Development of methods and components for future industrial energy supply with flexibility

by Sophie Knöttner

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Vienna, July 2024

Sophie Knöttner

Abstract

The importance of flexibility from industrial sources is increasing with the transformation of the energy system and industrial production. The need for industrial energy supply systems to become more sustainable is also rising. This work concentrates on integrating flexible and innovative energy supply technologies into industrial energy systems. Mixed-integer linear programming is applied and extended by new formulations to achieve this aim.

This work presents techno-economic analyses of flexible energy supply for industrial use cases under various conditions. With its energy-intensive production process, the paper and board manufacturing industry is the basis for these analyses. The work answers various questions considering different levels of the industrial energy system as well as site-independent energy supply levels. An overview of how flexibility can be integrated into decision variables, constraints, and the objective function of optimization problems is given. Operational aspects such as rolling time horizons for ongoing adaptation to fluctuating framework conditions are considered. Long-term structural measures such as sector coupling or independence from individual raw materials are also considered. The economic analysis of the calculated results quantifies the economic challenges that a transformation of the energy system entails.

In summary, the methods developed and demonstrated in this work contribute to a comprehensive decision-making basis for determining how the energy supply in industrial plants will develop in the future transformation process.

Kurzfassung

Vor dem Hintergrund großer Herausforderungen der Transformation des Energiesystems sowie der industriellen Produktion, steigt die Bedeutung von Flexibilität auch aus industriellen Quellen zunehmend. Gleichzeitig nimmt aber auch die Anforderung an industrielle Energieversorgungssysteme zu nachhaltiger zu werden. Diese Arbeit umfasst die Integration von flexiblen und innovativen Energiebereitstellungstechnologien in industrielle Energiesysteme. Dazu wird die Methode der gemischt-ganzzahligen lineare Optimierung verwendet und neue Formulierungen werden entwicklt.

Für industrielle Anwendungsfälle, die Charakteristiken des energie-intensiven Produktionsprozesses der Papier- und Kartonherstellung aufweisen, werden in den Publikationen, die zu dieser Arbeit gehören für verschiedene Rahmenbedingungen techno-ökonomische Analysen der flexiblen Energieversorgung vorgestellt. Ausgehend von den verschiedenen Fragestellungen, die unterschiedliche Ebenen des industriellen Energiesystems sowie standort-unabhängige Ebenen berücksichtigen, kann ein Überblick gegeben werden, wie Flexibilität in Entscheidungsvariablen, Nebenbedingungen sowie die Zielfunktion von Optimierungsproblemen integriert werden kann. Dabei werden sowohl betriebliche Aspekte wie rollierende Zeithorizonte für eine laufende Anpassung an fluktuierende Rahmenbedingungen, berücksichtigt, aber auch langfristige strukturelle Maßnahmen wie Sektorkopplung oder die Unabhängigkeit von einzelnen Rohstoffen. Die ökonomische Analyse der berechneten Ergebnisse, quantifiziert die wirtschaftlichen Herausforderungen, die eine Transformation des Energiesystems mit sich bring.

Zusammenfassend tragen die Methoden, die in dieser Arbeit entwickelt und demonstriert werden, dazu bei, dass eine umfassende Entscheidungsgrundlage für die Transformation zukünftiger, industrieller Energiesysteme unter Berücksichtigung von verschiedenen Flexibilitätstypen geschaffen werden kann.

Acknowledgments

Sometimes, it can take a considerable amount of time to achieve the desired result! When I look back on my path to my doctorate, it was obviously more of a marathon than a sprint. Today, I am very happy that I have finally completed this work. I had the opportunity to develop my research further, learn a lot, and meet inspiring people during this process. And I have received so much support along the way, for which I would like to express my gratitude.

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Contents

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Research summary

The first chapter of this work, Research Summary, presents and summarizes the background of the core publications of this thesis. This chapter consists of five sections, which are described below. First, the motivation and underlying initial situation are described in *Introduction*, Section 1. In Section 2, *Context*, the relevant theoretical background and literature for this thesis, including the related publications, are addressed in the fields of mathematical programming, mixed-integer linear programming, often referred to as MILP, flexibility, and industrial energy supply systems. In Section 3, the *Problem Statement* is introduced, including this thesis's research objectives and sub-questions. The corresponding and applied *Research Approach* is presented in Section 4. Thus, the fourth section is concerned with linking the four core publications of this thesis and the two main fields of interest identified in the *Problem Statement* (Section 3). Finally, in Section 5, a *Conclusion* for the work and contributions of this thesis is drawn.

1 Introduction

The **availability of reliable and affordable energy** is one key criterion and prerequisite to successfully operating industrial core processes of good manufacturing. Depending on the industrial sector and the respective country, energy costs can even contribute to 10-20% of the total costs in production (European Commission et al. 2020). These sectors with high shares of energy costs related to production costs are often referred to as *energy-intensive* industries. In general, energy intensity is defined as a performance indicator for the relation between the quantity of energy required per unit output or activity (Office of Energy Efficiency and Renewable Energy 2023). Typical examples are companies in the sectors *Iron and Steel*, *Pulp and Paper*, *Chemistry*, or *Non-metallic minerals*. Due to high energy costs, various challenges and opportunities have emerged for the energy supply, particularly in these sectors. A significant rise in energy costs causes a relevant increase in production costs and, thus, most likely, a price increase of industrial goods for final customers. Thus, a main requirement for the industrial sector in the ongoing transition process is to increase sustainability and lower emissions from industrial production and industrial energy supply while keeping the industry competitive.

An Austrian and Central European perspective on industrial energy supply and opportunities and burdens for the industrial sector in these regions is discussed below.

Based on developments from the 1990s to the 2000s, several changes have been made in regulatory and legislative frameworks. Examples are liberalization of the electricity market, unbundling of energy supply and grid infrastructure, or facilitated market access. These developments are summarized, e.g., by Österreichs Energie (2023), the representation of interests of the Austrian energy industry. The developments increased the attractiveness for smaller parties and not just large energy supply companies to participate in trading, e.g., in (short-term) energy markets. In general, the incentives to exploit (industrial) flexibility increased.

Incentive 1 — Negative Electricity Prices Since 2008, and with increasing frequency since then, negative electricity prices occurred in short-term electricity markets. *Next-Kraftwerke*, the operator of one of Europe's largest virtual power plants, compared annual hours with negative electricity prices for Central European countries from 2017 to 2022 (Volkert 2023). Results show that the German short-term electricity market recorded the highest value of 509 hours in 2022, followed by Ireland with 374 hours in 2020. Reasons for this are, e.g., guaranteed feed-in tariffs for renewable power generation in combination with increased renewable power generation in Europe, e.g., a high capacity of installed wind power in Northern Germany and Denmark, but also production from photovoltaic in Southern Germany or hydropower in Central and Eastern Europe. Also, periods with low electricity consumption, e.g., national holidays or reduced industrial operation during the COVID-19 pandemic, can contribute to negative prices. The occurrence of negative prices, as described above, increased, while the need for new sources providing ancillary services also increased. Higher renewable shares in the energy system lead to both an increased need for balancing power as well as an increased need for congestion management and redispatch provision. These two applications of flexibility in grid services can be distinguished regarding the following criteria (Traninger et al. 2023):

i Time of delivery — while redispatch is a preventive measure to avoid congestion in the grid, balancing service is a reactive measure to maintain the balance between generation and consumption

ii Geographics — while for balancing service, the actual location in the grid is of minor importance, the position of the flexibility source has a high significance and a direct impact on the effectiveness of the measure

iii Economics — while balancing service was already traded as a market-based product in the past, only cost-based remuneration has taken place for redispatch.

This results in new incentives for exploiting industrial flexibility. From a systemic perspective, (new) efficient and low-cost flexibility sources are crucial as the costs of flexibility measures to ensure reliable grid operation are indirectly passed on to customers at various consumption levels via grid usage charges. While the before-mentioned developments pose driving factors for increased industrial flexibility, there are also incentives and necessities to change industrial processes and energy supply toward more sustainable systems.

Incentive 2 — Legislative Changes In the late 2010s, new aspects relevant to the future (industrial) energy supply emerged in a legislative context. Climate change mitigation measures, e.g., greenhouse gas emission, primary energy consumption reduction, and higher shares of renewables, have been part of the discussion, especially in the scientific literature over decades. To show the role of the industrial sector as a greenhouse gas emitter, several relative and absolute numbers will be given in the following. Presented figures are derived from a common data source — Our World in Data — with a consistent calculation scheme, definitions, and units (Ritchie et al. 2017). For Austria, further specific numbers are derived from the *Austrian Climate Protection Report* (Zechmeister et al. 2022). Due to the data availability (status autumn 2023), data from 2020 forms the basis for the following analysis.

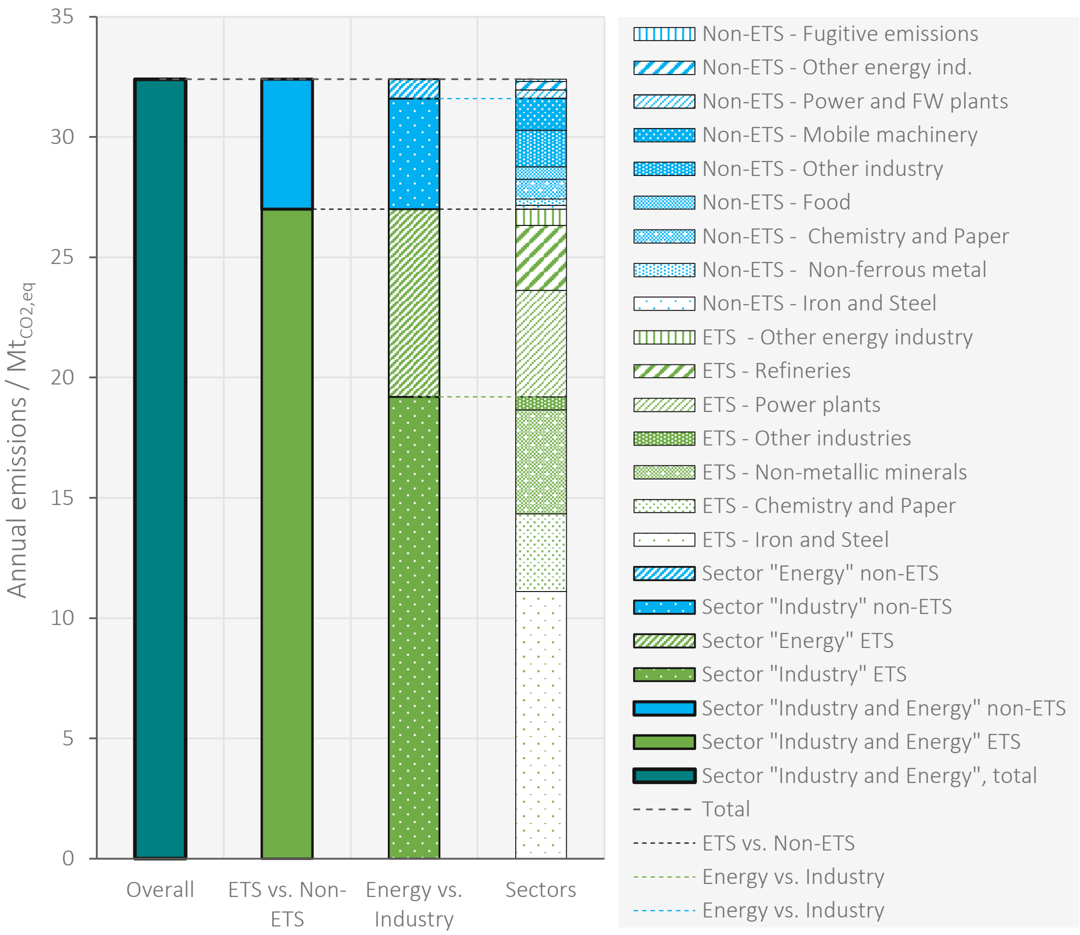

Figure 1: *Visualization of different aggregation levels of emissions from the sectors industry and energy for 2020 in Austria. Data source: Zechmeister et al. (2022).*

In Austria in 2020 73.5 Mt_{CO2eq} (Zechmeister et al. 2022) and 60.04 Mt_{CO2} (Ritchie et al. 2017; Friedlingstein et al. 2022) have been emitted when accounting only production-based emissions. For 2019 and 2021, the production-based emissions are 9.5 and 4.2% higher than in 2020, respectively (Ritchie et al. 2017; Friedlingstein et al. 2022). This effect results, e.g., from reduced industrial production and energy supply during the initial phase of the COVID-19 pandemic (Zechmeister et al. 2022). When accounting for consumption-based emissions in 2020, the CO_2 emissions were approximately 27% higher than the production-based emissions (Ritchie et al. 2017; Friedlingstein et al. 2022).

In 2020, the sectors industry and energy accounted for 27 Mt_{CO2eq} in Austria, including also the harmful effect of further greenhouse gases than CO_2 converted to an equivalent harmful effect of CO_2. This value equals 36.7% of total Austrian emissions — remark: emissions from aviation are not included in the calculation of these figures. A comparable scale can be observed for worldwide emissions. Ritchie presented for worldwide emissions of CO_2-equivalent in 2016 the following values: a share of 24% for energy use in the industry, a share of 5.2% for the production of chemicals and cement, and a further 13.6% for fugitive emissions from energy production and unallocated fuel combustion (Ritchie 2020).

A detailed look at the Austrian energy- and industry-related **scope 1 emissions** in 2020 is shown in Figure 1, which is based on the numbers presented in the *Austrian Climate Protection Report* (Zechmeister et al. 2022). Scope 1 emissions are understood as direct greenhouse gas emissions from sources owned or controlled by the company, by the European Commission (2019a). In Figure 1, the total emissions for *energy and industry* are shown at different aggregation levels. The first distinction in the second bar is between emissions from sites included in the emission trading system (ETS) (indicated with *ETS*) and sites not included in the ETS (indicated with *non-ETS*). Figure 2 gives an overview of the industrial sites and units included in the ETS. This summary is derived from the EU Directive on establishing a scheme for greenhouse gas emission allowance trading within the Community European Parliament and Council (2003). The second category includes, for instance, several industrial sites with smaller production capacities that are not part of the ETS. It also includes plants for the incineration of hazardous waste and municipal waste as well as public energy supply with overall fuel heat output below 20 MW and biomass heating plants. The second level of aggregation in the third bar further distinguishes between the subsectors *energy* and *industry*. However, the emissions attributed to the industry originate largely from on-site energy supply and burning of fuels. In the last bar, a more precise breakdown is shown for different groups of emitters, such as specific industrial sectors or company types from the energy sector.

The biggest emitters are (i) ETS-sites of the sectors iron and steel, (ii) non-metallic minerals, (iii) chemistry and paper production as well as, (iv) power plants considered in emission trading, and (v) refineries. Energy-related emissions result mostly from the firing of natural gas but also other fossil fuels such as coal or oil in boilers or kilns.

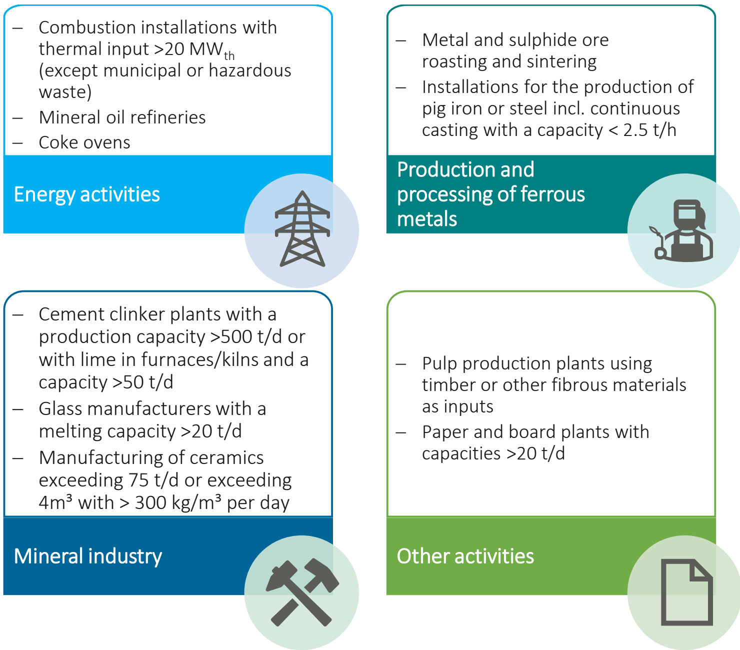

Figure 2: *Overview on activities included in the Emission Trading System. Source: (European Parliament and Council 2003).*

For the process-related emissions, the main emitters are steelmaking, refineries, cement production, and processing of other non-metallic minerals.

In the last decades, goals for reducing CO_2 emissions were hardly defined on a binding legislative basis. The Green Deal — a common European roadmap for sustainability in all sectors (European Commission 2019b) — was featured in 2019 and represents a new incentive for change and transition in Europe. In its subsequently elaborated modules, e.g., the European climate law, the "fit for 55" package (Wilson et al. 2023a) or the carbon border adjustment mechanism (Wilson et al. 2023b), the pressure for (structural) changes in the European industrial production sector has risen lately.

Also, customers' awareness of sustainability, climate neutrality, and decarbonized integrated production chains is subject to strong change. In general, a more holistic approach to decarbonization can be observed. For example, the relevance of considering complete value chains as well as taking scope 3 emissions[1] into account increased. Customers and movements have been mentioned as *new agents of change* for example, in the Horizon 2020 project *REINVENT — Realising Innovation in Transitions for Decarbonisation* (Bulkeley et al. 2022). The adapted requirements from two stakeholder groups, legislative and customers, are increasing pressure on industrial decision-makers to change production systems towards decarbonized, resilient, and sustainable systems.

[1]All indirect greenhouse gas emissions that are not included in scope 2 and occur in the up-and downstream value chain of the reporting company (European Commission 2019a)

Incentive 3 — Political Developments Recent political developments in Europe further pushed those trends, increased incentives and needs for flexibility, and the higher relevance of decarbonized (industrial) energy supply portfolios. The latest developments of the Russian-Ukrainian war in February 2022 and the subsequent energy crisis in Europe highlighted the relevance of switching from fossil sources, specifically natural gas, to alternative energy supply variants. Among other measures, it was highlighted by the *International Energy Agency* that decarbonization of flexibility sources and providing new flexibility sources, especially in power grids, is going to have a significant contribution to overcoming the dependency on the Russian natural gas supply (IEA 2022).

The developments described above emphasize the relevance of more resilience, flexibilization, new technologies, and decarbonization in industrial sites. In this context, decision-support tools pose a significant measure to overcome the burdens today's industry faces. Both for design and operational decisions, the mathematical programming method evolved to be an indispensable tool for industrial flexibility and decarbonization.

2 Context

The energy system, in general, is undergoing fast and frequent changes. Also, industrial production is confronted with a transition process that has increased speed lately. New requirements are coming up as presented in Section 1.

Part of the transition process is the integration of new components in industrial energy supply chains efficiently and flexibly. Those can include new supply options, such as new contracts or fuels, sector coupling, or the integration of innovative technologies. Integration is possible in completely new, also referred to as green-field, plants but also existing, also referred to as brown-field, industrial sites.

Here, a range of questions occur. Should a new component, such as thermal or electric storage, boiler, or energy source, be integrated? What size or capacity shall be ideally used if a new component is integrated? Additional questions arise when multiple timesteps are considered and thus the system's operation. Shall the new and existing components be operated, and when are the optimal operation and downtime periods? These questions are often summarized as *unit commitment problem*. Furthermore, how does an optimal operation profile of existing and new components look? This is usually referred to as *economic dispatch*. These questions can be answered with mathematical *optimization* models for the *operation* and *design* of industrial energy systems, which is the focus of this thesis.

In general, the method of mathematical programming can also be applied to further industrial challenges and questions. Besides the former mentioned *design and operational optimization*, further industrial optimization applications are *Heat Exchanger Network Synthesis* and *Scheduling*. In *Heat Exchanger Network Synthesis* models, the optimal heat recovery for a given set of hot and cold streams is determined. *Scheduling* problems aim at finding an optimal sequence of tasks in production systems.

Against the backdrop of the introduced changes in the energy sector, mathematical optimization answering industrial energy supply design and operation questions, as presented in this thesis, became a powerful tool with several advantages. For example, such advantages are explained, e.g., in Kallrath (2013). One significant advantage of using a mathematical optimization model as a **decision-support tool** in industry is the increased knowledge and awareness of the analyzed (sub)system. This increased system and process knowledge results from the formulation and setup of the model itself and all tasks required to achieve this goal. Also, such optimization models **provide quantitative assessments** to support decision-making. Last but not least, once a comprehensive model is set up, several variations of this model can be **calculated as scenarios** without the need to redefine the model or rebuild a new model for every new scenario. For these scenarios, settings and parameters in the (original) model are varied.

However, by appropriate modeling, not only technical characteristics but also logical aspects can be integrated into the optimization process. A relevant example is the concept of flexibility. Nevertheless, flexibility is more complicated to assess than other criteria, such as costs or emissions. To include flexibility in industrial optimization applications, it is necessary to understand the different types of flexibility as well as the drivers of these types, and adapt all components of optimization models appropriately.

The following subsections present the applied methods and elaborated issues in this thesis. Starting with an overview of design and operation optimization with mixed-integer linear programming, the concept of flexibility is also discussed from different perspectives. Finally, an overview of technologies and their relevance for (i) industrial energy supply and (ii) flexibility of energy supply systems is presented.

2.1 Mixed-Integer Linear Programming for Design and Operation Optimization of Industrial Energy Systems

Mixed-integer linear programming is a common approach to formulating mathematical optimization models and provides decision support for industrial actors. Compared to other programming approaches, e.g., linear programming without integers or non-linear (integer) programming, mixed-integer linear programming has several advantages.

- By introducing integer variables, more detailed modeling, in terms of technical characteristics and considering logical decisions, is possible compared to *linear programming*. However, this higher level of detail typically goes hand in hand with higher complexity and computational resources required.
- It also has advantages compared to *heuristic optimization models*. First, mixed-integer linear programming guarantees convergence towards a global optimum. Second, for every step within the optimization process, the solution accuracy can be determined with the indicator *optimality gap* (Wolsey 1998).
- Finally, the available solvers for mixed-integer linear programming formulations are typically rather efficient especially compared to solvers for *(mixed-integer) non-linear programs*. Thus, mixed-integer linear programming typically requires less computational resources than non-linear models (Epelle et al. 2020). Those efficient mixed-integer linear programming solvers have greatly improved over the last decades (Koch et al. 2022). Common, commercial examples for **mixed-integer linear programs** are, for instance, *Gurobi* (Gurobi Optimization 2021) or *CPLEX* (Cplex 2009). Well-known, open-source solvers are, for instance, *Cbc* (John Forrest et al. 2023), or *HiGHS* (Huangfu et al. 2018).

