatch, as, e.g. presented in [71] implies perfect information and forecasts, and assumes the presence of an optimal control strategy such as a plant-wide MPC. However, to obtain meaningful design and investment decisions, the actual prevailing control concepts and operational strategies must also be implemented sufficiently in the corresponding optimization problem. Thus additional formulations to represent the respective interrelations, rules, and restrictions need to be incorporated into the optimization model. While this is a rather uncommon practice in design optimization, it is newertheless selectively adopted in operational applications. For example, Antunes et. al. [130] present and discuss different MILP models to account for thermostatic loads in demand response of HVAC systems. If the SOC of a buffer storage serves as a controlled variable, a very compact formulation reflecting a two-point control behavior is given by Eq. (4.6).

$$\frac{SOC_{LB} - \boldsymbol{SOC^t}}{SOC_{UB} - SOC_{LB}} \leq \boldsymbol{u^{t+1}} - \boldsymbol{u^t} \leq \frac{SOC_{UB} - \boldsymbol{SOC^t}}{SOC_{UB} - SOC_{LB}} \tag{4.6}$$

[12] Assumption of Austrian electricity mix

The activation variable $\boldsymbol{u}$ of a supply unit assumes 1 when the component is activated and 0 when switched off. Reaching a certain lower bound SOC_{LB} of a connected storage, requires the activation of the supplier. In this case, the left term of the inequality is greater than 0, and the right term greater than 1, which means that u must change from 0 to 1 in the next time step. If the upper bound SOC_{UB} is exceeded, the right term is smaller than 0 and the left term is smaller than -1, which means that u must assume zero in the next time step. If the SOC is between its two bounds, the left term is between -1 and 0 and the right term is between 0 and 1. Since $\boldsymbol{u}$ is a binary variable which can only assume 0 and 1, this means that it cannot change in this intermediate range. For accounting a corresponding behavior while simultaneously optimizing the design capacity of the storage unit, it must be acknowledged that in this case also the lower and upper bounds are representing variables (see Eq. (4.1)). As the above Eq. (4.6) then becomes a nonlinear expression, the following robust BIG-M formulation, is therefore applied for linearization.

$$\boldsymbol{SOC}^{\,t} - \alpha_{max}\boldsymbol{CAP} \leq \left(1 - \boldsymbol{u}^{t+1}\right)M \tag{4.7}$$

$$\alpha_{min}\boldsymbol{CAP} - \boldsymbol{SOC}^{\,t} \leq \boldsymbol{u}^{t+1}\,M \tag{4.8}$$

$$\boldsymbol{J_C} = \sum_{t}^{N_t - 1} \left|\boldsymbol{u}^{t+1} - \boldsymbol{u}^{t}\right| c_{slack} \tag{4.9}$$

Here, Eq. (4.7) ensures that the generator switches off when the SOC exceeds the upper charging bound $\alpha_{max}\boldsymbol{CAP}$, while Eq. (4.8) activates the generator when the SOC falls below the lower barrier $\alpha_{min}\boldsymbol{CAP}$. Eq. (4.9), which actually minimizes the number of state changes of $\boldsymbol{u}^{t}$, forces the devices to remain in charging or discharging after a switch-on or switch-off while permitting the condition changes according to Eq. (4.7) and Eq. (4.8). Thereby, c_{slack} denote slack costs and M represents a positive constant which needs to be larger than the occurring variables.

Boundaries The systems boundaries regarding energy demands, prices and ambient conditions are listed above in Section 4.4. However, the considered investment costs are a very crucial input for the design optimization process and are listed in Table 4.2. Regarding energy and investment costs, high variations could be observed in recent times without addressing possible reasons and impacts. This affected the prices for electrical energy, natural gas as well as investment costs which all have a highly significant influence on optimal design. Due to the strong fluctuating economic framework conditions, it is not expedient to obtain information on the optimal design from a single optimization. Therefore, optimization runs were carried out for different scenarios. Table 4.3 additionally lists the specific operating parameters that are assumed for the components to be integrated.

Table 4.2: Investment costs of new components, Data sources: [128, 131, 132]

Component	Investment Costs		CO_2 Impact	O&M	Technical Lifetime
	Fixed	Size Specific			
Steam heat pump	30.000	800.000 €/MW	20 tCO2/MW	2,5%	20
HT heat pump	30.000	700.000 €/MW	20 tCO2/MW	2,5%	20
Chiller	30.000	850.000 €/MW	25 tCO2/MW	2,5%	20
Photovoltaic system	5.000	500 €/m²	350 kgCO2/m²	1,5%	20
Solar Thermal	20.000	350 €/m²	100 kgCO2/m²	1,5%	20
Steam storage	20.000	60.000 €/MWh	10 kgCO2/m²	1%	20
Stratified storage	20.000	750 €/m³	10 tCO2/MWh	1%	20
Cold Storage	20.000	50.000 €/MWh	15 tCO2/MWh	1%	20
Battery	5.000	300.000 €/MWh 150.000 €/MW	300 tCO2/MWh	1%	10

Table 4.3: Opertional parameters of new components

Generation Unit	Min Size	Max Size	Minimum Part Load	Energy Conversion	Ramp Up/Down	Min Time Up/Down
Steam heat pump	0 MW	6 MW	40%	COP: 2.6	100% / 30min	30 min
HT heat pump	0 MW	6 MW	40%	COP: 4	100% / 15min	30 min
Chiller	1.5 MW	6 MW	30%	COP: 3.2	100% / 15min	1h
Photovoltaic system	0 MW	1.5 MW	20%	η=0.2	100% / 15min	15min
Solar Thermal System	0 MW	2 MW	20%	η=0.5	100% / 15min	15min

Storage Unit	Min Size	Max Size	Min SOC	Max SOC
Steam storage	0.0 MWh	15 MWh	85% (Vol)	95% (Vol)
Stratified thermal energy storage	100 m³	1000 m³	10% SOC	90% SOC
Latent Energy Storage	1.3 MWh	10 MWh	10% SOC	90% SOC
Battery	0 MWh	20 MWh	5% SOC	95% SOC

4.5.4 Design Studies

With the possibility of integrating new technologies, these studies determine the optimal energy supply strategies for the respective industrial processes from a long-term perspective. Thereby, this use case especially provides an opportunity to evaluate the specific impact of various aspects on optimal design and operational performance. Precisely, in the respective scenarios, distinctions are made with regard to the prevailing operating and control strategy, minimizing total annual costs or emissions as well as different depreciation periods of investments:

- **Scenario A**: This scenario aims to determine the optimal economic design in the long term. The technological lifetime of the units is regarded as deprecition time. The price for natural gas is assumed to 220€/MWh (average in 2022) and a CO_2 price of 50€/ton is assumed. The objective is the minimization of costs, which takes into account investment costs, operation and maintenance costs, costs of CO_2 emissions and costs of energy purchase.
- **Scenario B**: This scenario addresses the entrepreneurial practice of considering shorter depreciation periods for investment decisions and is intended to show their economic impact in comparison with the long-term perspective. In this context, reference is made to Rathgeber et al. [68] who particularly refer to high interest rates of 10% and short payback periods of 5 years in industrial investments highlighting the considerable deviations from the effective lifetimes of technologies of several decades. Consequently, in this Scenario B, a depreciation time 5 years is adopted while all other conditions remain the same.
- **Scenario C**: This scenario serves as a reference for evaluating environmental performance and provides the design with minimal environmental impact by considering only the minimization of CO2 emissions in its objective function.
- **Scenario D**: In contrast to the Scenarios A, B and C, which implicitly assume the existence of optimal plant-wide control and perfect prediction, in reference to Section 4.5.3, Scenario D determines the optimal design taking into account a conventional 2-point control for the generation units. This is established by introducing the formulations presented from Eq. (4.7) to Eq. (4.9) to the respective units.
- **CRES**: This base case scenario, assumes a two-point controlled original system without considering the integration of new technologies to minimize costs and is used as a baseline for comparing overall costs and emissions

4.5.5 Results and Comparison

For comparing the design scenarios, Figure 4.17 and Figure 4.18 present the respective optimal capacities of generation and storage units, while the corresponding total costs and emissions are provided in Figure 4.19 and Figure 4.20. First and foremost, to highlight the potential savings associated with the integration of new technologies, the long-term economically optimal Scenario A is compared with the base case revealing significant cost savings of nearly 40% in combination with an emissions reduction of more than 61%. However, the different scenarios show significant disparities and indicate to significant performance shortfalls. Concerning the enterpreneurial practice of short-term thinking reflected by Scenario B, an increase in operational expenditures (OPEX) of 15% compared to Scenario A is showcased.

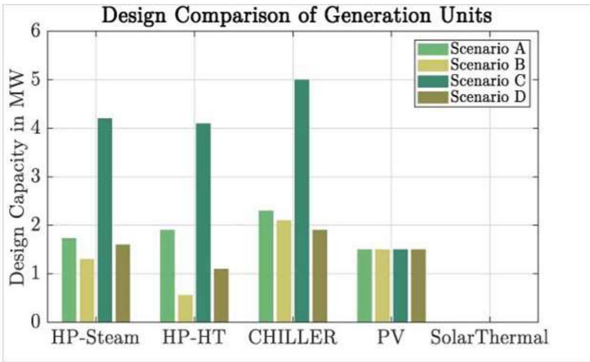


Figure 4.17: Scenario specific optimal Capacities of generation untis

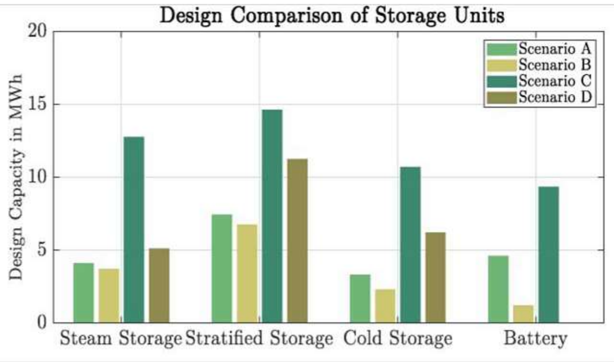


Figure 4.18: Scenario specific optimal Capacities of generation untis

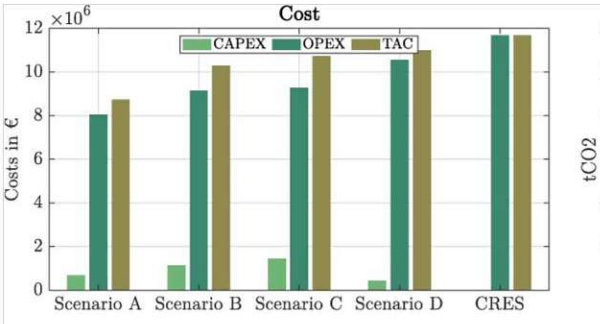


Figure 4.19: Scenario specific annual Costs

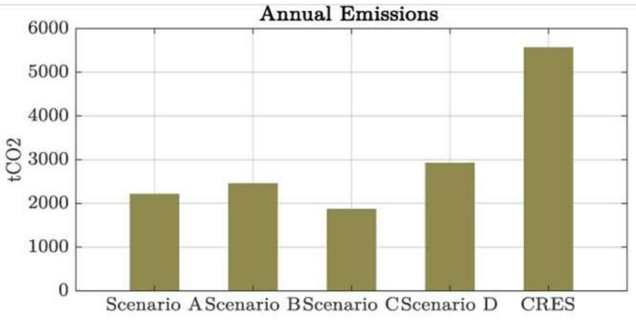


Figure 4.20: Scenario specific annual emissions

Considering component design, in Scenario B consistently smaller capacities are observed in comparison to Scenario A with the most significant differences in the HT-HP and the battery. When considering the total annual costs increase of 19,4%, also revealing higher cumulative annualized capital expenditures (CAPEX), however, the shorter amortization period must be taken into account, which limits direct comparability with regard to CAPEX and TAC.

The comparison between Scenario A and Scenario D provides an opportunity to analyze the long-term impact of plant-wide predictive optimal control, which allows for more strategic utilization of units and consequently also affects optimal design. Thus, compared to Scenario D, Scenario A clearly demonstrates the long-term benefits of plant-wide optimal control which is expressed in cost savings of about 23% and a 25% emissions reduction. These considerable savings potentials thus illustrate the strong influence of operating systems on the cost-effectiveness and efficiency of investments in new technologies. At this point, special reference is given to the case study in Chapter 5, which comprehensively examines the performance improvements and operational differences between conventional and plant-wide optimal control. Chapter 5 can therefore be regarded as a complementary study, though it addresses the issue from the operational side.

Most evidently, the environmental minimum Scenario C suggests significantly larger optimal dimensions of all units compared to all other scenarios, thereby achieving an emission reduction of about 17% at a cost increase of 20.7% compared to Scenario A. Both Scenarios A and C in combination show that economic and environmental goals can be achieved simultaneously with these technologies if they are operated appropriately.

Regarding the optimal capacities, Scenario D is characterized by smaller generation units, larger thermal energy storage units and no cost-effective integration of batteries is recognized. Generally, it is emphasized that the PV plant is present at maximum size in every scenario and, interestingly, no solar thermal system is implemented in any of the scenarios. Observing the respective annual costs provided in Figure 4.19, in general, significantly higher annual OPEX in relation to the cumulative annuities of the investments are particularly noticeable. In this respect, however, it is important to remember, that also the components already present in the energy system are inducing energy costs which are therefore not exclusively attributable to the designed components. The associated emissions, presented in Figure 4.20, show similar characteristics to the OPEX which can be attributed to the aspect, that these are almost exclusively related to the purchase of electricity from the grid. However, when comparing to the CRES-Scenario as a base-case, significant reductions are recognized in both TAC and even more in annual emissions.

The corresponding operational progression of the Scenarios A – D are presented specifically focusing on the energy carriers steam and power according to the graphs from Figure 4.21 to Figure 4.28. Yet the differences in the utilization due to different capacity dimensions are immediately observable. With regard to the used energy sources, Scenarios C and Scenario D entirely operate without the activation of fossil technologies, while these are occasionally used in the other scenarios. With regard to scenario D, it must be emphasized, that the additionally implemented control rules favor the heat pumps over fossil generators and district heating, which also has a decisive influence on the design and the corresponding operation. On the basis of the power balance of Scenario D shown in Figure 4.28, the discrete switching cycles of the heat pumps can be recognized. Comparing Scenarios A-C, it becomes evident, that larger capacities are leading to more pronounced production shifts to times of low power prices, which is also reflected by an intensified cyclical storage utilization. This effect is most pronounced under Scenario C. In addition to potential savings in cost, energy consumption, and CO_2 emissions, the study also indicates a considerable substitution of fossil energy sources through the integration of new technologies. Apart from the emission minimal Scenario C, where no fossil fuels are used at all, in Scenario A, on-site fossil fuel generation contributes less than 5% of the total energy production.

4.5.6 Final Capacity Selection

While the scenarios discussed all propose different optimal designs, with the goal of long-term optimal economic performance, the capacities from Scenario A, as summarized in Table 4.4, are adopted for the subsequent tasks and studies.

Table 4.4: Capacities of the new integrated components

HP Steam	HP HT	Chiller	PV	Stratified Storage	Steam Storage	Cold Storage	Electrical Storage
1.7 MW	1.9 MW	2.2MW	1.5MW	7.4 MWh	4.0MWh	3MWh	4.6 MWh

Comparison of Operational Progressions

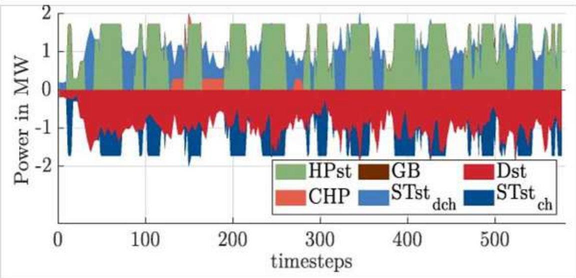


Figure 4.21: Steam Balance Scenario A

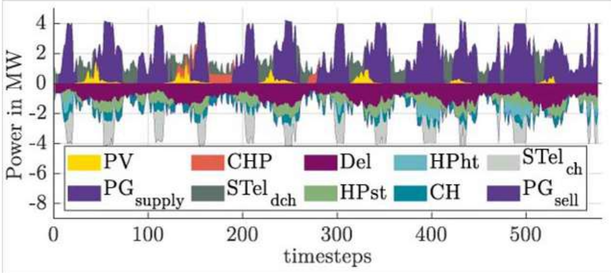


Figure 4.22: Power Balance Scenario A

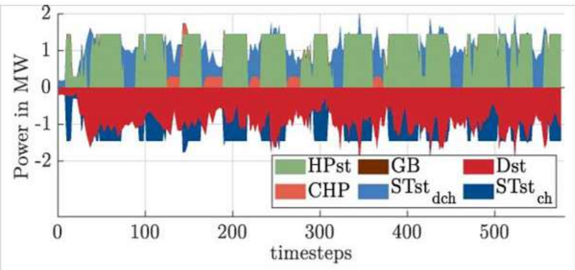


Figure 4.23: Steam Balance Scenario B

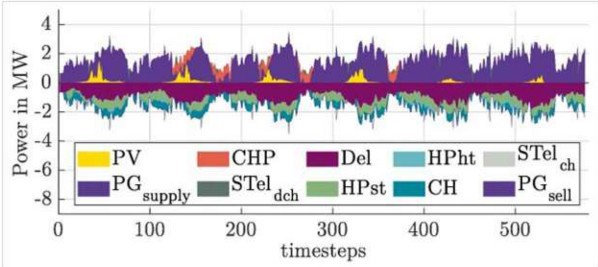


Figure 4.24: Power Balance Scenario B

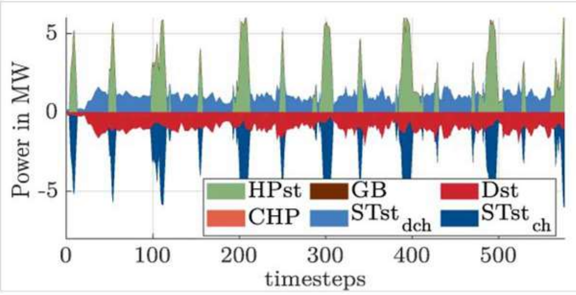


Figure 4.25: Steam Balance Scenario C

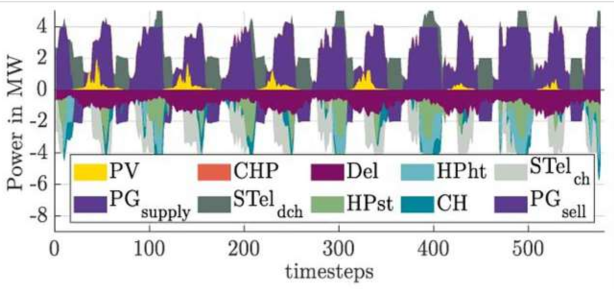


Figure 4.26: Power Balance Scenario C

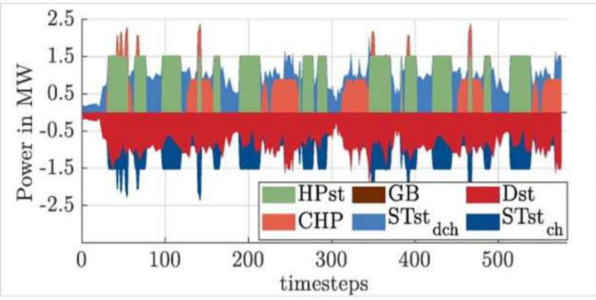


Figure 4.27: Steam Balance Scenario D

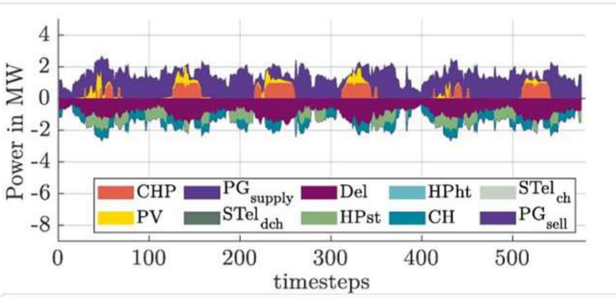


Figure 4.28: Power Balance Scenario D

Change is the law of life. And those who look only to the past or present are certain to miss the future.

JOHN F. KENNEDY

5 Holistic Management and Control of an Industrial Multi-Energy System

Aim and Scope This chapter covers practically the entire thematic, theoretical, and methodological spectrum of this work and is to be considered the most extensive part of the research contribution. In a comprehensive case study, the EMCS presented in Chapter 3 will be applied to the multi-component industrial energy system of the RES derived in Chapter 4 to demonstrate and evaluate its performance in holistic management and control. The necessity of advanced energy management systems and their contribution for overcoming the challenges of the energy transition have already been addressed in Chapter 1. Moreover, in Chapter 2 an overview of the scope of scientific publications on this topic was discussed with subject to the conceptual and methodical perspective as well as savings potentials evaluation. Among the main outcomes, an identified research gap was that specific applications of the published methods to real or realistic systems covering performance characteristics and evaluation of savings potentials were not, or only insufficiently addressed. The overarching scientific interest in this assessment resides in the consideration of a complex and multi-component energy system, an area that could only be rarely investigated so far. In diverse multi-component systems, there are evidently several different flexibilities that can be utilized either individually or in targeted bundling to optimize the operation. Consequently, greater performance improvements and savings potentials may be expected compared to simpler systems. By comparing to a state-of-the-art reference control concept, the improvement potential is assessed in a comprehensive scenario analysis. One aim of this chapter is to demonstrate the practicability and usability of the developed modeling methods for energy management and control applications, especially for complex multi-energy systems. Moreover, the further objective is to evaluate the performance and savings potential of the method in application to a complex energy system.

5.1 Case Study

The evaluation of performance, operational improvements, and potential savings achievable through the implementation of predictive energy management for a holistic control of industrial multi-energy systems is a complex and non-straightforward task, which can be examined in many dimensions and from various perspectives. It encompasses a wide range of aspects, from high-level objectives such as total operational costs or energy requirements to intricate details like precise control of individual units or variables making it extensive and multifaceted. Furthermore, such an evaluation of performance and savings cannot be universally quantified due to the significant dependence on the composition of the energy systems or specific operational conditions such as energy markets, local climate, and renewable generation capacity. Additionally, the accuracy of forecasts and exploitable flexibilities of the considered systems play a crucial role in assessing performance and potential savings. Moreover, very importantly, also the reference management and control concept, which the EMCS is compared to, has a very decisive influence on the investigation. Flexibilities on the local energy supply system can occur through substitutable energy sources (e.g. electricity is purchased from the power grid or is produced by the CHP based on gas) or technologies (e.g. a heat pump instead of a gas boiler) or temporal displacement through storages. Potentially, flexibilities can also be achieved on the consumption side through shiftable loads or scheduling of processes, which are, however not considered in these studies where process demand is considered as given.

Stepwise Approach For overcoming these associated implications and challenges, this study presents an integrative, step-by-step approach that systematically and comprehensibly evaluates the performance and associated savings potential that can be achieved through the use of predictive, plant-wide operational optimization and control.

Initially, the methodological an technological basis is defined which includes the definition of the conventional rule-based reference control concept (CRCC), serving as a performance benchmark as well as the two considered plant configurations, the CRES as the conventional baseline and the RES representing the technological state of the art. Therefore both systems are modeled in MATLAB-SIMULINK in order to be selectively operated by both control concepts as illustrated in Figure 5.1.

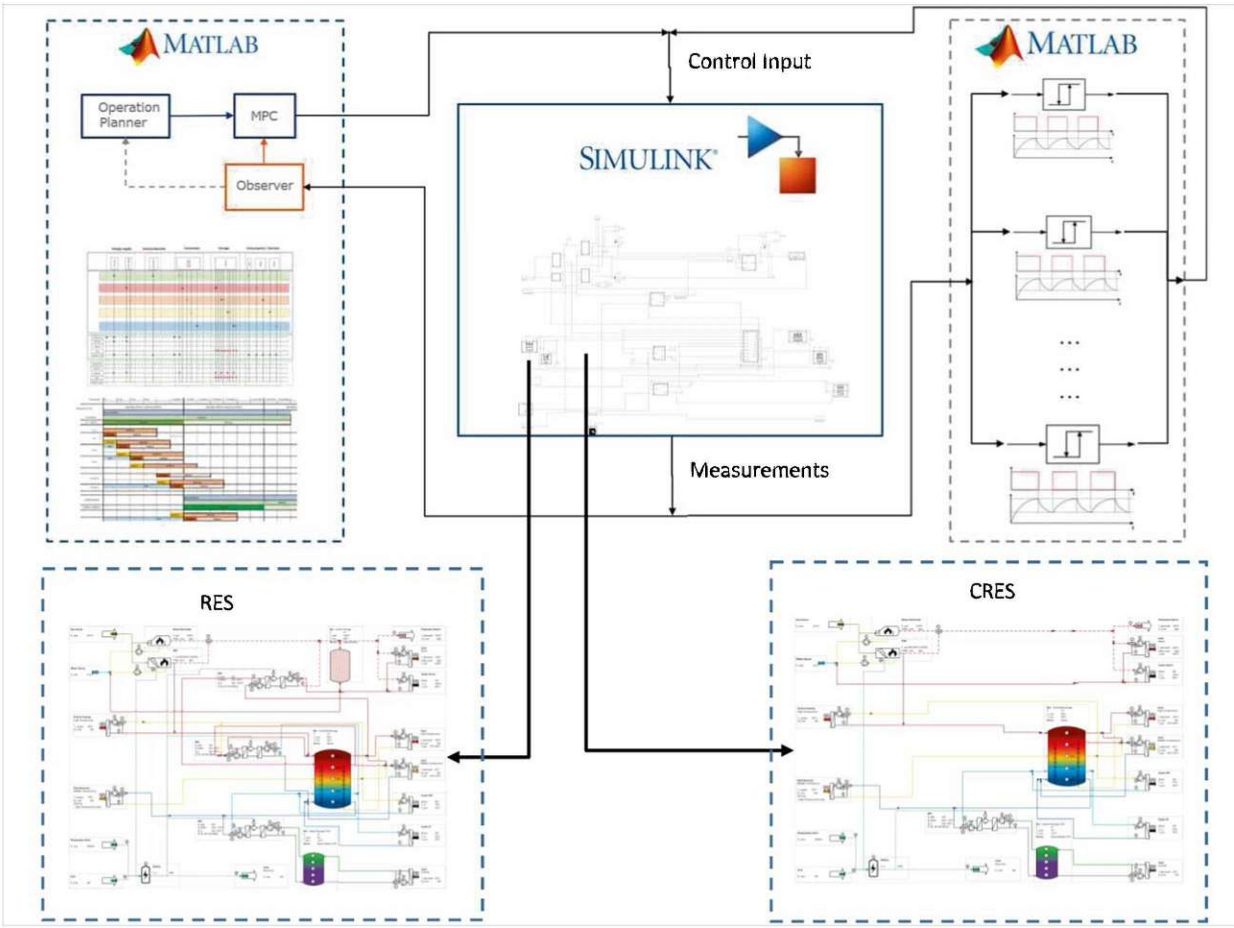


Figure 5.1: Overview and interrelations of the different system and control scenarios

The first assessment step determines the overall savings and potential improvements of the EMCS versus the CRCC for both plant configurations based on three different seasonal scenarios. The main focus is placed on the strategic utilization and control of units to minimize operating costs. Furthermore, detailed analyses are conducted to assess the effects of crucial factors, including inaccuracies in forecasting, methodological parameters such as the length of prediction horizons, weighting factors, and adherence to projected energy procurement schedules.