The general workflow of solving optimization problems can be divided into the following tasks:

Problem formulation An experienced applicant with the relevant domain knowledge formulates the equations describing all components of the considered system. Attention is paid to using the proper variable types and equations (e.g., linear, non-linear, etc.) so that the formulation corresponds to the relevant problem class.

Problem translation The equations set up by the user are then brought in a form a specific solver can process in the next step. This process can be done with toolboxes for general programming languages, e.g., Yalmip (Löfberg 2004) for Matlab (The Mathworks Inc 2016) or Pyomo (Hart et al. 2011; Bynum et al. 2021) for Python. Alternatives are specific modeling languages such as AMPL (A Mathematical Programming Language) or GAMS (General Algebraic Modeling Systems).

Problem solution This step is performed with a solver that uses appropriate algorithms to solve the given problem with a specific structure. Examples of common solvers have been presented above. Algorithms implemented in those solvers are, for example, the simplex method, the barrier interior point method, the branch and cut algorithm, or cutting planes.

Interpretation of results In this step, again, the applicant gets in action and interprets the values for the defined decision variables, the value of the objective function, and further derived performance indicators.

Industrial energy supply in a modular mixed-integer linear programming framework

The following is an overview of a modular and, thus, adaptive approach to setting up mixed-integer linear mathematical optimization models for industrial design and operational optimization. As presented by Kallrath (2013), optimization models consist of the following key objects:

Variables These are also called decision variables and are understood as initially non-determined values for time series or scalars. Variables represent direct and derived decisions that are made within the course of the optimization to minimize or maximize a previously defined criterion that is formulated as the objective function. Different variable types are possible. Examples of variable types are, e.g., continuous variables, integer variables, or binary variables. Furthermore, so-called slack variables can also be included in models to allow an efficient detection of unfulfilled constraints.

Constraints The limitations and requirements of the depicted system are expressed as mathematical equations in the optimization model. In such constraints, customized, predefined, and predetermined parameters, e.g., lower and upper bounds for decision variables, can be applied, and the technical and logical characteristics of components in the system can be expressed.

Objective Function The objective is a defined criterion that shall be minimized or maximized and is expressed as a function of the set-up decision variables and defined parameters.

A general formulation for mixed-integer linear programs is presented by Kallrath (2013) and shown in Eq. (1).

$$
\begin{aligned}
\min \quad & f(\mathbf{x}, \mathbf{y}), \\
\text{subject to} \quad & \mathbf{h}(\mathbf{x}, \mathbf{y}) = 0, \\
& \mathbf{g}(\mathbf{x}, \mathbf{y}) \geq 0, \\
\mathbf{h} : X \times V \to R^{m_e}, \quad & \mathbf{g} : X \times V \to R^{m_i}, \\
\mathbf{x} \in X \subseteq R^{m_c}, \quad & \mathbf{y} \in V \subseteq Z^{m_d}.
\end{aligned} \tag{1}
$$

For mixed-integer linear programs, the objective function to be minimized $f(\mathbf{x}, \mathbf{y})$ as well as m_e equality and m_i inequality constraint functions $h_e(\mathbf{x}, \mathbf{y})$ and $g_i(\mathbf{x}, \mathbf{y})$ in Eq. (1) are linear functions. Furthermore, $\mathbf{x}$ and $\mathbf{y}$ are m_c continuous and m_d integer decision variables. In the further course of this section, all integer decision variables are binary decision variables with $V = \{0, 1\}^{m_d}$.

When translating real industrial energy supply systems into (simplified) mathematical optimization models, the overall system can be divided into the subsequent main components. It can be distinguished between **units**, which are understood as components with ports that can be connected and related to each other in the second main component — the **nodes**. With those two main component groups, which are described in the following, a modular framework is enabled.

Units in optimization models Typically the components of type *unit* either provide, convert, or consume energy. Thus, most of the modeling equations for the component *unit* consider technical details. However, also logical conditions can be modeled for the component *unit*. *Units* usually have all three key objects of optimization models — variables related to that unit, constraints to model the behavior and characteristics of the specific unit, and a contribution to the objective function. In the following descriptions, the different types of units are described and their relevance for this thesis and the publications of this work with a focus on the core publications Papers 1-4 in Chapter Outlook for further research) is discussed. Also, the most relevant equations — concerning this thesis — to model industrial energy supply systems in mathematical optimization are presented. Thus, in general, the considered time horizon is denoted by set $\theta = \{1, ..., T\}$, and the time is indexed by t. For simplicity reasons, it is assumed in the next paragraphs that the total duration of a year is considered in the optimization model with a timestep duration of Δt =h.

Adaptable in- and outputs of the considered system These are often also referred to as supplies or demands and have either in- or output ports. Often only one port is required and used in modeling those components. Thus, at least one time series of decision variables is required, e.g., $sup_s(t)$ for the supply of an energy source s out of set σ or $dem_d(t)$ for the demand d out of set δ. These units often represent the considered system boundaries — consumed energy sources from external providers and demands of the production process or external entities that are fulfilled. Typical examples of sources and demands included in the core publications of this thesis (Panuschka et al. 2018; Panuschka et al. 2019; Knöttner et al. 2022; Knöttner et al. 2024) are electricity from spot markets, including grid connection or renewable generation, fuels such as natural gas, biomass, or renewable gases, as well as steam, power, or district heating demands.

Conversion and storage units These units typically have ≥ 1 in- **and** outputs modeled with several timeseries of continuous and binary decision variables. These variables are related to each other to model the technical characteristics of the unit. A typical set of operational decision variables for an energy conversion unit u out of set υ are:

- Binary decision variable to model the online state of the unit for every timestep $on_u(t)$
- Binary, e.g. in Morales-Espana et al. (2013b), or continuous decision variable, constrained so that it can only take values of 0 and 1, compare Morales-Espana et al. (2013a), to model the start-up of the unit for every timestep $su_u(t)$
- Binary, e.g., in Morales-Espana et al. (2013b), or continuous decision variable, constrained so that it can only take values of 0 and 1, compare Morales-Espana et al. (2013a), to model the shut-down of the unit for every timestep $sd_u(t)$
- Continuous decision variable(s) to model energy-related in- and outputs of the unit for every timestep. Typical examples are fuels $f_u(t)$, electric power $p_u(t)$ and heat $q_u(t)$. Depending on the type of unit, further decision variables might be required.

For design decisions to be made in the optimization model, further scalar decision variables for integrating the unit i_u and its capacity cap_u are added to the model.

For storage units, typically, similar scalar design decision variables are used. For operational behavior, at least time series for charging power $c_u(t)$, discharging power $d_u(t)$ and the state of charge $soc_u(t)$ are required. Depending on the complexity of the storage system, even more variables might be necessary.

Typical examples included in the core publications of this thesis (Panuschka et al. 2018; Panuschka et al. 2019; Knöttner et al. 2022; Knöttner et al. 2024) are different types of boilers or turbines, heat pumps as well as thermal storage and electric storage such as batteries.

The following paragraphs give an overview of **typical constraints and contributions to the objective function**. All of the following equations are applied at least in one of the core publications that build the basis of this thesis. Such constraints and objective contributions are used to model and express the characteristics of supplies, energy conversion units such as boilers, turbines, heat pumps, etc., and energy storage in combined operation and design optimization problems. In the case of exclusive operation optimization for some of the following equations, tighter and more compact formulations would be possible.

Integration and capacity of new conversion and storage units The required equations (Halmschlager et al. 2022) for the integration and capacity decision of new units such as boilers or turbines are shown in the following.

$$i_u \cdot par_{u,\text{cap}}^{\min} \leq cap_u \leq i_u \cdot par_{u,\text{cap}}^{\max} \tag{2}$$

$$C_{\text{invest}} = a \cdot \sum_{u \in \upsilon} (c_{u,\text{fix}} \cdot i_u + c_{u,\text{spec}} \cdot cap_u), \tag{3}$$

where a is the so-called annuity factor considering the depreciation period N in years and the corresponding interest rate r. The calculation of the annuity factor is shown in Eq. (4). The unit's investment costs are further modeled with a fixed cost factor $c_{u,\text{fix}}$ and a specific cost factor $c_{u,\text{spec}}$. In the special case that the new component has neither a minimum size nor a fixed cost factor, the modeling does not require variable i_u.

$$a = \frac{(1+r)^N \cdot r}{(1+r)^N - 1} \tag{4}$$

In addition to non-recurring investment costs, which can be converted into annual costs using the annuity factor, see Eq. (3), annual costs can also be incurred for maintaining the operating status. These fixed operation costs $C_{\text{fixoperation}}$, e.g., for service and maintenance, are usually expressed as a percentage of the investment costs per year, e.g., $par_{u,\text{fixop}} = 5\%_{\text{inv}/a}$.

$$C_{\text{fix,operation}} = \sum_{u \in \upsilon} par_{u,\text{fixop}} \cdot (c_{u,\text{fix}} \cdot i_u + c_{u,\text{spec}} \cdot cap_u) \tag{5}$$

This feature is included in two core publications of this thesis: Knöttner et al. 2022 and Knöttner et al. 2024.

Logic constraints for operation of conversion units The following formulation was first published in 1962 by Garver (1962) and has been applied as a constraint in several tight and compact mixed-integer linear programming formulations, e.g., a general tight and compact formulation (Morales-Espana et al. 2013b), a tight and compact formulation of start-up and shut-down ramping (Morales-Espana et al. 2013a) and a tight and compact formulation for the power-based unit commitment problem (Morales-España et al. 2015). This constraint guarantees that the start-up and shut-down variables take appropriate values for unit operation condition changes between the on- and offline state. Furthermore, this formulation forces the decision variables su_u and sd_u to take binary values even when defined as continuous variables in the range of $[0, 1]$ (Morales-Espana et al. 2013a). Eq. (6) is highly relevant for units with a high number of timesteps for the start-up. In optimization problems with a timestep duration of one hour, boilers with solid fuels have long start-up and shut-down durations. For shorter timesteps, boilers with liquid and gaseous fuels or heat pumps and turbines typically have start-up durations longer than one timestep, too.

$$on_u(t) - on_u(t-1) = su_u(t) - sd_u(t). \tag{6}$$

The variable indicating the online state on_u can also be used to express variable operation costs of the conversion units related to every timestep that the unit is online. Such costs are incurred, for example, for personnel costs caused by ongoing plant operations. Thus, the are referred to as staff costs C_{staff}

$$C_{\text{staff}} = \sum_{t\in\theta} \sum_{u\in\upsilon} (c_{u,\text{staff}} \cdot on_u(t)), \tag{7}$$

where $c_{u,\text{staff}}$ are the specific costs for every hour of operation of unit u.

Typical formulations for start and shutdown costs, in the following, referred to as start costs C_{start} can be modeled with the other two binary decision variables su_u and sd_u.

$$C_{\text{start}} = \sum_{t\in\theta} \sum_{u\in\upsilon} c_{u,\text{startup}} \cdot su_u(t) + c_{u,\text{shutdown}} \cdot sd_u(t), \tag{8}$$

where $c_{u,\text{startup}}$ and $c_{u,\text{shutdown}}$ are the specific costs for starts and shutdowns of unit u.

Minimum up- and down-time constraints: Energy conversion units $u \in \upsilon$ are modeled with minimum up and down times $\tau_{u,\text{up}}$ and $\tau_{u,\text{down}}$ in periods. The formulation in Eq. (9) and Eq. (10) for units with minimum up and down times and start-up costs is proposed by Rajan et al. (2005).

$$\sum_{k=t-\tau_{u,\text{up}}+1}^{t} su_{u,k} \leq on_u(t) \quad \forall t \in [\tau_{u,\text{up}}, T] \tag{9}$$

$$\sum_{k=t-\tau_{u,\text{down}}+1}^{t} sd_{u,k} \leq 1 - on_u(t) \quad \forall t \in [\tau_{u,\text{down}}, T] \tag{10}$$

This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024.

Generation

$$q_u(t) \leq par_{u,\text{cap}}^{\max} \cdot on_u(t) \quad \forall t \in \theta, \tag{11}$$

$$q_u(t) \geq cap_u \cdot par_{u,\text{partload}}^{\min} - par_{u,\text{cap}}^{\max} \cdot par_{u,\text{partload}}^{\min} \cdot (1 - on_u(t)) \quad \forall t \in \theta, \tag{12}$$

For the special case of exclusive operation optimization, the generation, e.g., of heat $q_u(t)$, can be modeled with Eq. (13). This tight and compact formulation ensures that the output equals zero at the beginning and end of the unit's online state. Furthermore, part-load characteristics are ensured with this constraint.

$$\begin{aligned} &cap_u \cdot par_{u,\text{partload}}^{\min} \cdot (on_u(t) - sd_u(t+1)) \leq q_u(t) \leq \\ &cap_u \cdot par_{u,\text{partload}}^{\max} \cdot (on_u(t) - sd_u(t+1)) \qquad \forall t \in \theta, \end{aligned} \tag{13}$$

where $par_{u,\text{partload}}^{\min}$ and $par_{u,\text{partload}}^{\max}$ are parameters indicating the relative minimum and maximum part-load share related to the unit's capacity.

In addition to Eq. (5) and Eq. (7), a third operational expense type for energy conversion (and storage) units can occur. This variable operational costs term $C_{\text{var,operation}}$ includes operational costs related to the produced energy of that unit. It is calculated by using the parameter $c_{u,\text{varop}}$ for specific costs of produced energy in unit u and can be given for instance, in €/MWh$_{\text{el}}$ or €/MWh$_{\text{th}}$. As the energy vector of produced energy might vary for different units, the general decision variable dv is used in the following equation. This variable indicates the produced power per timestep. Thus, the model's timestep duration Δt must be included in the cost function to ensure the correct units.

$$C_{\text{var,operation}} = \Delta t \cdot \sum_{t \in \theta} \sum_{u \in \upsilon} (c_{u,\text{varop}} \cdot dv_u(t)) \tag{14}$$

This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024.

Ramping Also, constraints for changing generated outputs, such as heat or power in two consecutive periods, are implemented. Here, two modeling attempts are possible. First, using parameters for absolute ramping limits in MW per timestep is possible. Second, setting up the constraint with relative changing limits in percent of installed capacity is applicable. The latter formulation is shown in Eq. (15) where $par_{u,\text{ramp}}^{\text{up}}$ and $par_{u,\text{ramp}}^{\text{down}}$ are the maximum relative ramp-up and ramp-down changing rates of unit u. The following equation is shown for a unit providing heat but can also be applied to other outputs, such as electric power.

$$-par_{u,\text{ramp}}^{\text{down}} \cdot CAP_u \leq q_u(t) - q_u(t-1) \leq par_{u,\text{ramp}}^{\text{up}} \cdot CAP_u \quad \forall t \in \{2, ..., T\} \tag{15}$$

This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024. However, as the first two consider exclusive operational optimization, ramping constraints and especially valid parameters for ramping are significant there.

Conversion As the generic term for this plant group of *conversion units* already indicates, the input-side energy sources are converted into other energy sources in these plants. Thus, additional constraints are required to express the relation between the in- and outputs of the respective unit. The actual constraint depends on the technology of the actual unit — e.g. whether it is a boiler, a turbine, a heat pump, etc. A general and simple example with the conversion factor par_u^{cf} of unit u is shown in Eq. (16).

$$f_u(t) \geq par_u^{\mathrm{cf}} \cdot q_u(t) \tag{16}$$

In the example in Eq. (16) the conversion factor par_u^{cf} corresponds to the inverse efficiency $\frac{1}{\eta_u}$ of unit u. For technologies with higher complexity, the binary operation variables could also be included in the conversion constraints.

This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024.

Storages For storage modeling, a formulation for generic and ideal deterministic storages is described in Pozo et al. (2014) with the following characteristics and parameters:

- Constant charging $par_{u,\mathrm{charge}}^{\mathrm{eff}}$ and discharging $par_{u,\mathrm{discharge}}^{\mathrm{eff}}$ efficiencies apply for the entire storage range
- No hysteresis in charging or discharging is considered.
- Charging and discharging occur at constant power within one optimization timestep
- No up or down ramp limitations occur. Any value is possible between no and full loading $par_{u,\mathrm{charge}^{max}}$ and discharging $par_{u,\mathrm{discharge}^{max}}$, respectively.)

$$\begin{aligned} soc_u(t) = &(1 - par_{u,\mathrm{storage}}^{\mathrm{eff}}) \cdot soc_u(t-1) + \\ &\Delta T \cdot \left(par_{u,\mathrm{charge}}^{\mathrm{eff}} \cdot c_u(t) - \frac{1}{par_{u,\mathrm{discharge}}^{\mathrm{eff}}} \cdot d_u(t) \right) \quad \forall t \in [2, T] \end{aligned} \tag{17}$$

$$par_{u,\mathrm{soc}}^{\min} \cdot CAP_u \leq soc_u(t) \leq par_{u,\mathrm{soc}}^{\max} \cdot CAP_u \tag{18}$$

$$0 \leq c_u(t) \leq par_{u,\mathrm{chargemax}} \tag{19}$$

$$0 \leq d_u(t) \leq par_{u,\text{dischargemax}} \tag{20}$$

Contributions to the costs can be modeled analogously to the formulations for energy conversion units presented above for investment costs and operations costs. Staff costs cannot be modeled due to the absence of binary operation variables for the storage. However, if such a cost contribution is required in modeling, binary decision variables and the respective contribution to the costs can be included in the model.

This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024.

Supplies Like the limitation of heat or power generation in conversion units, the supply sup_s of source s is constrained. The most common way is to limit it by an upper bound, as shown in Eq. (21).

$$0 \leq sup_s(t) \leq par_{s,\text{cap}}^{\text{max}} \quad \forall t \in \theta \tag{21}$$

For more complex requirements, further constraints are possible. Some examples are extensions of existing upper limits, including fixed and/or variable, specific costs for this extension, which could be modeled.

Usually, for the *supply* components in a model, cost contributions occur for the consumed amount of the respective supply. In the context of energy supply systems, typically, energy costs occur. Energy costs typically vary over different time horizons, including years, seasons, months, or even (quarter-) hours. Thus, the specific energy source costs $c_{s,\text{energy}}$ are explicitly included as a time series.

$$C_{\text{energy}} = \Delta t \cdot \sum_{t\in\theta} \sum_{s\in\sigma} c_{s,\text{energy}}(t) \cdot sup_s(t) \tag{22}$$

Another often modeled contribution to the cost function is costs for energy consumption that are related to the highest value of consumption over the considered period. Practical examples are grid usage fees for grid-bound energy carriers — besides an energy-related share that can be included in $c_{s,\text{energy}}$ they often also have a power-related cost component $c_{s,\text{power}}$.

$$C_{\text{power}} = \sum_{s\in\sigma} c_{s,\text{power}} \cdot \max(sup_s(t)) \tag{23}$$

This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024.

Further constraints Depending on the context, several further constraints are possible. A non-exhaustive collection with examples from the energy supply sector is listed below:

- Dependency of the operation of two or more units (e.g., heat recovery boilers must not operate if gas turbines are shut down). This feature is included in all four core publications of this thesis: Panuschka et al. 2018, Panuschka et al. 2019, Knöttner et al. 2022 and Knöttner et al. 2024.
- Overall emissions from different sources are limited with a specified bound. This feature is included in Knöttner et al. 2024.

The supply component, however, can be further adapted. Further cost parameters, e.g., staff costs with time-dependent cost time series or emission costs, can be integrated into the supply components described here. While staff costs would probably be modeled in a separate supply component, emission costs are usually directly related to an energy-carrier-specific conversion factor (e.g., in kilograms of carbon dioxide per kilowatt-hour of the energy source) to the consumption of a specific source.

Nodes in optimization models Normally nodes consist only of constraints and are often used to model energy balances and relations. In the integrated constraints of the nodes, the nodes' left and right sides are related to each other; see Eq. (24) where the relation between the left and right side is generally expressed as •.

$$\sum_{dv} dv_{n,\text{lhs}}(t) \quad \bullet \quad \sum_{dv} dv_{n,\text{rhs}}(t) \forall \quad t \in \theta \quad n \in \nu \tag{24}$$

The possible options for this relation (•) are (i) equality (==), (ii) inequality with the left side smaller equal (≤) than the right side, or (iii) inequality with the left side greater equal (≥) than the right side.

A useful feature, especially in model creation, testing, and debugging, is the definition of non-physical helper variables, often also referred to as slack variables. Slack variables sl are defined for both the left-hand side (subindex $_{\text{lhs}}$) and right-hand side (subindex $_{\text{rhs}}$), see Eq. (25) and Eq. (25).

$$sl_{n,\text{lhs}}(t) \geq 0 \qquad \forall \quad t \in \theta, \quad n \in \nu \tag{25}$$

$$sl_{n,\text{rhs}}(t) \geq 0 \qquad \forall \quad t \in \theta, \quad n \in \nu \tag{26}$$

Consequently, Eq. (24) needs to be updated to the final formulation of the equation in each node n, Eq. (27). The newly introduced slack variables allow closing a previously non-closed balance (constraint) of the right and left sides of a node. A practical example would be providing additional energy if more energy is required (left side) than provided (right side). Thus, these variables are indispensable in model setup, testing, and debugging.

$$sl_{n,\text{lhs}}(t) + \sum_{dv} dv_{n,\text{lhs}}(t) \quad \bullet \quad sl_{n,\text{rhs}}(t) + \sum_{dv} dv_{n,\text{rhs}}(t) \qquad \forall \quad t \in \theta \quad n \in \nu \tag{27}$$

These slack variables usually do not have a physical counterpart. Thus, an overarching aim is to keep them as small as possible — ideally zero. The following approach is chosen to realize their minimization during the solving process. The introduced slack variables contribute to the objective function with a high specific cost parameter M leading to $C_{\text{slack}} >> C_{\text{energy}}$ for slack variables ≥ 0 which indicates an infeasible system. This is also referred to as *big-M-formulation* and shown in Eq. (28).

$$C_{\text{slack}} = M \cdot \sum_{n \in \nu} \sum_{t \in \theta} (sl_{n,\text{lhs}}(t) + sl_{n,\text{rhs}}(t)) \tag{28}$$

Objective function The following cost function, the total costs (TC) in a defined period, represents a typical objective function in optimization. TC can be, e.g., total annual costs in design optimization or daily costs in operational optimization. The objective of TC is applied in all four core publications of this thesis and is thus shown in greater detail below. While in Panuschka et al. 2018 and Panuschka et al. 2019 only operational costs contribute to TC, in Knöttner et al. 2022 and Knöttner et al. 2024 also annualized investments are included to include design decisions.