Additionally, the two-layer EMCS is compared with a single-layer MPC to emphasize the methodological benefits of the approach as well as the comparison of economic and environmentally optimal operation. The assessment is concluded by a comparison with the ecologically optimal scenario. Through the variety of different studies, a broad and comprehensible evaluation can be provided which depicts the EMCS operational performance from different perspectives and outlines both particular benefits as well as common challenges to overcome.

Reference to Experimental Tests It needs to be acknowledged, that experimental performance evaluations on real systems provide unparalleled informative value, expressiveness, and credibility compared to simulation studies. However, there are inherent disadvantages and limitations such as high implementation costs, limited availability and accessibility of laboratory resources, safety concerns, and the time-consuming nature of real-time evaluations restricting the number of feasible studies. Consequently, laboratory tests often focus on small-scale systems, accepting a limited scope of investigations and findings. On the other hand, advanced planning and control methods, such as the EMCS, demonstrate their full functionality when applied to comprehensive and versatile energy systems as typically found in real industrial plants. However, establishing such multi-component technical facilities for testing in real operational environments like laboratories is very challenging and practically impossible. While this case study deals with the comprehensive simulative evaluation at a complex plant, the conducted laboratory test in the course of the research project EDCSproof [2] is repeatedly remembered, which offered to address practical issues related to the implementation on real components and process control systems. Thus both contributions can therefore be considered as complementary activities.

5.1.1 Use Case

Before introducing the various evaluation scenarios, a brief reference to the use case, comprehensively described in Chapter 4, is given. The so-called Conventional Reference Energy System (CRES, Figure 4.6) includes on the one hand several components and subsystems that are common in current industrial energy supply systems in the respective sector. Furthermore, the integration of new state-of-the-art technologies such as High-Temperature Heat Pumps (HTHPs) and Thermal Energy Storages (TES) at suitable positions was assessed to improve system performance, which also introduces additional flexibility into the system. The CRES represents the base case for comparison in order to evaluate the effect of flexibility in combination with the application of the EMCS in terms of savings evaluation. Considering the central aspects to be focused upon, varying energy prices have an impact on the patterns of power consumption. Moreover, the production of the PV-systems is reliant on the temporal profile of solar irradiation, and the recovery of waste heat is influenced by process-related limited availability. Thus, for efficient plant operation, the flexibilities of diverse storage and conversion units need to be strategically managed. This ensures the maximization of self-generated energy utilization and optimal timing for energy procurement.

5.1.1 Simulation Model

In order to effectively test the EMCS, it is essential to create simulation models that represent the behavior of all individual components in the RES with sufficient accuracy. Referring to the derivation Chapter 4, it is emphasized at this point that the complete system does not exist in reality in its integral form. Nonetheless, each component of the CRES can find at least one real counterpart in the project partners' existing plants. These served as valuable sources for the creation of the respective models by providing access to beneficial technical data and operational information. Subsequently, these simulation models were implemented and assembled according to the approach explained in Chapter 3 to form the complete plants.

The individual models were parameterized and validated using real measurement data from the industrial plants if sufficiently available. Nonetheless, it is important to note that the capacities of the components in the RES vary from those found in the actual plants (see Section 4.1.3). Additionally, the sampling intervals of actual measurements was very unequal and in some instances, very coarse. Model validations for thermal storage and HT heat pump were performed based on plant data from Plant B [133]. The models of the steam system were parameterized using data from Plant A. However, complete data was only available on an hourly basis thereby decreasing the relevance of any validation The model of the steam heat pump was provided by the EDCSproject partner AIT. Since these components did not exist in any plant or only limited data was accessible, the models for the photovoltaic system, the battery and the Ruth steam storage were taken from literature. Regarding the simulation models, the steam system is particularly notable, representing a system of communicating steam vessels in which both the system pressures and temperatures change dynamically. For a comprehensive description of both optimization and simulation models for all specific components, please refer to the Appendix A.1.

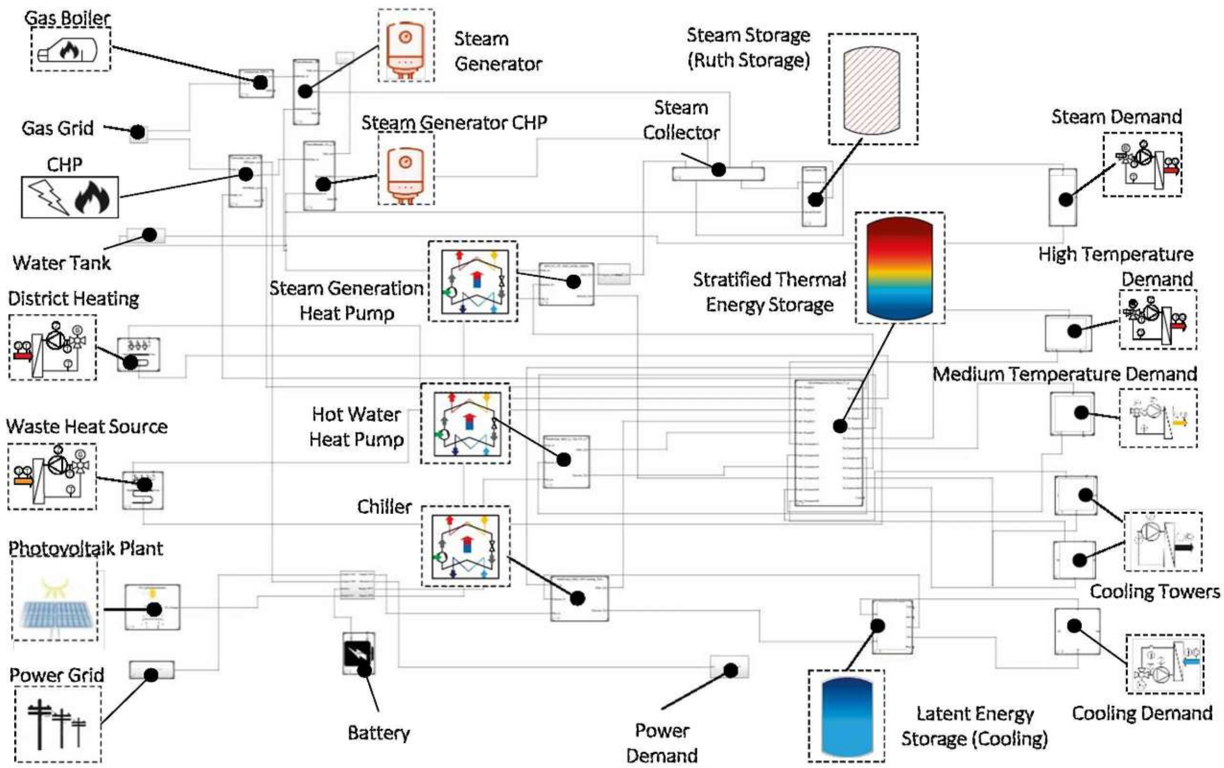


Figure 5.2 Simulink Simulation Model of the RES

With regard to the operational environment, three seasonal scenarios are examined, which differ in terms of the consumption patterns of the processes, the energy prices of the grid-connected energy sources, and the environmental conditions such as outdoor temperature and solar radiation. It's worth noting that these scenarios were also employed to determine the design and configuration of the RES. In the subsequent case studies, the simulation model, shown in Figure 5.2 is to be regarded as central element which can be operated either by the EMCS or the conventional reference control concept (CRCC) as depicted in Figure 5.1. Considering potential actions and interventions, the actuating variables of the controllable units are to be specified so that the delivery of the required energy to consumers in the appropriate quality, without exceeding or violating technical capacities. The consumption processes themselves are to be considered as non-regulable units that strictly extract energy according to the respective demand profiles. For all scenarios and studies, the same initial conditions and starting times were assumed. The Simulation Studies were executed in MATLAB [129] using the Simulink Simulation environment.

5.1.2 EMCS Control

It is highlighted that the perfomance evaluation of the EMCS, which is fundamentally described in Section 3.6, is the central objective of this case study. In this respect, it is particularly referred to the respective illustration of the fundamental architecture, (see Figure 3.13), the model implementation for the two-layer receding horizon optimization (see Figure 3.14 and Figure 3.16) as well as the operational principle (Figure 3.17). As the performance evaluation specifically compares the EMCS with the CRCC, both concepts are discussed below, with particular emphasis on the operating principles to highlight the significant differences in plant control.

Within the EMCS, the OP determines the optimal long-term operation schedules according to the superior operational objectives, such as cost- or environmental optimality, based on forecasts of respective operational environments. The task of the MPC is then to transmit appropriate control signals to the real units (or their simulation models) in order to realize the optimal schedules, for which in addition also the measured plant operation is essential. The observer also acts as a central coordination unit concerning the measurement of plant operation and processing information to the optimization models in the OP and MPC. According to the overall superstructure-based model implementation, depicted in Figure 5.3, both rely on the same plant models but use different objective functions due to their different main tasks. For the OP it becomes imperative to consider extended prediction horizons to effectively determine the optimal operation strategies considering essential operational boundaries such as weather conditions, energy prices, and process demands. Typically, these variables change in time frames ranging from a few hours to days. In contrast, when it comes to implementing the corresponding optimal trajectories at the individual units, precise control is required, which consequently necessitates finer time steps in the MPC.

Thus, for the selection of suitable time parameters, it is crucial to consider minimizing the number of time steps to ensure efficient and expedient calculations. Typically prediction horizons of 24-48h are an appropriate choice for the OP, mainly depending on the temporal variations of the boundary conditions, the complexity of the plant, and considered processes. In the OP, time-step lengths of 15 minutes or hours, according to the billing periods in energy markets, proved to be suitable. For the MPC shorter time step lengths in the range of minutes are recommended, with a lower limit of 15 minutes typically observed for prediction horizons [2, 45].

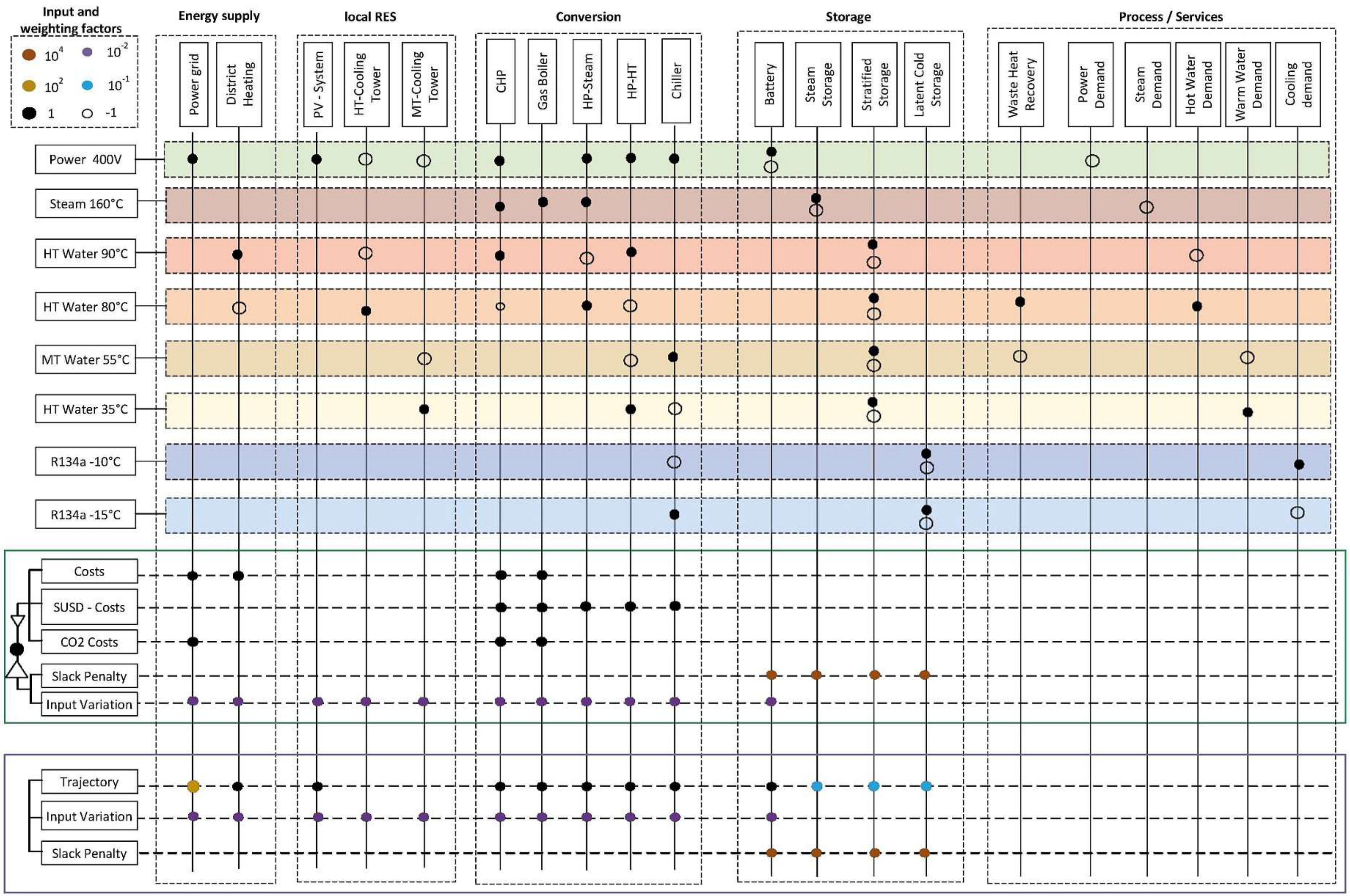


Figure 5.3: Two-layer superstructure model of the RES within the EMCS

The selection of appropriate execution intervals is mainly influenced by the frequency of new forecasts or measurements along with the projected calculation times. Particularly in the context of real-time online optimization, it is crucial for the optimization process to be completed in time. In the specific application on the RES, a time step length of 15 minutes with an execution interval of 2 hours was selected in the OP while in the MPC both time step length and sampling time were set to one minute. In order to adequately participate and utilize day-ahead power markets, prediction horizons of 36 hours are typically necessary. However, with a predetermined price profile provided by the energy supplier, effective planning can still be achieved even with a reduced horizon of 12 hours. In subsequent studies, an extended and a reduced prediction parameter set-up scenario was considered to facilitate performance comparisons. In the extended scenario, a prediction horizon of 36 hours was utilized in the OP, while the MPC employed a prediction horizon of 45 minutes. Conversely, the reduced scenario employed prediction horizons of 12 hours in the OP and 15 minutes in the MPC. The minimization of energy-related operational costs represents the superior objective in the higher controller level of the OP in most scenarios and comparisons. However, in the course of this evaluation, also emission minimization was applied in the respective scenario.

Regarding the particular optimization of the individual units, it is emphasized that the primary objective is not to employ the most comprehensive, detailed, and accurate models for optimization but rather to demonstrate that the Energy Management and Control System (EMCS) has the capability to yield significant improvements in operational energy planning, even when using simplified models. Accordingly, except of crucial parameters such as capacities and part load limitations, the individual optimization models were not specifically parameterized, adjusted or enhanced to exactly match the simulation models.

Both, the EMCS and the reference control method are implemented in individual simulink components in the shape of MATLAB functions. While the functioning of the EMCS is comprehensively described in Chapter 3, a brief description of the conventional reference control concept is given in the following section.

5.1.3 Conventional Reference Control Concept (CRCC)

Within the CRCC, the individual units are subjected to their own distinct control rules tailored to their specific characteristics. In contrast to the EMCS, these rules exhibit a methodological deficiency in considering future events or possible future consequences of current actions. Instead, they only rely on past events in order to execute operational actions. If applicable and accessible, respective control strategies and parameters were derived from the actual real components used in the industrial partners' plants. These control strategies are largely attributed to the concept of hysteresis control, with the state of charge (SOC) of a connected storage serving as the controlled variable. However, certain individual units employ their own distinct operating strategies. For example, the CHP unit operates in an "electricity-driven" manner, thus it is consistently activated once a specific power demand threshold is reached. Depending on the actual power demand it operates either at full load, 50% part load, or switched off. Additionally, it is also shut down in the event of a certain surplus in steam production. For the new components in the RES, which are currently not present in any of the investigated facilities, the following control rules were applied:

- The battery is operated with the aim of increasing self-consumption, charging in the event of surplus generation, and discharging in the event of a shortage in self-generation.
- The high-temperature heat pump operates in a similar manner to the gas-fired steam boiler, with the pressure in the steam distributor serving as the controlled variable. However, the heat pump is desired as the preferred choice for operation and is consequently switched on earlier and switched off later.
- As the heat pumps in the RES are each connected to storages at both its sources and sinks, both storage levels must be regarded for control. Thereby the activation follows the storage at its sink if the storage at the source is within a certain range. Nevertheless, the chiller exclusively considers the cold storage, as there is no other component persistent for control.
- The District Heating controls the same temperature level in the stratified storage tank as the high-temperature heat pump. However, the high-temperature heat pump is preferred and the district heating thus acts as a backup, which is switched on later and switched off earlier.

Since the CRCC fails to consider variable energy prices in its control actions, a constant electricity price is assumed, which corresponds to the mean value of the variable electricity price in the respective season.

5.1.4 Scenario Overview and Performance Indicators

Basic Scenarios In a first step a high-level evaluation is carried out to assess general savings potentials and obtain fundamental insights into the overall functionality of the EMCS in comparison to the CRCC. The primary focus is placed on analyzing the disparities in operation and the utilization of different units, including respective operational costs, energy consumption, and emissions. These scenarios, in which perfect information is assumed are categorized based on the following aspects:

- Two control concepts: To assess the potential performance improvement offered by an EMCS application compared to CRCC
- Two plant configurations: To analyze the influence of new technologies, the conventional configuration of the CRES is compared to the extended configuration of the RES, which incorporates new components such as heat pumps, thermal and electrical storage, and a PV, thus exhibiting more flexibility
- Three seasonal scenarios with different boundaries for a more comprehensive investigation

Detailed Analysis of Prediction Characteristics and Methodical Parameters This part provides a comprehensive insight into essential operational performance characteristics and functions featured by the EMCS such as prediction timespans, accuracies, and susceptibility to forecast errors. The following aspects and issues will be addressed in more detail.

- The Impact of forecast errors and optimization parameters on performance

- Compliance with the power-grid purchase schedule (with special regard to the load and congestion management of power grids)
- Trajectory progression priorities and characteristics
- Performance comparison of the two-layer EMCS with a single-layer MPC

Comparison of the Cost-Minimal with the Emission-Minimal Operation The main aim of comparing economic and environmental perspectives is to especially identify discrepancies and linkages indicating the accounting of environmental factors within economic frameworks and the corresponding influence of technology

The main performance indicators are the savings potential of the EMCS compared to the reference control concept, as well as the accuracy of the realized plant operations in relation to the desired predicted trajectories provided by the OP. From the base scenarios, where perfect forecasts and predictions are assumed for the EMCS, the main findings on the potential improvement through new technologies and energy management in terms of energy efficiency, CO_2, and cost savings are derived. Therefore, the EMCS operation is compared with the reference the CRCC for both the RES and the CRES for all three respective seasonal periods.

In the case of perfect forecasts and predictions, planning deviations appear exclusively through model inaccuracies (linear descriptive optimization models are subject to more simplifications than procedural, nonlinear simulation models). This means that the deviation between the perfect trajectories and the realized operation is purely a systematic or methodical deviation. Since the measures for correcting these deviations, which are carried out by the MPC, always require the expenditure of additional energy and consequently additional costs, the planning quality can consequently be quantified very well by comparing overall energy consumption or costs. Subsequent to the base case evaluations, the influences of prediction quality as well as control and other methodological parameters (e.g. receding horizon) are analyzed in further detailed studies. Thereby, the base case operation of the EMCS is considered as a reference. From a high-level perspective, global operational indicators such as total energy consumption or total costs can be used very well as benchmarks for evaluating the quality of the operation. In addition, certain operational effects, and anomalies are also analyzed based on detailed, specific investigations.

5.2 Results and Discussion

Explanation and Remarks on Graphical Illustrations In the respective progression graphs, which mainly intend to provide insight into the distribution of generation and consumption of the various energy sources over time, the different suppliers are shown on the positive y-axis, and the consumers are shown on the negative side. These graphs are particularly suitable for comprehensive, overarching evaluations of the operation of the various interrelated units. However, due to the stacking, the representations of more distant progressions are superimposed by those of the previous ones, which makes them less practical for detailed observations. The bar charts present the energy costs as well as the energy production of all producers in comparison with the energy consumption of all consumers in cumulative form covering all energy carriers. Suppliers delivering energy and consumers extracting energy occur on the respective positive y-axis. On the other hand, suppliers extracting energy (e.g.

grid feed-in or cooling towers) as well as energy services that actually deliver energy to the system (e.g. in the case of a cooling demand), are shown as negative contributions. In all area charts, each unit is indicated by its specific color, regardless of which variables or states of the respective units are accessed and analyzed. It should be noted that energy costs are only attributed to generators or suppliers. Conversely, since no costs are accounted by consumers, these do not appear in the cost diagrams at all. Negative costs, which are represented in cumulative form on the negative y-axis, are to be regarded as revenues and therefore need to be deducted from the energy costs. The abbreviations of the various units used in the legends of the figures are listed in Table 5.1.

Table 5.1: abbreviations used in the legends of the figures

CHP	Combined Heat and Power unit	HPcl	Heat Pump Cooling
CTht	Cooling Tower high temperature	HPht	Heat Pump high temperature
CTmt	Cooling Tower medium temperature	HPst	Heat Pump stem
Dcl	Demand cooling	PG	Power Grid
Del	Demand electricity	PV	PhotoVoltaic Plant
DH	District Heating	STel	STorage electricity (Battery)
Dht	Demand high temperature	STcl	STorage cooling (Latent energy st.)
Dmt	Demand medium temperature	STES	Stratified Thermal Eenergy Storage
Dst	Demand steam	STst	Storage Steam (Ruth Storage)
GB	Gas Boiler (steam generation)	WHR	Waste Heat Recovery

5.2.1 Analysis of Operational Improvements in Relation to Conventional Control

Focusing on the primary objective of evaluating operational improvements and associated savings in relation to conventional control, a comparison of the three seasonal scenarios was conducted on both plant configurations to provide a sufficient and comprehensive basis for evaluation. It is assumed that the EMCS operates based on accurate forecasts and utilizes variable power prices, while the CCRC employs constant prices to prevent unintended adventitious cost distortions.

To facilitate a clear comparison between the two control concepts and plant configurations, the scenarios are systematically presented in tabular form, focusing on the energy source balances, where each of the units is indicated by its respective color. If not specified otherwise, the summer scenario is considered. As indicated, the chars from Figure 5.4 to Figure 5.11 compare the two operation concepts on the RES, and Figure 5.12 - Figure 5.19 depict the CRES operations. The graphics with the uneven numbers, each shown on the left, correspond to EMCS operation while the even numbers on the right represent the CRCC. The fundamental operational differences become apparent already on a high-level comparison. Considering the CRCC operation, immediately notable capacity variations are observed indicating the prevailing control principle, while the EMCS exhibits rather continuous progressions, particularly of the controllable units. Despite these fundamental differences, all processes can be sufficiently supplied without experiencing any shortages in all scenarios. However, there are significant disparities in terms of energy input and costs between the two concepts.

RES

EMCS	CRCC

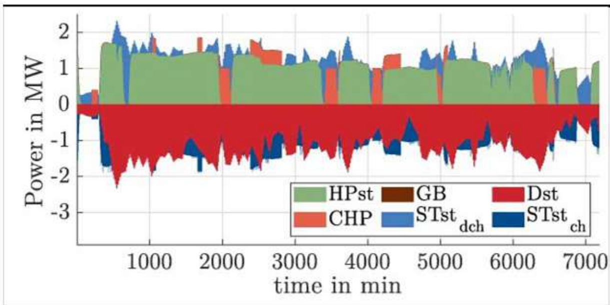


Figure 5.4: Steam Balance EMCS

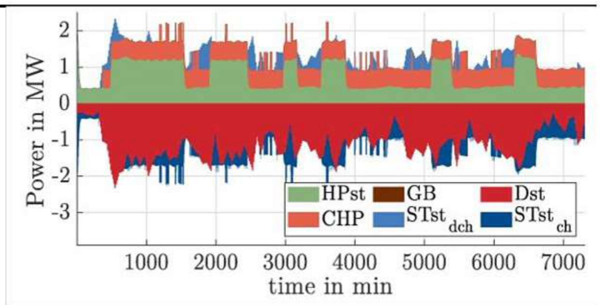


Figure 5.5: Steam Balance CRCC

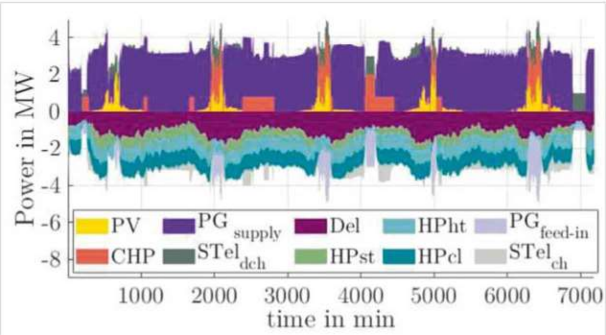


Figure 5.6: Electricity Balance EMCS

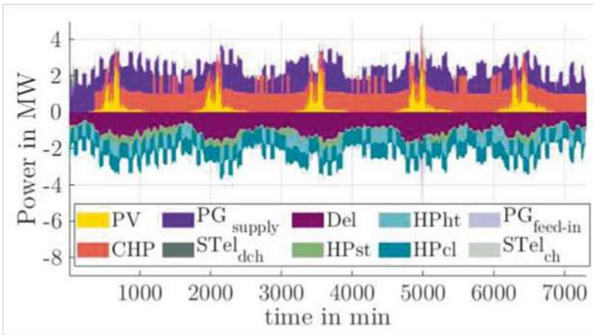


Figure 5.7: Electricity Balance CRCC

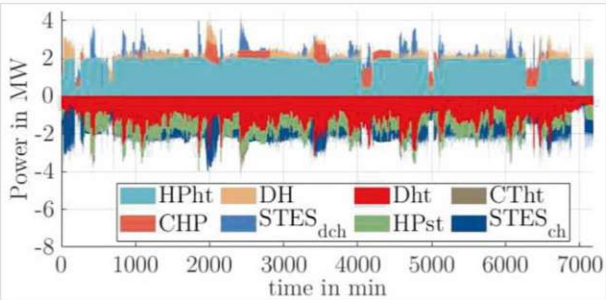


Figure 5.8: Hot Water Balance EMCS

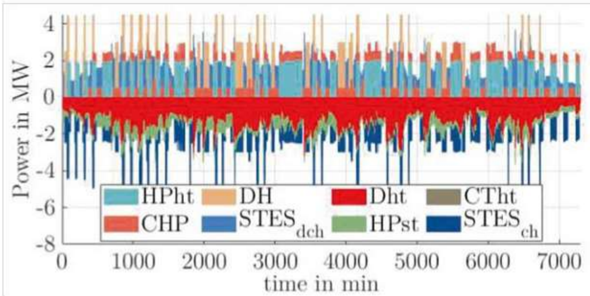


Figure 5.9: Hot Water Balance CRCC

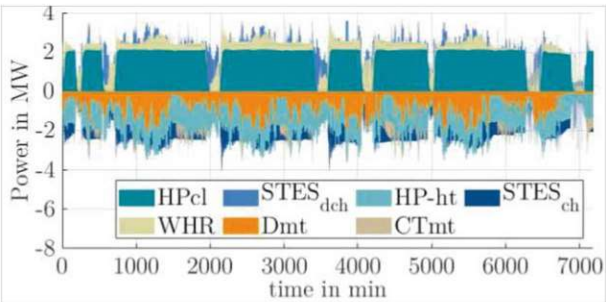


Figure 5.10: Medium Temperature Water Balance EMCS

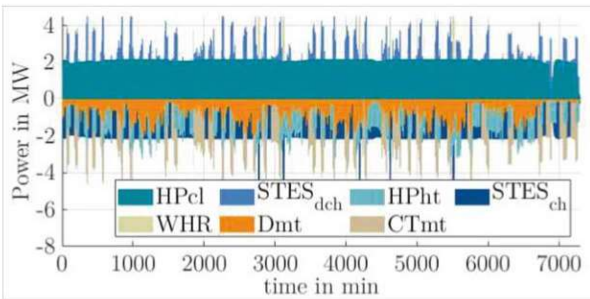


Figure 5.11: Medium Temperature Water Balance CRCC

CRES

EMCS	CRCC

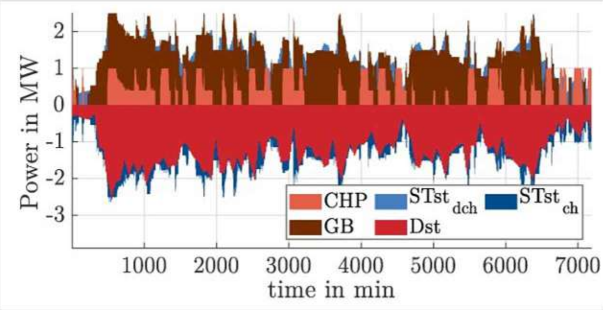


Figure 5.12: Steam Balance EMCS

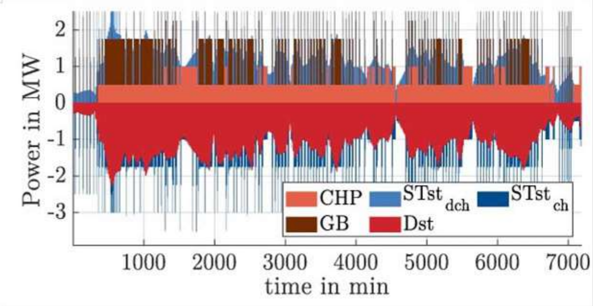


Figure 5.13: Steam Balance CRCC

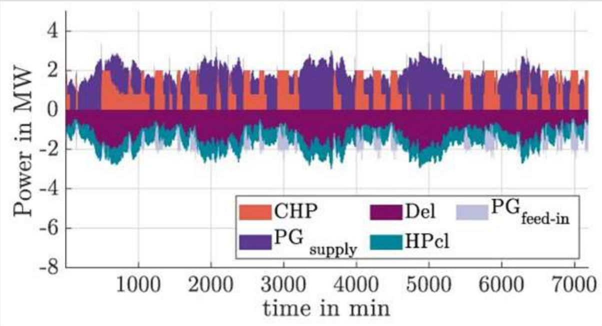


Figure 5.14: Electricity Balance EMCS

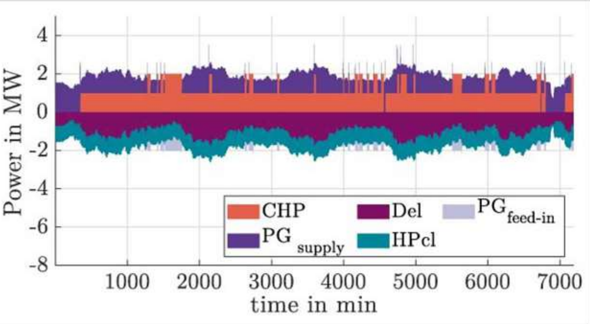


Figure 5.15: Electricity Balance CRCC

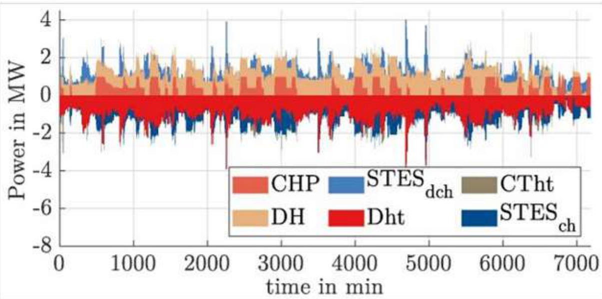


Figure 5.16: Hot Water Balance EMCS

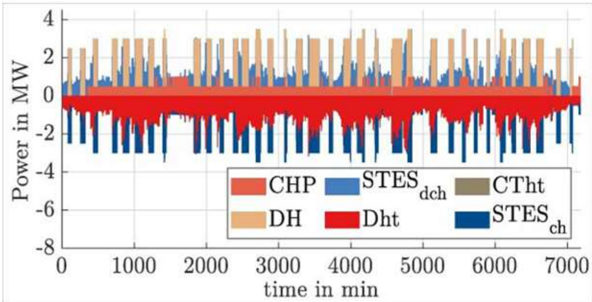


Figure 5.17: Hot Water Balance CRCC

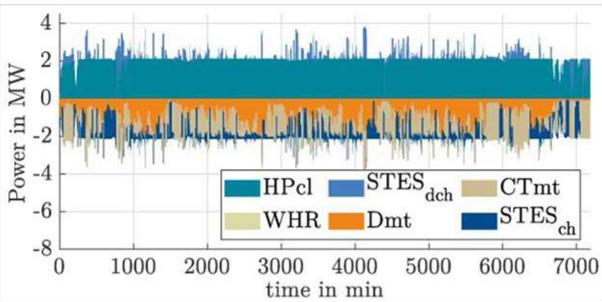


Figure 5.18: Medium Temperature Water Balance EMCS

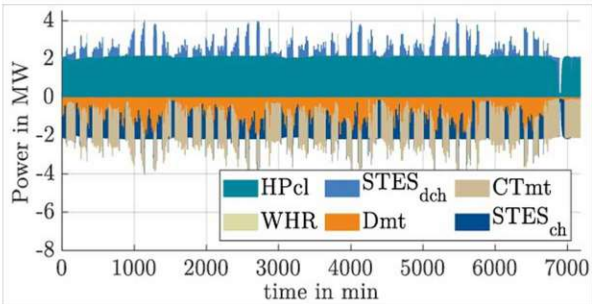


Figure 5.19: Medium Temperature Water Balance CRCC

For a high-level comparison of the EMCS with the CRCC on the RES, Figure 5.20 presents the cumulative energy supply and demand distribution of both scenarios while Figure 5.21 shows the distribution of cumulative costs. In total for all units, a reduction of 26% in energy supply corresponding to a cost saving of 21.6% is observed what is mainly attributable to the significant reduction in CHP utilization. Due to less flexibility and consequently fewer options for operational improvements, correspondingly lower savings are estimated at the CRES. However, according to Figure 5.23, still a cost reduction of 11.1% can be perceived, corresponding to a 10.1% reduction in energy use according to Figure 5.22. When comparing energy use, it is crucial to acknowledge that various energy forms, which are different in terms of specific exergy content as well as costs, are being compared in a cumulative manner. Additionally, it is important to refer to the expalanations and remarks on the graphical illustration at the beginning of Section 5.2. Accordingly, a negative demand represents an energy input that can be reused by the system.

Especially at the RES, it can be recognized that the predictive operation facilitated by the EMCS effectively manages consumption peaks and fluctuations through the utilization of existing storage facilities, without necessitating the explicit activation of additional generation capacities. Conversely, a detailed examination of the CRCC reveals an opposite situation the activation of additional capacities results in generation surpluses, leading to the storage facilities primarily being filled during peak consumption periods instead of being utilized to cover them. When considering the utilization of individual units, notable differences can be observed, particularly in the case of the CHP unit. In accordance with the practices of industry partners, the CHP is operated based on subjective preferences, following an "electricity-driven" strategy in the CRCC. In contrast, the EMCS exclusively considers economic aspects, leading to a distinct utilization pattern. Particularly considering the CHP connection to four different energy carriers, it is crucial to adopt a broader perspective rather than a distinct level. Considering the CRES, which exhibits fewer generation alternatives, a closer examination reveals that besides the CHP, there is also a higher utilization of district heating as well as significantly larger waste heat release.

In contrast, the EMCS rather uses the gas boiler and grid-based electricity more frequently, which turns out to be more cost-effective. Furthermore, it is noticeable that at the medium temperature balance, interestingly, great operational alignment between the EMCS and the CRCC can be recognized, while the energy balances show significantly different unit utilizations. This indicates that the system exhibits less flexibility in that part but also that the CCRC may work sufficiently at these conditions. Focusing on the RES, it becomes evident that heat pumps are the preferred choice for heat generation, while the CHP functions primarily as a backup and is rarely activated. With regard to the heat pumps, it is recalled that they are each connected to storage tanks at both the source and sink, which requires that both storage levels are to be considered for operation. In this respect, the advantages of the predictive and planning-orientated functional capabilities of the EMCS, enabling a continuously high and efficient operation of all three heat pumps, become especially apparent. This consideration also indicates that the optimal operation of the three heat pumps is closely coupled. With regard to storage management, operational usage requirements and applications have already been examined that go beyond a pure arbitrage and economic shifting of energy purchase. Above all, this comparison already illustrates the integral interrelationships in the energy management of industrial processes and indicates the importance of a holistic approach and control with regard to efficient and sustainable operation.

RES

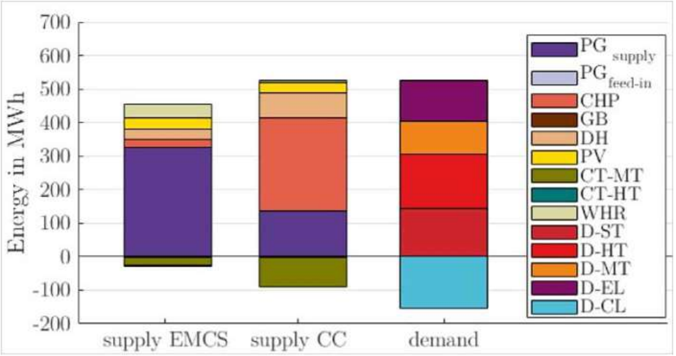


Figure 5.20: Comparison of cumulative energy supply and demand for the RES

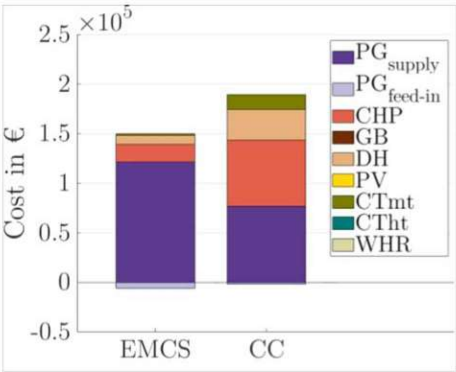


Figure 5.21: Comparison of energy cost distributions for the RES

CRES

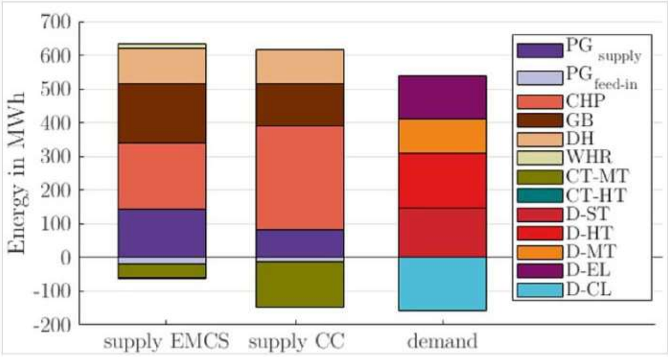


Figure 5.22: Comparison of cumulative energy supply and cumulative demand for the CRES

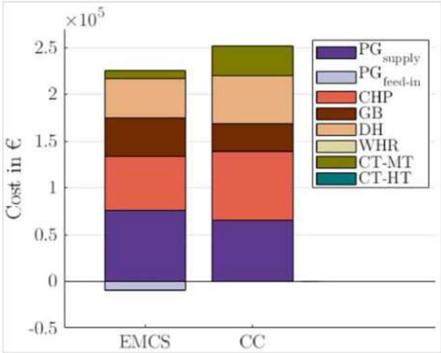


Figure 5.23: Comparison of energy cost distributions for the CRES

The corresponding EMCS-operation scenarios for the seasonal scenarios of transition and winter for both configurations, RES and the CRES, can be found in the same form in the Appendix A.2.

Executive Summary of Basic Scenarios The most important indicators for evaluating operational performance and associated savings on a high level are operational costs, energy use, and emissions, which are compared in Figure 5.24, Figure 5.25, and Figure 5.26, respectively. Evidently, the RES operated by the EMCS shows the most favorable operation for all seasons, however, the effects are differently pronounced. According to Figure 5.24, the cost savings through the EMCS range between 15,6% (winter) and 21,6% (summer) for the RES, and between 4,8% (winter) and 11,1% (summer) for the CRES. Examining the different indicators, emission reductions are the most prominent in particular at the RES, showcasing that the corresponding technologies are effectively aligning both environmental and economic objectives. At the RES the emission savings range between 45.6% (transition) and 48.8% (summer), while in the CRES these are significantly lower accounting for 8.2%, (summer) and 14.6% (winter).

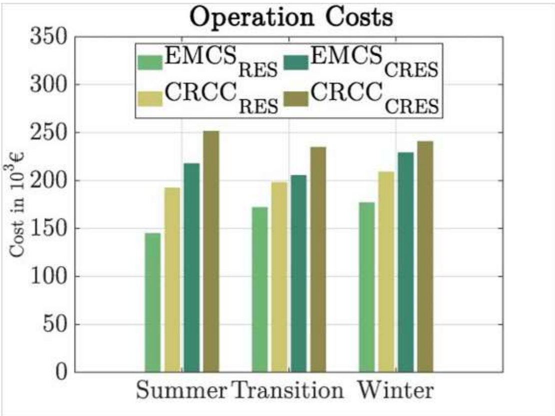


Figure 5.24: Comparison of energy costs

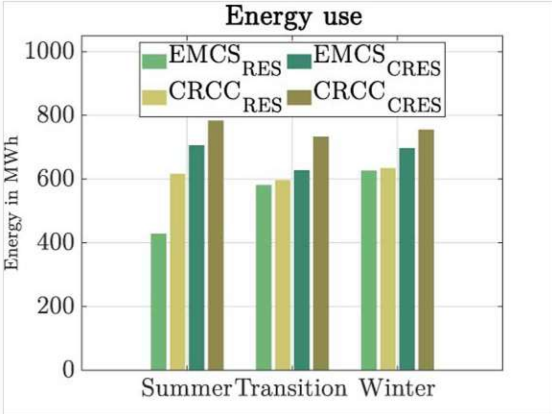


Figure 5.25: Comparison of energy use

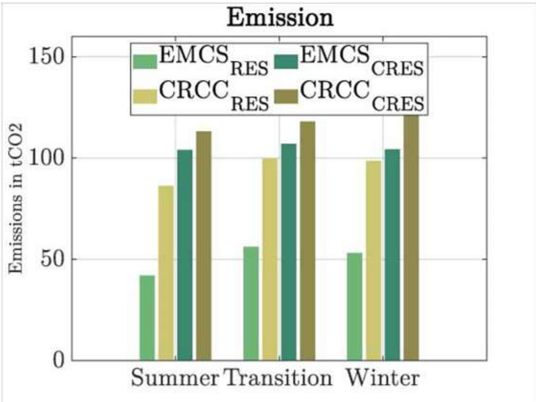


Figure 5.26: Comparison of emissions

Regarding the comparison of energy use, it is crucial to acknowledge that different energy forms, which show differences in terms of exergy content as well as specific costs, are being compared cumulatively. In summary, the EMCS proves to be particularly effective in application to the more flexible RES. The inclusion of components such as heat pumps, energy storage, and renewable generation facilitates cost-effective operations and substantially reduces the reliance on fossil gas to a negligible level. This also represents a situation in which environmental and economic aspects can be realized similarly as will be discussed in more detail in the subsequent section 0. Inversely, the technological options and advantages in the RES become in particular effective when utilizing the EMCS. Focusing on the CRES, which has significantly lower flexibility and technological options for using renewable energy, considerably lower improvement potential is observed. However, despite the constrained options for enhancement, the adoption of predictive control can still facilitate reductions in cost, energy consumption, and emissions. Comparisons across the different plant configurations show that the RES under conventional control operates mostly superior to the EMCS-operated CRES. The biggest difference is clearly identified between the EMCS-operated RES and the conventionally controlled CRES. Thus, especially in the investment decisions of industrial operators the integration of an advanced predictive Energy management system is highly advisable. In general, it can be deduced that EMCS extracts the full potential from systems, but is still inferior to technical limitations. Especially in systems that rely on renewable-based components and exhibit flexibilities, correspondingly high savings were examined to be achieved by applying the EMCS. While the energy use is rather related to available sources and existing technologies, respective costs are evidently substantially influenced by economic conditions.

5.2.2 Detailed Analysis of Methodical Performance and Prediction Characteristics

While the previous analyses rather focused on the evaluation of operational differences and related savings potentials in reference to conventional control and design, the purpose of the following sections is to provide a comprehensive insight into essential operational characteristics and functions provided by the EMCS such as prediction timespans, accuracies and susceptibility to forecast errors. Since perfect forecasts, which were assumed in the basic assessment, are evidently not existent in reality, it is of particular importance to assess the impact of forecast inaccuracies on the predictions and operational performance of the EMCS. In establishing a robust and reliable operation, inaccuracies and deviations can be counteracted by methodical measures such as enlarging planning horizons or shortening sampling time. However, the calculation effort increases with the number of time steps. The following list gives a brief description of the subsequent examinations and respective scenarios.

- Initially, four different scenarios are considered, where the operation in the presence of forecast errors is compared with perfect forecasts in each case for longer and shorter prediction horizons. In this respect, please refer to the explanation in Section 5.1.2. Accordingly, the index 36/45 denotes a prediction horizon of 36 hours in the OP and 45 minutes in the MPC. Similarly, the index 12/15 stands for a 12-hour prediction horizon in the OP and 15 minutes in the MPC. The index 0 indicates perfect predictions, while the index E stands for imperfect forecasts. For each scenario, the desired OP trajectories are displayed alongside their corresponding realized operations. This study provides initial evidence on the accuracy and achievement of the desired operational planning and additionally evaluates the impact of forecast errors on costs and plant operations.
- While the scenarios are first considered and assessed rather on the plant level, successively the effects of prediction inaccuracies on a particular supply unit are analyzed. As it constitutes the most significant portion of energy costs and is susceptible to high price fluctuations, the electricity purchase is picked for this investigation. This evaluation is intended in particular to demonstrate the function of the EMCS of precise schedule compliance, which can be achieved very practicably through parameter setting in the objective function.
- Following this analysis, a subsequent examination provides a more profound insight into the impact of weightings and parameter setting within the objective function, with a particular focus on model-specific model implications.
- Additionally, the methodical advantages of the two-layer EMCS concept are assessed by a comparison to the operation of a single-layer MPC.

Forecast Inaccuracies Before the respective studies are analyzed, the approach employed to incorporate forecast errors is explained. Despite very accurate weather forecasts as well as advanced predictions of energy prices, particularly for the near future, the existence of forecast inaccuracies is ultimately evident. Additionally, besides the profound operational experience of plant operators, the dynamic nature of business operations significantly complicates precise predictions of energy consumption. In order to appropriately incorporate prediction errors within the methodological framework, comprehensive knowledge of their frequency and magnitude is vital. Although there is considerable operational knowledge available from Industrial partners plants, identifying forecast errors based on existing data or industry partners' operational experience presents a challenge. This is primarily attributable to the current operational practice, where observations and forecasts of crucial boundary parameters, such as weather conditions or energy prices, are not routinely conducted and used. Regarding prediction of the energy consumption, it was only possible to fall back on the operational staff's rough estimates.

Error Estimation Approach To compensate for the lack of information, the following practical considerations are used to derive estimates for the deviation of forecast from actual observed data. The forecast error is assumed to be composed of a fundamental component ΔErr_{fund}, which is expressed either as an increase or a reduction to the real profile, and a stochastic fluctuation represented as a superimposition of normally distributed random numbers $No(0, \Delta Err_{stoch}{}^{2})$. The magnitude of the fundamental part ΔErr_{fund} is obtained by analyzing the deviations of the daily mean values. Additionally, the stochastic fluctuations ΔErr_{stoch} are derived as relative deviations of each time step in relation to the respective average daily profile. According to these assumptions, the modified error-included profiles introduce stochastic elements into the real progressions. For the fundamental part, the direction of increase or decrease is randomly selected and might change only once a day. The corresponding modification function z_{err}^{t} of the original value z^{t} is stated in Eq. (5.1). Initially, both parts are zero for the current time of prediction and are gradually increasing until their maximum magnitudes are reached at a certain time t_{max} which then remain constant. Table 5.2 states the respective derived error estimation parameters based on the data profiles presented in Chapter 4, in quantitative terms. To provide a practical insight, the charts in Figure 5.27 - Figure 5.30 exemplarily show the constructed, modified predictions together with their original profiles..

$$z_{err}^{t} = z^{t}\left(1 + min\left(1, \frac{t}{t_{max}}\right)\left(rand(sign(\mu))\ \Delta Err_{fund}^{t} +\ No^{t}(0, \Delta Err_{stoch})\ \right)\right) \tag{5.1}$$

Table 5.2: specific error estimation parameters of the indiviudal time series

Data	Fundamental error ΔErr_{fund}	Stochastic fluctuation ΔErr_{stoch}
Demand Electricity	10.1%	14.36%
Demand Steam	20.68%	28.35%
Demand High Temperature Water	15.42%	32.36%
Demand Medium Temperature Water	34.53%	37.98%
Demand Cooling	7.62%	10,01%
Solar irradiation	23.48%	28.12%
Ambient Temperature	11.62%	7.12%
Power Price	9.62%	8.21%

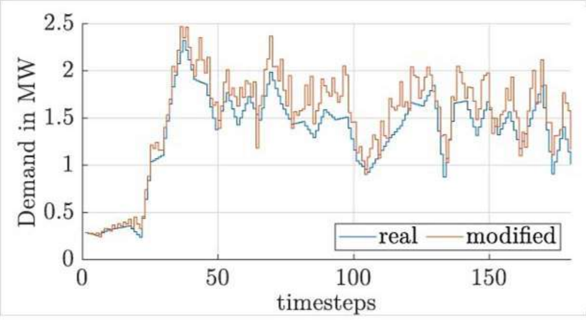


Figure 5.27: Prediction error example of Steam demand

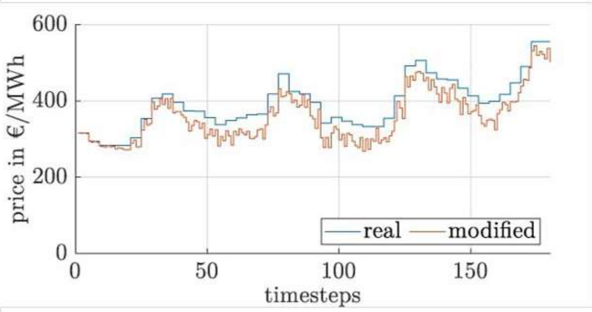


Figure 5.28: Prediction error example for Power prices

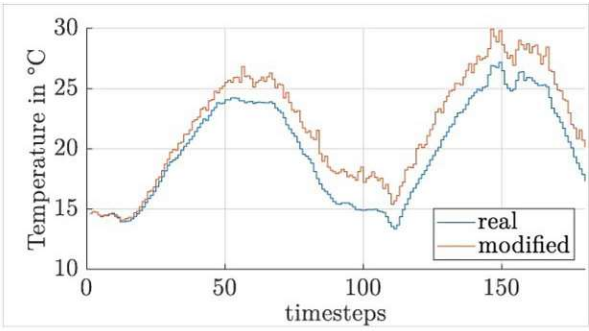


Figure 5.29: Prediction error example for ambient Temperature

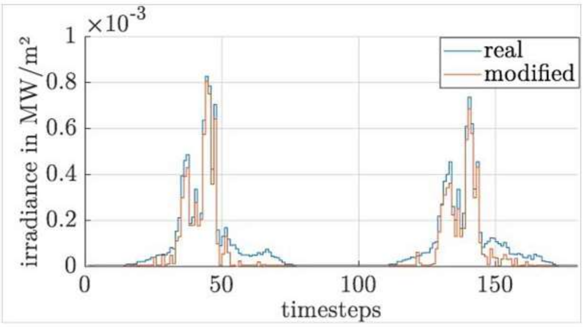


Figure 5.30: Prediction error example for solar irradiance

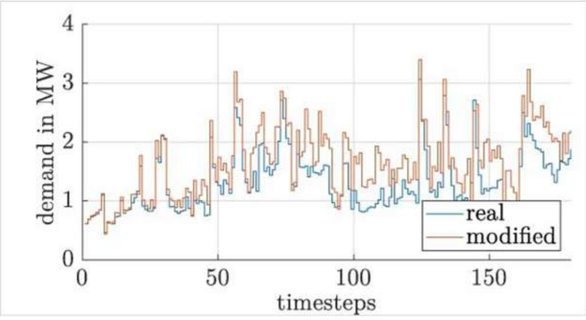


Figure 5.31: Prediction error example for High-temperature Heat Demand

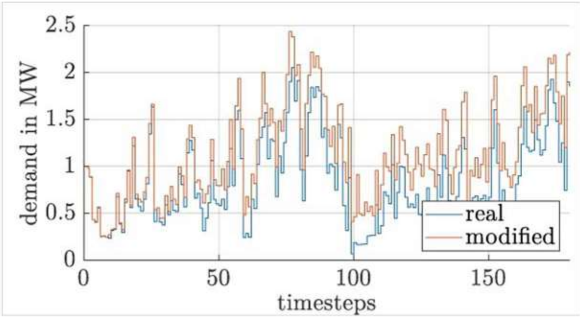


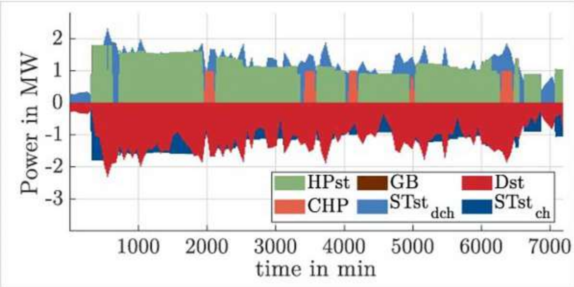
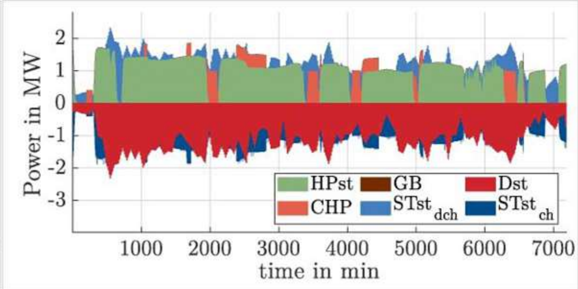
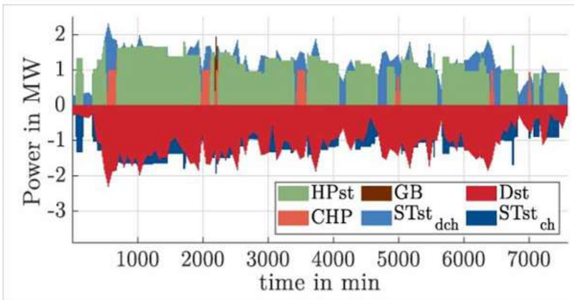
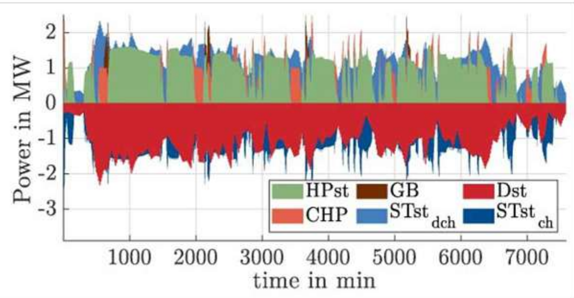
Figure 5.32: Prediction error example for Medium-temperature Heat Demand

Impact of Forecast Errors and Prediction Horizons The following evaluation compares the operation in the existence of prediction errors with perfect predictions for both prediction horizon combinations 36/45 and 12/15. Accordingly, this study addresses the question of how well the proposed operational strategies can be executed at the plant, and additionally examines the influence of forecasting errors and the length of the planning horizons.