In Eq. (29), a year is considered as the period for which the TC are evaluated. However, other objective criteria not applied in this work but also of high significance for industrial optimization can also be formulated as objective functions. Common examples are:

- *maximizing profits* — including e.g. aspects such as material and energy costs, production volumes (decision variable), and earnings from sales
- *minimizing material consumption* — including e.g. aspects such as production volumes (decision variable) and specific material needs for production
- *minimizing emissions* — including e.g. aspects such as energy supply (decision variable) and if relevant also production volumes (decision variable or parameter) for production-related emissions occurring for example in the iron and steel sector or for production of ceramics.
- *maximizing output* — including e.g. aspects as production volumes (decision variable).

$$\min \quad TC = C_{\text{invest}} + C_{\text{fix,operation}} + C_{\text{staff}} + C_{\text{start}} + C_{\text{var,operation}} + C_{\text{energy}} + C_{\text{power}} + C_{\text{slack}} \tag{29}$$

$$\begin{aligned}
\min \quad TC = & \underbrace{a \cdot \sum_{u \in \upsilon} (c_{u,\text{fix}} \cdot i_u + c_{u,\text{spec}} \cdot cap_u)}_{C_{\text{invest}}} + \\
& \underbrace{\sum_{u \in \upsilon} par_{u,\text{fixop}} \cdot (c_{u,\text{fix}} \cdot i_u + c_{u,\text{spec}} \cdot cap_u)}_{C_{\text{fix,operation}}} + \\
& \underbrace{\sum_{t \in \theta} \sum_{u \in \upsilon} c_{u,\text{staff}} \cdot on_u(t)}_{C_{\text{staff}}} + \\
& \underbrace{\sum_{t \in \theta} \sum_{u \in \upsilon} (c_{u,\text{startup}} \cdot su_u(t) + c_{u,\text{shutdown}} \cdot sd_u(t))}_{C_{\text{start}}} + \\
& \underbrace{\Delta t \cdot \sum_{t \in \theta} \sum_{u \in \upsilon} c_{u,\text{varop}} \cdot dv_u(t)}_{C_{\text{var,operation}}} + \\
& \underbrace{\Delta t \cdot \sum_{t \in \theta} \sum_{s \in \sigma} c_{s,\text{energy}} \cdot sup_s(t)}_{C_{\text{energy}}} + \\
& \underbrace{\sum_{s \in \sigma} (c_{s,\text{power}} \cdot \max(sup_s(t))}_{C_{\text{power}}} + \\
& \underbrace{M \cdot \sum_{n \in \nu} \sum_{t \in \theta} (sl_{n,lhs}(t) + sl_{n,rhs}(t))}_{C_{\text{slack}}}
\end{aligned} \tag{30}$$

2.2 Flexibility

The trend of increasing incentives for industrial flexibility has already been addressed in the introduction and will be analyzed and discussed in the subsequent subsection. A clear definition, interpretation, and understanding of flexibility of all involved parties are relevant prerequisites for applying and exploiting flexibility. However, a literature review brings up several challenges and pitfalls with the concept of flexibility. The following shows some examples of flexibility in energy and industrial production systems, a discussion of difficulties in using the term *flexibility*, and examples of existing classification approaches.

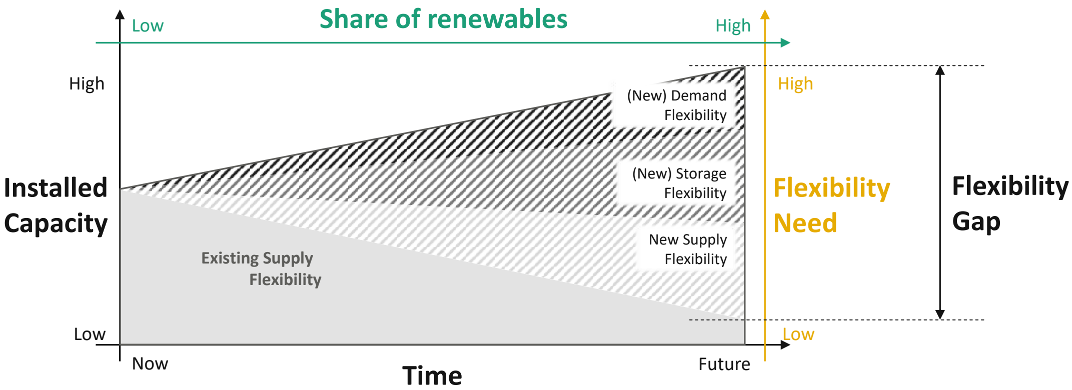

Figure 3: *Visualization of flexibility gap from the power supply system perspective. Source: Knöttner et al. (2024), figure adapted from (Papaefthymiou et al. 2014).*

Wording, definitions and perspectives

An essential and relevant criterion for flexibility in energy systems is **the perspective** from which it is assessed and analyzed. From a high level, e.g., the power (grid) system level, it is assessed as a key feature for successful decarbonization of (electric) energy supply. Phrases, terms, and keywords often used in this context are *grid services*, *fluctuating renewable energy supply*, *thermal power plants*, and the so-called *flexibility gap*. The latter describes how decreasing numbers of conventional thermal power plants and growing shares of renewable electricity generation lead to a significant increase for new flexibility sources and is visualized in Figure 3.

However, if the perspective of industrial companies is considered, flexibility is often used not only for energy supply but also for product types and batch sizes. Furthermore, it is used for other energy carriers than electricity too. The overlaps and differences in the understanding of flexibility from different perspectives are shown schematically in Figure 4.

As indicated in Figure 4, flexibility from demand assets and storages pose possible overlaps of flexibility from the power supply system perspective and the industrial energy system perspective. However, not all aspects of flexibility indicated in Figure 4 overlap. Still, the term *flexibility* is applied to many concepts — presented here and beyond Figure 4. In addition, using the following terms (Degefa et al. 2021) as synonyms or strategies and measures for flexibility occurs often. This synonymous application of the following terms for flexibility might lead to misunderstandings.

- Demand-side management
- Demand (side) response
- Energy storage

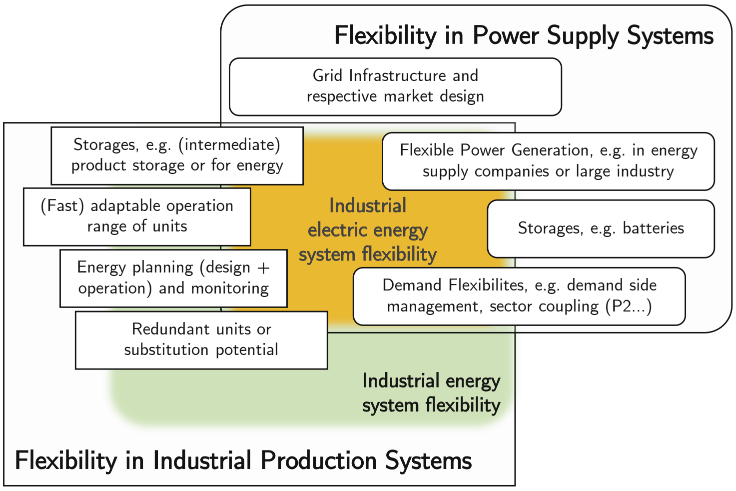

Figure 4: *Exemplary but not exhaustive set of measures to provide flexibility in power supply systems. Source: Knöttner et al. (2024), summarized upright based on (IRENA 2018) and (Papaefthymiou et al. 2014) and measures to increase flexibility in production systems based on (Pierri et al. 2020).*

- Flexible generation

Demand-side management and demand (side) response are partly applied synonymously. However, there are also publications clearly distinguishing between those two – often identifying demand response as a sub-group of demand side management. Although often identified as a demand-side management strategy, in this work *increasing energy efficiency* is not defined as a flexibility measure. On the one hand, efficiency measures are typically one-time measures. They are not activated frequently (Degefa et al. 2021), which makes them inappropriate candidates for readily available flexibility. On the other hand, there are diverse interactions between flexibility and efficiency, making case-by-case assessments necessary. Increasing energy efficiency and increasing flexibility can be countermeasures. This is the case if operation points are changed towards less efficient operation due to the flexibility measure (Degefa et al. 2021).

Furthermore, flexibility, typically of single units, often comes with the part-load operation or fast ramping and over-capacities (Weeber et al. 2017). Part-load operation, fast ramping, or over-capacities do not increase efficiency for many technologies. However, as energy efficiency is reducing the overall load, its impact can be seen as beneficial due to a reduction of the flexibility gap (see Figure(3)) while, at the same time also, the required flexibility resource size could be reduced.

Different studies emphasize the relevance of a **common and clear definition** currently missing. This results in a lack of a common understanding of flexibility. Several definitions are shown below to emphasize the difficulties of having a common understanding.

A general definition of suiting flexibility in different contexts was already given in 2000 by Golden et al. (2000). They identified that flexibility had become an important or even essential requirement. However, when analyzing how information technology impacts flexibility in organizations, they identified no clear definition supporting their work. Therefore, they came up with the following suggestion:

> *...flexibility is defined as 'the capacity to adapt' across four dimensions; temporal, range, intention and focus ...*
>
> (Golden et al. 2000)

Another rather general definition, although made in the context of power supply systems, is presented by Cochran et al. (2014)

> *... put simply, power system flexibility refers to a power system's ability to respond to both expected and unexpected changes in demand and supply ...*
>
> (Cochran et al. 2014)

Another rather general definition from the power system perspective has been presented in a study by IRENA (2018). This definition is as follows:

> *... the capability of a power system to cope with the variability and uncertainty that generation introduces into the system in different time scales, from the very short to the long term, avoiding curtailment of VRE and reliably supplying all the demanded energy to customers ...*
>
> (IRENA 2018)

In the before-mentioned VDI standard (Verein Deutscher Ingenieure e.V. 2020) the following definition of *energy flexibility* is given:

> *... ability of a production system to adapt quickly and in a process-efficient way to changes in the energy market ...*
>
> (Verein Deutscher Ingenieure e.V. 2020)

A systematic approach to flexibility is chosen by Degefa et al. (2021). They published an overview of 16 different power supply system flexibility definitions between 1995 and 2019. Furthermore, they defined three necessary criteria a flexibility definition should have: type of flexibility source, duration of activation, and incentive for flexibility. They analyzed existing definitions regarding those three criteria and assessed them for a majority, either too general or too narrow. Another disadvantage of the current definitions they identified is the orientation of most towards a certain stakeholder group. Degefa et al. understand flexibility as an ability of a flexibility resource (Degefa et al. 2021). Their definition is:

> *… The ability of power system operation, power system assets, loads, energy storage assets, and generators to change or modify their routine operation for a limited duration and respond to external service request signals without inducing unplanned disruptions. …*
>
> (Degefa et al. 2021)

From the presented definitions, one can conclude that flexibility has mostly been assessed from a power supply system perspective in the past. Industry plays an increasingly significant role in power supply systems. However, the industrial perspective on flexibility is more extensive than the contribution to the power supply system. Luo et al. (2022) presented a conceptual framework to evaluate the flexibility of chemical processes going beyond the definition of flexibility from the power supply system perspective. In their work, they summarize five general types of flexibility that can be applied to both the industrial production system itself but also to the industrial energy supply system:

- Feedstock flexibility (vary change in quality or quantity of inputs)
- Product flexibility (enable different product properties)
- Volume flexibility (ability to modify throughput)
- Scheduling flexibility (adaptation to resource allocation)
- Production flexibility (enable to change production schemes)

Furthermore, Luo et al. (2022) show that when speaking of flexibility, three cases can occur. First, use different terms for one concept (e.g., fuel and load flexibility for flexibility regarding changes for input and output streams). Second, only one specific term is applied for one concept (e.g., scheduling flexibility as adjustment ability of resource allocation to different production cycles). Third, the same term is used for different concepts (e.g., plant flexibility summarizes all flexibility types in one plant.)

Classifications for flexibility from the power supply perspective

When comparing definitions of flexibility and flexibility types from different perspectives and references, one can see that creating one single comprehensive overview that includes all aspects of flexibility becomes quite challenging. Nevertheless, the drive to classify, systematize, characterize, etc., consistently is huge. Several publications aiming to find comprehensive conceptualization have been presented (Verein Deutscher Ingenieure e.V. 2020; Degefa et al. 2021; Luo et al. 2022; Tristán et al. 2020; Blue et al. 2020). The relevance of suitable classifications and understanding of all included parties is indispensable, especially if flexibility from medium to small actors (e.g., industry) shall play a significant role in the future.

An exhaustive approach for a taxonomy of **energy flexibility in the power supply system**, the practice, and the science of classifications, is presented by Degefa et al.

(2021). According to them, a taxonomy can build the basis of organizing and identifying flexibilities taking different perspectives into account.

First, they show how several previous classification approaches for flexibility in power supply systems have been set up.

Generally, flexibility resources can be classified according to the **flexibility characteristics**, where technical and economic characteristics are distinguished. Examples of the former are quantitative, qualitative, and controllability parameters. The quantitative parameters are often directly applied in the modeling of physical units and include, for instance, ramping capacities and minimum on- and offline times (recovery times). Such technical, quantitative parameters and (performance) indicators are also presented and categorized in Dotzauer et al. (2019) when they assess demand-driven power generation from biogas plants. The latter include typical costs related to the flexibility resources distinguishing between capital and operational expenditures for the flexibility. Capital expenditures can be required for technology investment and installation or to set up relevant communication. Operational expenditures are caused by activation costs or costs for fuels or other energy carriers.

A common, already more extensive classification approach is the grouping based on the **flexibility resources**. Subgroups of this classification can be classified according to:

- Their place in the electricity supply chain: supply, demand, networks, storage, or markets
- Their roles of flexibility in the power supply system: concept 1 — sources and enablers, concept 2 — technical and organizational measure
- Their direction of load shifting: advance of energy consumption, delay of energy consumption, advance or delay of energy consumption, reduction of energy consumption
- Their mathematical properties for modeling: buckets — power and energy-constrained integrators (e.g., refrigeration units), batteries — power and energy-constrained integrators with a certain filling level by a certain time (e.g., electric vehicles), or bakeries — a batch process with a required finish time (e.g., large industrial sites)

Another approach is grouping by **other aspects of flexibility**. Some examples of possible subgroup classifications are based on (i) the control mechanism (central vs. distributed), (ii) the offered motivation (price- vs. incentive-based), (iii) the decision variable (schedule the activity vs. control the power in real-time), (iv) their availability (potential resource, actual resource, reserve, market-available reserve), (v) the need (power, energy, transfer capacity vs. voltage), (vi) the activation method (explicit vs. implicit), and (vii) the activating actor (transmission system operators, distribution system operators, or commercial parties).

Based on their analysis and the identified existing classifications, they propose their own (more) comprehensive classification approach. Degefa et al. (2021) suggest the following classification for **flexibility solutions** incorporating several aspects presented above.

1 Flexibility resources with the subgroups of flexibility assets (demand, supply, and storage) and operational flexibility

2 Enablers with the subgroups market, regulation, grid hardware, and grid interconnection

Although this work does not include all energy systems perspectives, as mentioned above, it shows how to approach a comprehensive classification. Thus, this approach shows potential for future expansion for more levels of the energy system.

Integration of flexibility in mathematical programming

The challenge of integrating flexibility in mathematical programming applications can be summarized as follows. First, a clear definition is lacking. Second, flexibility is a relative feature of a system (either a unit or a set of units). Thus, integrating flexibility directly into an objective function is not straightforward. Several approaches can be found in the literature aiming at the integration of flexibility in optimization. Typical strategies here are the following:

Include technical flexibility in component modeling Features such as ramping speed, the operation range of the unit, or minimum on- and offline times are implicitly integrated into the optimization model by formulating the corresponding constraints.

Calculation of operating scenarios Within the optimization model several operating scenarios are considered simultaneously and therefore certain flexibility types can be included directly in the optimization model.

Post-optimization performance indicators For different configurations, performance indicators are evaluated from the optimal solution. These performance indicators are compared, and thus, conclusions on more or less flexible configurations can be drawn

2.3 Technologies for Industrial Energy Supply and their Relevance for Flexibility

The core publications of this thesis include energy supply technologies and relevant components and influencing factors at different layers of an industrial site. These are visualized in Figure 5 and can be described as

(i) industrial process level requesting electricity, heating, and cooling,

(ii) on-site energy supply such as storages and energy conversion technologies (boilers, heat pumps, turbines, etc.),

(iii) off-site energy supply, including technologies, grids, regional renewable production and

(iv) as an additional layer: further stakeholders leading to legislative, social, or other influences on the holistic energy supply system.

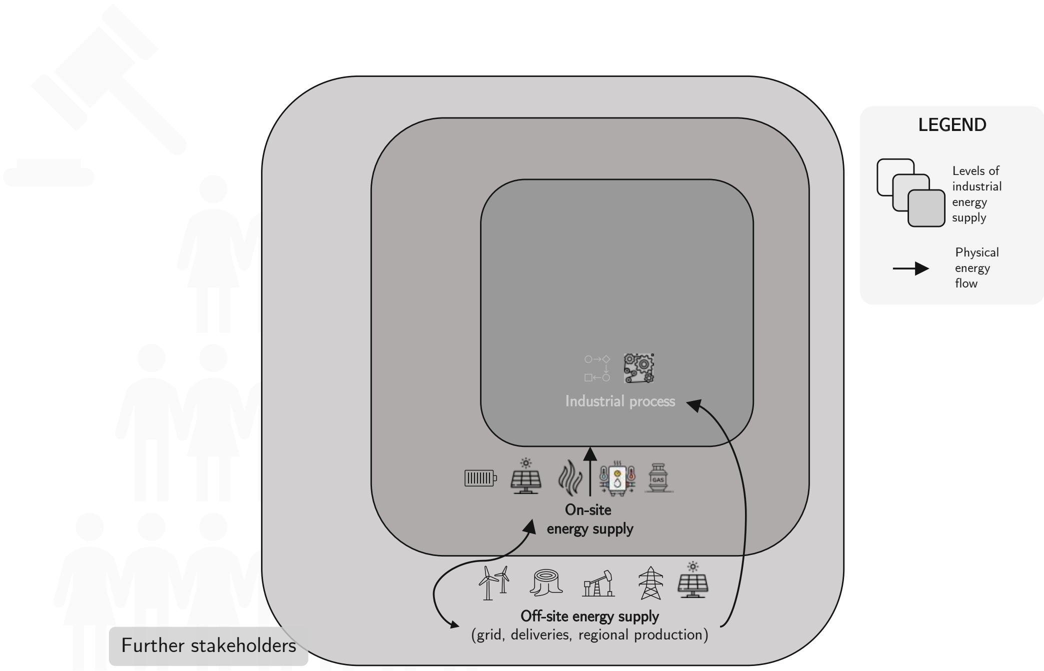

Figure 5: *Stratified visualization for energy supply-related industrial layers.*

Typical examples and an indication about the respective flexibility of established and new energy supply components in industrial systems and their relevance for flexibility are shortly described in Subsection 2.3. More details are summarized in Appendix A of this work.

Typical industrial energy system components

In the past, common technologies in industrial energy supply systems were, for instance, grid connection for electricity or fuels, direct heat consumption from external heat or steam suppliers, and boilers for liquid and gaseous fuels. Boilers for solid fuels, e.g., coal, biomass, or internal and external residues, can also be found in specific industrial sectors, e.g., wood and bark boilers in the wood-processing or pulp and paper industry. This boiler subgroup is characterized by little operational flexibility (a change of the operation point of heat production) compared to liquid or gaseous fuel-fired boilers.

Due to changing frame conditions on electricity and balancing service markets leading to new incentives for flexibility in the power systems, a boiler sub-group, the so-called power-to-heat boilers, can be found more often in industrial energy systems. In those flexible operating, fast-ramping units, electricity is used instead of fuel to provide hot water or steam at the required temperature. With this technology, which is considered as a demand from the perspective of the power supply system, different contributions to flexibility can occur. They are often used to provide ancillary services to the electricity grid. Also, (energy) production flexibility is possible when the energy carrier provision of the power-to-heat boiler can be substituted, e.g., with a gas boiler. This results in feedstock (fuel) flexibility of the overall energy supply system. Benefits from this flexibility type are often realized by generation adaption to spot market prices.

Further typical examples, especially in large industrial sites, often from energy-intensive sectors, are steam or gas turbines or combined cycle units. Depending on the actual realization, their degrees of freedom and, thus, their flexibility for process supply and energy markets differ.

Depending on the process needs also, chillers (e.g., in the food or chemical sector) as well as kilns (usually in the metal or non-metallic mineral sector) can be found in industrial energy systems. Those units are often strongly linked to the production process (kilns) or quality aspects (cooling), which limits the flexible operation.

Renewable power generation such as hydro-power or photovoltaics has also been included in industrial energy supply systems, subject to the available local and regional potentials. Such technologies, often characterized by fluctuating generation profiles, often require increased flexibility from the remaining energy supply system.

On-going developments and an increasing interest in partly counteracting goals such as flexibility, efficiency, competitiveness, sustainability, and decarbonization have enlarged the options for applied energy sources and energy supply technologies. Thus, from a modeling perspective, the integration and formulation of new technologies and features might be required. A non-exhaustive list of energy supply system technologies with increasing importance can be found in the following. Multi-fuel boilers allowing the usage of different fuels, (large) renewable power-purchase agreements requiring even more flexibility in demand and generation as well as direct and indirect heat recovery, often driven by the goal of sustainability and efficiency increase.

Further, energy sources and supply technologies not considered in the papers belonging to this thesis but with (increasing) relevance and interest for industrial applications are, e.g., geothermal heat supply — directly or as the source for heat pumps –, and hydrogen-related technologies such as electrolyzers and fuel cells.

Modeling features for industrial energy system technologies

The basic mathematical optimization formulations for operation and design modeling of different technologies presented above in Subsection 2.1 can be used for a wide range of the described technologies. Furthermore, strategies of how to include flexibility in mathematical optimization are shortly discussed in Subsection 2.2. By applying features such as generation and ramping in a model, the first strategy presented above *include technical flexibility in component modeling* and thus a relevant aspect of flexibility has already implicitly been included in several existing optimization formulations.

Several of those presented features and formulations have originally been proposed and used for typical units from the power generation sector in classic unit commitment and economic dispatch problems, e.g., for combined heat and power plants with boilers, gas turbines, and steam turbines. These technologies are also the technological main focus of Paper 1 (Panuschka et al. 2018) and Paper 2 (Panuschka et al. 2019) of the core publications in this thesis.

However, in general, the formulations presented are generic, focusing on features of technologies and sources. Thus, they are adaptable to a large set of industrial energy supply technologies, including innovative new technologies. Examples included in publications of this thesis of such technologies with upcoming relevance for future industrial energy supply are,e.g., photovoltaic modules, (high-temperature) heat pumps, multi-fuel boilers, but also contractual structures such as power-purchase agreements for renewable generation systems. They are modeled, e.g., in core publications Paper 3 (Knöttner et al. 2022) and Paper 4 (Knöttner et al. 2024) of this thesis.