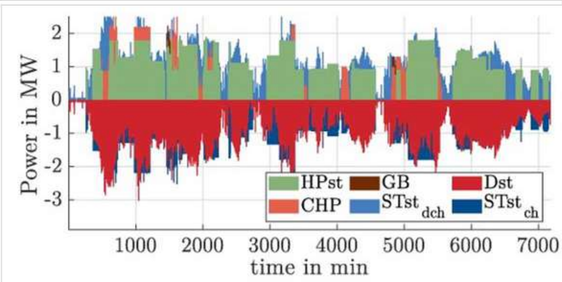
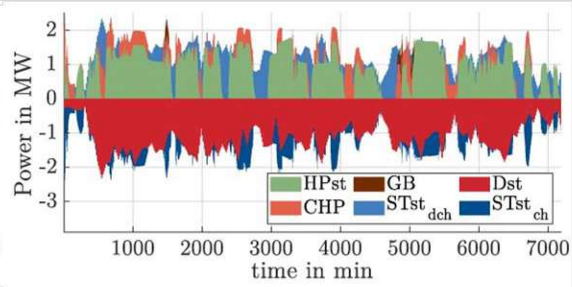
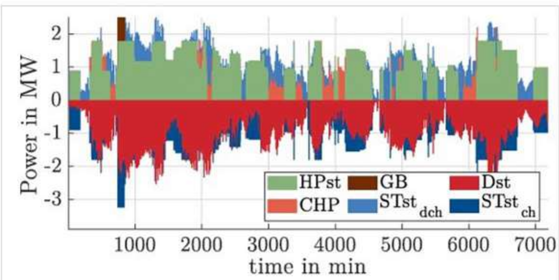
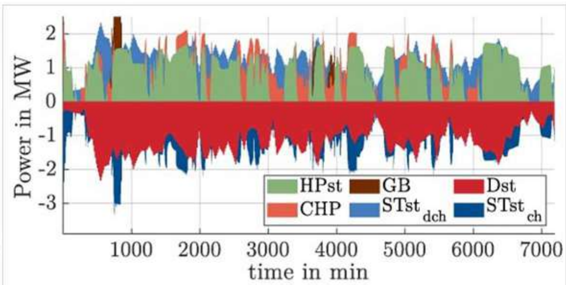
For a concise analysis, only the steam balances, shown from Figure 5.33 to Figure 5.40 are compared to highlight key insights. Thereby different operations can be observed very conveniently based on a few representative components. The steam-generation heat pump (HP-ST), the CHP, and the gas-fired steam boiler (GB) are available for steam generation, while the steam storage (STst) decouples generation from consumption and thus further increases the flexibility of operation. However, the use of the heat pump is affected on the one hand by the availability of energy at its heat source as well as the fluctuating electricity prices. The CHP can only generate steam, power, and hot water at the same time, which also causes dependencies, while the gas-fired steam boiler is not affected by any restrictions.

The corresponding progression graphs, depicted from Figure 5.33 to Figure 5.40, present the different operational progressions and provide a practical and lucid basis for analyzing the various scenarios. The left side represents the optimal schedules determined by the OP, which are based on perfect forecasts in the two upper scenarios while in the two scenarios shown below inaccurate predictions were assumed. On the right side, the respective realized operations are shown respectively. When compared with the operation at perfect forecasts, the existence of forecast errors reveals considerably more pronounced disparities between the desired OP trajectories and the realized operation, which is particularly noticeable by rather unsteady progressions. Considering the operation of individual units, differences are most clearly reflected by the steam heat pump (HP-ST) shown in green and the CHP in orange. Evidently, the heat pump is the preferred alternative but at the same time, it can be recognized that its operation is unevenly deployed in different scenarios. Moreover, a selective utilization of the CHP is obrservable, while the steam boiler is very infrequently activated. Essentially, the frequency of the CHP use can be interpreted as an operational quality indicator as it is utilized more often in case of prediction deviations compared to accurate planning. While at the 36/45 set-up and perfect forecast, the CHP is hardly needed at all, an increasing utilization is observed in the other scenarios. With perfect prediction, the planned operation can be realized very well in both set-ups 36/45 and 12/15. Differences appear mainly in a slightly different utilization of the steam-generating heat pump (HP-ST) and more frequent use of the CHP. Although storage facilities are available as a compensation measure, the CHP is still utilized. Due to its constant generation costs, this is particularly effective during periods of high electricity prices or when power purchase thresholds exist. It is important to emphasize that exceeding a power purchase threshold of 4 MW results in a notable cost escalation due to the subsequent shift in grid utilization class. Obviously, if alternative measures are more cost-efficient, the exceeding of this threshold is avoided. Thus, additionally, also the activation of the gas boiler can be noticed in rare cases, but slightly more at the short prediction horizon.

Perfect forecast

	Operational Planning (OP)	Realized Operation (RO)
OP 36, MPC 45	 Figure 5.33: OP of the 36h/45min-Setting	 Figure 5.34: RO of the 36h/45min-Setting
OP 12, MPC 15	 Figure 5.35: OP of the 12h/15min-Setting	 Figure 5.36: RO of the 12h/15min-Setting

Inaccurate forecast

OP 36, MPC 45	 Figure 5.37: OP of the 36h/45min-Setting	 Figure 5.38: RO of the 36h/45min-Setting
OP 12, MPC 15	 Figure 5.39: OP of the 12h/15min-Setting	 Figure 5.40: RO of the 12h/15min-Setting

Regarding the distribution of cumulative costs, presented in Figure 5.41 and Figure 5.42, it is evident that the realized operations consistently incur slightly higher costs than the respective operational planning. The observed discrepancy can be attributed to the requisite adjustments made by the MPC to realize the optimal schedules. Comparing the OP predictions with the realized operations, these adjustments lead to the incurrence of additional costs, which consequently exhibit margins of 17.1% (36/45) and 11% (12/15) in the case of perfect prediction, and 9.2% (36/45) and 14% (12/15) when considering prediction errors. While the 36/45 realizes the most economic operation with perfect prediction, it interestingly also records the largest cost increase in relation to its OP forecast. The causes may relate to many aspects, but above all this also clearly indicates, that the OP predictions may be very ambitious compared to the realized operation. However, the fact that the other scenarios show lower cost increases is rather attributable to suboptimal OP predictions than to a better functioning MPC. Considering cost minimization as the overall objective, the aforementioned values may also be interpreted as indicators of a systematic or methodological error. These are particularly meaningful in the case of perfect prediction, where they are almost entirely attributable to inaccuracies of the optimization models used for prediction. At this point it is emphasized that the overall cost increase can be reduced or amplified by the weightings in the target function of the MPC, which will be comprehensively examined below (see the investigation from Figure 5.66 to Figure 5.77.)

By observing Figure 5.41 together with Figure 5.42, it can be derived that the shorter prediction horizon of 12h in the OP, despite perfect prediction, results in an inferior operational planning corresponding to a cost increase of 11% compared to 36h. In the realized operation, this results in a final cost increase of about 7%. This underpins the previous observation, that limited information on future events, resulting from a shorter prediction horizon, is responsible for a planning-related cost increase. However, the shorter prediction horizon of 15 minutes in the MPC may be a suitable choice at perfect prediction.

The existence of forecast errors mitigates the validity and reliability of the desired operational trajectories, which are depicted in Figure 5.37 and Figure 5.39. Together with the respective realized operations shown in Figure 5.38 and Figure 5.40, valuable insight into how the EMCS compensates for forecast errors is provided. In comparison to the base cases of perfect prediction, for the realized operation a cost increase of 3.5% at the 36/45-setting is observed, whereas the increase at the 12/15-setting is slightly higher at 7.7%. However, it needs to be considered that at the 12/15-setting, already the OP-prediction was less cost-optimal.

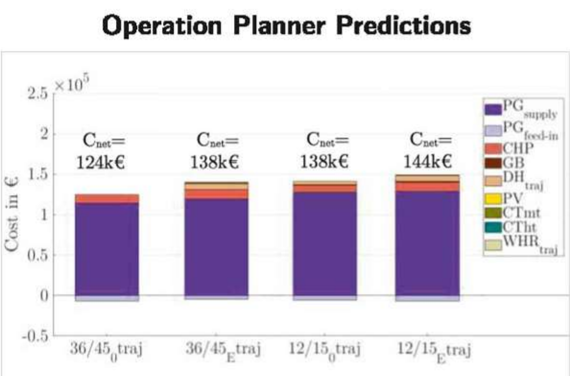


Figure 5.41: Cumulative Costs according to the operational planner predictions

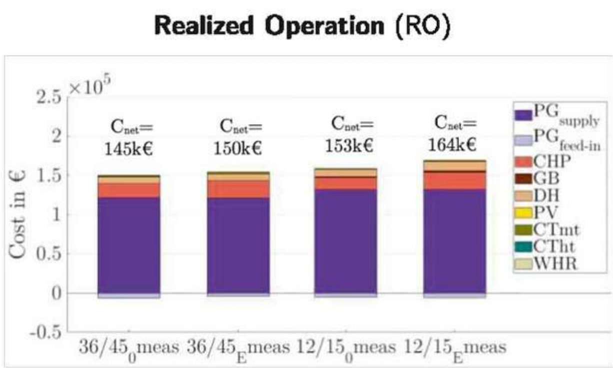


Figure 5.42: Cumulative Costs of the realized operations

Interestingly, the cost increase compared to the OP prediction was lower at the 12/15 setting. In a direct comparison, the scenario with long prediction horizons is about 6% more cost-effective to operate at perfect prediction and 9% at imperfect forecasts. Conclusively, the shorter planning horizon in the OP entails a lack of information on future events and the associated restricted planning scope implies a cost increase. Even when assuming perfect predictions, the cost increase due to the incomplete consideration of future events can not be compensated by the MPC. Nevertheless, the operational and financial impacts can be significantly mitigated by employing longer planning horizons, which facilitate a more effective anticipation and adaptation to potential deviations from forecasts. However, besides the operational advantages, it is important to note that the 36/45 setting entails a doubling of the computational effort required. Conclusively, the following main findings can be stated:

- A longer OP prediction horizon may achieve a more efficient operation due to a more complete consideration of future events. At least with a prediction horizon of 12 hours, the potential of forecasting can only be insufficiently utilized
- With imperfect prediction, it is especially sufficient to use a longer prediction horizon in both, OP and MPC. Thereby, imperfect forecasts can be compensated with an almost negligible increase in costs of 3.5 percent.
- At perfect prediction, the shorter prediction horizon of 15min in the MPC is a suitable choice.
- Especially at perfect forecast, the costs of OP predictions tend to be overly ambitious compared to the realized operations.

Emphasizing on the importance of optimization parameters in enhancing operational performance, the assements particularly demonstrates the compensating for prediction errors by using longer prediction periods.

Implications on Power Consumption Patterns Given that energy procurement from the power grid constitutes the most significant portion of energy costs and is susceptible to high price fluctuations, the analysis will specifically examine the effects of prediction inaccuracies on electricity purchase patterns. In contrast to the previous comprehensive perspective, this detailed observation exclusively concentrates on one specific optimization variable. The following graphs in Figure 5.43 and Figure 5.44 compare the power purchase curves in the case of perfect prediction with those where prediction errors were assumed, respectively for the two optimization settings 36/45 and 12/15. On a qualitative level, in both cases, largely consistent trends between the two curves are recognizable most of the time. However, also significant deviations can be observed at certain times, emphasizing the suboptimal power purchasing induced by imperfect forecasts.

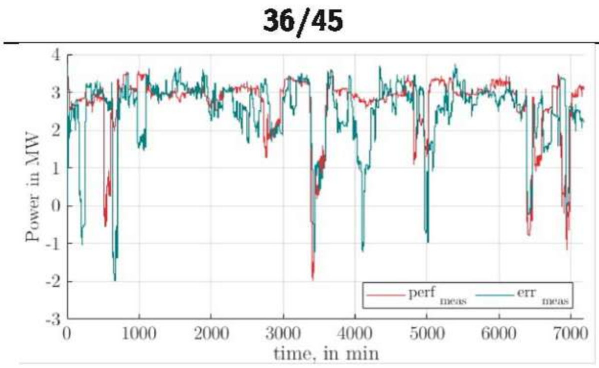


Figure 5.43: Comparison of power purchase patterns with perfect and inaccurate prediction for the 36/45 setting

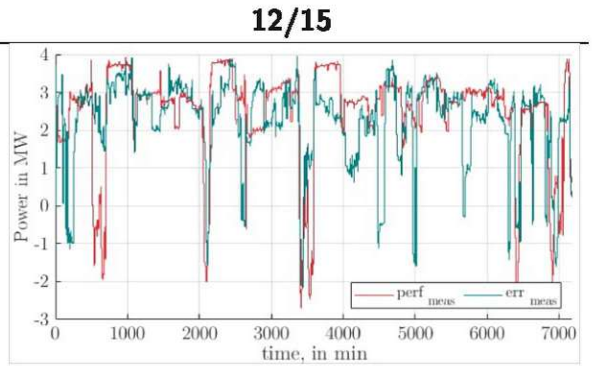


Figure 5.44: Comparison of power purchase patterns with perfect and inaccurate prediction for the 12/15 setting

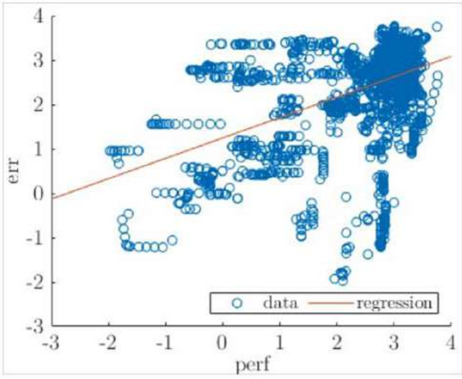


Figure 5.45: Scatter plot for the evaluation of the correlation between the two progressions of the 36/45 setting.

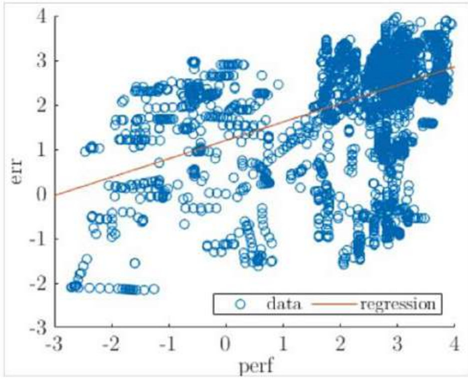


Figure 5.46: Scatter plot for the evaluation of the correlation between the two progressions of the 12/15 setting.

Comparing these deviations, larger discrepancies are observed for the shorter prediction horizons in Figure 5.44. Additionally, the scatter plots shown in Figure 5.48 and Figure 5.49 offer a quantitative assessment of the correlation between the two curves to underline the observed impressions. Exhibiting a coefficient of determination of R^2=0.33 and a standard deviation of σ=0.89, in comparison to R^2=0.23 and σ=1,2755, a stronger correlation can be attributed to the scenario with longer prediction times.

At this point, it is important to repeat that variations in operating costs do not solely arise on the purchase of electricity, but are rather distributed over various substitutive energy sources as shown in Figure 5.56. However, especially for the RES, electricity constitutes the primary energy source and, additionally, exhibits the most significant price variations. Consequently, the electricity purchasing strategy is crucial to minimize operational costs.

Assessment of Compliance Capabilities to Power Purchase Schedules Initially, referring to the preceding comparison, it is crucial to emphasize that decisions on electricity purchase could selectively be made according to internal preferences primarily reflecting the minimization of energy costs, without any external restrictions. However, for the safe operation of power and energy transmission networks, the ability to precisely and accurately comply with specific predefined procurement schedules may represent an essential requirement for large-scale consumers such as industrial plants in the future. With special regard to balancing and congestion management in power grids, this vital feature will be further examined in the following analysis. Transmission grids already represent crucial technical bottlenecks in the energy system. Particularly given the challenges discussed in the introduction, with further increases in fluctuating, decentrally distributed power feed-in, this will require even more precise planning of transmission capacities in the future. For large consumers such as industrial companies, this means that they may have to announce and adhere to their planned electricity procurement schedules for a certain period of time in advance in order not to jeopardize the security of electricity supply. This is an enormous challenge, especially when taking into account complex, multifaceted energy systems, which is de-facto impossible without holistic control. The capabilities and advantages of holistic energy management and control systems are particularly evident when it comes to such requirements.

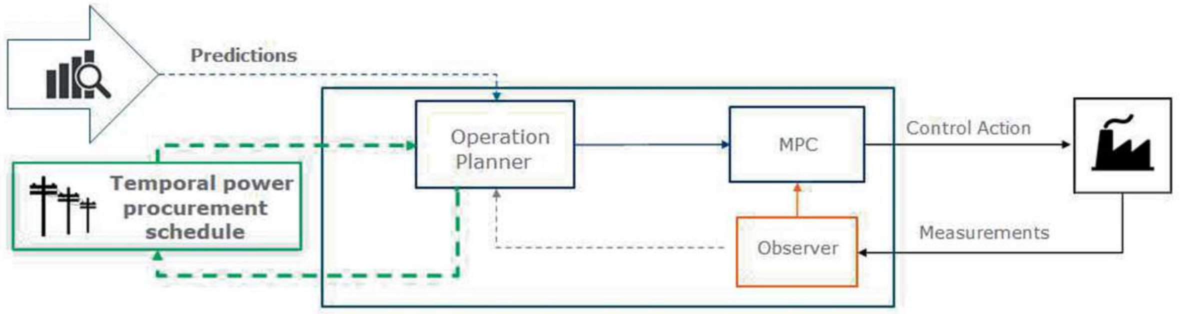


Figure 5.47: EMCS interaction with the grid operator to ensure a reliable power procurement

Consequently, the following study provides insight into the performance of the EMCS for schedule compliance. Therefore, compared to the previous scenarios, the previously determined power procurement schedule is considered to be committed and thus a deviation is additionally explicitly penalized in MPC. As illustrated in Figure 5.47, the power procurement schedules are taken once (in the 36/45 scenario) or twice a day (12/15) from the most recent OP calculation, where once again imperfect forecasts are assumed. This means that they deviate from the actual optimum, but still have to be adhered to, which of course involves certain additional costs.

Figure 5.48 and Figure 5.49 demonstrate that a very accurate compliance of the projected and realized power purchases can be achieved with both prediction horizon settings. The scatter diagrams in Figure 5.50 and Figure 5.51 show a high correlation that indicates a very accurate compliance through the introduction of the respective trajectory progression in the objective function. The progressions express coefficients of determination of R^2=0.95 and R^2=0.92 as well as standard deviations of σ=0.22 and σ=0,31 for the 36/45 and the 12/15 scenario, respectively.

However, of particular interest are the corresponding plant operations shown from Figure 5.52 to Figure 5.55, which provide evidenve on the operational means by which compliance is achieved. Comparing the two scenarios, similar operational patterns can be observed as before, such as slightly more fluctuations in steam supply and increased use of CHP at shorter prediction horizons. It is to be noted that both the CHP and the gas boiler are utilized, which indicates a rather complex control task. As shown by the cost comparison in Figure 5.56, the measure of power supply compliance is related to an increase in energy costs of 10.3% (36/45) and 13.2% (12/15) compared to an unconstrained power purchase.

36/45	12/15

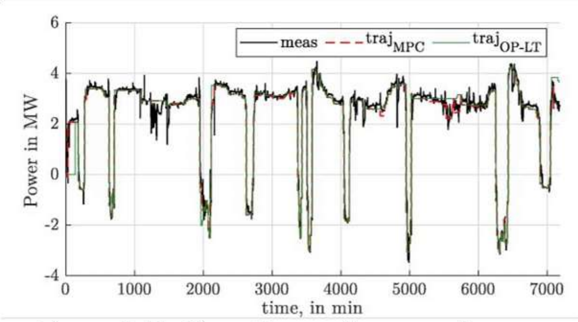


Figure 5.48: Compliance of measured power purchase with specified procurement schedules for the 36/45 scenario

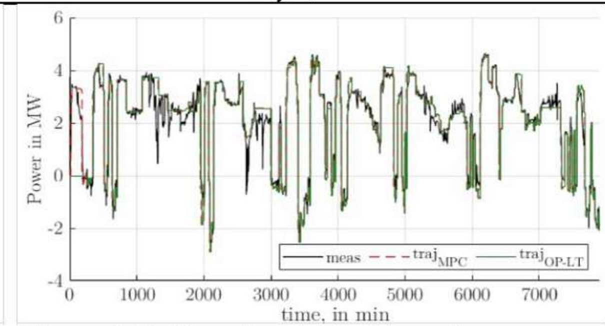


Figure 5.49: Compliance of measured power purchase with specified procurement for the 12/15 scenario

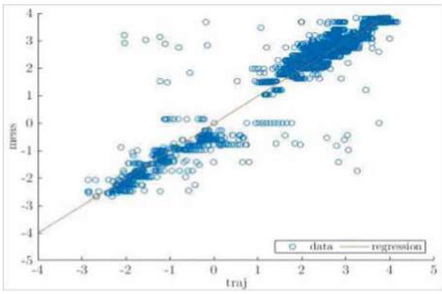


Figure 5.50: Scatter plot of the correlation between the two progressions of the 36/45 setting. (R^2=0.97, σ=0.33)

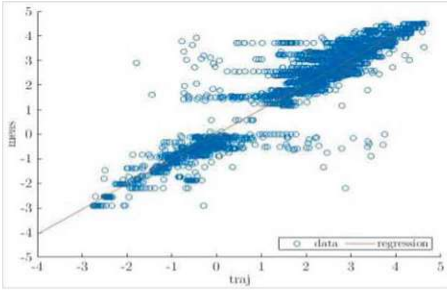


Figure 5.51: Scatter plot of the correlation between the two progressions of the 12/15 setting. R^2=0.91, σ=0.46)

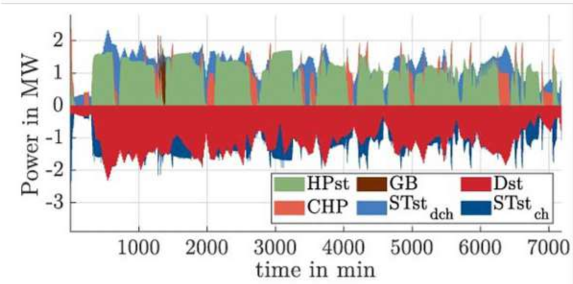


Figure 5.52: Steam balance at power schedule compliance for the 36/45 setting

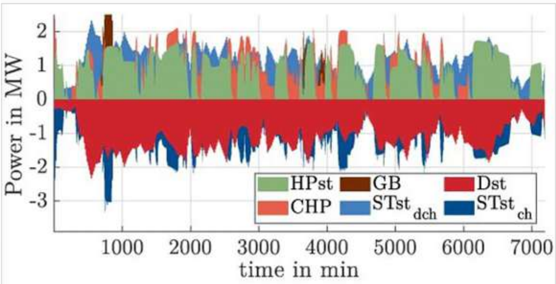


Figure 5.53: Steam balance at power schedule compliance for the 12/15 setting

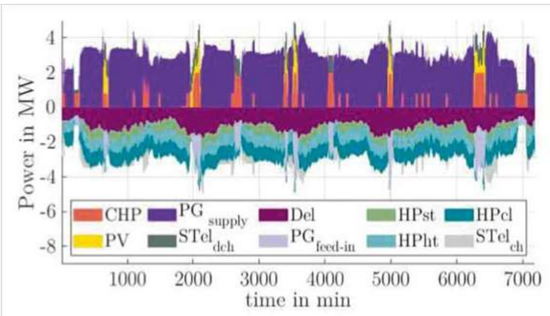


Figure 5.54: Electricity balance at power schedule compliance for the 36/45 setting

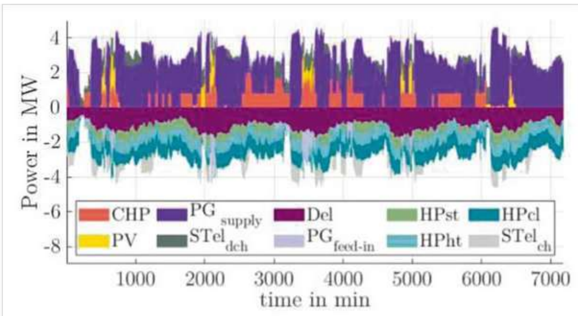


Figure 5.55: Electricity balance at power schedule compliance for the 12/15 setting

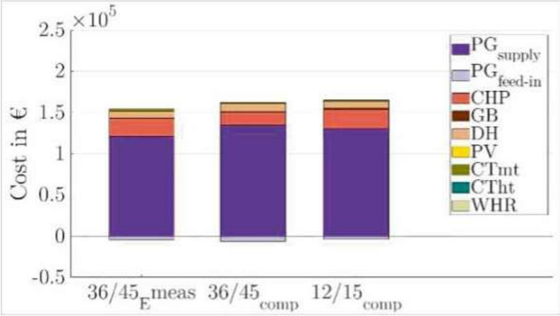


Figure 5.56: Comparison of cummulative costs at power schedule compliance

Analysis of Trajectory Progression Parameters As comprehensively explained in Chapter 3, the hierarchical optimization in the EMCS is systematically realized by specifying the optimal long-term trajectories determined by the OP, which are then complied by the MPC. While in the previous analyses, emphasis was placed on rather higher-level aspects, where this procedure was of relatively limited focus, the following analysis provides a comprehensive methodological evaluation of the specific functional principle. Particularly considering the respective methodical implementation within the MPCs objective function, the impact of using different weightings to prioritize certain units or state variables for improving overall performance will be comprehensively examined. Initially, specific practical considerations are examined to introduce the subsequent study.

Within the EMCS, the determination of the optimal operation and the corresponding trajectories is accomplished by optimization models, which are evidently subjected to certain simplifications and abstractions. Additionally, considering the inherent existence of forecast inaccuracies, the perfect realization of the desired optimal operation of one unit may inevitably result in slight deviations in the immediately connected units. Consequently, this indicates the existence of potential conflicts within trajectory tracking between generation, consumption, and interconnected storage units.

Since the continuous adjustment of control signals to optimally achieve the intended overall plant operation is the main task of the MPC, this affects the methodological challenge to reconcile conflicting criteria within its objective function (see Eq. (3.43)). To overcome this challenge, alternative methodological approaches may be pursued. The most straightforward method suggests treating all tracked variables equally. However, this strategy assumes a perfect and equitable scaling amongst all individual components and their respective contributions, which may often be challenging to achieve in practice.