3 Problem Statement

Current challenges for industrial energy supply were described in the introduction. Among others, mathematical optimization, especially mixed-integer linear programming, evolved to be a promising method to answer questions concerning future developments, e.g., increased flexibility needed or required decarbonization and efficiency increase. Not only (future) operations in existing but also in new or retrofitted energy systems raise several questions.

Flexibility in Industrial Optimization: The term flexibility is widely used in contexts of (electric) power systems, industrial energy systems, and industrial production processes. For several reasons, e.g., increasing share of renewable electricity generation or independence of fossil fuels, flexibility in industrial systems has become more important over the last years. An exemplary (but still incomprehensive) list of measures of how flexibility can be included in mathematical optimization is:

- involving fluctuating prices, generation, or demands in the model (e.g. **Paper 1 - Paper 4** (Panuschka et al. 2018; Panuschka et al. 2019; Knöttner et al. 2022; Knöttner et al. 2024)),
- defining and modeling a (comprehensive) superstructure with a wide range of industrial supply options (e.g. **Paper 1 - Paper 4** (Panuschka et al. 2018; Panuschka et al. 2019; Knöttner et al. 2022; Knöttner et al. 2024)),
- considering prediction uncertainty or analyzing the impacts of storage integration (e.g. **Paper 2** (Panuschka et al. 2019)).

The fact that different approaches are possible to consider various types of flexibility leads to a need for a more general and holistic perspective on industrial energy flexibility in mathematical optimization. Such contribution shows high relevance to answering questions in the transition of (future) industrial energy systems. Thus, the following research objective and corresponding subquestions are derived.

Objective: *Develop a framework for flexibility in mixed-integer linear programming concise with holistic perspectives on industrial flexibility*

> ***Question 1:*** *How can various aspects of flexibility, such as technical and organizational flexibility, simultaneously?*
> ***Question 2:*** *How is it possible to include different types of flexibility within a generic structure or framework, respectively?*
> ***Question 3:*** *How do incentives for different types of flexibility interact with the different possible optimization applications (e.g., design and operation optimization, scheduling, etc.)?*

A comprehensive literature review was first performed to reach the proposed objective. Based on this review, various flexibility properties with high relevance for optimization models were elaborated. Two properties need to be emphasized. Flexibility is (i) a relative criterion. A configuration can always just be more or less flexible compared to another. Defining one absolute parameter that can be used as an optimization objective is difficult. Furthermore, flexibility is (ii) triggered by incentives, such as minimizing costs, which can be used as an advantage in optimization. Based on those findings, a framework was elaborated with sequential optimization runs and different operating scenarios, which allows the inclusion of various types of flexibility. For a simplified but generic use case from the pulp and paper sector, derived from knowledge built up in previous work on decarbonization and flexibilization of the Austrian pulp and paper sector, the energy source flexibility and potential additional costs for flexible systems were assessed.

Components in future industrial energy supply systems: Challenges in decarbonization and energy system transition raise the importance of measures such as heat recovery and sector coupling, but also new technologies in industrial energy supply. Several examples of such technologies — also applied in the core papers of this thesis — are described in the Appendix A. These technologies include, e.g., power-to-heat assets or multi-fuel boilers, both interesting candidates for decarbonization and flexibility in energy markets with price fluctuations and for sector coupling. Also, existing technologies, such as solid fuel boilers for biogenous fuels or steam turbines, can contribute to decarbonization or flexibility. Formulations including such technologies and their characteristics are necessary to set up the corresponding mixed-integer linear programming models. Consequently, the following objective was defined for this work:

Objective: *Integrate relevant components and technologies for decarbonization and flexibility and their technical features for future industrial energy supply in mixed-integer linear programming models.*

> ***Question 1:*** *Can the formulations map the relations of ≥ 1 in- and outputs with different degrees of freedom in their operation?*
> ***Question 2:*** *How can thermodynamical properties be included in the modeling of large industrial plants?*
> ***Question 3:*** *How can characteristics of heat recovery and sector coupling be included?*

In the presented generic industrial use cases of **Paper 1 - Paper 4** (Panuschka et al. 2018; Panuschka et al. 2019; Knöttner et al. 2022; Knöttner et al. 2024), oriented at the energy-intensive industry production schemes, component models for a wide range of technologies, e.g., energy conversion units, heat recovery, or sector coupling, have been formulated for operation and design optimizations. Thus, linearized but technically detailed formulations of technologies and technology-specific features were proposed and described, especially in **Paper 1 - Paper 3** (Panuschka et al. 2018; Panuschka et al. 2019; Knöttner et al. 2022).

4 Research Approach

The overarching theme of this thesis is the future of industrial energy supply, including, on the one hand, new technologies in industrial energy and production systems typically related to investment and new system designs. On the other hand, technology-independent measures, such as increased efficiency or flexibility with given assets, change the operation of a system and can contribute to significant and required changes, e.g., towards more sustainability. Both the medium- to long-term existing and the emerging challenges emphasize the importance of supportive tools to decide on designs but also operational strategies for competitive, affordable, and secure energy supply in industrial production sites in the future. Mathematical programming is one option for supporting decision-makers, operators, or other parties involved in answering questions about current and/or future industrial energy systems.

The advantages and possible associated disadvantages of applying mathematical programming are: The level of detail in mathematical programming is promising for conceptualization but unsuitable for detailed engineering. The dimensions considered in mathematical programming allow a direct linking of technical systems to economics (or ecological results) by the defined objective function and integration of external factors, e.g., in constraints. This often goes along with simplifying technical details, e.g., due to the mixed-integer linear characteristic of the formulated equations. However, non-linear formulations often struggle with reduced solver performance, high computational effort, and long calculation times.

Not only do the challenges and drivers for a transition in industrial energy supply differ, but also the possible optimization applications. Thus, a visualization and tabular overview were developed on how industrial energy flexibility interacts with and can be integrated into industrial optimization problems. The basis for this representation was a literature review, together with the author's knowledge from setting up optimization models in the context of previous and further core (and additional) publications of this thesis.

The additional tabular summaries focus on (i) how different optimization applications consider the different layers in industrial energy supply and (ii) how different types of flexibility and their corresponding objective functions can be included in different optimization applications.

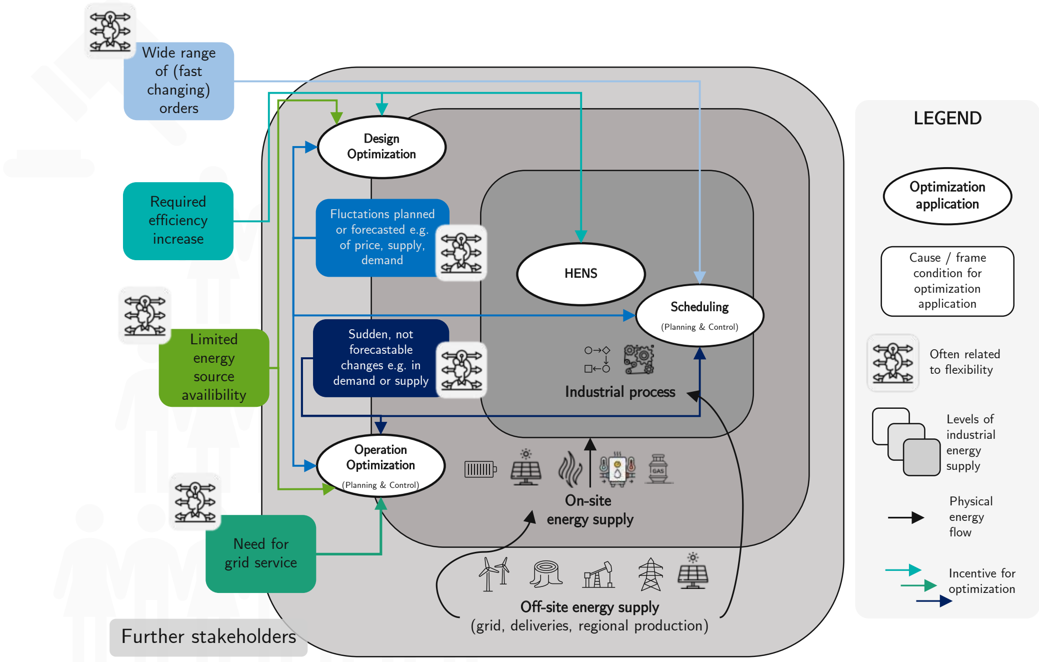

Figure 6: *Stratified visualization for industrial levels, incentives, and reasons to provide flexibility and different optimization applications.*

First, the relevant dimensions of industrial energy supply systems, already introduced in Figure 5, are shown as grey areas in the layered visualization in Figure 6. The core process of an industrial production site itself — the industrial process is shown as the innermost layer, which can have heating or cooling but also medium requirements such as steam or hot water. The next layer is the layer of on-site energy supply, which can typically include boilers, turbines, energy storage, heat pumps, on-site photovoltaics, etc. The next layer includes off-site energy supply options such as necessary grid infrastructure and bilateral agreements, e.g., power-purchase agreements for (regional) fluctuating, renewable energy supply, etc. This third layer is surrounded by further stakeholders, which typically do not have a direct impact on the physical energy supply and consumption but have an impact on the overall system, e.g., through laws, regulations, or pressure to provide decarbonized products from a customer group. Furthermore, in this Figure, different, typical optimization applications in industry are shown in white ellipses, overlapping with the before-mentioned layers of industrial energy supply they mainly cover. Another aspect introduced in colored squares in Figure 6 are incentives to take advantage of the system's flexibility. Colored arrows also indicate which type of optimization problem (e.g. design, operation or scheduling) these incentives are / can be typically included.

Figure 6 does not only allow a comprehensive (but without claim to completeness) representation of the following topics of interest: (i) mathematical programming for industrial applications, (ii) industrial flexibility, and (iii) future industrial energy supply. It also addresses the research objectives and subquestions presented in Section 3 of this thesis. Briefly summarized, the stated subject areas of the research objectives are (1) industrial flexibility in mathematical optimization and (2) future industrial energy supply technologies in mathematical optimization. Consequently, the classification and interactions of the (core and some further) publications of this thesis with the formulated research objectives can be described based on Figure 6. Therefore, Figure 7, an adapted version of Figure 6, was created, where the number in the blue circles indicates the number of the core publication in the Publication chapter, which deals with that specific aspect in the figure. A similar graphical summary is shown for the co-author publications in Publication Chapter. In the following subsections, the two research topics presented in Section 3 concerning the contributions in the core publications of this work are addressed.

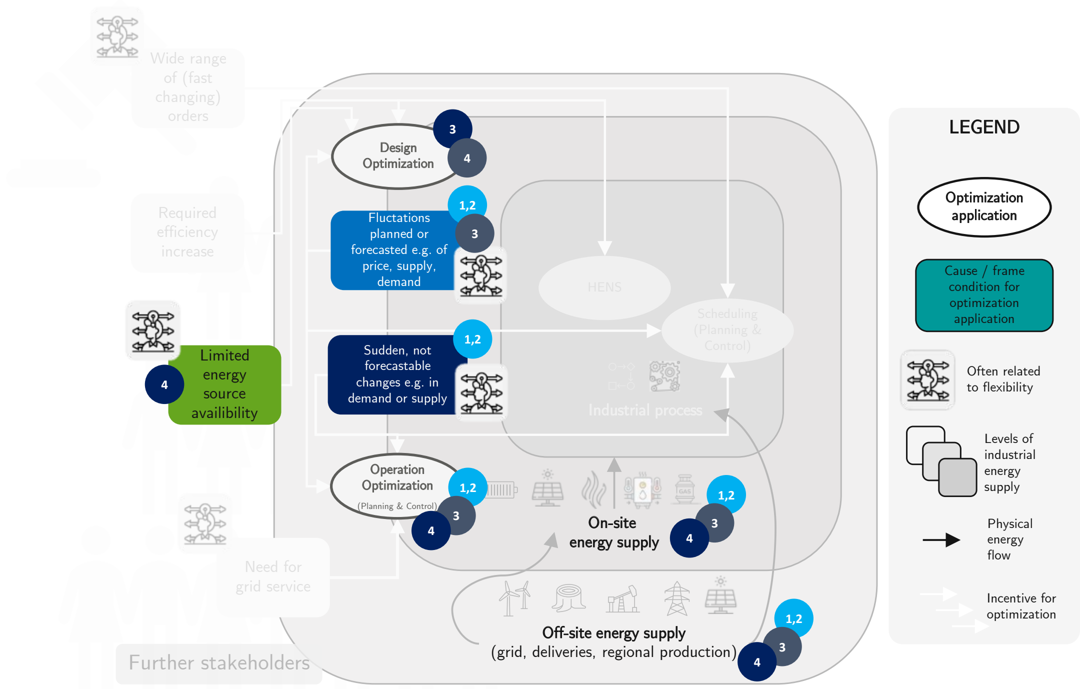

Figure 7: *Adapted stratified visualization for industrial energy supply and consumption levels, incentives, reasons to provide flexibility, and different industrial optimization applications. The visualization is supplemented by an indication of the core publications (1-4 in blue circles) of this thesis in the particular aspects of the representation that are taken up in the respective publication.*

4.1 Flexibility in industrial optimization

The importance of flexibility in industrial production systems as a competitive advantage or even as an indispensable feature has increased over the last few years. Industrial energy supply systems, especially in the energy-intensive industry, do not only supply the production, which is the plant's core business, but they are used to generate economic benefits too, e.g., on different electricity markets, e.g., short-term or ancillary services. This is often named industrial flexibility, although various concepts can be summarized in this term.

In general, both technical and organizational flexibility can be considered in mathematical optimization. This can also be anointed *different hierarchical levels* of flexibility. While technical flexibility is typically a feature of a single component, organizational flexibility is realized with smart operation strategies for these units. So mathematical optimization has the potential to cover both aspects.

In Section 2.2 the following three strategies to consider flexibility in optimization have shortly been introduced:

- Include technical flexibility in component modeling
- Calculation of operating scenarios
- Post-optimization performance indicators

The first strategy of integrating the technical flexibility of a single unit by including parameters and constraints to specify a technology is included in **Paper1** (Panuschka et al. 2018), **Paper2** (Panuschka et al. 2019), **Paper3** (Knöttner et al. 2022), and **Paper4** (Knöttner et al. 2024) of this work. The second strategy is considered, for example, in **Paper 2** (Panuschka et al. 2019), where storage sizes are varied in the scenarios and the impact on overall energy costs is analyzed. Strategy three highly depends on the type of considered flexibility. As flexibility is a relative feature it is often combined with strategy two to evaluate and compare different solutions after the actual optimization. Combining strategies two and three is realized, for example, in the Pareto-front inspired approach developed and presented in **Paper 4** (Knöttner et al. 2024).

Organizational flexibility can often be integrated into optimization by setting up the problem as an optimization model. Simplified, the potential of organizational flexibility lies in the adaptable operation of different technical components and (sub)systems that provide an advantage over unadapted operations.

Here, a strong interaction occurs between the underlying incentive, the type of flexibility, and the formulated constraints and objective functions in the problem. Thus, based on the analysis in the course of **Paper4**, it was summarized how different incentives for flexibility and, further, types of flexibility could be linked. This summary is shown in Table 1.

In **Paper 1 & Paper 2**, the organizational flexibility of the proposed system was used

Table 1: *Interaction between flexibility type and integration into optimization by suitable objective functions as well as a selection of requirements that need to be fulfilled for the specific type of flexibility in various optimization applications, Source: Knöttner et al. (2024)*

Flexibility type	**Typical objective function**	**Selection of requirement to integration flexibility types for**			
		Operation optimization	Design optimization	Scheduling	Heat recovery network synthesis
Fuel flexibility (Feedstock flexibility)	No explicit obj. function, often: min *Cost*	Often not expressed explicitly but implicit by parametrization of available technical unit flexibility: ramping or minimum on- and off-line time of units	Often not expressed explicitly but implicit by parametrization of available technical unit flexibility: ramping or minimum on- and off-line time of units	Hardly considered	Hardly considered
Market flexibility	min *Cost*	Forecasts (prices, demands, self-production), Realize rolling horizon optimization	Forecasts (prices, demands, self-production)	Forecasts (prices, orders)	forecasts (Prices)
Grid support e.g. balancing or redispatch (product flexibility)	min *Cost* max *Profit*	Typically needs a two-step approach. Step 1: determine baseline without support Step 2: determine support possibilities	Often only with probabilities due to lower temporal resolution	Hardly considered	Hardly considered
Planning with fluctuating sources (e.g. renewables or batch demands) (feedstock or volume flexibility)	min *Cost*, max *Self-sufficiency*	Forecasts, technical flexibility expressed in model (e.g. ramping)	Limited computational resources require typ. periods, technical flexibility expressed in model	Include temporal profile of availibilities / prices which is included as parameter	Use multi-period stream table
Adaption to unforeseen changes (volume flexibility)	min *Cost* or max *Product*	Realize rolling horizon, iterative calculation, fast solving times, Eventually stochastic optimization or storage operation constraints	Often integrated by calculation for a scenario set where possible ranges are considered	Realize rolling horizon, iterative calculation, fast solving times, Eventually stochastic optimization or storage operation constraints	Often found with parametrization and integrated by calculation for a scenario set
Adaption to customer wishes product(ion) flexibility	max *Profit*	Hardly considered	Hardly considered	Important incentive to set-up this type of optimization,	Hardly considered

to determine the best economic result for fluctuating demand profiles and energy prices. This can be summarized as integrating market flexibility and planning with fluctuating sources in a model to minimize costs for an operation optimization model. Here, a specific focus was laid on the requirements to be considered when short-term fluctuations of time series and a rolling time horizon characterize the optimization task. Some examples that need to be considered are (i) integrating electric grid fees related to the maximum power consumption in one timestep in a billing period and (ii) the integration of slow-starting units in a rolling time horizon.

In **Paper 3** the integration of fluctuating profiles on the demand side as well as different customer expectations, were the main drivers causing a need for operational flexibility in the supply system. The latter is integrated into the model by considering sector coupling (combined district heating and industrial heat supply). Here, a far longer period compared to Paper 1 and Paper 2 is considered. However, the optimization application is enlarged to include combined design and operation optimization. In this work, the duration of a year is represented by determined representative weeks with corresponding weights. One main finding, also relevant when discussing operation flexibility, is the relevance of performing combined considerations for industrial optimization in general and sector coupling in particular. Therefore, the choice of system boundaries for modeling and the included components in the system have a decisive influence on the quality of the result.

Finally, in **Paper 4**, building up on a broad knowledge base about industrial flexibility, a new concept of including flexibility in optimization was proposed, aiming at integrating the "relative" character of flexibility. In this work, the approach was applied to a use case with feedstock (fuel) flexibility. The overarching concept behind that formulation is to relate flexible solutions to a baseline, e.g., solutions found for a clearly defined objective function of minimizing total costs, as presented in Papers 1-3. By setting up a multi-step approach, first, the basic solution was determined, followed by a solution fulfilling a soft criterion such as the ability to minimize all used energy sources in a supply system in different sub-scenarios while only one set of design parameters is possible (in case of fuel flexibility to increase the resilience of an energy system regarding fuel failures or limitations).

Especially, the work in **Paper 4** and the summary in Section 2.2 highlight that an overall, holistic understanding and assessment concept of industrial flexibility is lacking. This thesis has contributed to the topic of a holistic assessment of industrial flexibility by conceptualizing and classifying it within the application of different flexibility types in mathematical optimization. Nevertheless, not all facets of this topic are already related to each other and elaborated.

4.2 Components in future industrial energy supply systems

Future-proof industrial production systems do not only include improved cross-technological features, e.g., flexibility, as described before. Also, altered and new components compared to the status quo will be part of the industrial energy systems, covering all different layers of industrial supply and consumption. These components include technological innovations, new contractual concepts for energy supply, and enhanced sector coupling.

However, new and adapted technologies for the production process are beyond the scope of this work. Thus, this work does not include technologies such as direct reduction in iron and steel production, carbon capture to reduce geogenous emissions in the cement production process, or olefin production by sustainably produced methanol. Within the work for this thesis, a focus was laid on future-proof components, especially in the layers for on- and off-site energy supply, see Figure 7. The following contributions, in chronological order, regarding industrial energy supply technologies relevant to future industrial systems were made within the core publications of this thesis.

In **Paper 1 & Paper 2**, encouraged by analyzing flexibility options in industry and exploitation possibilities of flexibility on (short-term) energy markets, a focus was laid on current supply technologies in the energy-intensive industry. Thus, a typical use case based on a use case from the pulp and paper sector was set up. There, characteristic energy-intensive production sector supply units were included in a rolling horizon operational optimization. The rolling horizon framework was chosen to consider the characteristics and effects of short-term energy markets in the optimization. Setting up a rolling horizon framework included the following features of the model: (i) considering a relevant period of historical operation, especially for units with long start-up, shut-down, or minimum on- and offline duration; (ii) fixed decision for start-ups, once the duration between the actual timestep to the first online timestep is smaller than the start-up duration

The energy supply units in those two publications are gas turbines, heat recovery boilers with additional firing, back-pressure, condensation steam turbines, often with steam extraction, boilers for solid fuels or sector internal residues, and thermal (steam) storages. To allow a precise formulation, the following steps were performed: (i) definition of required operation decision variables of a unit, (ii) determination of degrees of freedom a unit has in its operation, and (iii) dependencies between the decision variables of a unit. For the last step, thermodynamic properties, including stochiometric air needs, typical excess air ratios, isentropic compression or expansion, etc., were included to derive the linearized dependencies between the considered operational decision variables.

In the following core publication of this thesis, **Paper 3**, the importance of decarbonized and more efficient energy supply options was moved into the center of attention and motivation. Thus, the modeling work focused on different excess heat recovery options and how interfaces with external consumers could be included.

Finally, in **Paper 4**, increasing flexibility to reduce dependency on long-term cheap fossil fuels was considered. Based on the analysis of real industrial plants in energy-intensive production processes, the relevance of boilers for residuals, both internal and external, was detected. Such boilers are often realized as multi-fuel boilers in industry. Due to their increasing relevance, photovoltaic power purchase agreements have also been introduced. This has been realized by expanding the supply component with fixed generation profile forms, which are scalable in their maximum output.

The development of component models within this thesis also applicable in further industrial optimization tasks is valuable against the backdrop of the major challenges of our time. Strategies to set up models, considering technical but also organizational aspects can help to understand the development of future pathways for the operation and design of industrial sites. However, transferring theoretic findings from optimization models to reality is still challenging.

i First, industrial sites are usually heterogenous. Thus, industrial optimization models are typically case-specific. Although replicable component models are formulated the actual task of modeling still needs previous processes, e.g., an often time consuming system analysis as a base for model set-up and parametrization.

ii Second, integrating results from operation optimization is often hindered by complex adaptations of, e.g., existing process control systems and the necessary communication between different systems.

iii Third, the feasibility of optimal decarbonized design suggestions is often limited compared to conventional systems.

Those drawbacks cannot be overcome with better optimization approaches. Further supportive measures will be necessary to fully exploit the positive effects mathematical optimization can bring.

5 Conclusion and Outlook

Given major challenges, such as transforming the energy system and industrial production, the importance of increasing sustainability and flexibility in industrial energy systems is high. Thus, in this work, adaptions of mixed-integer linear programming formulations are developed with the aim of (i) integrating relevant components and technologies for decarbonization and flexibility and their technical features for future industrial energy supply in those mixed-integer linear programming models and (ii) deriving a framework for flexibility in mixed-integer linear programming, which is concise with holistic perspectives on industrial flexibility.

The formulations and conceptualization of relevant aspects developed in this work include the following main contributions:

- Linearized operation optimization formulations for conventional energy supply technologies derived from thermodynamical parameters have been presented and demonstrated for rolling horizon optimization formulations (**Paper 1** Panuschka et al. 2018 and **Paper 2** Panuschka et al. 2019).
- Optimal design and operation for various sector coupling configurations for combined industrial and different district heating energy supply generations have been evaluated. The role of heat recovery and heat pumps in such sector coupling applications is assessed (**Paper 3** Knöttner et al. 2022).
- Presentation of incentives for industrial flexibility and integration into different mathematical optimization applications (see 2).
- Generic formulation for integrating various flexibility types in optimization models for industrial energy supply systems (**Paper 4** Knöttner et al. 2024).

5.1 Main conclusions on flexibility and innovative technologies in industrial energy supply systems

In general, the work done in this thesis emphasized that the mathematical programming method has a great potential to assess questions of the ongoing transition in the industrial and energy sectors. The following qualitative and quantitative results are obtained for the paper-industry-inspired use cases analyzed.

- The integration and operation of conventional thermal storages depend on the electricity-steam-demand-ratio in systems based on combined heat and power energy supply technology.
- In the past (approx. until 2021), observed emission certificate price levels have been so low that even a price increase of 100 percent does not change the optimized results for operation in conventional energy systems based on combined heat-and-power technologies.

- For sector coupling and industrial energy supply, the choice of optimal heat recovery technologies and storage integration depends on the actual characteristics of the demand to be met.
- Costs for both, investment and operation, increase for sector coupling applications, and increased flexibility and sustainability. However, the cost increase could be significantly limited with case-specific optimal designs.

A comprehensive overview of the topic of flexibility in the energy system has been given. Different strategies for including flexibility in mathematical programming have been applied to the publications of this work. With increasingly challenging requirements for industrial energy supply systems, especially on a regulatory level, it is also important to consider aspects beyond the technological characteristics of energy supply systems. This has already been partly covered in this thesis by integrating, e.g., contractual details such as power purchase agreements.

5.2 Outlook for further research

The concepts, e.g. the adaptions and extensions of optimization formulations and the defined flow charts for solving the corresponding problems, presented in this work are promising to address relevant challenges in the energy system transition. Actual solutions depend on the specific structure of industrial sites and their frame conditions. Thus developed models must be parametrized and adapted to the use cases to determine explicit measures for a transition in industrial energy plants.

Furthermore, additional and more specific (scenario) calculations and analysis of the interaction with different stakeholders in the energy system are required to quantify the impact of industrial flexibility in the energy system transition general methods. In this work, for example, the characteristics of different generations (1^{st}-4^{th}) of district heating networks have been considered. However, including further parts of the energy system, e.g., the operation of electric grids, can be a possible and relevant next step.

Another issue for future research and work is the lack of a holistic assessment of flexibility in energy systems beyond the horizon of power systems, e.g., in the form of a taxonomy. Degefa et al. (2021) propose such a taxonomy for power systems. However, a taxonomy that includes the input of all relevant stakeholders on flexibility is missing. Compared to Degefa et al. such an extended taxonomy should not only consider the power system perspective on industrial flexibility but also industry-intern needs for flexibility.

In conclusion, the aspects addressed in this work are highly relevant to the current challenges of decarbonization and a transition towards more sustainable production systems. Analyzing existing and advanced technologies — concerning technology readiness — shows that the range of options for a more sustainable future is promising. However, technical, organizational, or economic burdens often hinder exploiting the full (sustainable) potential. Thus, beyond the focus of this thesis, the following further fields of action could also be identified and need to be mentioned here to allow for a holistic perspective on the subject. Promoting cultural changes has a huge potential to exploit existing flexibility potentials. Often, industrial sites with a low to medium energy intensity lack awareness and acceptance of new and innovative operational routines promoting increased flexibility. Furthermore, technology development needs to accelerate if decarbonized technologies such as industrial high-temperature heat pumps, storages in general (e.g., thermal or electrical), as well as renewable gases shall become technically and economically feasible alternatives to technologies in current supply systems.

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Publications

In this Chapter, all relevant publications for this thesis are presented. First, the *core publications* are introduced chronologically, corresponding to the publication date. The core publications include three journal papers and one conference paper. Second, *further contributions* are presented, including three co-author publications and other scientific contributions, such as contributions to scientific studies, a selection of presentations, and supervised academic work. For the core publications, the full papers are presented as well as a summary and my contribution to the publication, which is based on CrediT author statement [2]. Further contributions relevant to this thesis are only described briefly.

Paper 1

Modelling of Industrial Energy Systems for Flexibility Increase via Operation Optimization with Mixed-Integer Linear Programming

in the course of the SEE.SDEWES2018 - 3rd South East European Conference on Sustainable Development of Energy, Water and Environment Systems in collaboration with René Hofmann.

An oral presentation was given in Novi Sad on July 2^{nd}, 2018. This conference paper was invited for publication in a Special Issue of the Energy Conversion and Management journal. The enhanced journal paper is included as Paper 2 in this thesis.

In this work, for the first time, a general modeling approach for typical industrial energy supply units in the energy-intensive industry, including gas and steam turbines as well as firings considering thermodynamic parameters, is presented. The modeling approach builds upon the concept that different components of industrial energy supply systems can have different degrees of freedom in modeling regarding the in- and outputs. Depending on the number of degrees of freedom of specific units, conversion factors between the different in- and outputs are derived from the thermodynamic parameters. The method is shown for an industrial plant model derived from characteristics in the Austrian pulp and paper industry considering two different electricity tariff structures. Cost savings can be obtained for fluctuating electricity prices from the day-ahead spot market compared to a fixed tariff structure. Furthermore, a change in resulting storage loading and discharging trajectories can be observed for fluctuating day-ahead electricity prices.

My contribution: Conceptualization, Methodology, Writing - Original Draft, Writing - Review & Editing, Visualization

Panuschka, Sophie; & Hofmann, René. (2018). Modelling of Industrial Energy Systems for Flexibility Increase via Operation Optimization with Mixed-Integer Linear Programming. in Proceedings of the 3rd South East European Conference on Sustainable Development of Energy, Water and Environment Systems

Paper 2

Impact of thermal storage capacity, electricity and emission certificate costs on the optimal operation of an industrial energy system

published in Energy Conversion and Management in collaboration with René Hofmann.

In this work, the general modeling approach for typical industrial energy supply units in the energy-intensive industry, including gas and steam turbines and firings considering thermodynamic parameters, is enhanced for another steam turbine type and a power-based formulation. To show the opportunities and potential of the proposed formulation, it is applied for a use case derived from characteristics of the energy-intensive pulp and paper sector. For this use case, (i) the impact of electricity-steam-demand-ratio on optimal storage integration is observed, (ii) the operation changes for double emission certificate costs in conventional systems are analyzed, and (iii) a 5% cost reduction for thermal storage accounting for 7% of generation capacity.

My contribution: Conceptualization, Methodology, Software Programming, Writing - Original Draft, Writing - Review & Editing, Visualization (ev. Formal analysis)

Panuschka, Sophie; Hofmann, René (2019): Impact of thermal storage capacity, electricity and emission certificate costs on the optimal operation of an industrial energy system. In: Energy Conversion and Management 185, S. 622–635.

URL: `10.1016/j.enconman.2019.02.014`

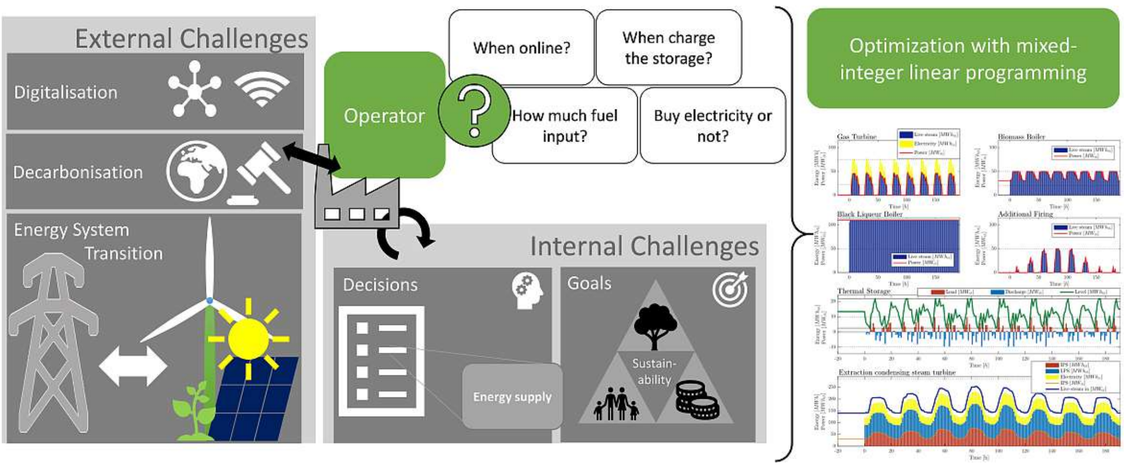

Figure 8: *Graphical Abstract Paper 2*

Paper 3

Impact of recent district heating developments and low-temperature excess heat integration on design of industrial energy systems: An integrated assessment method

published in Energy Conversion and Management in collaboration with Benedikt Leitner and René Hofmann.

In this work, design and operation optimization for sector coupling of residential and industrial heat supply was analyzed. For both sectors, relevant future trends were considered, e.g., direct and indirect heat recovery, renewable fuel boilers, and low-temperature district heating grids. The impact of progress in the district heating sector was analyzed for six scenarios. The cost increase for sector coupling was between 2 - 39% compared to exclusive industrial supply. However, the lowest cost increase did not coincide with the lowest additional energy supply. Thus, synergies as corresponding temperature levels between energy supply for all domains have been identified as crucial criteria for economic success. This work highlights the relevance of combined considerations for industrial optimization in general and sector coupling in particular.

My contribution: Conceptualization, Methodology, Writing - Original Draft, Writing - Review & Editing, Visualization

Knöttner, Sophie; Leitner, Benedikt; Hofmann, René (2022): Impact of recent district heating developments and low-temperature excess heat integration on design of industrial energy systems: An integrated assessment method. In: Energy Conversion and Management 263, S. 115612.

URL: `10.1016/j.enconman.2022.115612`

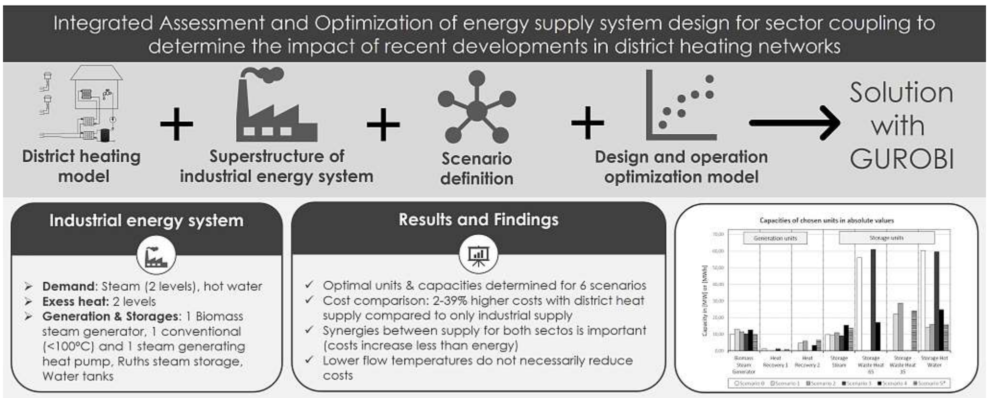

Figure 9: *Graphical Abstract Paper 3*

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Impact of recent district heating developments and low-temperature excess heat integration on design of industrial energy systems: An integrated assessment method

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ABSTRACT

One of today's biggest challenges is taking effective measures to mitigate negative effects and consequences of human-made climate change such as sector coupling and excess heat valorization. In this work, sector coupling of residential and industrial heat supply are considered in an optimization-based design and operation evaluation for industrial energy supply systems with the aim of minimizing costs and determining the impact of on-going developments and progresses in district heating systems. The developed method is applied to a use case with a superstructure for the industrial energy system including a biomass-fired steam generation unit, two heat pumps and various thermal storages, generic industrial load profiles for steam, hot water and excess heat and simulation-based district heating load profiles. The most relevant results reveal that depending on the district heating setting total annual costs, including fuel costs and annualized investments, increase between 2 and 39% compared to no additional district heating supply by the industrial energy supply system. However, the lowest cost increase does not coincide with the lowest additional energy amount. Thus, synergies such as corresponding temperature levels between energy supply for all domains have been identified as crucial criteria for economic success. Also, unit integration for excess heat recovery occurs always combined with thermal storages adapting the temporal occurrence of excess heat. Results for the evaluated use case highlight the importance and relevance of combined considerations for sector coupling measures. Thus, methods, as presented in this work, can contribute crucial information for future assessments. However, further development of the model, e.g. a larger set of generation technologies, and further use cases with other temperature levels, demand profiles are identified as relevant next steps.

1. Introduction

1.1. Background and challenges

One of today's biggest challenges is taking effective measures to mitigate negative effects and consequences of human-made climate change. The recent publication *Global Carbon Budget 2021* within the framework of the Global Carbon Project published updated climate change related indicators and numbers. To give some examples, which emphasize the importance of fast and effective climate change mitigation, some findings from Friedlingstein et al. [1] are stated here:

- the assumed emissions in 2021 will return to pre-pandemic levels of 2019 and thus earlier than expected.
- the remaining carbon budget for a limited temperature raise of probably not more than 1.5 °C accounts for the emitted amount at 2021 levels for 11 more years.

On a global level, binding climate and energy policy goals and targets are stated in the framework of the Paris Agreement. On European level, in redwithin the package of the European Green Deal it is emphasized to take action in order to preserve Europe's natural environment.

A closer look into regulatory framework reveals an increasing pressure on all sectors to contribute to climate change mitigation measures. This requires:

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Nomenclature

Acronyms

BM-SG	biomass fired steam generator
COP	coefficient of performance
DH	district heating
DHW	domestic hot water
EBH	electric booster heater
HEX	heat exchanger
HP	heat pump
IEH	industrial excess heat
IESS	industrial energy supply system
RS	Ruths steam storage
SG	steam generator

Sets

UNIT	set of all supply units
use	set of usage shares at temperature level 85°C
θ	set of excess heat temperature levels
T	set of supply temperature levels

Parameters

β	maximum filling level of full storage (–)
$\Delta\tau$	time step duration (h)
η	efficiency (–)
ν	specific volume ($m^3\ kg^{-1}$)
a	annualization factor (–)
c	specific cost coefficient (€MW^{-1} or €MWH^{-1})
COP	coefficient of performance (–)
f	specific investment factors for heat pumps (–)
h	specific enthalpy ($MJ\ kg^{-1}$)
n	number of years for depreciation (–)
p	specific price of fuel (€MWH^{-1}))
r	interest rate (–)
T	Temperature (°C)
U_{avg}	heat transfer coefficient ($W\ m^{-2}\ K^{-1}$)
WH	Parameter in modeling excess heat load (MWH)
wh	Parameter in modeling excess heat load (%)

Subscripts

1	part stream 1
2	part stream 2
annual	amount for one year
BM	biomass
d	daily
DH	district heat
e	empty storage, end of discharging
el	electricity
F	flow, industrial perspective
f	full storage, beginning of discharging
fix	fixed cost
HEX	heat exchanger
HP	heat pump
HP1-3	heat pump specific investment
hydr1-3	hydraulic specific investment
i	index for chosen representative weeks
invest	investment cost
k	index for hours per week
max	maximum value
R	return, industrial perspective
ret	return, space heating perspective
RS	Ruths steam storage
SG	steam generator
sink	sink side of heat pump
source	source side of heat pump
spec	specific cost
ST	storage
sup	supply, space heating perspective
T	temperature level
use	usage share
w	weekly
y	yearly

Superscripts

’	water phase
”	steam phase
0	related to current timestep *t*
1	related to timestep $t-1$
4	related to timesteps $t-4:t-1$
base	offset for excess heat modelling
SH	space heating

Variables

$\dot{m}$	mass flow ($kg\ s^{-1}$)
$\dot{Q}$	thermal power (MW)
CAP	capacity of supply unit (MW or MWH)
ω_i	integer indicating weight of representative week (–)
ς	annual variation for excess heat (–)
C	cost (€)
D	energy demand (MWH)
dd	relative daily demand share related to one week (–)
dh	relative hourly demand share related to one day (–)
dw	relative weekly demand share related to one year (–)
EH	excess heat load (MWH)
m	mass (kg)
Q	thermal energy (MWH)
t	timestep (–)
w_i	integer indicating chosen representative week (–)
x	binary variable for unit existence (–)

- Limiting physical effects of climate change
- Acting aligned to regulatory framework

While the importance of such measures has been highlighted from the scientific community over years an important factor has changed recently. In the last years the regulatory framework on European level has changed. Thus, increasing sustainability has now become not a potential but mandatory aspect to remain competitive. ”Unsustainable measures” (e.g. investment in new, fossil energy supply systems) are not likely to be financially supported anymore in the near future anymore.

To decarbonize the hard-to-abate sectors in industry and transport technological solutions still need to be (further) developed, e.g. scale up or increase technology-readiness levels. However, for residential and low-temperature industrial heat supply several solutions are already possible or in advanced demonstration states, respectively. Examples for decarbonization of residential heating supply can be heat pumps (HPs), bio-based heating technologies - although it has to be mentioned that also this is a carbon neutral but not carbon free technology or non-fossil district heating (DH), e.g. provided from valorization of industrial excess heat (IEH). In this work, synergies between industrial and residential heat supply as well as valorization of IEH are analyzed. Thus, a method is proposed and applied to a generic use case for different configurations of DH networks. The following challenges have been identified when it comes to simulation and optimization-based evaluation of sustainability measures in industrial and residential heat supply. For instance, DH network modeling usually considers large numbers of components and connected buildings and, thus, requires a detailed modeling approach to represent. On the other hand, the complexity and diversity of industrial energy supply system design calls for a detailed analysis of each process. Here, a combined approach, dealing with the complexity of both subsystems, is shown and elaborates how to determine and analyse potential benefits and the impact from changes from 1^{st} to 4^{th} generation DH networks. In the following, an overview of current publications for DH developments, IEH applications and the combined analysis of those two is given followed by a summary of the contribution of this paper.

1.2. Literature review

Currently, for DH supply often fossil fired supply technologies such as combined heat and power supply unit are used. DH currently experiences a shift from traditionally centralized generation systems with high supply and return temperatures to decentralized systems with multiple supply units, e.g., solar thermal, and low supply and return temperatures. This is often referred to as 4^{th} generation DH or low-temperature DH [2] and developments are still on-going, highlighted by recent publications considering 4^{th} generation DH systems shown in the following. Merkert et al. [3] address the potential of sector coupling in order to react to volatile renewable energy generation and determine thousands of euros as savings in a case study where the grid is used as thermal storage. Fujii et al. [4] propose a design for a hypothetical 4^{th} generation DH grid in Northern Japan, where only 1^{st} and 2^{nd} generation DH grids can be found, and evaluate the usage of excess heat as primary energy source, which could replace more than 70PJ of currently fossil fuels.

For a successful industrial transformation path towards more sustainability, also for low-temperature applications, big challenges need to be overcame. The above-mentioned regulatory frame conditions require significant greenhouse gas emission reduction and increasing renewable generation shares as well as primary energy consumption reduction. Increased efficiency in existing energy systems can contribute to emission reduction. Also the integration of new units using renewable energy carriers contributes to this challenging goal. Recent developments in investment costs for technologies, e.g. photo-voltaic cells or electrical batteries, will increase the speed of such transformation pathways. Examples for this development are shown e.g. in Fu et al. [5] who report a cost reduction for photo-voltaic installations of factor 3–4 from 2010 to 2018 or in an analysis of battery costs in real terms (without further equipment) for electric vehicles which shows a decline of about 87% to 2019 [6]. To reduce primary energy consumption the relevance of using low-exergetic energy carriers due to limited amounts of high-exergetic energy carriers increases. Among others, this is addressed by Geyer et al. [7] who identify (high temperature] HPs as relevat contribution in decarbonized industrial energy supply. The importance of (high-temperature) HPs in the energy transition is also highlighted in the report on "Net zero emissions" by the international energy agency [8]. There, it is stated that according to the pathway net zero emissions until 2050 HPs with a monthly capacity of 500 MW heating power need to be installed. In those recent contributions, a special focus is laid on the (cascadic) use of energy and the concept of heat recovery, e.g. by means of high-temperature HPs.

In the following, publications considering DH and IEH together are presented. From a methodological point of view not only simulation tools are used but also optimization approaches or combined simulation–optimization methods adressing a wide range of aspects. An analysis of regulatory and organisational aspects using IEH for DH applications has been done especially for Scandinavian/ Northern regions and specific questions. Broberg et al. [9] analyse untapped IEH for DH potentials and potential benefits of realizing the third party access proposal in Sweden, which would facilitate IEH delivery to DH networks. Lygnerud and Werner [10] address one specific barrier for higher utilization rates: the associated risk for DH network operators and consumers due to potential activity termination, which they find to be one of two major reason for termianted heat delivery. However, they conclude that the risk of losing IEH for DH should be considered to be lower than often presumed in feasibility studies.

Furthermore, several publications focus on the analysis of country-specific potential of IEH for DH.

For a Swedish petro-chemical cluster a potential and feasibility study regarding the use of IEH for DH based on the pinch analysis is performed by Morandin et al. [11]. As it is done in this paper, they also address the competition between external excess heat usage for DH and local industrial efficiency measures. However, the present work distinguishes from this work by the focus of the optimization itself and as not a different set of DH configurations are considered

In several countries detailed estimations and quantification of potentials regarding the use of IEH in DH networks have been performed. Often the underlying motivation is based on a contribution to climate goals such the reduction of the primary energy use [12] and CO_2 reduction [13] in Denmark. Required data for a successful potential analysis are among others source and sink temperature, amount and potential users in its vicinity [12].