Specifically, it is important to acknowledge that various units may be subjected to varying levels of modeling granularity, simplifications and abstraction. Additionally, the forecasts of vital boundary conditions can differ significantly in precision. Furthermore, as more units become involved, the problem tends to escalate in complexity. An alternative method proposes a contrary approach by treating various units with distinct, predefined priorities.

Thus, rather than attempting to resolve conflicts by thoroughly establishing equality among variables, the aim is to avert conflicting criteria through the deliberate specification of priorities or hierarchies among the units. Despite the awareness that a respective prioritization is inherently subjective to a certain extent, rational considerations may nevertheless assist in their selection. For example, addressing the pertinent factor of model accuracy, the progression of a trajectory is anticipated to be more effective when a specific model representation exhibits sufficiently high accuracy.

In the development and implementation of the EMCS in the RES, both the equal weighting and distinct priority approaches were explored, where employing distinct priorities predominantly yielded superior performance in that particular case. To provide a comprehensive insight, the subsequent study delivers a comparative analysis of both approaches, specifically assessing the impact of different weighting schemes, which are identified as vital parameters for optimizing overall performance. At this point, it is important to acknowledge that during the rigorous and extensive setup and modeling process employed for conducting these simulation studies, the settings and weightings underwent iterative empirical refinement. However, it is also essential to note that these were not optimized in a mathematical or systematic context. Thereby, the best performance was achieved (for the summer load scenario) by implementing the following component-specific considerations and the respective parameters:

- Steam Storage, Stratified Thermal Energy Storage, and Latent Energy Storage: Lower weighting of trajectory progression (factor=0.1) as the optimization models exhibit deficiencies in precisely reproducing the nonlinear dynamic behavior of its respective more advanced simulation models. Additionally, the stratified and steam storage are comprehensively interconnected to several connected supply and consumption units. Thus, high penalty (slack) costs at the lower and upper capacity limits need to be applied to avoid potential violations of the operating limits.
- As the power grid is subjected to high price fluctuations and significantly affects energy costs, the importance of the trajectory is increased by a factor of 10.
- For the cooling towers the trajectory progression is neglected as these are considered as balancing units for the low-temperature thermal management and their power demand is considerably lower compared to their heat flows.

By comparing the time courses of balance graphs according to Figure 5.57 - Figure 5.64, generally, the equal weighting scenario exhibits recurring adjustments or downshifts, which causes fluctuating progressions of the controllable units. These fluctuations can be comprehended by examining the objective function of the MPC, which is mainly composed of the trajectory tracking contributions of all components.

Equal treatment of all units	Improved setting

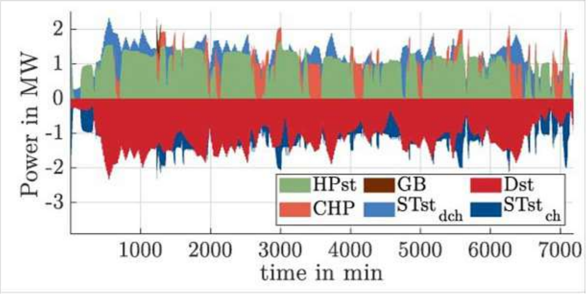


Figure 5.57: Steam Balance, equal setting

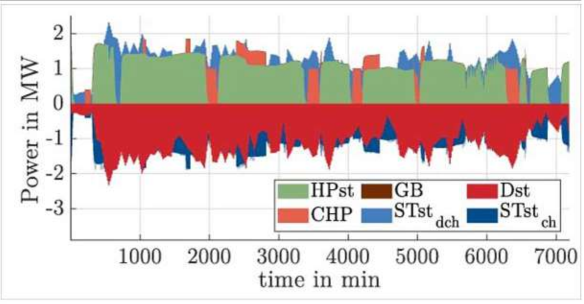


Figure 5.58: Steam Balance, improved setting

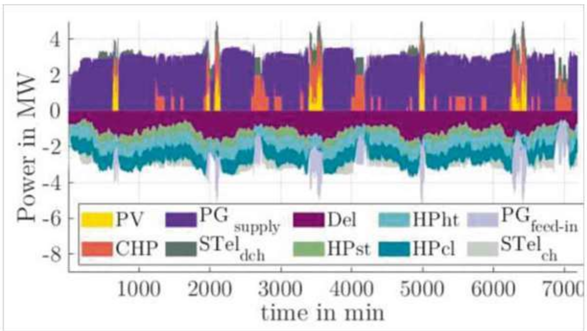


Figure 5.59: Power Balance, equal setting

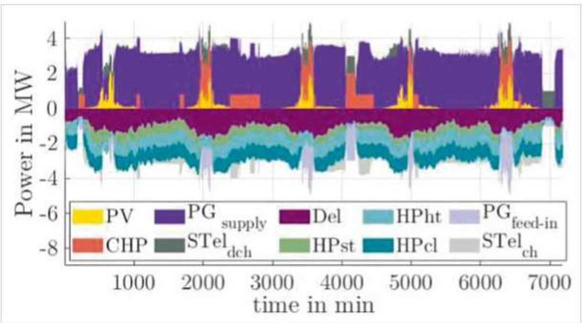


Figure 5.60: Power Balance, improved setting

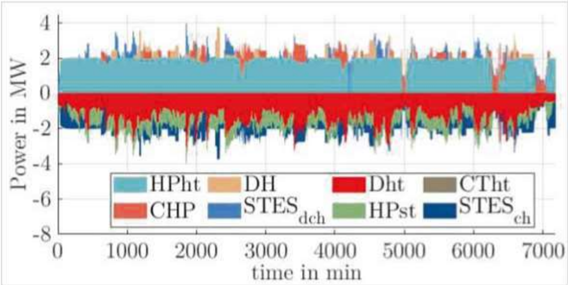


Figure 5.61: Hot Water Balance, equal

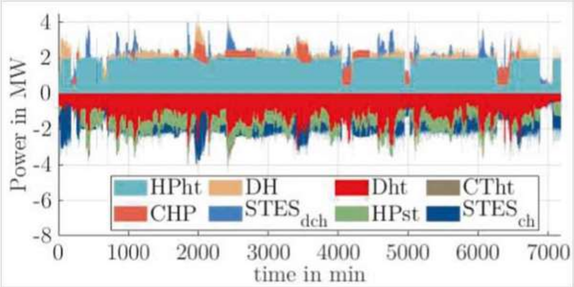


Figure 5.62: Hot Water Balance, improved

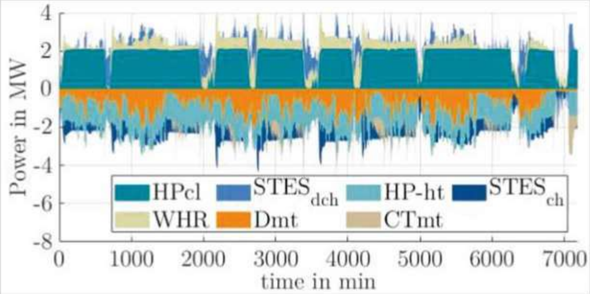


Figure 5.63: Medium-Temperature Water Balance, equal setting

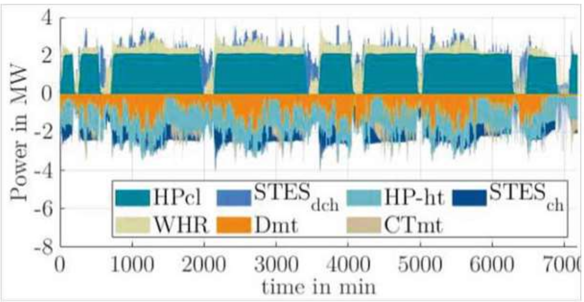


Figure 5.64: Medium-Temperature Water Balance, improved setting

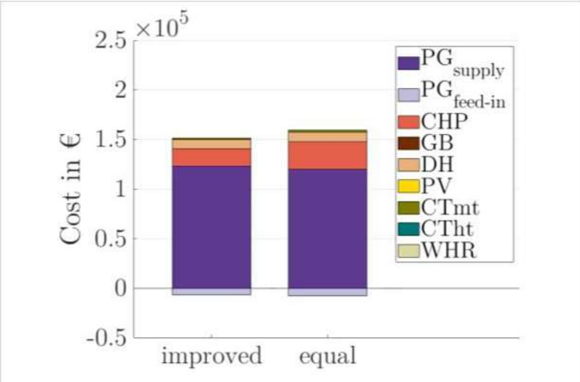


Figure 5.65: Comparison of cumulative costs

By deliberately allocating higher or lower weights, control dominance may selectively be channelized to specific variables or units, which show more substantial implications. (e.g. high costs, volatility, model accuracy, or critical boundary conditions). Thus, the focus on maintaining stability in the progression of critical variables, while avoiding the disproportionate influence of less impactful or reliable states, may lead to a more equitable and optimized operation. While so far the operational progressions of individual units have rather been evaluated as part of an energy balance than individually, a more detailed examination is presented below to further extend the previous comparison.

Initially, the graphs from Figure 5.66 to Figure 5.69 provide a detailed insight into a shorter observation period to illustrate the distinctive control behaviors in the example of two interconnected components, the high-temperature heat pump, and the steam accumulator. There, the OP trajectories are shown as red dashed lines while solid black lines represent the actual measured values.

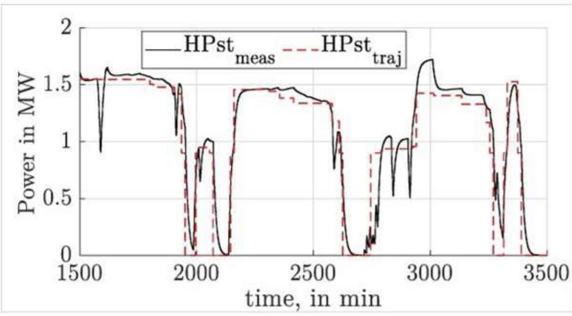


Figure 5.66: HP-ST, Equal Setting

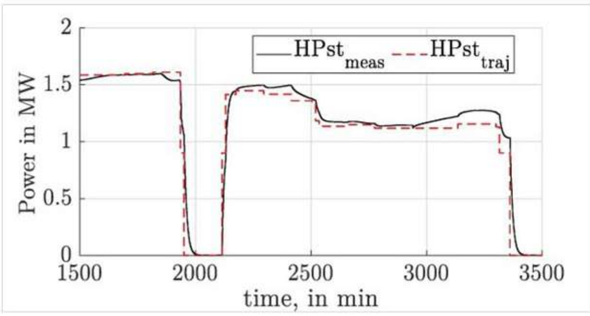


Figure 5.67: HP-ST, Improved Setting

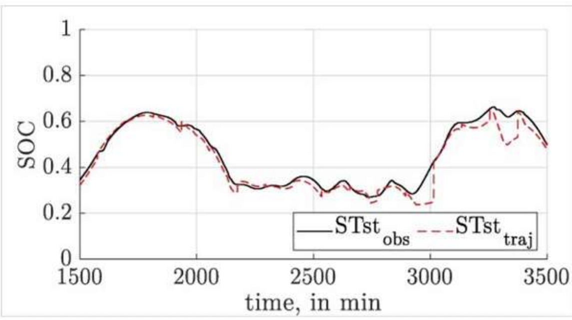


Figure 5.68: Steam Storage, Equal Setting

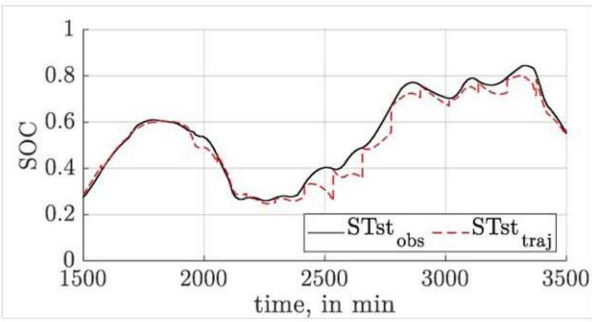


Figure 5.69: Steam Storage, Improved Setting

The equal setting strategy aims for both units to closely follow their respective trajectories, which is achieved quite well throughout long parts of the observation period. However, the heat pump repeatedly executes intermittent short-term up- and downshifts that indicate adaptation measures. Furthermore, the longer-term course also reveals occasional brief plant shutdowns and generation peaks. In contrast, the improved setting leads to a notably smoother and more continuous production curve of the heat pump indicating that its operation remains largely unaffected by deviations at the storage tank because of its elevated prioritization.

Analyzing the steam-accumulator utilization shows qualitatively similar long-term trends in both scenarios. In the equal scenario, both curves largely align, with exceptions during two brief periods where pronounced deviations and heat-pump oscillations suggest conflicting control events. In contrast, the storage in the improved setting exhibits recurring divergences between the planned trajectory and actual states indicating its lower importance. In summary, over the entire period comparatively consistent long-term trends in the storages utilization can be observed, however in the improved setting fewer adjustments of generating units produce slightly higher SOCs.

Extending the present comparison, in the following specifically the utilization of storage units is examined in more detail, particularly since they are very impractical to analyze by the frequently employed progression graphs of energy carrier balances. For better comparability, the operating diagrams show the respective SOC curves in normalized form, so that they only assume values between zero and one. Examining the operation diagrams depicted from Figure 5.70 to Figure 5.77, two predominant effects can be discerned by comparing the two scenarios. Obviously, a different trajectory progression weighting leads to certain deviating operational progressions. However, over the course of a full working week, no substantial deviations between the predicted and actual operations are evident in either scenario. Although assigning a reduced tracking priority allows larger deviations from the projected operation, these only occur in the short term which is predominantly attributable to the periodic adjustment of initial states with each periodic OP recalculation. The respective operating patterns can be observed more clearly in the progression cutouts shown in Figure 5.66 to Figure 5.69 above.

Consequently, this underscores the importance of periodic state adjustments for the avoidance of large discrepancies between predicted and realized operations. On the other hand, in all storage devices, peaks as well as qualitatively similar trends of the SOC progressions are recognized at approximately the same times, but with different pronouncements and amplitudes. This indicates that the long-term trends of charging and discharging may primarily be influenced by time-variable boundary conditions such as costs or energy demand, which are the same in both scenarios. Accordingly, the noticeable disparities may then be attributed to the different weighting approaches, which are associated with slightly different short-term executions of the long-term trends. From a methodological perspective, these observations underscore the necessity of incorporating even less accurate models for identifying long-term optimal trends. Moreover, in the short-term, the neglecting of less accurate models also reduces potential disturbances and thus facilitates more stable and reliable control actions. It needs to be emphasized, that the above analysis is not particularly restricted not to storage devices, however, they constitute the most significant devices in terms of temporal energy management, which is why the effects are most noticeable here.

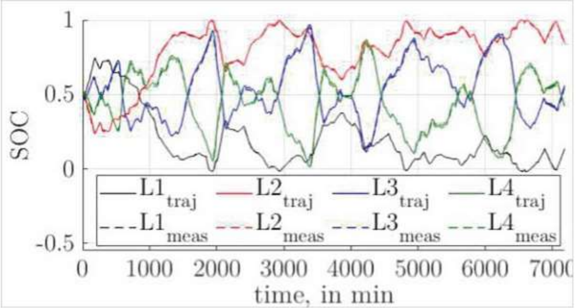


Figure 5.70: Stratified Storage SOC-curve, equal setting

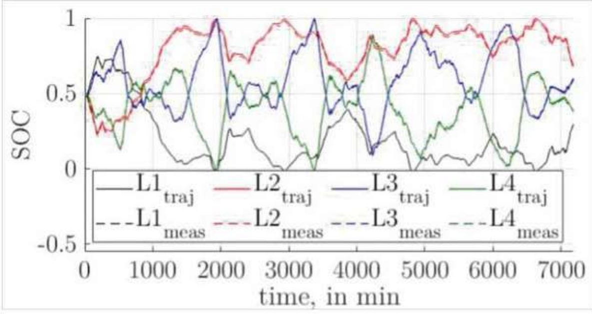


Figure 5.71: Stratified Storage SOC-curve, improved setting

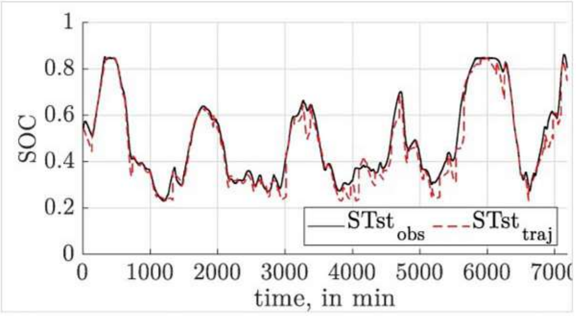


Figure 5.72: Steam Storage SOC-curve, equal setting

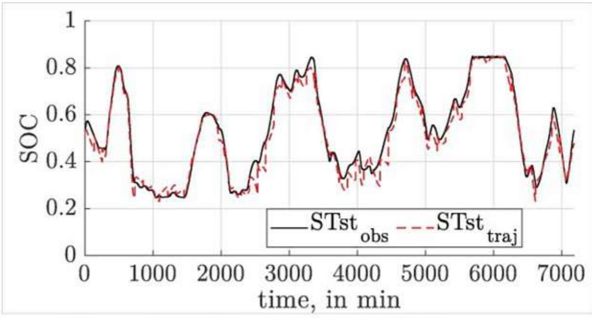


Figure 5.73: Steam Storage SOC-curve, improved setting

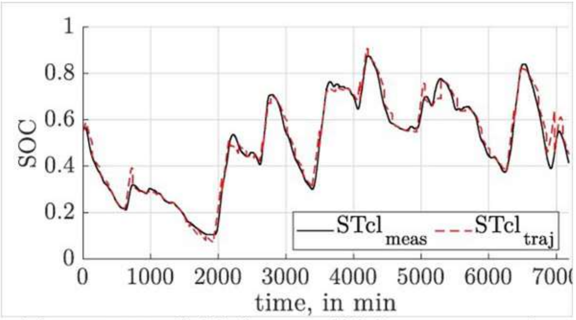


Figure 5.74: Cold Storage SOC-curve, equal setting

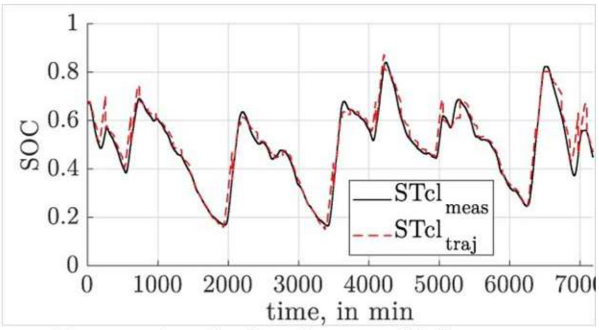


Figure 5.75: Cooling Storage SOC-curve, improved setting

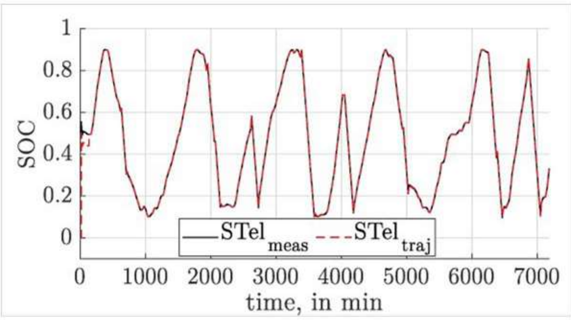


Figure 5.76: Electrical Energy Storage SOC-curve, equal setting

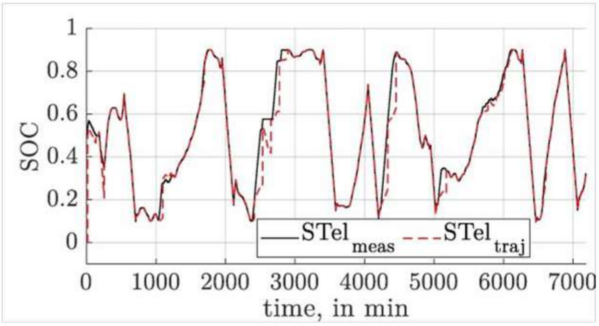


Figure 5.77: Electrical Energy Storage SOC-curve, improved setting

Selectively investigating the progressions of the different storage units, the most pronounced deviations between the OP trajectory and measured operation are observed at the steam storage (STst). The latent energy storage (STcl), shows a similar behavior, however, less frequent and pronounced. These insights reveal that the respective MILP-based optimization models fall short of accurately representing the specific nonlinear behavior to the same extent as the simulation model. On the other hand, less pronounced discrepancies are recognized for the stratified storage (STst) and the battery (STel), which indicates a better alignment of the models.

This comparative analysis provides a comprehensive and detailed insight into the functioning of trajectory progression and underscores the importance of methodological parameters. Moreover, it outlines that strategic fine-tuning enables to further exploit the improvement potentials of hierarchical optimization systems. In this respect, Fonseca et al. [134] emphasize the potentially effortful experimental parameter estimation by experts which reveals the importance of strategic rules to facilitate this task. Therefore, these specific observations together with the fundamental considerations offer general conclusions regarding the appropriate choice of weighting strategies and the determination of decisive parameters. However, these may be strongly related to the respective use cases, which may vary substantially among real industrial processes. Despite the aspiration for leaner and less elaborate implementation in real-world environments, however, this study also reveals challenges indicating additional implementation effort.

Comparison of a Single-Layer MPC vs. the Two-Layer EMCS The reasons and benefits of partitioning energy management and control tasks into multiple hierarchical levels have been previously discussed. However, these preliminary deliberations primarily centered around practical, logical, and rational considerations, with limited reference to specific examples, experiences, or information due to a scarcity of relevant literature. Consequently, the subsequent study intends to tackle this gap and compares the performance of the two-layer EMCS to a single-layer receding horizon optimizer that integrates MPC and OP.

In this context, particular emphasis is placed on the selection of the number of time steps for the single-layer MPC. As the number of variables in the respective MILP approximately grows linearly with the number of time steps, the computational time exhibits a more pronounced increase, potentially non-polynomial, as MILP problems are NP-hard in the general case. As a result, single-layer optimizers encounter a tradeoff between shorter time step lengths and longer prediction horizons. On the one hand, in order to effectively perform energy management strategies, it is imperative to establish extended prediction horizons that span longer durations. On the other hand, shorter time step lengths offer advantages for enhancing control performance. Additionally, while longer sampling times proportionally allow extended computation times and thereby enable an increase in the number of time steps, these are particularly unfavorable for mitigating the consequences of component outages and technical failures, where prompt detection and response are vital. Thoroughly reflecting on the previous consideration and placing a superordinate focus on safety, a time step length of two minutes was chosen for the single-layer MPC. Considering the excessive computational effort, the prediction horizon of 4 hours, corresponding to 120 time steps, practically represents an upper feasible limit. It needs to be emphasized, that there were instances, where the optimization problem could not attain the desired solution quality within the respective time- or iteration limits.

By comparing the respective progression graphs depicted from Figure 5.78 to Figure 5.85, clear differences in the utilization of the individual components are observed, which is especially reflected in the lower utilization of the heat pumps, and more frequent use of the CHP and heat sources such as the steam generator and district heating. Within this context, it is crucial to emphasize that the operation of heat pumps is not only influenced by time-varying power prices but also significantly impacted and potentially constrained by the utilization of connected storage systems.

Furthermore, it is evident across all units that their utilization is less uniform. Generally, a reduced time horizon might restrict the consideration of future events on current actions as well as well as the possibility to spread control actions over a longer period in a more balanced way. This may also account for the increased short-term utilization of less integrated, controllable generators. Additionally, (despite the absence of the desired trajectory) the objective function of the single-layer MPC encompasses various different terms and contributions, potentially leading to a proliferation of conflicting criteria. Moreover, in a single-layer MPC, short-term control actions also ultimately affect the medium-term optimal operation. In this sense, all units have equal weightings, allowing for the identification of similar operating and behavioral patterns as seen in the corresponding upper scenario.Therefore, longer planning periods play a pivotal role in mitigating such restrictions, which are of particular relevance for enhancing the overall utilization of heat pumps. Apart from operational deficiencies, which are related to a cost increase of 14.8%, the single-layer MPC necessitates more than three times the computation time compared to the EMCS in the 36/45 scenario, and roughly six times compared to the 12/45 scenario.

Single Layer MPC | **Two-Layer EMCS**

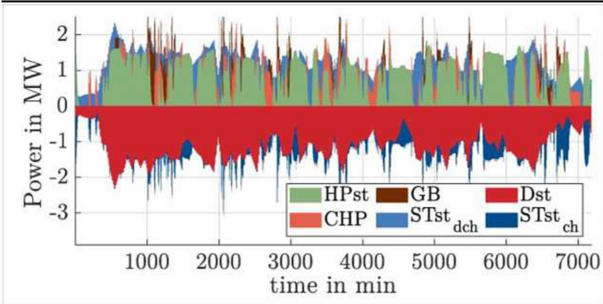


Figure 5.78: Steam Balance - Single MPC

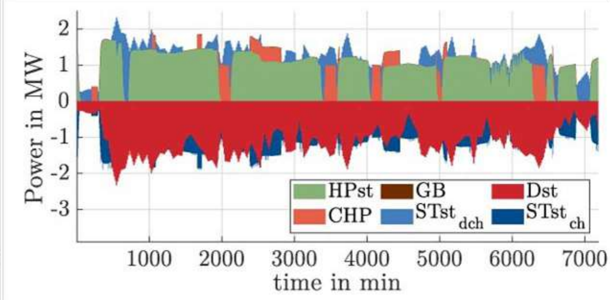


Figure 5.79: Steam Balance - EMCS

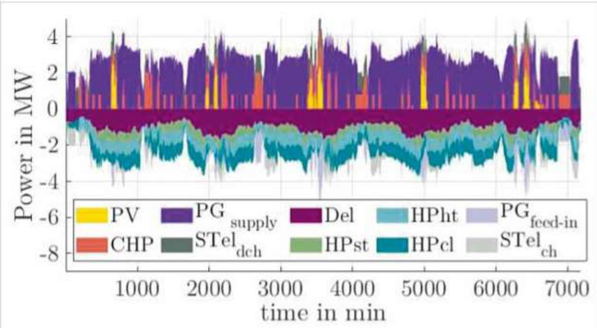


Figure 5.80: Power Balance - Single MPC

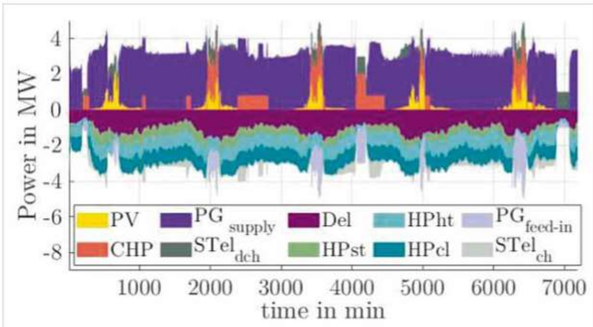


Figure 5.81: Power Balance - EMCS

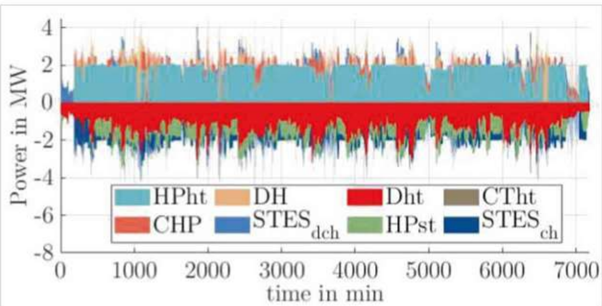


Figure 5.82: Hot-Water Balance - Single MPC

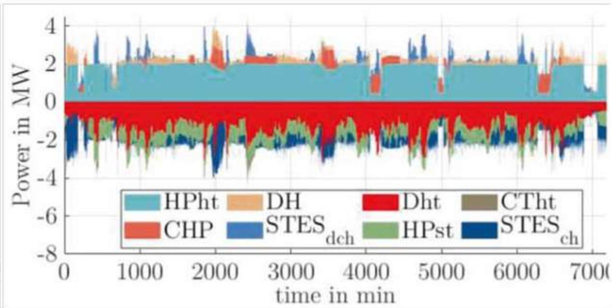


Figure 5.83: Hot-Water Balance - EMCS

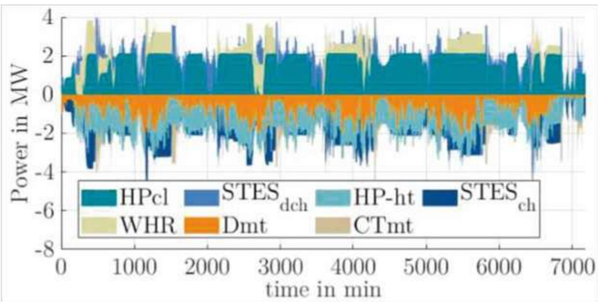


Figure 5.84: Medium Temperature Water Balance - Single MPC

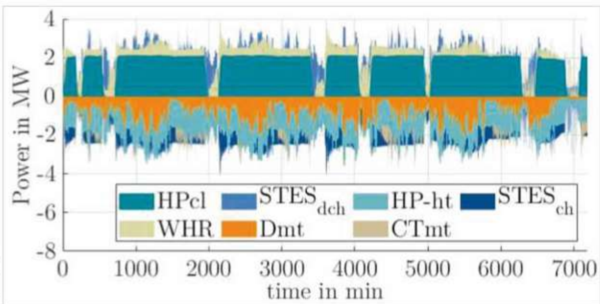


Figure 5.85: Medium Temperature Water Balance - EMCS

5.2.3 Environmental Aspects and Sustainability

In the previous analyses, the principle of cost minimization was utilized as the overarching objective, as operational decisions and energy management strategies within industrial enterprises primarily pursue business interests according to the prevailing market-economic conditions. However, especially aiming toward sustainable development, it is imperative to shift the focus from a purely individualistic micro-economic perspective to a holistic societal context that encompasses the broader implications of the comprehensive biospheric environment. In this concern, environmental pollution needs to be deemed of at least equal importance as economic welfare. Particularly, in the introduction the decarbonization of industrial energy supply has been emphasized as a central motivation for this work, serving as a crucial measure in mitigating climate change. Thus, potential opportunities and benefits provided by the EMCS are finally examined from an environmental perspective focusing on CO_2 emissions. Therefore, the minimum emission operation scenario for both RES and CRES configurations are introduced as central references for comparison and evaluation. The main aim of comparing economic and environmental perspectives is to identify particular discrepancies and linkages indicating the accounting of environmental factors within economic frameworks and the corresponding influence of technology. At this point, it should be recalled that a CO_2 price of 50 €/tCO_2 in the form of a tax was already assumed in the economic studies. For conciseness, the subsequent comparison concentrates on power and steam, representing the energy carriers with the highest exergy content and cost impacts, consequently exhibiting the most significant discrepancies.

The corresponding energy balances are illustrated from Figure 5.86 to Figure 5.93 and the cummulative cost and emissions are shown from Figure 5.94 to Figure 5.97, additionally including the conventional control scenario as reference for comparison. The two plant configurations show very different comparative patterns.

Initially, the CRES is discussed, as there are more significant differences to be observed, with one particularly noteworthy characteristic: While in the economic case, the CHP is more frequently used, the environmental operation shows a preference for the steam boiler compared to the CHP. Despite the CHP's characteristic to utilize waste heat from electricity generation, resulting in enhanced overall efficiency, the cumulative emissions turn out to be higher due to the comparatively lower emissions associated with grid-based electricity coupled with district heating and gas-based steam generation. This can be observed by comparing the differently pronounced respective sections in the bar charts of Figure 5.96 and Figure 5.97. The emission minimization at the CRES results in an average carbon intensity of 125.9 gCO_2 per kWh process energy, which corresponds to emission reductions of 22 tCO_2 (-21.1%) and 31 tCO_2 (-27%) in comparison to cost minimization and conventional control, respectively. In terms of costs, this corresponds to cost increases of 35 k€ (11.5%) and 8 k€ (3.3%).

However, in contrast to these discrepancies noted for the CRES, strong operational consistency is observable for the RES, ultimately indicating the significant influence of technology for meeting environmental goals.

Emission Minimal | **Cost Minimal**

RES

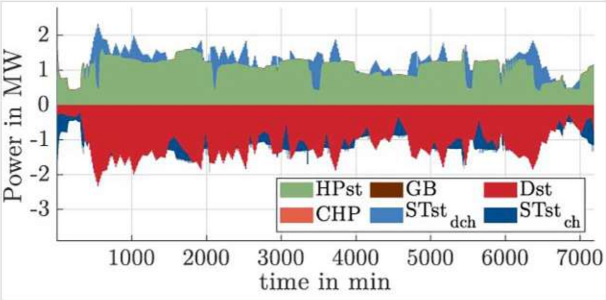


Figure 5.86: Steam Balance environmental

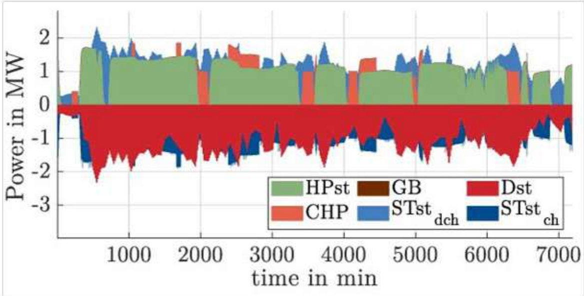


Figure 5.87: Steam Balance economical

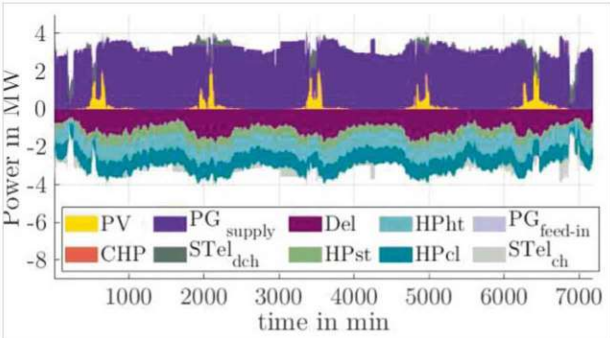


Figure 5.88: Power Balance environmental

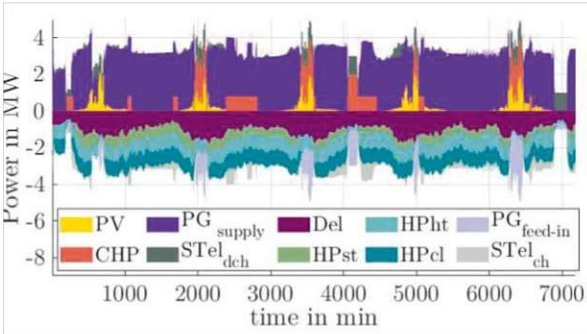


Figure 5.89: Power Balance economical

CRES

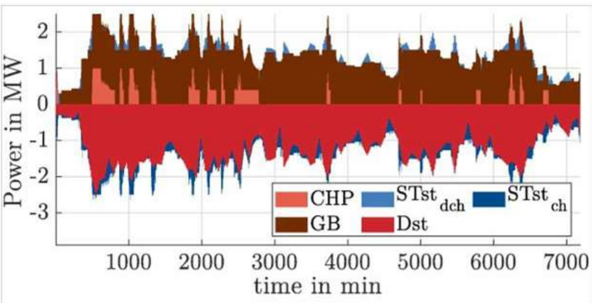


Figure 5.90: Steam Balance environmental

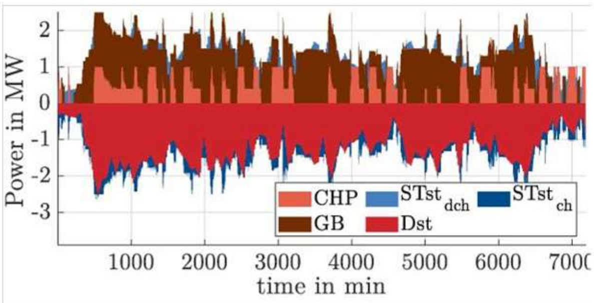


Figure 5.91: Steam Balance economical

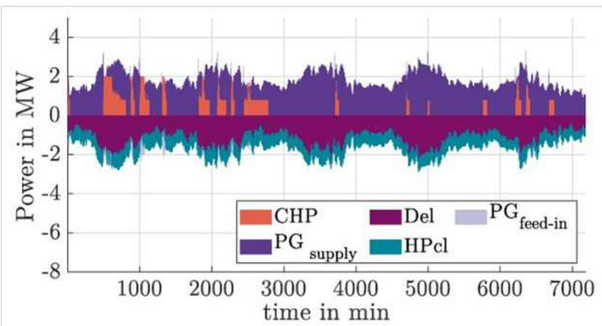


Figure 5.92: Power Balance environmental

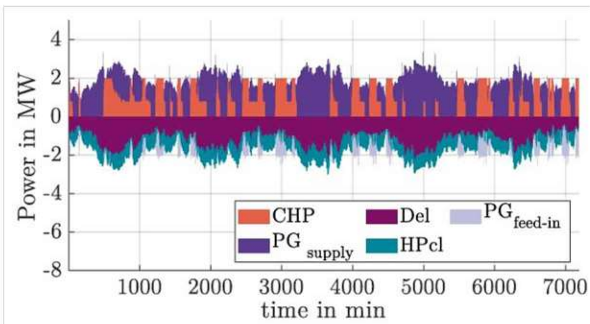


Figure 5.93: Power Balance economical

RES | **CRES**

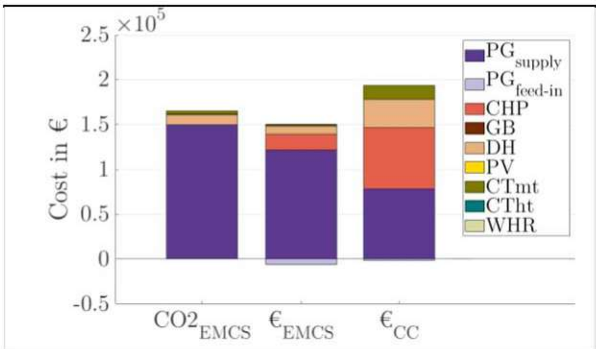


Figure 5.94: RES - cost comparison

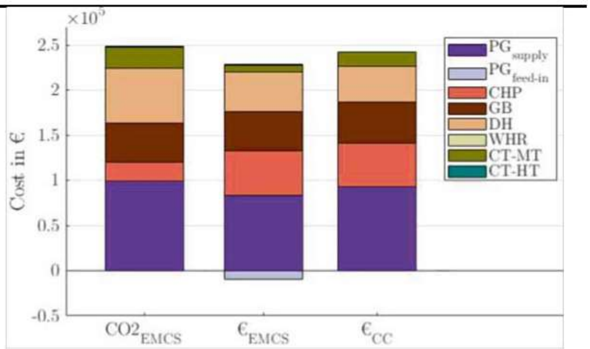


Figure 5.95: CRES - cost comparison

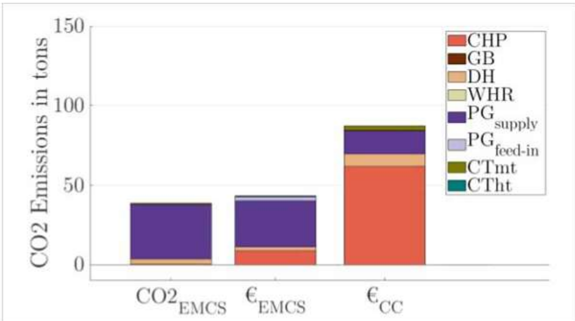


Figure 5.96: RES - emission comparison

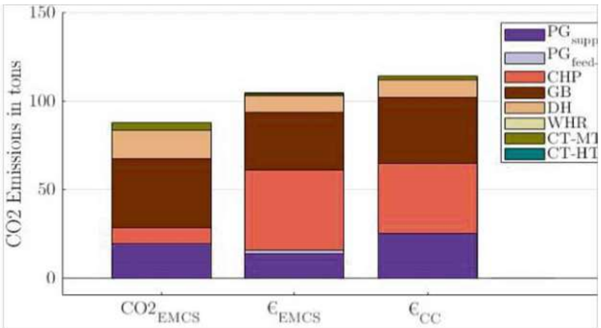


Figure 5.97: CRES - emissions comparison

Compared to the economic optimal operation, emission minimization at the RES results in a comparatively low emission reduction of 1.2 tCO_2 (2,8%) due to the already very low average carbon intensity, which finally amounts to 62.1 gCO_2 per kWh process energy, accompanied by a cost increase of 11.9 k€ (7.8%). By relating the emission savings of the minimum emission operation to the associated cost increases, an insight into the marginal costs of the respective operational emissions savings can be provided. Due to the already very low emission level, these are much higher at the RES accounting for 9916.7 €/tCO_2 compared to 1346.3 €/tCO_2 at the CRES. Most notably at the RES, the emission minimal scenario prominently entirely excludes the use of fossil-based technologies and the remaining emissions are exclusively attributable to the grid-based power.

The implementation of the EMCS to the RES demonstrates that through the utilization of appropriate technologies, ecological and economic aspects may closely align, which is in accordance with the principle of sustainability. Above all, however, it is emphasized that the substantial performance improvement of the RES compared to the CRES is not solely attributable to the technological design but, on the contrary, enabled by the operation through the EMCS. This becomes evident in comparison with conventional control, which is associated with more than twice as high emissions, according to Figure 5.96 and Figure 5.97. In this context, the EMCS needs to be regarded as assistive technology as it rather represents a digital tool than an energy component. As previously mentioned, by this comparison the impact of technology on sustainability advancements is effectively highlighted and exemplified.

It should be noted, however, that this comparison is limited to operational capabilities due to fixed system configurations, and therefore only evaluates current operational options rather than providing a comprehensive analysis of CO2 reduction potential. Such a comprehensive assessment requires the consideration of multiple aspects at different levels, including investment opportunities, the evaluation of various suitable technologies (both hardware and software), environmental factors, economic frameworks, and the enterpreneural business perspective (e.g., accounting periods for capital expenditures). In this respect, reference is made to the design optimization for the RES configuration in Chapter 4, which provides a more comprehensive long-term assessment indicating significantly higher emissions reductions of mor than 17%.

5.3 Concluding Remarks on Performance Evaluation

At this point, it is worth referencing to the challenges in assessing savings potential of a holistic optimal control, which was outlined at the beginning of this chapter and the step-by-step approach to address these implications. While the initial baseline scenarios provided information on general performance improvements, the numerous further studies not only substantiate these high-level results, but also provide a much more comprehensive insight into the functionality and showcase new capabilities associated with an EMCS application in a broader operational environment. The variety of different aspects and methodological characteristics also show what the individual capabilitites are based on and what mututal influences need to be taken into account that are not immediately apparent.

Every success is the mother of countless others.

HERNY FORD

6 Conclusion and Outlook

Synthesizing the central findings acquired through the presented methodology, conclusively a coherent overview of the research work and its principal discoveries is provided, specifically reflecting the primary research questions and their implications for the broader scientific context. Accordingly, the conclusion first discusses methodological aspects to gradually focus on the thematic implications gained through the respective use case. In addition, potential methodical improvements, adaptions, and extensions, as well as other new opportunities created by these contributions for further advancing the topic, will be addressed.

6.1 Conclusion

6.1.1 Methodical

Emphasizing the holistic treatment of energy systems, the novel optimization superstructure for the generic definition of plant-wide optimization problems, presented in Chapter 3, represents the central methodological element of the research work. It was developed with a special focus on generic applicability while at the same time enabling intuitive, streamlined, and user-friendly modeling and implementation. This is accomplished through the utilization of components, distribution networks, and ports as a selective set of standardized modeling objects. Thereby specific plant-wide properties, such as energy carriers or objective criteria, are defined globally at the superstructure level, while process-related properties and technical data are specified at the individual component models. Standardized ports serve interfaces to ensure a consistent and mutual inheritance of specifications. Moreover by employing integrated generic functions a direct and seamless formulation of optimization problems is facilitated, which is especially advantageous as energy systems become more complex. The development and structural arrangement were significantly enhanced by the expertise of technology partners and practical experience gained during the laboratory implementation in the collaborative research project. Especially regarding the desired application of complex versatile energy systems, the formulation as MILP ensures efficient and reliable solvability while requiring comparatively little computational resources. Therefore, the following main assumptions were adopted for establishing linear models: Dynamic behavior, inertial effects, and spatial dimensions are neglected in networks where consequently only constant thermodynamic states are assumed. Consequently, energy conversions and storage can only occur within components.

The EMCS framework for simultaneous online operational optimization and control, which performs a two-stage hierarchical optimization, represents a deliberate extension of the superstructure and the ultimate novelty of the work. Advantageously, it therefore inherits all the modeling properties of the superstructure. The functional division of long-term energy management and short-term control to separate optimization levels is particularly advantageous since the subproblems are to be solved on different time scales. Thereby the coupling of both levels is established in a soft-constrained manner by trajectory tracking of selected state variables, realized within the objective function at the short-term control level. Consequently, the different levels use the same or very similar plant models; however, the composition of the objective function differs significantly. The generic streamlined modeling through the superstructure is intended to minimize implementation effort thus providing a decisive advantage compared to the state of the art. Its primary objective is to enable seamless integration while ensuring compatibility for the implementation in real-world technical facilities. Therefore, adopting first-principle component modeling proved beneficial particularly for appropriately representing the state variables of the real components to the models. This serves as a central foundation for enabling a continuous reconciliation and ensuring a synchronized control performance when used as an online energy management system. Additionally, the use of theoretical modeling enables low parameterization effort with significant data to be obtained from technical data sheets and descriptions.

However, beyond these key features, as shown by the case study, the significant impact of methodological parameters on functional performance is recognized, which is an essential issue in terms of implementation effort. Most notably, the specification of weightings in trajectory tracking is crucial to avoid or resolve potentially conflicting criteria. In this regard, two approaches are discussed and experimentally compared, with a particularly focus on model accuracy, operational limitations, and costs, in order to derive reasonable weighting strategies. However, a comprehensive performance investigation of weighting concepts in a systematic and consistent manner was beyond the scope of this work. Referring to the desired features of easy and streamlined applicability in real environments, these cannot directly be demonstrated with this work. However, the ideas and logic of the approach enable to present the entire optimization problem in a clear and structured manner as presented in Figure 3.7 and Figure 4.16 thus offering a comprehensible and convincing indication.

Concerning the central methodological goal of broad applicability, the two use cases provide evidence of the beneficial use of the optimization framework at different organizational levels of energy management. While the application of the optimization framework within EMCS demonstrates its particular suitability for multi-level optimization of complex multi-energy systems, the basic assumptions and simplifications may be less appropriate for other types of problems and issues. For instance, at its current stage of development, the approach is less suitable for typical synthesis problems or detailed process-specific issues, which is mainly attributable to the adopted assumptions for linearization. However, the basic framework has the potential to be conveniently modified, enhanced, or methodically integrated by implementing component-based extensions or interfaces. Since expanding the performance demonstration to multiple plants is not feasible within the scope of this dissertation, the use case was designed in a more general and comprehensive way. It includes the characteristics of three real industrial plants in conjunction with a review of current conventional system design and prospective technological advancements. Thus, a broader perspective could be obtained to derive more generalizable insights, especially relevant to the particular subsector.

6.1.2 Thematic

In the transition to a sustainable energy supply facilitating the use of renewable sources, industrial enterprises operate in a diverse, multi-faceted and dynamic landscape, influenced by environmental, economic, technological, and regulatory conditions. The associated interdependencies introduce complexities and uncertainties, particularly effecting long-term decision-making, and thus hinder or decelerate systemic changes. In this regard, this dissertation utilizes an integrative, stepwise approach based on two complementary use cases to comprehensively assess the potential for energy savings and operational improvements at various decision-making levels.

In the first use case, aimed to demonstrate the application on a design optimization, the developed framework was utilized for the optimal integration of sustainable technologies into existing systems, thereby displaying the corresponding financial implications and reductions in carbon dioxide emissions. The approach stands out from common single-perspective design optimizations by extensively analyzing various scenarios to investigate the impact of different operational objectives, economic perspectives, and, most importantly, control concepts on optimal design. For this particular unique scenario, a conventional two-point plant control is incorporated into the model, what is often overlooked in design optimizations that implicitly assume optimal plant control. Since such operational practices are not yet standard in real industrial facilities, it follows from this assumption that the theoretically determined optimal design is inherently suboptimal under real-world conditions. For this specific use case, adopting conventional control results in consistently smaller generation units and larger storages, resulting in a more than 20% more expensive energy supply. In comparison to the conventionally controlled state-of-the-art system, the selective set of technological investments under optimal control enables a remarkable cost reduction of almost 30% and an impressive emission reduction exceeding 60%, thus significantly transitioning to sustainable energy sources. Furthermore, the analysis also addressed the common practice of considering short depreciation periods as the economic framework for new investments, consequently resulting in smaller component design and more than 10% higher annual operational energy costs. On pure economic optimization, the contribution of on-site fossil generation to the overall energy production is observed to be less than 5%. However, the environmental optimal configuration, completely eliminating on-site fossil generation would be associated with an increase of 20.7% in annualized energy costs. Focusing on energy technologies, the study highlights the importance of heat pumps as a substitute for controllable conventional fossil heat supply. However, the investigation also clearly indicates that their full CO_2-reduction potential can only be fully exploited in combination with storage systems and, in particular, with optimal control. Consequently, the design optimization essentially underscores the importance of holistic energy management and control revealing its long-term implications and potential for substantial savings.

Therefore, to advance the investigation on this issue, the optimization framework was subsequently incorporated into a two-layered optimization framework to provide a novel real-time capable energy management and control system (EMCS). The development of this viable tool can be regarded as the ultimate novelty of this work, with the intention of facilitating an efficient implementation in real industrial environments, leveraging the distinctive characteristics of the optimization framework. Hence, the respective second case-study presented in Chapter 5, conducts an extensive performance evaluation based on the energy system previously designed in Chapter 4. This evaluation encompassed not only the determination of overall savings potentials achieved through its application, but also an analysis of the systems capabilities on handling of forecast errors, the accuracy of planning, and the impact of crucial methodological parameters on its performance. Among the different seasonal scenarios, noteworthy cost savings, varying between 15% and 22% for the RES and 4% to 11% for the conventional system, were identified compared to the conventional control approach. Additionally, the emission savings achieved by the RES exhibit even more significant reductions, ranging between 40% and 50% across the seasonal scenarios. Referring to the assumption of optimal control in the design use case, this more detailed analysis reveals savings of a comparable range on the high-level perspective, however marginally lower. This comparison indicates that the control concept can almost exhaust the theoretical potential of the design optimization. In a more in-depth evaluation, the functional performance in the existence of forecast inaccuracies is comprehensively analyzed. While such inaccuracies are inherently associated with rising costs, however, these can be kept very low with an increase of less than 4% for the respective error scenario. Furthermore, when compared to a single-layer MPC, the two-layer EMCS operates with a notable reduction of 14.8% in energy costs. Focusing on the environmental perspective, the utilization of fossil fuels is very limited, accounting for less than 5% in energy use. Moreover employing emission minimization to the objective function, it could be demonstrated that the EMCS also enables to completely avoid on-site fossil energy use when applied to the RES, with the remaining CO_2 emissions solely attributable to the energy mix of the electricity supply. However, emission minimization is related to an increase in operational costs of 9%. Hence, when evaluating the operating costs in relation to the reduction of CO_2 emissions, this particular example clearly illustrates the trend of increasing marginal costs for CO_2 reduction as emission levels decrease. This observation aligns significantly with the outcomes obtained from the design optimization presented in Chapter 4. Evidently, the remaining emissions incurred to the purchased grid power largely depend on the proportion of renewable large-scale generation in the energy mix. In this context, the introduction already emphasized the necessity of increasing flexible consumption for facilitating a high share of fluctuating feed-in from renewable sources such as wind and PV. Hence, in particular, EMCS-operated energy systems may also contribute to further emission reductions, achievable through controlled and coordinated flexible consumption. In this context, the compliance to previously projected power purchase schedules was examined, demonstrating that these schedules could be realized precisely, expressing a coefficient of determination of 97%.

Emphasizing the higher-level comparison of the two plant configurations and control concepts it becomes clear, that the benefits of new technologies facilitating the use of sustainable energy sources become fully exploitable only through the application of the EMCS, indicating the importance of operations and control. In contrast, the improvement potentials at conventional design is considerably lower. Thus, for low to medium-temperature processes, a significant potential reduction in emissions of up to 60% compared to the current industrial state-of-the-art is revealed, which can be exploited by industrial companies through the adoption of currently available technologies. With respect to achieving the ambitious climate targets, this work demonstrates that major steps toward sustainability are already achievable through the use of available technologies, which become increasingly efficient the more these are combined.

6.2 Outlook

In its scope, this dissertation conducts a comprehensive and stepwise study investigating and demonstrating decarbonization measures and efficiency improvements in industrial enterprises. While substantial benefits and potential for improvement have been derived and exemplified by the presented approach, the full extent of its capabilities was only partially exploitable within the scope of this study.

For the EMCS, especially extending functional capabilities and features to enhance reliability and operational safety is crucial to effectively handle real-world application challenges. Foremost, this mainly involves abilities to react to unpredictable incidents such as component outages, failures in production process, or power supply blackouts. Despite of its significant importance, the management of such events strongly depends on plant- or process-specific characteristics and was recognized to be beyond the scope of this dissertation. However, developing and incorporating universal strategies to react, and manage such unforeseen events presents a highly compelling area for future research, potentially elevating the TRL of the EMCS. Regarding operational performance, the influence and performance effects of methodological and optimization parameters such as prediction horizons, sampling times or specific weightings within the objective function were investigated. Nonetheless, the respective findings rather indicate a fair potential for further enhancements and performance improvements, which are suggested to be elaborated and engineered in subsequent research.

Moreover, the diverse thematic landscape offers a variety of prospective opportunities for enhancing, incorporating, and coordinating energy management actions, potentially unlocking substantial synergies for improving the efficiency and economics of overall energy use. Respective opportunities range from long-term energy supply strategies to the coupling of consumption sectors, as well as the integral provision of system flexibilities for demand response to secure the large-scale power supply and operation of transmission grids. As depicted in Figure 6.1, the EMCS offers the capabilities to serve as central, integrated platform for the operational incorporation of diverse energy management actions. In accordance to the presented work, the EMCS combines the optimization of internal energy use with safeguarding operations by model-predictive control. On the supply side, a design optimization as presented in Chapter 4 can also be incorporated into the hierarchical optimization structure, as well as a portfolio optimization of energy purchase markets. As previously stated, providing demand response is essential for ensuring large-scale electricity supply, particularly with a high ratio of variable power producers. In this respect, the scope of action may also be expanded on the consumption side. While process scheduling was not investigated in this study, the modular structure permits a straightforward integration to leverage additional flexibilities. Furthermore, industrial companies often manage their internal logistics systems, providing a certain degree of flexibility in transport route planning. Given future transportation scenarios with significant electric and hydrogen mobility, this presents another opportunity for coupling and expansion in operational energy management. Finally, it is emphasized, that all respective subjects are presently investigated within our research unit Industrial Energy Systems, elaborating methods and solution approaches.