One important finding there, motivating the approach presented in this work, is that a majority of the IEH can be provided with lower socio-economic heating costs than the average Danish DH price or solar DH [13]. Regarding the most promising sectors the following sectors are found in their analysis: oil refineries, building materials and food production. Fang et al. [14] presented a holistic, universal, but in contrast to the present work not optimization-based design approach for IEH based DH, which was applied to a use case in Northern China. For the applied use case they find great correlations for the recovery of low grade IEH in low temperature DH networks.

In the following an overview of existing papers and literature with a focus on different assessment methods is given. Li et al. [15] address difficulties and burdens of spatial mismatch between low-temperature IEH sources and DH consumers. They identify the importance of energy consumption and pipe investment for comprehensive efficiency improvement. Thus, they propose an optimization approach for primary temperatures, which differs from the optimization approach presented in this paper, in the network and corresponding connection forms by using systematic models. The developed method is applied to a real case study and reveals better results than conventional systems withHPs using sources as sewage and ambient heat. This offers a promising potential of using low temperatures also in long distance DH systems.

An analysis approach with side-wide composite profiles related to the concept of pinch analysis is presented by Kapil et al. [16]. They consider the impact of fuel costs, electricity costs and distance between IEH sources and DH consumers to determine the economic performance of such an integrated energy system. The developed optimization framework is applied for a carried out case study. Another pinch analysis related formulation is proposed by Oh et al. [17] for a multi-period framework to determine the energy optimal integration of IEH into energy supply of different local energy systems. Thus, they also aim at an optimization approach to determine the best solution for heat recovery from IEH for among other e.g. DH supply. However, they do not consider a combined design optimization for industrial and DH demand as it is done in this work. Especially, as the operating range of HPs is enlarged towards higher temperatures due to technological progress, considering internal industrial heat recovery potentials becomes more and more important. In contrast to the before mentioned papers this heat recovery option is considered simultaneously with heat recovery for DH supply in this paper.

Djuricllic and Trygg analyse 83 manufacturing companies in Sweden with regard to their consumption potential for DH [18]. Thus, they consider an approach focusing on the opposite of several other studies. Relevant findings are that this would allow a reduction in greenhouse gas emissions, a lower dependence of DH supply on outside temperatures and consequently a better utilization of plants providing DH, in this case: combined heat and power supply unit. Especially, these last two findings highly motivate the approach followed in this paper: find a systematic, combined consideration, formulation and optimization of industrial and DH heat supply using IEH as a source for both. In general, the high sensitivity of economic parameters and frame conditions, found among others e.g. in [16] emphasize the need for fast and simple models to determine the impact of different settings, e.g. the combined DH and industrial energy supply, as presented in this work.

A recent literature review by Butturi et al. [19] gives a comprehensive overview of the work in the fields "eco-industrial parks" and "urban-industrial symbiosis" including optimization methods. Among others, one relevant conclusion is that energy symbiosis networks between industrial and urban areas are under-investigated and need further research. A closer look reveals that often the potential of DH supplied by IEH is determined. Nevertheless, also in this review for the other way around (impact of different DH networks characteristics on optimal energy system layout) no examples are presented. However, as it will become even more crucial in the future to consider new and innovative approaches in sector coupling in order to derive more flexible and efficient systems over all domains, which is highlighted by Gea-Bermúdez et al. [20], the authors identified the need to determine the impact of changes from 1^{st} to 4^{th} DH systems on design decisions in sector coupling with industry.

1.3. Contribution and goal

This work aims at analyzing the impact on optimal design of energy supply systems of on-going developments and changing characteristics and parameters in DH grids in case of combined heat supply for the DH and industry. Therefore, a design and operation optimization formulation is proposed with the aim of minimizing total annual costs including fuel and investment costs. To show the capability of the presented formulation six scenarios are evaluated for an industry-related case study. The following aspects are considered in the optimization model due to their increasing relevance in terms of economic, regulatory and environmental frame conditions: valorization of excess heat by means of thermal storages, conventional HPs ($\leqslant$100 °C), innovative steam generating high-temperature HPs and sector coupling of residential and industrial heat supply. As the above described challenges emphasize the need for a long-term strategy and corresponding decision support tools as presented in this work, the authors wanted to determine whether general remarks regarding design guidelines and conceptual insights for the application of technologies using low grade heat in the proposed setting could be derived.

The contribution of this work goes beyond the state of the art as, to the knowledge of the authors, no approach is presented using mathematical optimization measures to analyse the impact on optimal energy system design of on-going developments and therefore different configurations in DH networks (from 1st to 4th generation). The most important contributions, in chronological order regarding the remainder of the paper, are:

- presenting a method to assess developments in building stock and DH on design of industrial energy supply system (IESS) using a sequential dynamic DH model and a superstructure-based IESS design and operation optimization model for a decarbonized industrial heat and DH supply system
- showcasing the assessment method in an example application and deriving simple design guidelines for this elaborated use case
- highlighting the importance of an integrated assessment of DH and IESS design based on the evaluation and analysis of the results

2. Method

The presented method combines different approaches in energy system modeling. An overview of the applied methods and their interaction is visualized in Fig. 1. There, the order tasks performed in the actual calculation is shown.

Core of this work to determine the sector coupling potential for combined residential (via different DH options) and industrial heat supply was a mathematical optimization model. This model consisted of a superstructure approach with static frame conditions for the synthesis of the IESS. Binary and continuous decision variables were used determine optimal design and operation of the IESS which supplied both industrial and residential heat demand. Those three elements, system synthesis, design and operation have been identified as three crucial, interacting levels for energy system optimization by Frangopoulos et al. [21] and should be considered together [22], which was realized in this work. To take all interactions of this IESS superstructure into account further modeling approaches were required.

Thus, static frame conditions for the DH were defined. These included building energy system characteristics such as type of heating system, i.e., floor heating or use of radiators, and respective temperature requirements as well as design of DH piping, e.g., insulation thickness, hydraulic diameters, etc. In the next step, the detailed dynamic thermal–hydraulic simulation is performed for the combined DH grid and building models to assess the DH needs for a given scenario condition, i. e., mass flow rates as well as supply and return temperatures. Details are explained in Section 2.2. Results for these DH load profiles were used together with predefined, generic industrial load and excess heat profiles and evaluated in a set of scenarios for one specific case study. The scenarios are explained together with the case study in Chapter 3. In order to limit calculation duration the load profiles are reduced to a set of representative week. The applied formulation is presentend by Poncelet et al. [23] and shortly described in Section 2.3.

2.1. Optimization

In the following the defined IESS superstructure and the set-up of the optimization model applied to determine the optimal design and operation of the industrial energy system are described.

2.1.1. Superstructure of industrial energy supply system

Within the problem formulation step an extensive energy system was set-up. Nevertheless, within the optimization this full IESS superstructure might be reduced to a smaller system with the best economic performance compared to all alternatives available from the superstructure set-up. The chosen system shall fulfill the before described levels of demand. As the focus was determining the impact of additional DH supply with various characteristics and requirements on the design of an IESS with excess heat recovery, the predefined superstructure focuses on storage integration and heat recovery in order to deliver heat to the DH system. The choice within the solving process can be made from the following set of energy supply, conversion and storage units.

SG	Biomass fired steam generator (BM-SG) provides steam at the highest temperature which can be transferred to any demand at a lower temperature level
RS	Ruths steam storage (RS) charged with steam and operated between two steam temperature levels
STθ_1	Water tank storage for the excess heat with lower temperature
ST θ_2	Water tank storage for the excess heat with higher temperature
ST DH	Water storage at the industrial hot side of the DH HEX - can be implemented as pressurized storage or water storages with ambience pressure, depending on the temperature level
HP1	Heat Recovery Unit 1 (can be realized as Hp or HEX) using the excess heat stream with higher temperature as heat source. For readability reasons this unit is referred to as HP1 in the following, although integration as a HEX is possible.
HP2	Heat Recovery Unit 2 using the excess heat stream with lower temperature as heat source. In this work this unit is always considered as HP. Thus, it is referred to as HP2.

Fig. 2 represents one possible set-up of the IESS. Here, all possible units are integrated and heat recovery units are realized as HPs because

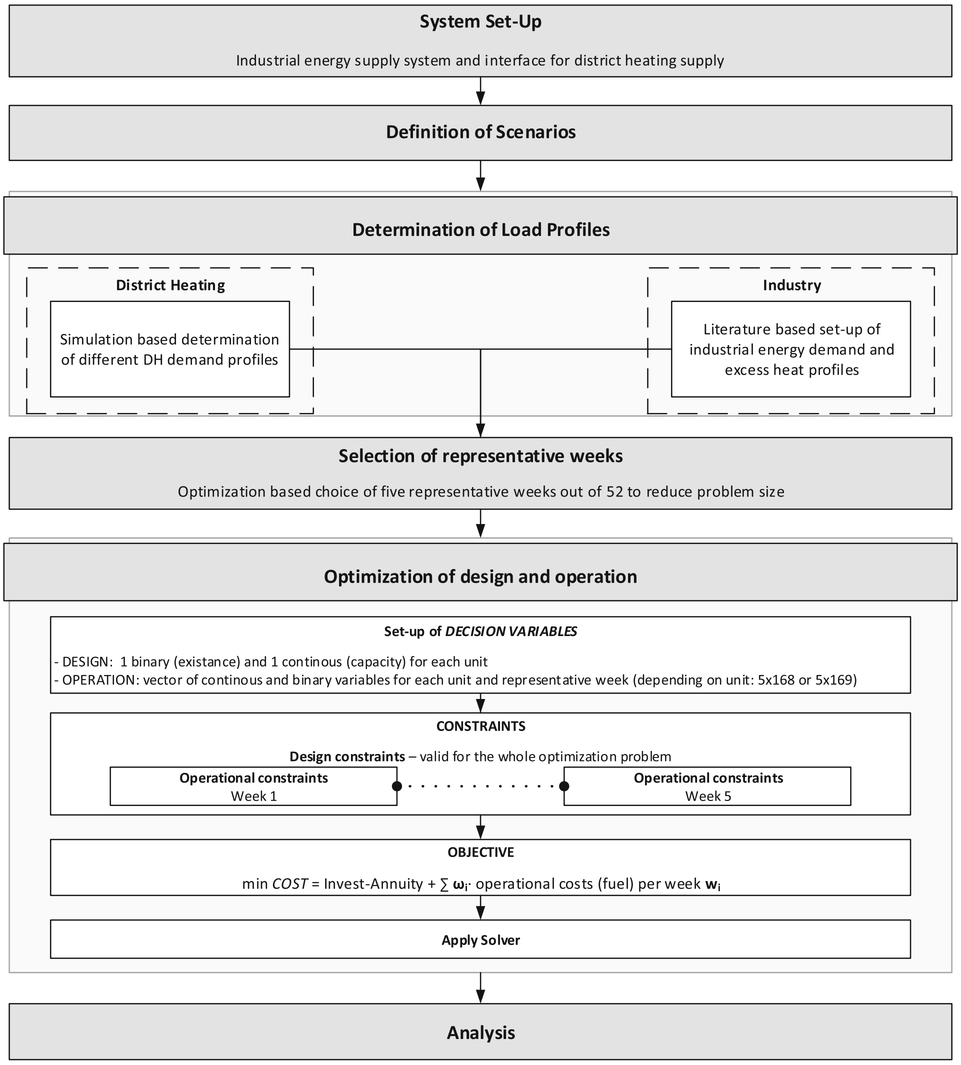

Fig. 1. Overview of the applied approaches in energy system modeling and the interactions of these approaches used in this work.

of the assumed temperature levels in Fig. 2. Furthermore, the hot water storage tank (⩾100 °C) is implemented as pressurized water storage in this supply system.

2.1.2. Formulation

Decision variables for both the design and operation determination are implemented.

- Design decision variables were defined in the following way.

  - To determine the optimal design for each unit one binary decision variable per unit was included to determine the existence of this unit in the chosen IESS.
  One continuous decision variable per unit was defined to derive the optimal capacity.

- Furthermore, for every time-step of the optimization time horizon operational decision variables are included.

  - For generation/conversion units binary decision variables were implemented expressing the on- and offline behavior of those, while continuous decision variables express the generated thermal power in the respective time-step.
  - In case of the storage units continuous decision variables are introduced to express the loading and discharging behavior.
  - In case of the RS further continuous decision variables are used to realize a consumption of the discharged steam on all levels with lower temperatures.

In general, the temporal resolution is defined as one hour in the industrial optimization problem and all according units in this work.

Steam Generation. The steam generator (SG) was modeled with the following features, according to the approach presented in Halmschlager et al. [24]:

- Minimum part-load operation (> 0)
- Limited ramping ability
- Minimum on- and offline times (> 1 h)

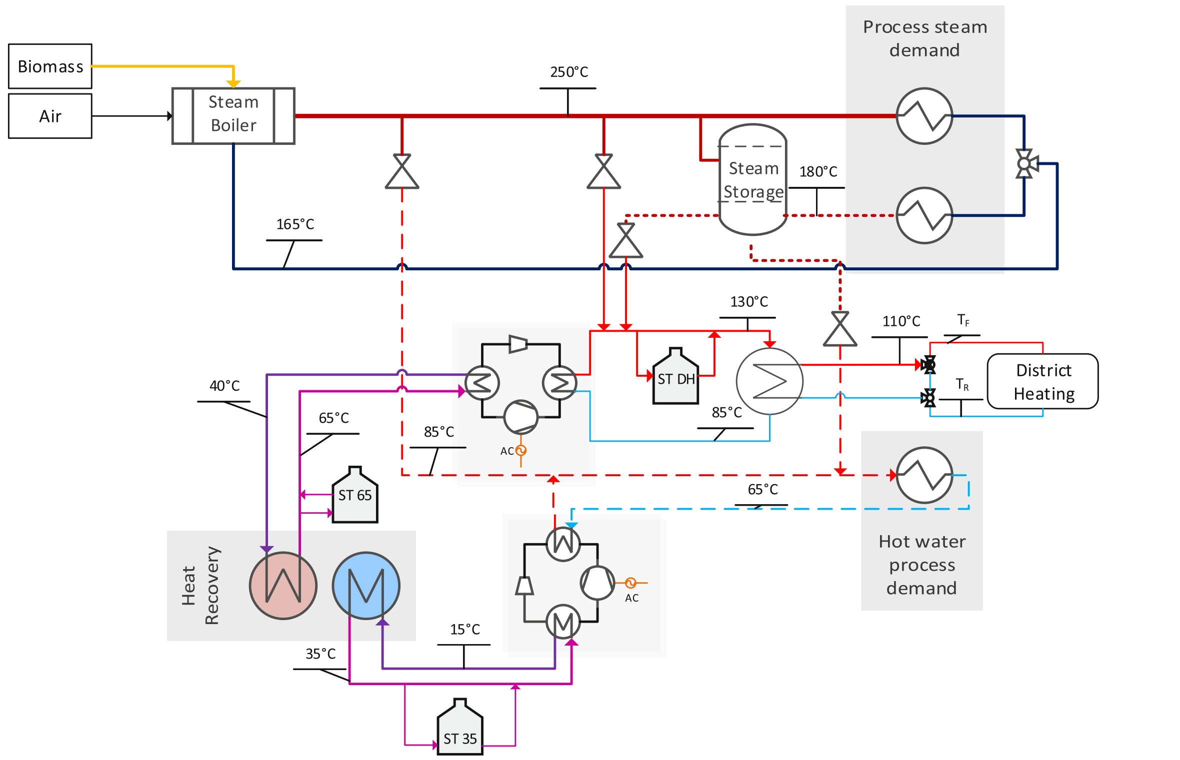

Fig. 2. Schematic example of visualization of one realization option of the industrial energy system design model with heat recovery configuration and predefined temperatures.

Due to the temporal resolution no start-up or shut-down capacities and durations were considered, as they are assumed to be comparatively small with regard to the time-step duration (⩽1 h). The relation between fuel input (mass flow) and steam output was implemented as a constant factor. This factor depends on thermodynamic parameters such as specific enthalpy, heating value, stochiometric air consumption and common air excess, as it is presented in Panuschka and Hofmann [25].

Heat Recovery. Heat recovery units 1 and 2 can be realized as HP or HEX. In the case of both heat recovery units were integrated as HPs, they were assigned to the heat sinks depending on the relation of the heat sink temperatures compared to the heat source temperatures. In other words, the higher sink temperature T_{sink} was provided by the HP connected to the higher source temperature T_{source}.

In this work the coefficient of performance (COP) of each HP was calculated as a function of respective T_{source} and T_{sink} as well as an assumed constant 2^{nd} law efficiency of 0.5. The COP was a constant input parameter in the optimization. Arpagaus et al. [26] reported that a majority of experimental data reveiled a 2^{nd} law efficiency between 0.4 and 0.6. However, the actual performance also depends on the operational load and system dynamics.

The HPs were modeled with the following features, according to the approach presented in Halmschlager et al. [24]:

- Minimum part-load operation (> 0)
- Minimum on- and offline times (> 1 h)

In order to allow operation with rather constant load conditions simple storage tanks were integrated at the heat source side of the potential heat recovery units in the IESS superstructure.

Storages. The thermodynamic characteristics for the RS were derived from the simplifications presented in Glück [27]. There, a relation between the maximum volume, V_{max}, and maximum discharged mass flow, m_{steam}, is presented, see Eq.(1).

$$m'' = \frac{V_{max} \cdot \beta}{\nu_f^{'}} \cdot \frac{h_f^{'} - h_e^{'}}{0,5(h_f^{''} + h_e^{''}) - h_e^{'}} \quad (1)$$

where V_{max} is the maximum storage volume, β is the maximum filling level when discharging starts and defined to be 0.9, ν and h are specific volumes and enthalpies for the water(′) and steam phase (′′) at the beginning (subindex ^{f}) and end (subindex ^{e}) of the discharging cycle (full and empty state).

With the following assumptions and Eq.(2) a maximum storage capacity Q_{RS} of 53 MWh^{th} was defined and implemented in the optimization formulation:

- A maximum storage volume of 300 m^3 (rule of thumb from engineering practice)
- Operating range between high temperature steam (full) and low temperature steam (empty), which results from the temperature settings in the IESS superstructure and a minimum pressure level of saturated steam above 2bar

$$Q_{RS} = m'' \cdot \frac{h_f^{''} + h_e^{''}}{2} \quad (2)$$

For all further storage tanks, which store water (either at ambient pressure or in pressurized condition) the maximum storage capacities were related to a maximum volume and the specific volume and enthalpy of the stored mass streams. All thermal storage units were modeled with losses in charging, discharging and storing cycles ($\eta < 1$).

2.1.3. Interface district heating and industry

In order to model the interface between the IESS and the DH supply the following approach was chosen. To simplify the interface it was assumed that the IESS provided the same flow temperature for the DH in every time-step. Thus, this temperature equals the maximum flow temperature in the DH simulation for the respective scenario. The actual, required flow temperature was then realized by admixing the return flow. Furthermore, on the industrial side of the HEX the temperature of the heating stream at the HEX inlet was 20K higher than the maximum flow temperature provided at the DH side of the HEX. This was defined in order to allow a supply security margin for heat exchange and heat supply in the DH network. Fig. 3 represents and describes this simplification.

2.1.4. Industrial demand and excess heat

Generic industrial demand and excess heat profiles were used in the proposed method and assumed to occur on different temperature levels.

Starting point for the generation of the demand profiles were normalized day, week and partly year profiles. The final demand profiles are generated by combining the normalized demand profiles and multiplied by the annual consumed energy for each temperature level and usage share, respectively. For all temperature levels the final demand profiles are given as load requirement $D_{T,use}(t)$ in MW^{th} for period t.

$$\sum_{t_d=1}^{24} dh_{T,use}(t_d) = 1 \quad \forall \quad T, use \tag{3}$$

$$\sum_{t_w=1}^{7} dd_{T,use}(t_w) = 1 \quad \forall \quad T, use \tag{4}$$

$$\sum_{t_y=1}^{52} dw_{T,use}(t_y) = 1 \quad \forall \quad T, use \tag{5}$$

$$D_{T,use}(t) = \frac{Q_{annual,T,use}}{\Delta\tau} \cdot dh_{T,use}(t) \cdot dd_{T,use}(t) \cdot dw_{T,use}(t) \quad \text{with} t \in [1; 8760] \quad \forall \quad T, use \tag{6}$$

where dh, dd and dw are the relative hourly, daily or weekly demand shares related to one day, week or year at temperature level T for the usage share use (only for $T = 85^\circ$) and $Q_{annual,T,use}$ is the annual heat in MWh for the respective temperature and usage share. $\Delta\tau$ is the duration of one time step in order to link load and energy requirement.

A similar approach is shown by Wolf [28], who used normalized load profiles, the annual heat energy and a base load factor to generate load profiles. Several normalized load profiles used in the approach presented in the present paper are derived from Wolf's publication. Further normalized load profiles are derived from published data from the Austrian standard load profiles for the industrial usage of natural gas [29]. These are usually used to predict the upcoming load of households and industrial processes in small enterprises without installed load measurement of the gas withdrawal from the gas grid, e.g. cooking or hot water.

The excess heat profiles $EH_\theta(t)$ were based on an exclusively generic approach including different shares related to process demand $D_{T,use}(t)$ and temperature levels T shown in Eq. (7). Use case specific details for excess heat occurrence at temperature level θ and technical integration are shown in Section 3.1.

$$EH_\theta(t) = \left(WH_\theta^{base} + \sum_T \left(wh^0_{T,\theta} \cdot D_T(t) + wh^1_{T,\theta} \cdot D_T(t-1) + wh^4_{T,\theta} \cdot \frac{\sum_{\gamma=1}^{4} D_T(t-\gamma)}{4}\right)\right) \cdot \varsigma(t) \tag{7}$$

This includes:

- An assumed offset WH_θ^{base} in MW^{th}
- Influences by the demand in the current and last hour(s), e.g. $wh^0_{T,\theta}$, $wh^1_{T,\theta}, wh^4_{T,\theta}$
- An annual variation, by $\varsigma(t)$, to simulate e.g. higher cooling demands and thus higher excess heat occurrence in summer.

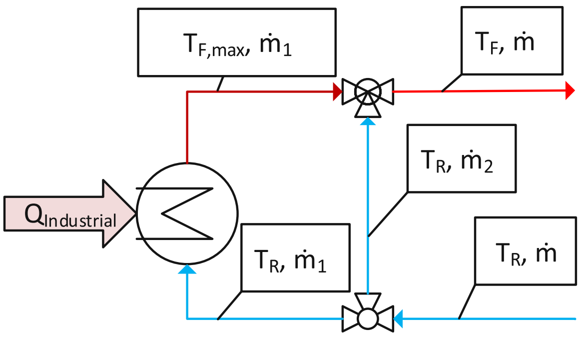

Fig. 3. Visualization of simplified modeled interface of industrial site provision and DH network with heat supplied by the IESS $Q^{industrial}$ and DH return (R) and flow (F) temperatures.

2.2. District heating

The modeling language Modelica [30] is used to model the DH network and the connected buildings. Modelica enables an acausal modeling approach with mathematical equations and is by design an object-oriented language. The openly available Modelica library DisHeatLib [31], using the open source IBPSA library [32] as a core, was used to model all relevant components of a DH network. This facilitates the reuse, extension and adaptation of existing models for various different systems.

The main purpose of the building model is to appropriately represent the mass flow rate of DH supply water and the corresponding return temperature. To this end, a dynamic single zone model combined with a radiator model is used for space heating and a domestic hot water (DHW) storage tank is used for DHW.

The buildings are modeled using one-dimensional reduced order models based on chains of thermal resistances and capacities to reflect heat transfer and heat storage [32]. The architecture of the model is based on the German Guidline VDI 6007 [33] that describes dynamic building models for calculation of indoor air temperatures and heating/cooling power. The four resistances, i.e., exterior walls, roof, floor and windows, are parameterized using U-values for wall, roof, floor and window, of multi-family building archetypes for Austria described in [34]. The indoor air temperature set-point is 22 °C during the day and 18 °C during the night, i.e., using a night set-back control. The heating system of each building is represented by a single radiator model that is based on the European Norm EN442 [35], taking into account the nominal mass flow rate, the nominal supply and return temperature and the nominal heating power.

A PI-controller is used to set the mass flow through the radiator according to the current room air temperature of the building.

As DHW profiles are highly dependent on actual user behavior, the water draw profiles were created using statistical means [36], incorporating basic assumptions on nominal flow rates. A one-dimensional model is used for the DHW tank. The hot water tank is modeled with stacked volume segments to account for stratification. For low-temperature DH scenarios, an additional electric booster heater is considered. Thus, if the temperature of the top tank layer is insufficient an electric heating rod increases the temperature to the prescribed DHW supply temperature.

The DH substation model consists of two individual DHW and space heating stations and a bypass valve, arranged in parallel. The DHW station consists of an electric booster heater (EBH) tank. The DHW demand draws a mass flow from the top of the EBH tank according to the respective profile. The space heating station uses a HEX with a constant effectiveness and a flow valve at the primary side. The valve is controlled such that an outside-dependent set point temperature at the secondary side is reached. All consumer substations are connected with the main DH network via service pipes.

The dynamic thermal–hydraulic DH network model includes time delays, heat dissipation and pressure drops of the piping network, mixing of flows from different pipes, supplies or substations and accounts for different controls in the system. It allows to represent complex thermal network behavior such as zero mass flows, varying temperatures, heat losses and time delays.

The main DH supply unit is modeled as an ideal heat source, with no limits on maximum/minimum power or ramp rate, and with a prescribed supply temperature T_{set}^{DH}. The delivered pressure lift of the electrically driven DH network pump is determined by the weakest point in the DH network, i.e., the building that is hydraulically the furthest away.

Details about implementation and experimental validation can be found in [37]. The temperature change and, thus, the heat loss of a fluid parcel depends only on its initial temperature, on its residence time in the pipe, the undisturbed ground temperature and the thermal resistance, i.e., insulation, of the pipe.

A medium model for water with constant mass density and constant specific heat capacity is used.

2.3. Representative week selection

For the combined IESS design and operation optimization the following inputs were used: load profiles (industrial and DH) and a predefined settings of the IESS. To include seasonal fluctuations annual profiles (8760 h) with a temporal resolution $\Delta\tau$ of one hour or even shorter (DH) were generated for all demand and excess heat profiles. However, in order to limit the computational effort the following simplification and thus reduction of the problem size was made:

- A set of five representative weeks $w = \{w_1, w_2, w_3, w_4, w_5\}$ with corresponding weights $\omega = \{\omega_1, \omega_2, \omega_3, \omega_4, \omega_5\}$ was selected from 52 weeks before the actual combined IESS design and operation optimization.
- This selection was optimization-based according to the method described by Poncelet et al. [23]. Thus, an optimization constrained by the requirement, that the sum of the weights must add up to 52, was formulated. The optimization objective was to minimize the deviation of the annual load curve of all load curves from these representative and weighted weeks and the actual annual load curve. This was formulated as quadratic objective function.

The subsequent operational optimization of the IESS including charging and discharging of thermal storage units was done for each of the representative weeks. For storage units it was defined, that the final filling level must not be lower than the initial filling level for each week. However, design parameters (e.g. unit capacities) were defined as decision variables once for the entire problem and had to stay unaltered for all five weeks.

3. Use case

In the following an overview of the derived scenarios, assumptions and input values for the previously described model is given.

3.1. Industrial demand and excess heat

Based on the above described method the following characteristics of industrial demand and excess heat profiles were chosen.

Process demand. Deriving industrial demand profiles was based on normalized load profiles with relative hourly, daily or weekly demand shares related to one day, week or year at specific temperature and usage levels. The industrial heat demand was assumed to occur at three different temperature levels of the set $T = \{250\ ^\circ\mathrm{C}; 180^\circ\mathrm{C}; 85^\circ\mathrm{C}\}$. With respect to the temperature level the demand can be fulfilled by saturated steam or hot water. Demands shares at 250 °C and 180 °C represent the required heat for production processes and do not correlate with ambient temperatures. Thus, their week profiles were assumed to be applicable for the total time horizon of the optimization (one year). In contrary, the demand at 85 °C consists of different, partly season dependent usage shares of set $use = \{clean, HW, SH\}$. This included cleaning processes, the hot water process demand and space heating demand. The former two do not underlie monthly variations as they were not related to the ambient temperature. Nevertheless, the space heating demand, the third share of the 85 °C demand, had have a weekly variation that is considered.

Excess heat. Two generic excess heat profiles on temperature levels 35 °C and 65 °C were assumed and derived from Eq. (7). The following shares were included. An offset for thermal power in MW^{th} (for details see Table 1) was considered to express e.g. a source providing a rather continuous excess heat delivery such as chillers. Furthermore, production process heat demand often leads to excess heat release. Thus, both profiles were related to the current and former demand on different temperature levels. It was assumed that the demand in the last four hours, in the last hour, and in the current hour influenced the excess heat profiles. One example, also summarized in Table 1, was that excess heat at 65 °C depended of 0.1% of the average heat demand at 250°C in the four hours before the excess heat occurs. Finally, both profiles were

Table 1
Parameters used to generate excess heat profiles. Percentages relate to the relative share of the demand at the corresponding temperature level in the respective time period.

		$\theta_1 = 65\ ^\circ\mathrm{C}$	$\theta_1 = 35\ ^\circ\mathrm{C}$
Offset WH_θ^{base}		0.2 MW^{th}	0.2 MW^{th}
T = 250 °C	$wh_{T,\theta}^4$	0.1%	–
	$wh_{T,\theta}^1$	0.1%	–
	$wh_{T,\theta}^0$	0.1%	–
T = 180 °C	$wh_{T,\theta}^4$	0.3%	0.2%
	$wh_{T,\theta}^1$	–	–
	$wh_{T,\theta}^0$	–	0.05%
T = 85 °C	$wh_{T,\theta}^4$	–	0.2%
	$wh_{T,\theta}^1$	–	0.05%
	$wh_{T,\theta}^0$	–	0.05%
Overlaid annual variation $\varsigma(t)$		$(1 - 0.1 \cdot cos(\frac{t \cdot 2\pi}{8760}))$	$(1 - 0.2 \cdot cos(\frac{t \cdot 2\pi}{8760}))$

overlaid with an annual variation to simulate higher cooling demands and thus higher excess heat occurrence in summer. There were to options for considering an annual variation. First, the excess heat occurrence could be related to the ambient temperature. Second, which was chosen in this paper, a cosine function with the function maximum in summer and the function minimum in winter was multiplied to the derived excess heat.

3.2. Scenarios

The whole IESS is set-up as superstructure with all connections between units enabled. Depending on actual temperature levels in a specific scenario some connections are "pre-chosen" and actual characteristics of some units are finalized before the optimization task starts. Whereas the temperature levels of the industrial demand, the steam generation and the excess heat storages are assumed to be the same in all scenarios, four different DH configurations are considered. Thus, the supply temperatures on the industrial side of the HEX, the connected thermal storage and the combination of HP and excess heat source vary over the scenarios.

These four DH configurations, which reflect the developments from second to fourth generation DH networks, are analyzed in six scenarios (S0-S5). Their differences are described in Table 2.

As a comparison benchmark scenario 0 (S0) is defined as base case without any DH supply. The first DH configuration, evaluated in scenario 1 (S1), represents a high temperature DH network supplying poorly insulated buildings. In the second DH configuration, a third generation DH network, is assumed with moderately insulated buildings and piping as well as with medium to high DH supply temperatures. This DH configuration is considered in scenario 2 (S2). DH configuration 3, evaluated in scenario 3 (S3), corresponds to a fourth generation DH grid with high building and piping insulation standards and low supply temperature levels. Configuration 4 differs only by the use of distributed EBH for DHW from DH configuration 3. This allows to even further reduce the supply temperature of DH. Thus, this configuration corresponds to the edge of fourth and fifth DH generation grids. Two scenarios, S4 and S5, consider this DH configuration 4.

In addition to Table 2, Fig. 4 and Fig. 5 show an overview of the enabled connections between the units in the IESS and the actual temperature levels in the scenarios. Furthermore, the previously shown IESS in Fig. 2 corresponds to the explicit superstructure with defined connections between excess heat and HPs in S1.

3.3. Optimization settings

Both optimization tasks from the applied methodology, see the flowchart in Fig. 1 – selection of representative weeks and determining the optimal plant configuration – are implemented in MATLAB R2016a [38] using the YALMIP Toolbox [39] and the solver Gurobi 8.0.1 [40] for all six previously defined scenarios (S0-S5).

For the first task of choosing the representative weeks the following settings are set: The maximum optimization time was defined as 1800 s unless a relative gap of 5% was reached before. For the second optimization, to derive the optimal system layout and operation, the maximum optimization time was set to 3600 s unless a relative gap of 0.5% was attained prior to the elapse of this period.

3.3.1. Objective function

The aim of the IESS optimization, to minimize costs C_{annual} for optimal plant layout and operation to fulfill both, the industrial and DH demand, is expressed in the objective function, see Eq. (8).

$$\min \quad C_{annual} = a\cdot\sum_{\text{unit}\in U} C_{\text{invest,unit}} + \sum_{i=1}^{5}\omega_i\cdot\sum_{k=1}^{168}\left(p_{BM}\cdot q_{BM}(t_{i,k}) + p_{el}\cdot e_{el}(t_{i,k})\right) \tag{8}$$

where p_{BM} and p_{el} are prices for biomass and electricity in €/MWh respectivly. $q_{BM}(t_{i,k})$ and $e_{el}(t_{i,k})$ are the consumed amounts of fuel (biomass) and electricity in every time-step t with running indices $i\in\{1, 2, 3, 4, 5\}$ for the five chosen representative weeks and $k\in\{1, 2, 3, \ldots, 168\}$ for the time-steps per week.

Investment costs are considered as annuities. Thus, the total investment, as sum of individual investment costs is multiplied with annuity factor a, see Eq. (10). Indivudual investment costs for all units $\in U$, where U is the set of all possibly integrated energy generation, conversion and storage units the investment costs are calculated as follows:

$$C_{\text{invest,unit}} = c_{\text{fix,unit}}\cdot x_{\text{unit}} + c_{\text{spec,unit}}\cdot CAP_{\text{unit}} \tag{9}$$

where $c_{\text{fix,unit}}$ and $c_{\text{spec,unit}}$ are fixed and specific investment costs for the specific unit. While the former are incurred in the costs as soon as the

Table 2
Overview of DH and industrial specifications in defined scenarios. For the heat recovery (HR) units respective heat source and heat sink temperatures, including the purpose of the heat sink, DH or industrial on-site use (Site), are shown for all scenarios together with calculated COP, where a 2^{nd} law efficiency of 50% is assumed. As the temperature lift in S1 happens to be higher than 50 K, a two-stage HP might be required in an implementation, which is not considered here.

		S0	S1	S2	S3	S4	S5
		DH specifications					
Buildings	U_{avg}	X	1.33	0.75	0.26	0.26	0.26
	SH	X	radiator	radiator	floor heating	floor heating	floor heating
	$T^{SH}_{sup}/T^{SH}_{ret}$	X	80/60 °C	65/40 °C	35/25 °C	35/25 °C	35/25 °C
	DHW	X	TES	TES	TES	TES + EBH	TES + EBH
	T_{sup}	X	110/90 °C	85/75 °C	65 °C	45 °C	45 °C
		Industrial specifications					
ST	T^F	85 °C	130 °C	110 °C	85 °C	65 °C	65 °C
	Sink	Site	DH	DH	Site + DH	DH	DH
	Pressurized	no	yes	yes	no	no	no
HR1	T^{source}	65 °C	65 °C	65 °C	65 °C	65 °C	65 °C
	T^{sink}	85 °C	130 °C	105 °C	85 °C	85 °C	65 °C
	Sink	HW	DH	DH	DH	Site	DH
	Unit	HP	HP	HP	HP	HP	HEX
	COP	8.95	3.10	4.73	8.95	8.95	—
HR2	T^{source}	35 °C	35 °C	35 °C	35 °C	35 °C	35 °C
	T^{sink}	85 °C	85 °C	85 °C	85 °C	65 °C	85 °C
	Sink	Site	Site	Site	Site	DH	Site
	Unit	HP	HP	HP	HP	HP	HP
	COP	3.58	3.58	3.58	3.58	5.64	3.58

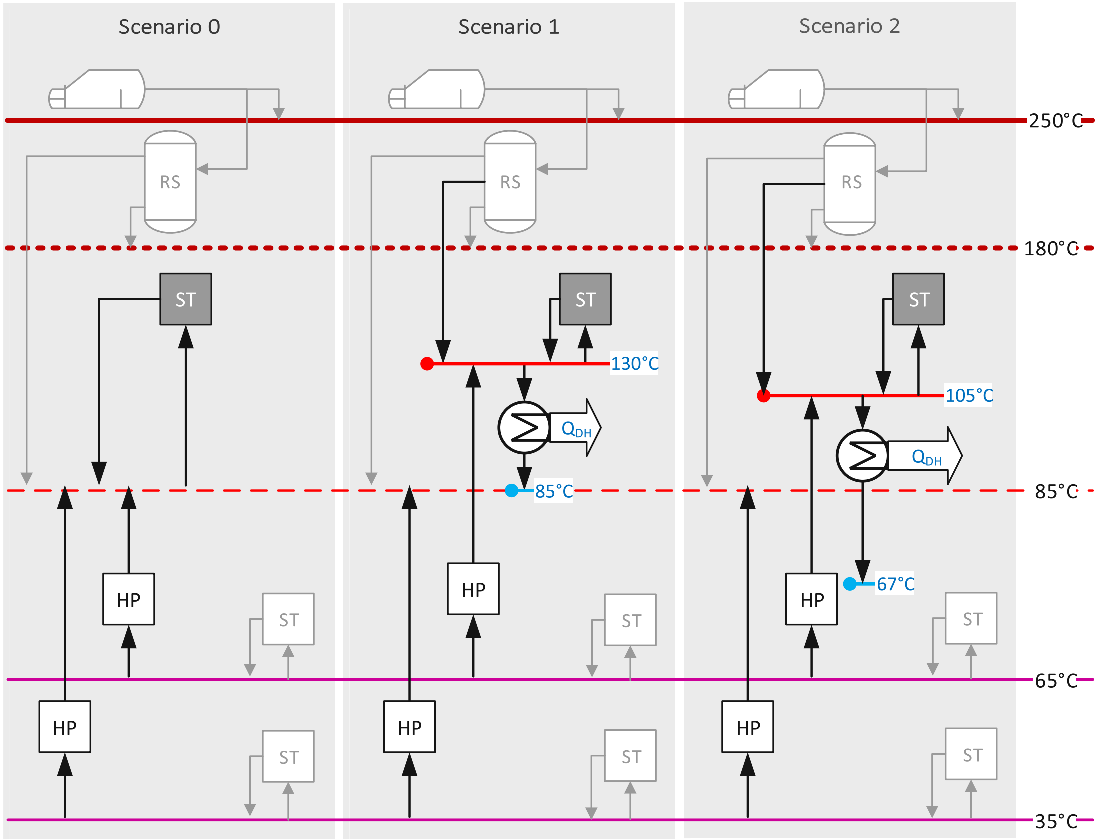

Fig. 4. Overview of temperature levels and unit connections in scenarios 0, 1 and 2 with a steam storage (RS), heat pumps (HP), various storage tanks (ST) where the (potential pressurized) storage for DH is colored in dark grey to allow a distinction to the excess heat buffer storage tanks at 35 and 65 °C. Units and connections which are not varied over the scenarios are shown in light grey and with light grey arrows. Supplied DH and the corresponding flow and return temperature levels on the industrial side of the corresponding HEX are colored in dark blue.

unit exists in the solution (binary decision variable $x_{unit} = 1$), the latter, specific costs, ensure that the unit has a higher total investment as its size (continuous decision variable CAP_{unit} in MW for generation units or MWh for storages) increases.

$$a = \frac{(1+r)^n \cdot r}{(1+r)^n - 1} \tag{10}$$

where r is the calculation interest rate (e.g. 0.05 for 5 %, which is assumed in this work) and n is the number of periods or years, which is assumed as 15 years in this calculation. An overview of the used economic parameters is given in A.

4. Results

In the following an overview of the determined representative weeks in all scenarios is given. Furthermore, the optimal system design for the scenarios is discussed. Thus, the scenarios are compared first. Finally, a detailed comparison for all units of the proposed IESS is presented.

4.1. Representative weeks

For the evaluated scenarios the representative weeks and their corresponding weights were determined in a pre-optimization task. The maximum optimization time was defined as 1800 s unless a relative gap of 5% was reached before. However, for all scenarios the optimization was stopped after 1800 s with final gaps in the range of 10.41 to 52.33%. Although these gaps seem to be rather big a closer look for the absolute number of the final objectives, which are in the range of 4.59E-05 to 4.39E-04, reveals that the result of this first optimization step, prior to the main optimization task can be assessed as accurate enough. An overview of the chosen weeks and the corresponding weights is summarized in Fig. 6.

4.2. Cost-optimal design

The results of the evaluated scenarios are discussed and presented in the following.

Overall comparison of scenarios.

In Fig. 7 the values of the objective (total annual costs) are shown for a first overview. There, the objective values are related to the basic scenario: **S0**, without DH supply, defined as 100%. Furthermore, Fig. 8 shows an overview of the absolute units' capacities in all scenarios. However, their absolute capacity varies over the scenarios. A more detailed quantitative analysis is revealed in Fig. 9 and 10. There, for each single unit of the generation and storage units their relative sizes are related to the highest value for the specific unit over all scenarios.

Scenario 0 and 3. Due to the temperature settings in **S0** both heat recovery units are realized as HPs in the superstructure. In contrast to the majority of the further scenarios both heat recovery units were integrated in the superstructure with the same sink temperature. A further difference to the other scenarios is the purpose of use of the hot water thermal storage. In the further scenarios this unit implemented to

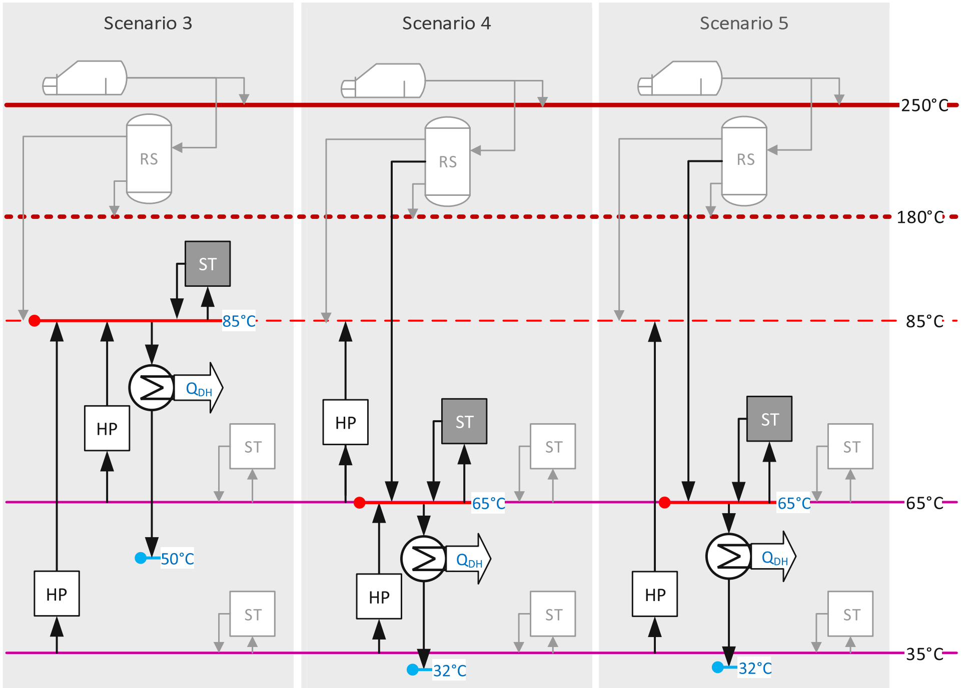

Fig. 5. Overview of temperature levels and unit connections in scenarios 3, 4 and 5 with a steam storage (RS), heat pumps (HP), storages (ST) where the (potential pressurized) storage for DH is colored in dark grey to allow a distinction to excess heat buffer storages at 35 and 65 °C. Units and connections which are not varied over the scenarios are shown in light grey and with light grey arrows. Supplied DH and the corresponding flow and return temperature levels on the industrial side of the corresponding HEX are colored in dark blue.

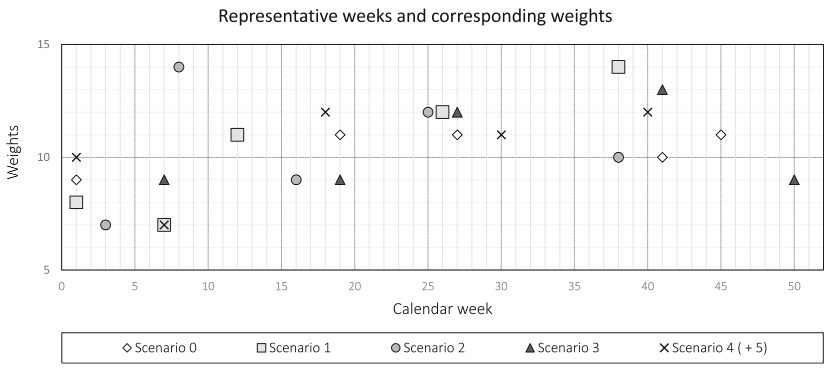

Fig. 6. Optimal choice of five representative weeks and their corresponding weights as input for the industrial energy system layout optimization. S4 and 5 are shown together, as they have the same demand profiles and thus also the same chosen weeks and weights and only differ in the enabled connections and units in the set-up of the IESS superstructure.

support the DH supply. However, in **S0**, it is realized as atmospheric hot water storage for the process hot water demand. Thus this storage can support the supply of hot water demand in **S0**. With this set-up the pre-definition (superstructure) of the energy supply system in **S0** is comparable to **S3**. There, also both heat recovery units are realized as HPs in the superstructure with the same sink temperature as both, DH and hot water demand flow, happen to have the same temperature requirement. Also, the DH storage provides hot water with this temperature. Hence, it can therefore support both, the fulfillment of DH and hot water demand requirements.