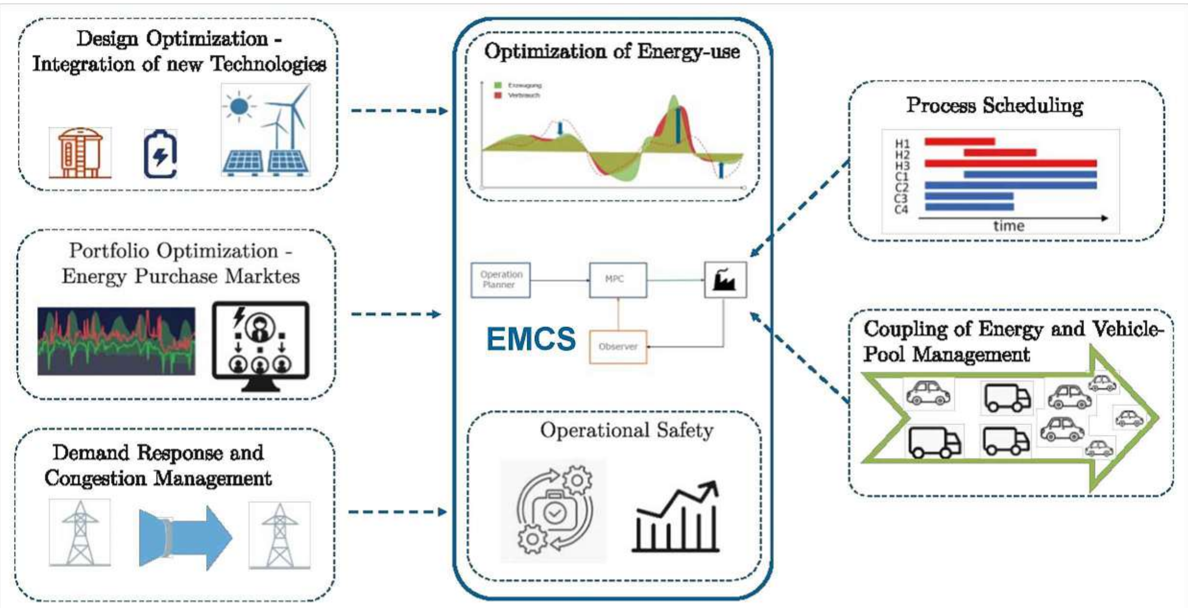


Figure 6.1: EMCS as integrated energy management platform

A. Appendix

A.1 Components Models

Since the research primarily focused on holistic, multi-component energy systems rather than on single units, the individual component models were of secondary importance to the central research objectives. However, modeling individual components is a crucial aspect of examining the research content and was a very elaborate and challenging task. Hence this section provides more comprehensive descriptions of the functional principles and modeling of the various units. Particularly, the optimization models represent key elements in the model-based optimization framework while the simulation model is crucial for the performance evaluation of the EMCS in Chapter 5. First, the operating principles and the connections of the units are introduced in order to provide a more detailed description of the optimization and simulation models. With regard to Chapter 5, the differences between the two models are of particular interest. In contrast to the optimization models, which are subjected to MILP formulations, the simulation models are designed to accurately capture components' non-linear and transient operational behavior. Thereby, it is emphasized that the primary objective was not to employ the most elaborate and detailed optimization models, but rather to demonstrate that the EMCS also has the capability to yield significant improvements even when using simplified models.

If accesible, the simulation models were validated using real operating data from the industrial plants in EDCSproof. Additionally, respective literature was consulted, which is also referenced in the following descriptions. In contrast, while the specific optimization models were parameterized with the corresponding technical data according to the first-principle approach, they were not explicitly validated with real data. However, the respective operational scenarios of the performance evaluation in Chapter 5 may also be interpreted as validation with the respective simulation models. For the determination of the thermodynamic state variables, the "coolprops" database for pure and pseudo-pure thermophysical fluid properties [135] was fundamentally adopted and incorporated in both in the simulation and optimization models. The order of description of the various components is chosen according to their importance and further use in the RES.

Heat Pump

A compression-expansion heat pump (HP), depicted in Figure A.1 converts thermal energy from a colder heat source to a warmer heat sink at the supply of electric power performing a clausius-rankine cycle. The cycle operation is driven by a mechanical compressor with the electric power supply as actuating input. As shown in Table A.1, this component comprises 4 thermal ports and one electrical ports.

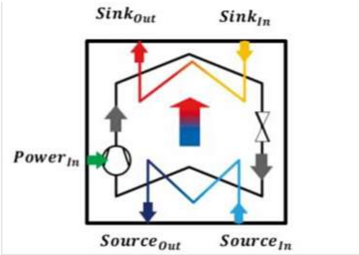


Figure A.1: Heat-Pump model

Table A.1: **Heat Pump - Optimization model overview**

	global					individual		
Ports	CS_{in}	CS_{out}	HS_{in}	HS_{out}	P_{in}	$Q_{HS,min}, Q_{HS,max}\ Q_{HS,RURD}$		
Type/Parameters	*thermal*	*thermal*	*thermal*	*thermal*	*electrical*	$\eta_{Comp}, \Delta T_{HS}, \Delta T_{CS}$		
Variables	m	m	m	m	P	Q_{CS}	Q_{HS}	U
UC Constraints							$\Gamma_L, \Gamma_R, \Gamma_S, \Gamma_T$	
Auxiliary Variables							u, v, w	

Representation in the RES The RES incorporates three different types of heat pumps in different locations. These differ in terms of thermodynamic operating conditions, generation capacities, process fluids and, consequently, different parameters of the cycle processes.

- The cooling heat pump chills a 50% water-propyleneglycol mixture from -10°C to -15°C at the cold side and provides up to 55°C on its hot side. By using the refrigerant R134a as internal process fluid, this unit reaches a COP of 3.2 at nominal power. The process characteristics are based on a real heat pump as existing in Plant B.
- The hot water heat pump supplies 90°C at the sink from a source temperature of 50°C, using the refrigerant R1234ze in the internal cycle resulting in a COP of 4 at nominal power.
- The steam generation heat-pump represent a novel technology in the RES system and exhibits an advanced two-stage cycle orientated on the configuration presented in [66] which comprises an internal HEX and an evaporation with a maximum saturated steam temperature of 165°C. At its cold side it intakes hot water of 90°C and reaches a COP of 2.6 at nominal power.

The generation capacity refers to the heat output at the hot side (heat sink) $\dot{Q}_{HS}$ representing the characteristic system state and consequently also the controlled operational decision variable.Therefore the control input $\mathbf{U}_{HP}$ is to be regarded as normalized heat generation according to Eq. (A.1).

$$\dot{Q}_{STout} = \mathbf{U}_{GB}\ \dot{Q}_{ST,max} \tag{A.1}$$

Optimization Model While the simulation models are desired to more precisely reproduce the transient system dynamics, following a detailed nonlinear first-principle approach, the linearized optimization model is based on the assumption of quasi-static-changing steady states thus representing a 1DOF system. For a detailed derivation and description of the employed optimization model please refer to Section 3.3.1. The basic optimization models for the different heat pumps are the same with each having different model parameters, process fluids, and characteristics, respectively. The application of operational limitations for changing of states (ramping gradients) as well as minimum standstill and switch-on times can be perceived from Table A.1. For the explanation of the generic creation of UC constraints please refer to Section 3.3.

The simulation models were created and provided by the EDCSproof project partner AIT as Functional-Mockup Units (FMU) originally modeled in the simulation environment Dymola[13]. The description, parameterization and validation of these FMU Simulation models, which were explicitly allowed to be used in this work, is documented in [133]. The heat pump for cooling and hot water generation assume a single-stage compression-expansion cycle as depicted in Figure A.2: Heat-Pump model illustration shown in the Modelica GUI. The heat transfer is temperature controlled by varying mass flow. The corresponding circulation pumps for the process fluids are integrated in the heat pump models including the respective PID-controlled mixing-valves.

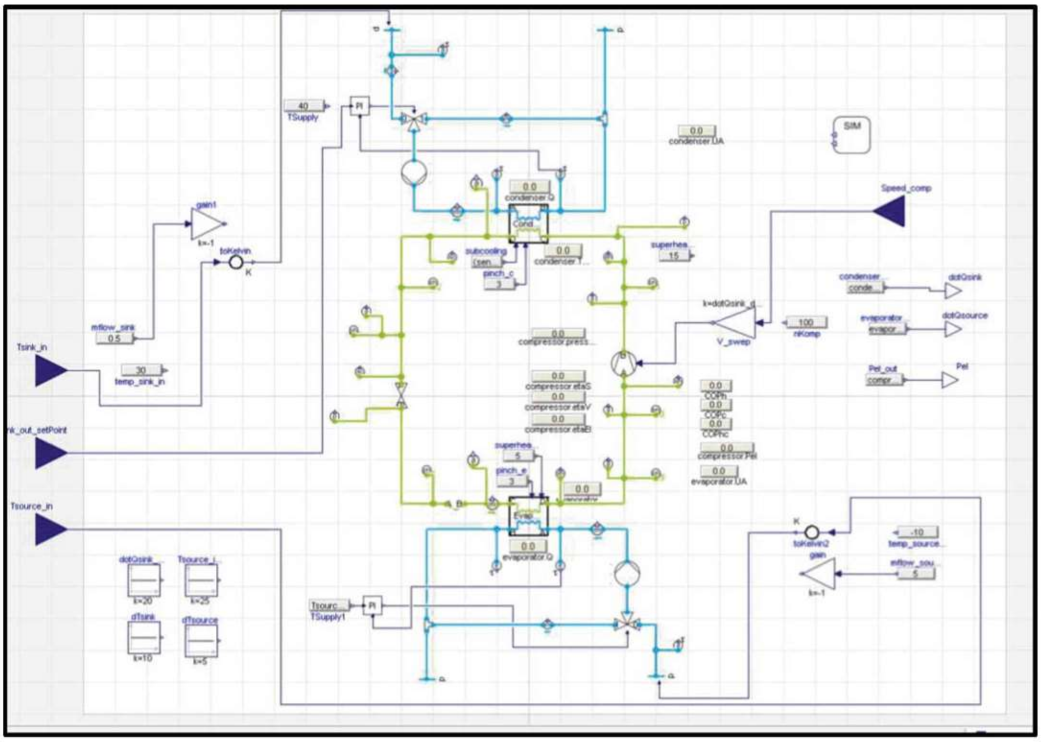


Figure A.2: Heat-Pump model illustration shown in the Modelica GUI

[13] https://www.3ds.com/products-services/catia/products/dymola/

Ruths Steam Storage Model

The Ruth steam storage is largely filled with saturated water and in the remaining space saturated steam in the remaining space at the top, as depicted in Figure A.3. If the storage is charged, the water level and pressure in the tank increase and post-condensation takes place. Conversely, the water level and pressure decrease when steam is withdrawn, and post-evaporation occurs as the heat of evaporation is extracted by the water phase. Pressure and temperature always correspond to the respective saturated state. The operation of this steam accumulator is a transient highly nonlinear thermodynamic process. As shown in Table A.2, this component comprises an input and output for steam and two additional ports for the input and output of liquid water, which regulate the filling level, if necessary.

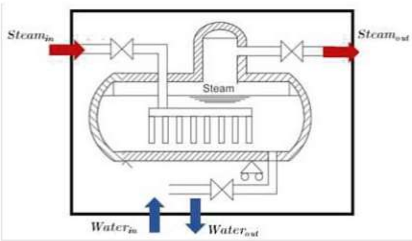


Figure A.3: Ruth Steam Storage model

Table A.2: **Steam Storage - Optimization model overview**

	global				individual	
Ports	ST_{in}	ST_{out}	LW_{in}	LW_{out}	$SOC_{min}, SOC_{max}, h_{SW}$	
Type/Parameters	*thermal*	*thermal*	*thermal*	*thermal*	$m_{SW,mas}, m_{SW,min}$	
Variables	$\dot{m}$	$\dot{m}$	$\dot{m}$	$\dot{m}$	m_{SW}	SOC
UC Constraints						Γ_L
Auxiliary Variables						u

Representation in the RES This unit appears once in the RES, however it is not existing in any of the EDCSproof original plants.

According to Eq. (A.2) the state of charge (SOC) is defined as enthalpy content above the minimum filling level of the saturated water phase $\boldsymbol{m_{SW,min}}$. This state also corresponds to the saturated water's minimum specific enthalpy $\boldsymbol{h_{SW,min}}$, temperature $\boldsymbol{t_{SW,min}}$ and pressure $\boldsymbol{p_{SW,min}}$. Thereby it is emphasized, that due to the much higher density of liquid water compared to steam and the fact that the tank is largely filled with saturated water ($\boldsymbol{m_{SW}^t}$), the heat capacity of the steam phase is neglected in the determination of the SOC.

$$\mathrm{SOC} = m_{SW}\ \boldsymbol{h_{SW}} - m_{SW,min}\, h_{SW,min} \tag{A.2}$$

In the optimization model, the storage is represented based on following simplifying assumptions in order to achieve a linear representation: The steam and water phase represent two different states, which are in direct contact within an open system. Equivalent to the SOC definition, the heat capacity of the steam phase is neglected. Likewise, a constant temperature, and consequently also a constant pressure and enthalpy are assumed. Based on these assumptions, the accumulator can be represented in a simplified way as a thermal reservoir with variable volume at constant thermodynamic properties. Thus, the basic model can be represented by the simple relationships shown by Eq. (A.3) - (A.5). Accordingly, the normalized water mass content is considered as SOC. The input and output port of liquid $\boldsymbol{LW_{in}}$ and $\boldsymbol{LW_{out}}$ are not considered in the optimization model as a constant enthalpy is assumed.

$$\boldsymbol{m_{SW}^{t+1}} - \boldsymbol{m_{SW}^{t}} = \boldsymbol{\dot{m}_{STin}^{t}} - \boldsymbol{\dot{m}_{STout}^{t}} \tag{A.3}$$

$$SOC_{min} \leq \boldsymbol{SOC} \leq SOC_{max} \tag{A.4}$$

$$\boldsymbol{SOC} = (\boldsymbol{m_{SW}} - \mathrm{m_{SW,min}})\, h_{SW} \tag{A.5}$$

In the simulation model, the transient behaviour is modeled using the approach presented in [136] with assuming equilibrium conditions for the evaporation process. The approach of Glück[14] was utilized to determine the exact size of the storage, which resulted in a tank volume of 150 m³ meters for the 4 MWh steam storage.

[14] https://berndglueck.de/waermespeicher.php

Gas-fired Steam Generator

The gas-fired Steam geneator, depicted in Figure A.4 consumes fuel, such as natural gas or biomass, and converts the chemical energy in thermal energy in the form of live steam. This unit has thermal ports for the water intake, steam output and exhaust air outlets, as well as fuel input port. According to Table A.3, this unit comprises inputs for fuel and water and outputs for exhaust gas and steam.

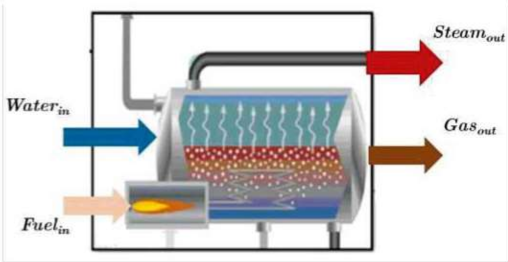


Figure A.4: Gas-fired Steam generator model

Table A.3: **Gas-fired steam generator - Optimization model overview**

	global				individual
Ports	LW_{in}	ST_{out}	$Fuel_{in}$	Gas_{out}	$Q_{ST,min}, Q_{ST,max,}, Q_{ST,UT}\ Q_{ST,DT}$
Type/Parameters	*thermal*	*thermal*	*fuel*	*thermal*	$Q_{ST,RURD}, \eta_{Comb}, \lambda_{comb}, h_{Air}$
Variables	m	m	m	m	U_{GB}
UC Constraints		$\Gamma_L, \Gamma_R, \Gamma_S, \Gamma_T$			
Auxiliary Variables		u, v, w			

Representation in the RES This unit is part of plant A and C, and appears once in the RES. The model is based on the component of plant A.

The generation capacity is referred to the steam production $\dot{Q}_{STout}$ representing the main operational state and consequently also the controlled operational decision variable. Therefore the control input $\mathbf{U}_{GB}$ is to be regarded as normalized steam production according to Eq. (A.6).

$$\dot{Q}_{STout} = \mathbf{U}_{GB}\ \dot{Q}_{ST,max} \tag{A.6}$$

In the optimization model, the evaporation process is simplified to take place in a zero-dimensional node at constant temperature and pressure. The combustion is simplified and assumed quasi-static using an overall combustion efficiency at a constant fuel-air ratio λ_{comb}, which is also applied in the simulation model. The considered operational limitations are also indicated by Table A.3.

$$\dot{Q}_{STout} = \dot{m}_{Fuel}\,(h_F + Hu_{Fuel}\ \eta_{Comb} + \lambda_{comb} h_{Air}) \tag{A.7}$$

$$\dot{m}_{Steam}\,(h_{ST} + h_{LW}) = \dot{Q}_{STout} \tag{A.8}$$

The simulation model reproduces the steam generation process in a detailled, dynamic manner, by modeling a two-state pressurized boiler in which the same model as for the ruth steam storage is adopted and extended with a heat input. (Please refer to [136]). Thereby it considers a fixed filling level set point using a PID-controller for maintaining the respective water supply. The combustian process uses the same formulation of the Optimization model.

Combined Heat and Power Unit

The CHP unit, depicted in Figure A.5, consumes fuel, such as natural gas or biomass and converts the chemical energy in both electrical and thermal energy at two different temperature levels. According to Table A.4, this unit comprises inputs for fuel, cooling water and water for steam generation as well as outputs for electric power, steam, cooling water and exhaust gas.

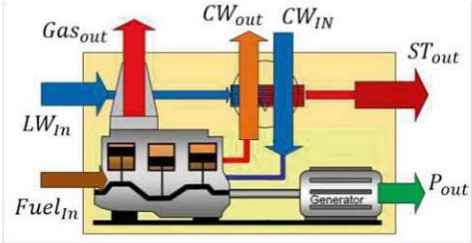


Figure A.5: CHP model

Table A.4: **Combined Heat and Power Unit - Optimization model overview**

	global							individual			
Ports	CW_{in}	CW_{out}	LW_{in}	ST_{out}	$Fuel_{in}$	Gas_{out}	P_{Out}	$P_{min}, P_{,max}\ P_{,RURD}, P_{UT},$			
Type/Parameters	*thermal*	*thermal*	*thermal*	*thermal*	*fuel*	*thermal*	*electrical*	$P_{DT}, r_{P2H}, r_H, \eta_{Comp}, h_{Air}$			
Variables	m	m	m	m	m	m	P	Q_{CW}	Q_{ST}	Q_{Tot}	U_{CHP}
UC Constraints							$\Gamma_L, \Gamma_R, \Gamma_S, \Gamma_T$				
Auxiliary Variables							u, v, w				

Representation in the RES This unit appears once in the RES and is originally part of plant A on which the model is based on.

The units capacity is represented by the electrical power generation $\boldsymbol{P}$ representing the characteristic system state and consequently also the controlled operational decision variable. Therefore the control input $\mathbf{U}_{CHP}$ is to be regarded as normalized Power generation according to Eq. (A.9).

$$\mathbf{P} \ = \mathbf{U}_{CHP}\ \mathrm{P}_{max} \tag{A.9}$$

In the optimization model, the evaporation is simplified to take place in a zero-dimensional node at constant temperature and pressure. The combustion is simplified and assumed quasi-static using an overall combustion efficiency at a constant fuel-air ratio in both the simulation and optimization model according to Eq. A (A.10). The electric power output and the total thermal heat output are related with the power to heat-ratio $\boldsymbol{r}_{P2H}$ as shwon by Eq. (A.11). The steam generation is modeled similarly to the gas-fired steam generator. Additionally, the low temperature heat generation due to engine cooling is also assumed as zero-dimensional quasi-static process at constant inlet- and outlet temperatures. The parameter $\boldsymbol{r}_H$ denotes the share of total heat distribution to the different heat outputs fort Steam ($\dot{\boldsymbol{Q}}_{ST}$) and Cooling Water ($\dot{\boldsymbol{Q}}_{CW}$) according to Eq. (A.13) and Eq. (A.17). The applied UC-Constraints for the operational limitations can also be perceived by Table A.4.

$$\dot{\boldsymbol{Q}}_{Heat,tot}\ (1 + r_{P2H,v})\ \eta_{\ tot,v} = \dot{\boldsymbol{m}}_{Fuel}\ (h_{Fuel} + \ \mathrm{Hu}_{Fuel}\ \eta_{Comb} + \lambda_{comb} h_{Air}) \tag{A.10}$$

$$\boldsymbol{P} \ = \dot{\boldsymbol{Q}}_{Heat,tot}\ r_{P2H,v} \tag{A.11}$$

$$\dot{\boldsymbol{Q}}_{Heat,tot}\ r_{H,ST} = \dot{\boldsymbol{Q}}_{Steam} = \dot{\boldsymbol{m}}_{\mathrm{ST}} \left(h_{ST,out} - h_{LW,in}\right) \tag{A.12}$$

$$\dot{\boldsymbol{Q}}_{Heat,tot}\ r_{H,CW} = \dot{\boldsymbol{Q}}_{CW} = \dot{\boldsymbol{m}}_{\mathrm{CW}} \left(h_{CW,out} - h_{CW,in}\right) \tag{A.13}$$

The simulation model reproduces the steam generation process, equally to the gas boiler. It considers a two-state pressurized boiler in which the same model as for the ruth steam storage is extended with a heat input. (Please refer to [136] Equally to the gas boiler a fixed filling level set point is achieved using a PID-controller for maintaining the respective water supply.

Thermal Consumer and Supplier

Thermal consumers represent the heat transfer points to the lower distribution networks of the corresponding temperature levels or individual heat-consuming processes. When used as heat sources, their function is similar, except that heat enters the system.

Table A.5: **Thermal consumer and supplier – Optimization model overview**

	global		individual
Ports	*In*	*Out*	m_{max}
Type/Parameters	*thermal*	*thermal*	
Variables	m	m	$\dot{Q}$
UC Constraints			Γ_L
Auxiliary Variables			

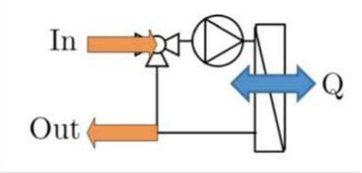


Figure A.6: Heat consumer and supplier

Representation in the RES Thermal consumers and heat sources are the most common components in the RES and occur at least once in each temperature levels. Usually, system boundaries are usually attached to these components, such as Feed-in, purchase schedules or costs.

The optimization model, simply comprises the heat balance according to Eq. Fehler! Verweisquelle konnte nicht gefunden werden.. Thereby, depending on the input and output properties, $\dot{Q}$ is positiv in a heat supply and negative in a consumer.

$$\dot{Q} = \dot{m}\, cp\, (h_{out} - h_{in}) \tag{A.14}$$

In the Simulation model variable temperatures are possible, thus a minimum inlet temperature must also be maintained. If this conditions is not complied with, the heat transfer to or from the process is interrupted. In addition, a certain maximum mass flow rate is considered, which may restrict the feasible heat transfer.

$$T_{in} > T_{in,min} \tag{A.15}$$

$$\dot{m} \leq m_{max} \tag{A.16}$$

Stratified Thermal Energy Storage

The stratified thermal energy storage, depicted in Figure A.7, stores water in layers of different temperatures. The thermal stratification occurs naturally, due to variating temperature-dependent water densities. Warmer water tends to rise to the top, while colder water remains at the bottom. In both models, optimization and simulation, the stratification is represented with a finite number of discrete elements, with each layer having an input and output port as shown in Table A.6.

Table A.6: **Stratified thermal energy storage - Optimization model overview**

			individual	
Ports	LW_{in}	LW_{out}	SOC_{min}, SOC_{max} T_{aml}	
Type/Parameters	*thermal*	*thermal*	V_l, $\Delta h_{l,min}$, k_f, k_l	
Variables	m	m	m_{LW}	SOC
UC Constraints				Γ_L
Auxiliary Variables				u

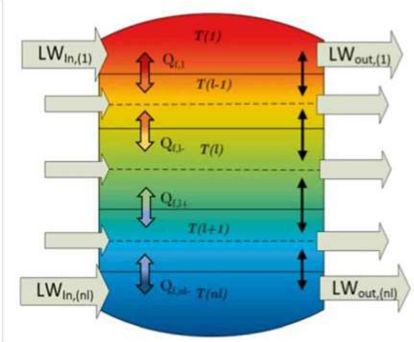


Figure A.7: Stratified Thermal Energy Storage model

Representation in the RES This unit appears once in the RES an exists in all of the EDCSproof industrial plants.

Due to its different temperature levels, which are each connected to different suppliers and consumers, for each temperature level an own state of charge is considered. According to Eq.(A.17) these SOCs refer to the available enthalpy at the respective temperature level above the return temperature from the consumers $T_{out,cons,l}$.

$$\mathrm{SOC}_l = m_l\,(h_l - h_{(T,out,cons,l)}) \tag{A.17}$$

For optimization, the storage tank is modeled with a finite number of discrete elements with constant temperature and variating mass (CTVM). Under the assumption of perfect stratification, there is no mixing and consequently no mass transfer between the layers. This means that the faces of the individual layers are moving. Furthermore, it is assumed that the respective ports of the layers are homogeneously distributed in the vertical centers of each layer. In this way, the circular surface areas $Ar_{f,l+}$ and $Ar_{f,l-}$ of the upper faces f,l+ and the lower faces f,l- of each layer can move close to location of the connections of the respective lower and upper layers. The minimum vertical distance to the ports of the adjacent layer is denoted as $\Delta h_{l,\,min}$. The respective contraints are presented form Eq. (A.18) to Eq. (A.23).

$$m_{l,lb} \le \sum_{l=1}^{l} m_l \le m_{l,ub} \tag{A.18}$$

$$m_{lb}^{l} = \begin{cases} \dfrac{V_t\left(l - \frac{l}{2} - \Delta h_{l,\,min}\right)\rho}{n} & otherwise \\ 0 & l = 1 \end{cases} \tag{A.19}$$

$$m_{ub}^{l} = \begin{cases} \dfrac{V_t\left(l + \frac{l}{2} + \Delta hl\right)\rho}{n} & otherwise \\ V_t\ \rho & l = n_l \end{cases} \tag{A.20}$$

$$\sum_{l=1}^{l} \frac{m_l}{\rho} = V_t \tag{A.21}$$

$$\Delta \mathbf{m}_l^{t+1} = \boldsymbol{m}_l^{t+1} - \boldsymbol{m}_l^{t} = \sum_{lin} \dot{\boldsymbol{m}}_{,l,lin}^{t} - \sum_{lout} \dot{\boldsymbol{m}}_{,l,lout}^{t} \tag{A.22}$$

$$\rho\ \boldsymbol{V}_t = \sum_{l=1}^{l} \mathbf{m}_l^t \tag{A.23}$$

As the storage has a fixed volume, the sum of the mass contents of all layers is constant and accounts to the total mass capacity as expressed by Eq. (A.23). Referring to Eq. (A.17) the constant layer temperatures in the optimizaion model show a direct correlation between the mass and the SOC of a specific layer. The density $\boldsymbol{\rho}$ is considered constant and inherited from the connected stream at the highest temperature level.

For simulation, a more precise model based on the stepped temperature distribution model in [137] is used which considers variating temperatures. In contrast to the optimization model, this approach considers vertical heatflows. The energy balance of a particular layer is stated in Eq. (A.24) in which the heatflux between the layers appears according to Eq. (A.39).

$$\boldsymbol{\rho}\ V_l \frac{\boldsymbol{dT_l}}{\boldsymbol{dt}} = \boldsymbol{m_{in}}\ (\boldsymbol{T_{in}} - \boldsymbol{T_l}) + \frac{\dot{\boldsymbol{Q}}_{f,l-}}{cp} - \frac{\dot{\boldsymbol{Q}}_{f,l+}}{cp} + \frac{k_l}{cp} Ar_l\ (T_{amb} - \boldsymbol{T_l}) \tag{A.24}$$

$$\dot{\boldsymbol{Q}}_{f,l-} = k_l Ar_{f,l-} (\boldsymbol{T}_{l-1} - \boldsymbol{T}_l) \tag{A.25}$$

Referring to Eq. (A.17), in constrast to the optimization model, the determination of the SOC in the simulation model also requires to consider the variable layer temperatures.

Latent Energy Storage

This type of latent heat storage, as incorporated in plant B, can be regarded as an extension of the stratified thermal energy storage concept. The sensible heat transfer fluid in the storage is filled with floating spherical elements containing a phase-change material (PCM) that has a melting point exactly reflecting the temperature range of the storage. Thus, its operating temperature range is typically much smaller than that of a stratified storage tank. As depicted in Figure A.9, the main storage capacity results from the phase transition of the PCM which in this case accounts for about 65% of total volume. Similar to the stratified storage, the model assumes a finite number of discrete elements. According to Figure A.10, potentially each layer can have an input and output port, however, in the RES configuration, only the top and bottom layers are connected, which significantly affects formulation the employed optimization model, shown in Figure A.8.

Table A.7: **Latent energy storage - Optimization model overview**

	global				individual		
Ports	HS_{in}	HS_{out}	CS_{in}	CS_{out}	SOC_{min}, SOC_{max} T_{amb}		
Type/Parameters	*thermal*	*thermal*	*thermal*	*thermal*	$V_{PCM}, \Delta hl_{PCM}$		
Variables	m	m	m	m	$\dot{m}_{ch}$	$\dot{m}_{dch}$	SOC
UC Constraints							Γ_L
Auxiliary Variables							

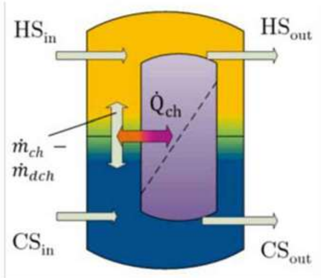


Figure A.8: Latent Energy Storage Optimization Model Illustration

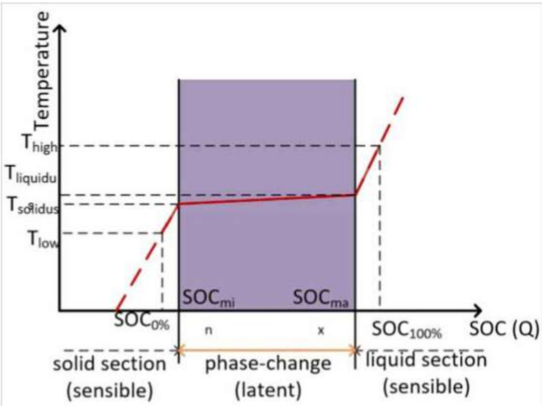


Figure A.9: Relation between the SOC and the storage temperatures during the latent phase transition

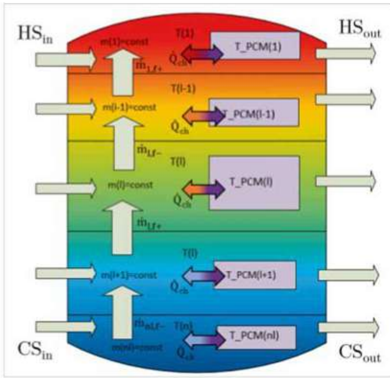


Figure A.10: Latent Thermal Energy Storage Simulation Model Illustration

Representation in the RES Plant B (See Chapter 4) already includes such a storage system, which was adopted and customized for integration into the RES. This mainly concerns the storage size and the PCM material. While the storage dimensions differs from the original component, the diameter of the PCM elements were preserved (d=108mm). Furthermore, in the RES the operating temperatures of the central cooling systems are slightly lower than those of the storage tank in its implementation in plant B. Accordingly, the phase-change properties of a respective suitable PCM were adopted. The data for different PCM materials were inquired from the manufacturer of the latent energy storage system from plant B.

Due to the much higher specific latent heat of the PCM (290kJ/kg) compared to the HTF (5,1kJ/kg at $\Delta T = 5K$), only the phase change of the PCM is considered for determining the State of Charge. Thus, the SOC can be defined by using the melted fractions of the different layers according to Eq. (A.26).

$$SOC = \sum_{l=1}^{n} M_{Frac,l}\, \rho_{PCM,l}\, V_{PCM,l} \Delta hl_{PMC} \tag{A.26}$$

The optimization model, is based on the simplified assumption, that the PCM is aggregated as a single interrelated storage capacity which is shown by Figure A.8. It also assumes only two layers of liquid, one hot and one cold, with fixed volumes and temperatures. Consequently, charging or discharging, creates a vertical flow of the HTF within the storage tank between the hot and cold levels which inherently assumes that the entire heat difference between the two temperatures of the HTF is transferred to the PCM. The vertical flow equals the difference between the charging and discharging flows ($\dot{m}_{ch} - \dot{m}_{dch}$). Thus Eq. (A.27) and Eq. (A.28) state the charging and discharging process.

$$\dot{Q}_{ch} = (\dot{m}_{ch} - \dot{m}_{dch})\, cp\, \Delta T \tag{A.27}$$

$$SOC^{t+1} - SOC^{t} = \dot{Q}_{ch}^{t} \tag{A.28}$$

$$SOC_{max} = V_{PMC}\, \rho\, \Delta hl_{PMC} \tag{A.29}$$

The simulation model is formulated as an extension of the stratified storage model according to Figure A.10. In contrast to the stratified storage model, it considers a constant mass in eacht layer and allows vertical flows of the heat transfer fluid. The PCM is treated separately for each layer and is assumed to be in heat exchange only with the HTF of the same layer. The heat transfer between the PCM and HTF is expressed by Eq. (A.31) where the heat transfer coefficient k is assumed to be constant. Likewise, the temperatures of the HTF and the PCM are considered uniform in each layer. Consequnetly, the HTF's energy balance of each layer is expressed as extension of the stratified storage modeling approach according to Eq. (A.30).

$$\rho\, V_l \frac{dT_l}{dt} = \dot{m}_{l,in}(T_{in} - T_l) + \dot{Q}_{f,l-} - \dot{Q}_{f,l+} + \frac{k_l}{cp} Ar_l (T_{amb} - T_l) - \frac{\dot{Q}_{ch,}}{cp} \tag{A.30}$$

$$\dot{Q}_{f,l-} = \dot{m}_{l,f-}(T_{l-1} - T_l),\quad \dot{Q}_{f,l+} = \dot{m}_{l,f-}(T_{l-1} - T_l) \tag{A.31}$$

$$\dot{Q}_{ch,} = \frac{k_{PCM}}{cp} Ar_{l,PCM} * \left(T_{l,liquid} - T_{l,PCM}\right) \tag{A.32}$$

$$Q_{PCM,l}^{t+1} - Q_{PCM,l}^{t} = \dot{Q}_{ch}^{t} \tag{A.33}$$

The PCM phase is modeled based on the respective modeling approach presented in [137] which considers the phase change of the PCM to occur in a small temperature interval, enclosed by the liquidus (melting) temperature $T_{Liquidus}$, representing a certain lowest temperature of the sensible region as fluid and the solidus temperature $T_{Solidus}$, assumed as highest temperatur of sensible region as solid. As depicted in Figure A.9, in between a small temperature interval (typically <5K), the phase change takes place, which is related to a significantly large enthalpy change.

$$\dot{Q}_l^t = Q_{PCM,l}^{t+1} - Q_{PCM,l}^{t} = V_{PMC,l}\, \rho\, cp\, (T_{PCM,l}^{t+1} - T_{PCM,l}^{t}) \tag{A.34}$$

Depending on the region, different values for the cp in Eq. (A.34) assigned. During the phase change, the PCM temperature takes values between $T_{Liquidus}$, and $T_{Solidus}$, which also determines the melted fraction M_{Frac}.

$$T_{PCM,l} > T_{liquidus} \quad \rightarrow \quad M_{Frac} = 0 \qquad cp = cp_{liquid} \tag{A.35}$$

$$T_{liquidus} T_{PCM,l} < T_{Solidus} \quad \rightarrow \quad M_{Frac} = \frac{T_{PCM,l} - T_{Solidus}}{T_{Liquidus} - T_{Solidus}} \qquad cp = \frac{\Delta h_{PMC}}{T_{Liquidus} - T_{Solidus}} \tag{A.36}$$

$$T_{PCM,l} < T_{Solidus} \quad \rightarrow \quad M_{Frac} = 1 \qquad cp = cp_{solid} \tag{A.37}$$

In the simulation model, the SOC can then be determined according to Eq. (A.26).

Representation of Electric components Before listing the models of electrical devices, it is emphasized that electrical energy is considered in less granular detail only based on power and energy.

Electrical Energy Storage (Battery)

A battery as electrical energy storage system functions as a device that stores electrical energy in the form of chemical energy. The functional principle can be broken down into the two primary processes of charging and discharging. During the charging process, electricity from the external source (grid or renewable energy system) flows into the battery, causing a chemical reaction within the battery cells that converts electrical energy into chemical energy. In the discharging process, the chemical energy stored in the battery is converted back into electrical energy and it is released to the connected electrical devices or grid.

Table A.8: **Electrical energy storage - Optimization model overview**

	global		individual
Ports	P_{in}	P_{out}	$SOC_{min}, SOC_{max}, P_{max}$
Type/Parameters	*electrical*	*electrical*	η_{ch} η_{dch}, η_{loss}
Variables	P	P	SOC
UC Constraints	Γ_L	Γ_L	Γ_L
Auxiliary Variables			

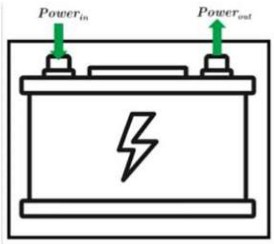


Figure A.11: Electrical energy storage

Representation in the RES The battery is incorporated in the RES as new component RES as it is not existing in any of the partners plants. The SOC simply refers to the stored electric energy.

In the optimization model, the electrical storage system is represented as a simple repository for electricity energy with the SOC as only state variable. As shown by Eq. (A.38) the charging and discharging is established by the control variable U that refers to the power flow to or from the batterie, which in that case assumes values between -1 and 1. The energy balance for the storage system is stated Eq.(A.39) and outlines the consideration of the charging and discharging efficiencies η_{ch} and η_{dch} as well as self discharging by the storage efficiency η_{loss}. Additionaly, the application of UC-Constraints is shown in Table A.8.

$$U\, P_{max} = P_{in} - P_{out} \tag{A.38}$$

$$SOC^{t+1} = SOC^{t}\, \eta_{loss} + P^{t}_{in}\, \eta_{ch} - P^{t}_{out}\, \frac{1}{\eta_{dch}} - \tag{A.39}$$

The simulation model is based on the equivalent circuit battery model provided by the model library in Simulink. It is incorporated and customized within the simulation structure to transfer the electrical charge and discharge power at the ports.

Photovoltaic Plant Model

A photovoltaic system converts the solar irradiation to electrical power. The units size is represented by the total panel area and the capacity is referred to the generation of electric power. Thus the solar irradiation limits the maximum usable power generation. The utilized share of this maximum usable power generation represents the controlled operational decision variable.

Table A.9: **Photovoltaic plant - Optimization model overview**

	global	individual
Ports	P_{out}	P_{min}, P_{max} ,
Type/Parameters	*electrical*	$Irr\ \eta_v\,\mathrm{Ar}$
Variables	P	U
UC Constraints		$\Gamma_{L,}$
Auxiliary Variables		

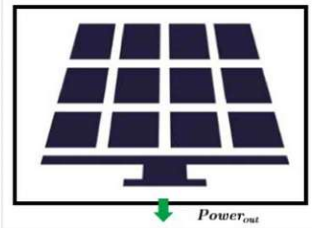


Figure A.12: Electrical energy storage

Representation in the RES The PV system represents the only local renewable power generation in the RES. During the project time, PV-Systems became part in all EDCSproof industrial plants.

The optimization model, assumes a constant efficiency for the converision of solar irradiation into electric power. Accordingly, Eq. (A.40) states the corresponding energy conversion constraint where U represents the utilization variable for available solar power.

$$\boldsymbol{P} = Irr\ \eta_v\,\mathrm{Ar}\,\mathbf{U} \tag{A.40}$$

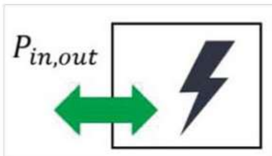
The Simulation model of the photovoltaic plant is based on the model presented in [138] which represents the effective module efficiency as a nonlinear function of the module temperature. The module temperature is calculated as a function of the outdoor temperature and solar irradiation under the assumption of steady state conditions.

Power Cnsumer and Supplier

Representation in the RES The internal consumption of electric power as well as the power purchase from the grid are considered as simple source or sink that contains only one variable representing the input or output of electric power.

Table A.10: **Power consumer and supplier - Optimization model overview**

	global		individual
Ports	*In*	*Out*	P_{max}
Type/Parameters	*electrical*	*electrical*	
Variables	P	P	U
UC Constraints	Γ_L	Γ_L	
Auxiliary Variables			



As shown by Eq. (A.41) together with Table A.10 the control variable U refers to the power supply or consumption $\boldsymbol{P}$.

$$\boldsymbol{U}\,P_{max} = \boldsymbol{P} \tag{A.41}$$

A.2 Operational Progression for the Seasonal Scenarios Transition and Winter

Transition Season

EMCS	CRCC

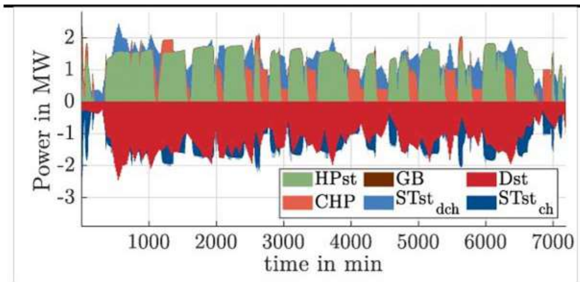


Figure A.13: Transition Season Steam Balance at EMCS operation

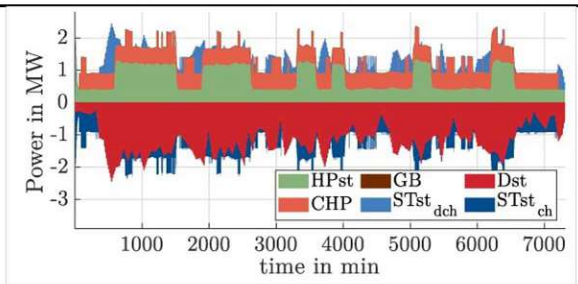


Figure A.14: Transition Season Steam Balance at CRCC operation

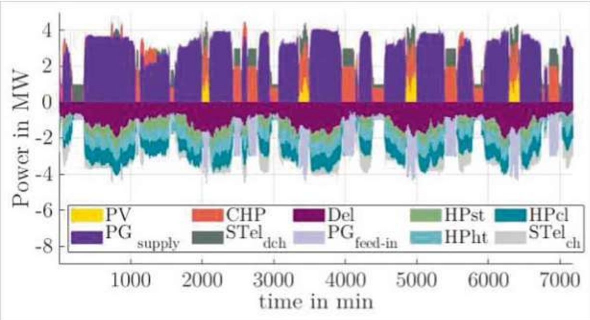


Figure A.15: Transition Season Power Balance at EMCS operation

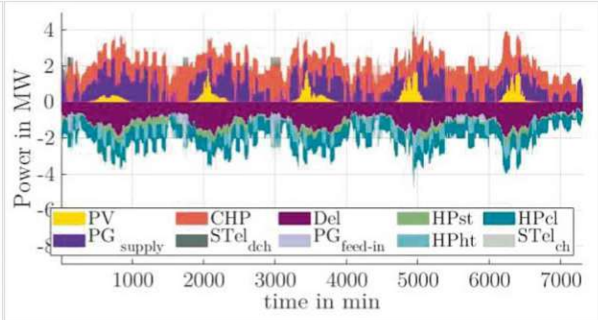


Figure A.16: Transition Season Power Balance at CRCC operation

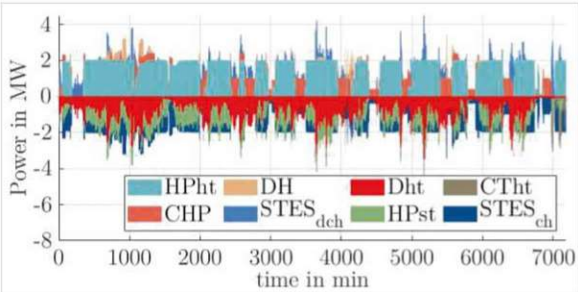


Figure A.17: Transition Season Hot-Water Balance at EMCS operation

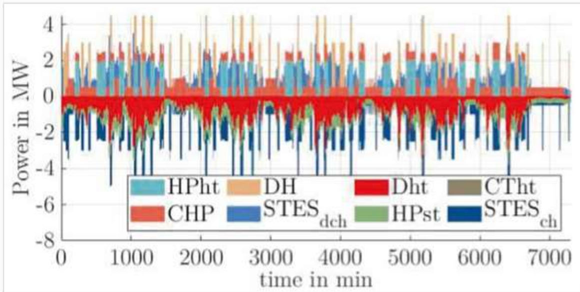


Figure A.18: Transition Season Hot-Water Balance at CRCC operation

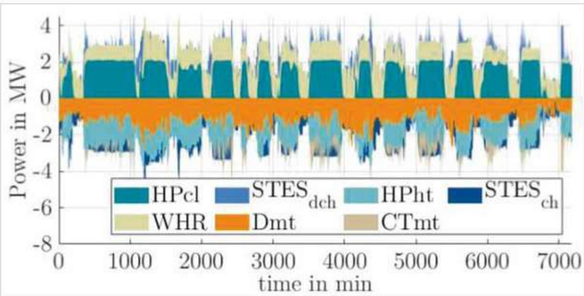


Figure A.19: Transition Season Medium Temperature Balance at EMCS operation

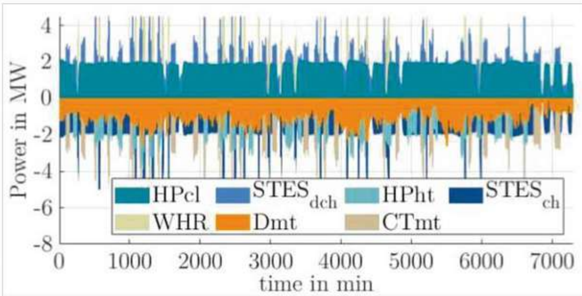


Figure A.20: Transition Season Medium Temperature Balance at CRCC operation

Winter

EMCS	**CRCC**

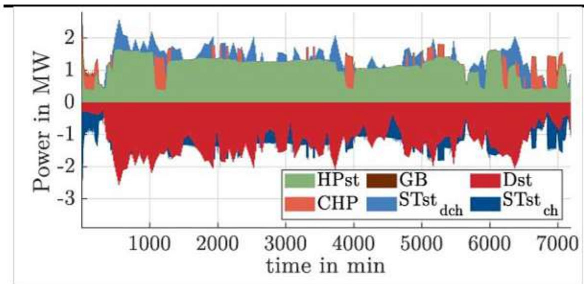


Figure A.21: Winter Season Steam Balance at EMCS operation

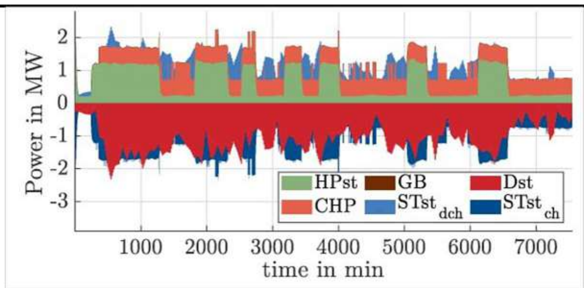


Figure A.22: Winter Season Steam Balance at CRCC operation

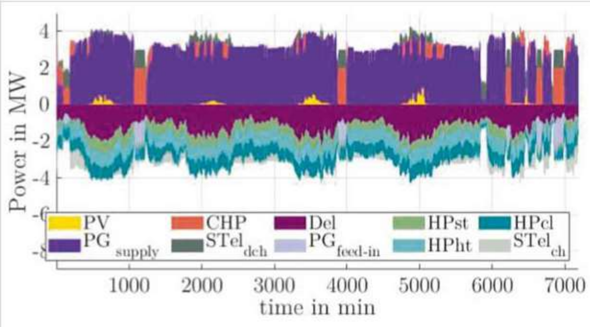


Figure A.23: Winter Season Power Balance at EMCS operation

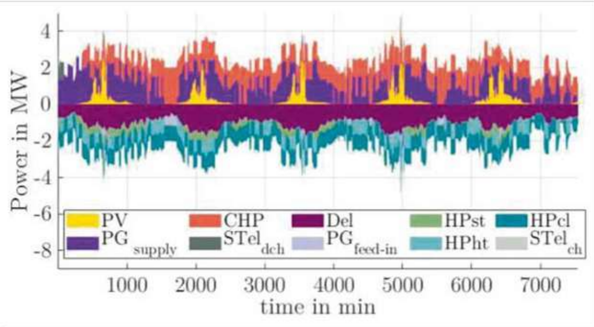


Figure A.24: Winter Season Power Balance at CRCC operation

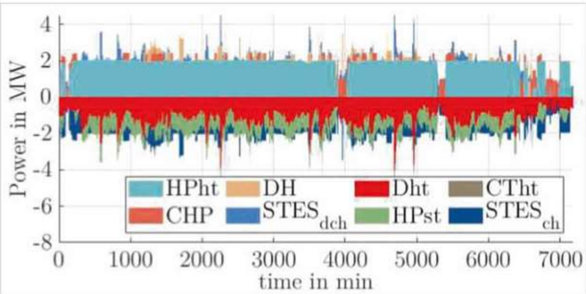


Figure A.25: Winter Season Hot-Water Balance at EMCS operation

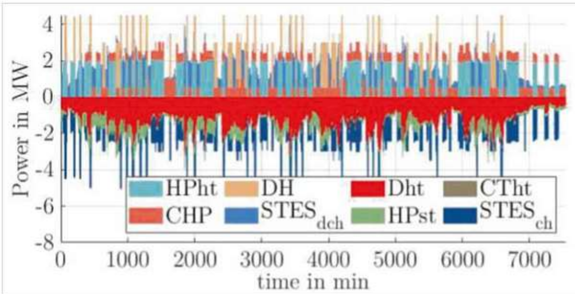


Figure A.26: Winter Season Hot-Water Balance at CRCC operation

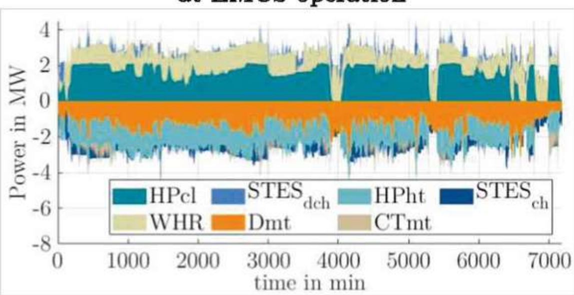


Figure A.27: Winter Season Medium Temperature Balance at EMCS operation

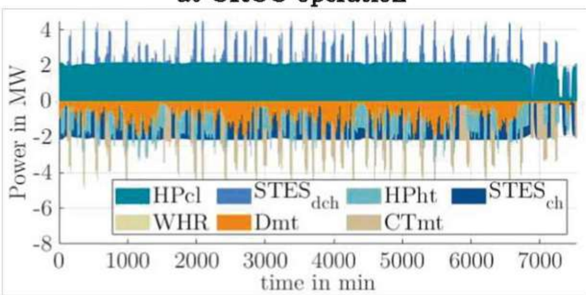


Figure A.28: Winter Season Medium Temperature Balance at CRCC operation

A.3 Complementary Academic Work

Presentations

Throughout my scientific career, I have had the privilege of presenting my research topic and discoveries to a professional audience at elective conferences, providing valuable opportunities to share insights and receive feedback from corporate and scientific experts.

- Schenzel K., Hofmann R.: „Management und Betriebssicherheit in komplexen Energiesystemen"; Talk: evon up2date, Schielleiten (invited); 2022-6-22
- Schenzel K: „Ganzheitliche Regelungskonzepte für komplexe Energieversorgungs-systeme"; Talk: Blickpunkt Forschung – Assistive Technologien, Wien (invited); 2022-10-12
- Schenzel K: "EDCSproof – Energy Demand Control System - Process optimization for industrial low temperature systems"; Project video presentation on Youtube; 2022-03-25, https://youtu.be/x0OLkcTbAm0

Scientific Reports

This dissertation was fundamentally conducted within the founded research project EDCSproof - Energy Demand Control System - PROcess Optimization For industrial low temperature systems. The public final report is available or can be made available via the corresponding project's website: https://www.nefi.at/de/projekt/edcsproof

Supervised Thesis

As project assistant I co-supervised the following master's thesis which was part of an industrial research project:

Steiner M: "Analysis and evaluation of decarbonization measures in synthetic resin production"; Supervisor: R. Hofmann, K. Schenzel, D.Huber; E302 – Institut für Energietechnik Thermodynamik, 2022;

Teaching Activity

Besides my project related research contributions, I was also given the valuable task of supporting the teaching activities at the Institute of Energy Systems and Thermodynamics with my practical experiences within the course:

302.074. Numerical Process Simulation of Thermal Power Plants. VU, 2.0 ECTS (2019, 2020, 2021, 2022, 2023)

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About the Author

Karl-Wilhelm Schenzel was born in 1987 and grew up in Bruck an der Leitha, Austria, where he graduated from secondary school in 2005 (Matura). He studied mechanical engineering at TU Wien and Chalmers University of Technology in Gothenburg. He finished his studies in 2015 at TU Wien.

Karl-Wilhem Schenzel started his professional career during his master's degree at ENRAG in 2012 developing innovative energy storage concepts in a research-orientated environment, where he collaborated with the Institute of Energy Systems and Thermodynamics for his master's thesis. Evolving from developing individual technologies, he expanded his expertise into designing holistic sustainable energy systems for communities and buildings at ILF Consulting Engineers Austria. His enthusiasm for innovation combined with his interest in mathematical optimization and his strong commitment to sustainable energy, were fundamental to his ambition to pursue a PhD in this field. Finally, at the end of 2018, he was granted this opportunity and therefore returned to the Institute of Energy Systems and Thermodynamics at TU Wien, while partially remaining in the ILF team. As a project assistant, his PhD work was centered on the EDCSproof and Industry4Redispatch projects, which culminated in this dissertation.

Beyond academia and professional activities, Karl-Wilhelm Schenzel is passionate in sports, experiencing nature and runs a winery with his family.