For both scenarios, **S0** and **S3** only the HP with 65 °C as sink is integrated. Furthermore, both units, BM-SG and HP, the optimization results show similar capacities. The BM-SG capacity is chosen to be 10.15 and 10.35 MW, respectively. The thermal heating capacity the HP is determined to be 1.2 and 1.25 MW respectively.

The analysis of the optimization objective revealed that the total annual costs are only 2.3% higher in **S3** compared to **S0** although an additional 3.6 GWh of DH are supplied. This value corresponds to an increase of (over all temperature levels aggregated) thermal energy supplied by the industrial energy supply system of 6.52% in **S3** compared to **S0**. For those two scenarios one can see, especially in Fig. 8, that both, the storage tank at 65 °C and the hot water storage tank, are sized rather big, related to all other units and scenarios. Altogether, this leads to the conclusion that synergies in energy supply due to an advantageous relation of demand levels, together with well-placed and sized energy storages allow comparably cost efficient combined

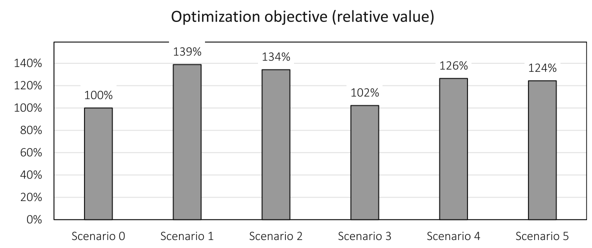

Fig. 7. Relation of optimization criteria "Total annual costs" in Scenarios 0–5 with total annual costs determined in Scenario 0 defined as 100% corresponding to 7,965,897.52 €.

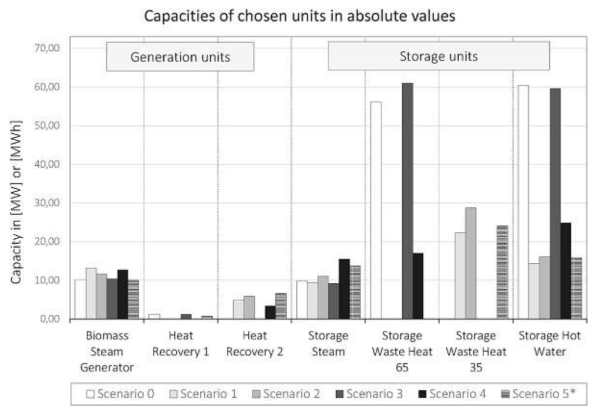

Fig. 8. Absolute size of the generation and storage units in all scenarios.

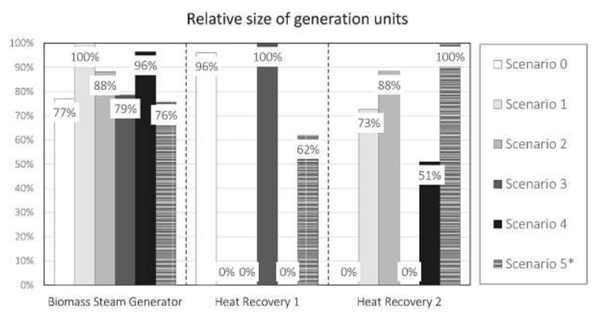

Fig. 9. Relative size of the generation units in all scenarios. For each unit 100% corresponds to the highest capacity found in the optimal solutions of all scenarios. Thus, 100% correspond to 13.17 MW for the BM-SG. For heat recovery unit 1 the maximum value corresponds to 1.25 MW, realized as HP for scenarios 0–4 and as direct heat recovery in **S5**, which is indicated by superscript *. In case of heat recovery unit 2, realized as HP in all scenarios, 100% correspond to 6.63 MW.

industrial and DH supply.

Scenario 1 and 2. For **S1** and **S2** with considerably higher DH flow temperatures compared to scenarios 3–5 the objective value of total annual costs increases by 39 and 34%, respectively. Meanwhile, the amount of supplied energy increases only by 31.67 and 21.28 %. However, for these two scenarios the flow temperature of DH supply is considerably higher than the hot water demand. Thus, not only the COP of the HP using excess heat with 65 °C to supply DH is low compared to the other scenarios, see Table 2. But also, the specific investment costs for this HP are higher, when the sink temperature exceeds 100 °C, see Table 3. As a consequence, one can see that the HP with 65 °C as source

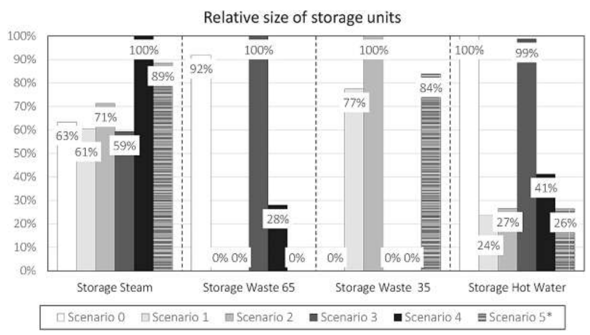

Fig. 10. Relative size of the storage units in all scenarios. For each unit 100% corresponds to the highest capacity found in the optimal solutions for all scenarios. Thus, 100% correspond to 15.49 MWh for the RS, to 61 MWh for the 65 °C and to 28.76 MWh for the 35 °C excess heat water storage and to 60.38 MWh for the hot water storage, used to supply heat for the DH demand. This last storage is realized as pressurized system for scenarios with flow temperatures ⩾100 °C (**S1** and **S2**). In **S0** and **S3** the hot water storage can also support the demand fulfillment of the hot water process demand due to equivalent temperature requirements.

Table 3
Overview of fixed and specific investment costs for energy generation, conversion and storage units in the IESS superstrucuture.

		Reference	Fix Cost c_{fix}	Specific Cost c_{spec}
		unit	€	€/Ref.unit
Generation	BM-SG	[MW^{th}]	100,000	300,000
	HP (general)	[$MW^{th,sink}$]	50,000	300,000
	HP (sink ⩾100 °C)	[$MW^{th,sink}$]	1.05·50,000	1.05·300,000
	Direct heat recovery	[$MW^{th,sink}$]	0.05·50,000	0.05·300,000
Storages	RS	[MWh_{th}]	100.000	100.000
	Warm water tank (35 °C)	[m^3]	15,000	400
	Warm water tank (65 °C)	[m^3]	30,000	400
	Pressurized hot water tank	[m^3]	100,000	1500
	Atmospheric hot water tank	[m^3]	$\frac{1}{3}$·100,000	$\frac{1}{3}$·1500

is not included in the energy supply system in **S1** and **S2**. The additional amount of supplied energy is mainly realized by higher BM-SG capacities. However, compared to **S0**, the site-demand supplied by the BM-SG can be reduced. This is enabled by the integration of heat recovery from 35 °C via a HP to supply the hot water process demand. Also the corresponding water storage tanks at 35 °C are realized as rather big aggregates to exploit the full potential of excess heat recovery at this temperature level. These results are also shown in Fig. 8 for absolute values of capacities of all units in all scenarios. and Fig. 9 for the relative capacities of the generation units in all scenarios compared to each other.

Scenario 4 and 5. While the additional costs in **S1** and **S2** are still easy to explain, the increase in costs in **S4** and **S5** compared to **S0** related to the additional required energy is surprising. Furthermore, in these two scenarios additional costs, not considered in the objective function, would occur for decentral electric booster heaters lifting the flow temperature to required levels, which are not considered so far. Specific costs for electric heating elements Nevertheless, several important conclusions, leading to the surprisingly higher costs compared to **S0** and **S3**, are:

- Comparably high capacities of the integrated HPs occur leading to higher investment costs and power costs
- Comparably high capacities of the cost-intensive RS. The highest and second highest capacity are found in **S4** and **S5** with 89%, respectively, followed by **S2** with 71% of the capacity found in **S4**.
- Higher losses are assumed to occur in those two scenarios. A detailed evaluation of this is shown in Section 4.4

4.3. Unit integration

In a comparison of Fig. 8, Fig. 9 and Fig. 10 one can see that the following three units are integrated in all six scenarios:

- BM-SG
- RS
- Pressurized or atmospheric hot water storage

The integration of those three units will be discussed in detail in the following paragraphs. This is followed by a summary for the integration of heat recovery units and storage units with direct connection to the heat recovery units.

Biomass steam generator. For the BM-SG the smallest capacity, result of **S5**, accounted for 76%, see Fig. 9, of the highest capacity obtained in **S1**. In **S1** both, the DH energy demand and the necessary flow temperature, are the highest compared to the other scenarios. In comparison, in **S5** the BM-SG capacity can be significantly reduced as both heat recovery options are integrated (one HP a one direct heat recovery unit). In general, several interesting observations regarding the capacity of the BM-SG can be concluded:

- Compared to **S0**, where no DH is supplied, the capacity of the BM-SG in **S5** is even a little smaller, see Fig. 9. Nevertheless, due to more integrated units higher total annual costs occur in **S5**, see Fig. 7.
- Compared to **S3**, where more energy is supplied for DH, the difference in capacity size of the BM-SG in **S5** only accounts for 3%, see Fig. 9.
- **S4** with the lowest energy demand and flow temperature for DH supply has the second highest capacity for the BM-SG, see Fig. 9. The capacity is only 2% than the maximum BM-SG capacity in **S1**. Compared to **S5** with the same demand characteristics the capacity is approximately one third higher.

Ruths steam storage and hot water storage. A different picture is revealed when comparing the capacities of the RS. Here, the highest capacity is obtained for **S4**, with already lower requirements of the DH grid regarding both: total energy demand and flow temperature level, see Fig. 10. The smallest capacity is obtained in **S3** with only 59% of the maximum value. This comparably small RS capacity comes along with a high capacity of the hot water storage, which can support the fulfillment of two energy demand requirements in **S3**. Thus it can be concluded, that the importance of a high capacity of the RS is not as big as in other scenarios.

However, the capacity of the hot water storage in **S3** is not the maximum capacity, this is obtained for **S0**, see Fig. 10. Nevertheless, in **S3** the hot water storage is only slightly smaller, accounting for 99% of the maximum capacity.

The lowest capacity values for the hot water storage are obtained in **S1**, **S2** and **S5** with 24, 26 and 27 %, respectively, see Fig. 10. For **S1** and **S2** the determination of the optimal capacity of the hot water storage is also influenced by higher specific investment costs for this unit compared to the other scenarios, as the hot water storage has to be realized as pressurized unit here. Thus, the economic disadvantage of integrating a bigger RS is not as high as compared with atmospheric hot water storage units. However, in **S5** a slightly different picture is shown. Here, the excess heat with 65 °C is enabled for DH supply via direct heat recovery, see Fig. 5. Thus, in case of integration the hot water storage would supply heat with 65 °C in the superstructure. Compared to the scenarios with heat recovery by HPs a smaller share of the DH can be provided with heat recovery as no additional electrical energy is used to supply the heat.

Another interesting aspect of this unit in **S5**, is that for direct heat recovery at 65 °C it would also be possible to buffer temporal differences between excess heat occurrence and energy demand with the water storage tank at 65 °C. This storage is linked to the source side of the heat recovery equipment in the superstructure. Due to this circumstance, it was already estimated prior to the optimization that only one of those two storage units would be integrated. The optimization confirmed this assumption and resulted in the integration of the storage tank linked to the DH interface for the defined frame conditions, see Fig. 10. However, this finding already leads to a detailed analysis of heat recovery and connected excess heat storages in the following section.

Heat recovery and linked storages. For the heat recovery units and optional, preceding water storages at 35 and 65 °C the following, general conclusions can be made:

- For all six scenarios only one HP is chosen to be integrated. Although, in **S5** both heat recovery units are integrated, only one HP is integrated as heat recovery unit 1 is realized as direct heat recovery unit (by means of an HEX) here.
- When a HP is integrated the corresponding water storage tank for the excess heat at the source side of the HP is also integrated. For direct heat recovery in **S5** no source-side water storage is included. However, the energy generated via direct heat recovery can still be stored and thus adapted to the DH demand the water storage linked to the DH interface, see above.
- HPs using the excess heat at the level of 65 °C are integrated in **S1** and **S3**, where they are enabled to supply hot water for the process demand (**S1**) or both, hot water and DH (3).
- In case of HP integration high usage degrees of the excess heat can be achieved. For HP1 excess heat usage levels account for 85 and 87% in **S0** and **S3**, respectively. For HP2 even higher shares of 97% (**S2**) and 98% (**S1**, **S4**, **S5**) are determined and obtained in the operational optimization.

From the combined implementation of HPs with corresponding excess heat buffers, one can conclude, that providing suitable temporal profiles of excess heat is an important requirement to re-use excess heat in industrial or DH energy supply systems.

4.4. Efficiency analysis

In another analysis step the efficiency of the energy supply system is determined for all scenarios. Thus, the following definition of the energy supply efficiency η is used: provided heat by the SG and the heat recovery units are compared to the required heat in the industrial process and the DH system, see Eq. (10)

$$\eta = \frac{Q_{industrial} + Q_{DH}}{Q_{SG} + Q_{HP1} + Q_{HP2} + Q_{HEX}} \tag{11}$$

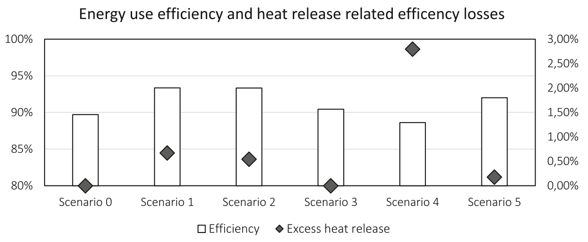

Fig. 11. Efficiency of energy supply.

Highest efficiency was seen for S1 and S2 (⩾93%), which also occur to have the highest total annual costs. However, it can still be concluded that combined provision of energy for industry and households can lead to high overall efficiencies, also in conventional DH systems. Regarding efficency, these scenarios are followed by S5 with approximately 93%. The lowest efficiency was achieved in S4 (⩽89%), while in S0 and S3 it was slightly below and above 90%, respectively. These values are shown as white bars in Fig. 11. While the majority of the losses can be explained by storage losses (heat losses while storing as imperfect insulation and losses while charging and discharging are assumed in the optimization model), for Scenarios 1,2,4 and 5 also "wasting heat" was observed. Especially, for low-load weeks (summer) heat was released to the environment in single hours. Regarding the total demand by industry and DH the heat release accounted for 0.18% in S5, 0.54% in S2, 0.67% in S1 and 2.8% in S4.

Especially, for S4 with surprisingly high costs (see before) and now also the highest relative heat release the following conclusion can be drawn. Optimal matching of excess heat streams and energy demand linked by heat recovery measures depend strongly on temperature levels, energy amounts and a well-suited system design. Here, the chosen superstructure approach already shows that the system design (compare S4 and S5 with equivalent demand characteristics) is a crucial criteria. S3 reveals that especially synergies between providing industrial and DH can be a promising contribution in the future, regarding economics without making compromises regarding the overall efficiency. Efficiency losses do not occur due to heat release to the enviroment for S3 but due to storage losses. Thus, it can be concluded that the optimization approaches, as presented in this work, can contribute to find well-suited IESS.

5. Conclusion

This work presents a method applied to an exemplary use case to assess the impact of DH developments on industrial energy system design when coupled generation of industrial and DH heat supply occurs. It consists of a two-stage approach based on a dynamic district energy system model considering building, substation and network details and a subsequent mixed-integer optimal design framework for the IESS. Thus, the impact of building, DH substation or pipe network measures are directly represented through first principle physical models. The method is applied to an example application. Thus, four different DH configurations are studied that showcase the impact of different building and pipe network measures in six scenarios.

Results for the elaborated use case show that especially synergies, e. g. in corresponding temperature levels, between industrial heat and DH demand lead to advantageous results. However, low temperature requirements in DH networks do not always lead to better overall economic performance in sector coupling. For the analyzed use case also the integration of small storages is found as important criteria to smooth and adapt temporal profiles of excess heat occurrence.

This work and the described findings showed the relevance and potential contribution of suitable, system layouts evaluated with optimization-based design and operation methods. The application of such approaches is emphasized by the findings in this work. Especially, as decision support for sector coupling approaches with several options and thus a high decision complexity, optimization-based approaches can offer good and fast estimates for optimal system layouts. Furthermore, they allow economic comparisons without time–costly detailed simulations for a high number of different system settings. However, this work has revealed future improvement potential for the presented approach. Integrating the following aspects in the overall formulation might lead to different, optimal results and pose an promising outlook for the work presented in this paper.

- Only a selection of renewable generation options is included in the IESS superstructure. Further, probably cheaper units available in the superstructure might change the optimal plant layout.
- Combined electricity and heat provision instead of exclusive heat provision could be evaluated.
- Synergies between cooling needs, which are not considered in this paper, and heat provision can increase the feasibility of HPs to a higher extent, compare the concept of heat recovery over the pinch point in grand composite curves of stationary or time-averaged pinch analysis methods, [41]
- In this work rather low excess heat temperature are assumed. Also, only one excess heat profile for each temperature level is considered. Changes in profiles, excess heat amount and temperatures have a high potential to change results found for this case study.

Also, the applied method has limitations, which need to be mentioned to understand the results in a correct way, such as:

- Due to the sequential combination of methods, it is limited to DH networks that are either completely supplied by an industrial energy system or to industrial supply systems that are not dynamically interacting with the DH network, i.e., where heat supply is not depending on network dynamics like pressure distribution.
- Capital expenditures considered in this work, see Section A, include conservative estimates of equipment costs but no detailed installation and integration expenditures. More detailed cost information can also alter the results for single or all district heating configurations

CRediT authorship contribution statement

Sophie Knöttner: Conceptualization, Method, Software, Formal analysis, Writing - original draft, Writing - review & editing, Visualization. **Benedikt Leitner:** Conceptualization, Method, Software, Formal analysis, Writing - original draft, Writing - review & editing, Visualization. **René Hofmann:** Conceptualization, Formal analysis, Writing - review & editing, Supervision.

Declaration of Competing Interest

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

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Appendix A. Economic parameters

The following prices for energy carriers (biomass and electricity) and coefficients for investments are used as input for the optimization. These values are also summarized in Table 3.

A.1. Energy carriers

For electricity no distinguishing of energy and power related costs is made for this first layout optimization run. An average price (energy + grid costs + taxes) of 90 €per MWh^{el} is assumed. This assumption is based on the following figures: An analysis of Austrian Energy Exchange hourly spot market electricity generation costs for 2020 revealed a cost range of −40.45 €/Mwh to 125.24 €/MWh with an average value of 33.09 €/MWh and a median of 32.67 €/MWh [42]. Furthermore, in Austrian commercial enterprises, for example, the generation costs amount for approx. 45 % of total electricity costs [43]. Nevertheless, exact figures depend on individual contracts between energy suppliers and industrial consumers. The biomass purchase prices is assumed with 50 € per MWh, which aligns with the upper limit of the range found in literature. The Austrian Biomass Association [44] provide a purchase price for firewood of about 45.0 €/MWh in 2019. In December 2020 lower prices are recorded (40.3 €/MWh for December 2020). An analysis of the price trajectory showed a slight price decline compared to the years before in Q1/2020, which might be caused by short-term economic effects of CoVid19. A German company specialized on heating systems state a price of 52 €/MWh for firewood [45].

A.2. Generation units

For the **BM-SG** specific investment costs (including costs for implementation, taxes, etc., between 280,000 (for ⩾90 MW) and 500,000 (for ⩽10 MW) €/MW are derived from findings for stoker boilers in a U.S. report by the Environmental Protection Agency. [46]. Also a cost range for biomass fired fluidized bed boilers is derived from there, which was found to be 340,000 (for ⩾90 MW) – 1,050,000 (for ⩽10 MW). Furthermore, within the framework of the EU-funded project PROMOBIO (Promotion to Regional Bioenergy Initiatives) fixed costs of 100,000 € and specific costs in the range of 300,000 €/MW are stated for a 2 MW biomass boiler [47].The latter, which is in the range derived from [46] is used in the work here.

For **HPs** the cost regression for industrial implementations derived by Wolf [28] is used.

$$C_{invest,HP} = f_{HP1}\cdot(CAP_{HP})^{f_{HP2}}\cdot f_{HP3} + f_{hydr1}\cdot(CAP_{HP})^{f_{hydr2}}\cdot f_{hydr3} \quad (A.1)$$

where CAP_{HP} is the heating power of the HP in kW, factors f_{HP1} and f_{HP2} are considered to determine material costs and factor f_{HP3} to determine costs of installation and planning. The second term of Eq.(A.1) considers costs for necessary hydraulics for the HP set-up, again for the materials as well as the installation and planning. The actual correction factors were determined by Wolf [28] in own calculations. For HPs two regressions are distinguished for below and above a heating power of 210 kW. In order to derive a linear function for this work investment costs were calculated according to Eq. (A.1) for a heating power in the range of 100–2,500 kW (equidistant increase of power of 100 kW). Then a linear regression formula, see Eq.(A.2) was derived with a coefficient of determination of 0.9979 for this range. For very small or very large HPs beyond this range the derived cost function will overestimate costs to a certain extent.

$$C_{invest,HP} = 54,134€ + 271,690€/MW_{HP} \quad (A.2)$$

For further calculations in this work values are rounded to 50,000 €and 300,000 €/MW^{HP}, respectively. For specific configurations further *sizing factors* are implemented. High-temperature heating demand (⩾100 °C) provided with HPs is considered by a cost increase of 5% (value assumed) for both values (sizing factor 1.05) compared to the basic HP (sizing factor 1). If the heat source temperature is already higher than the heat sink temperature, implementing a HEX is enabled in the model. Thus, also a cost regression presented by Wolf [28] was analyzed, where the HEX area is the reference unit. An analysis and comparison for the thermodynamic relations in the use case showed that the costs for direct heat recovery can be included in this work as approximately 5% (sizing factor 0.05) of the HP costs, which is implemented in the optimization formulation.

A.3. Storage units

The RS investment costs are assumed with a fixed component of 100,000 € and a specific cost share with the same value in €/MWh^{th}. This assumption is based on specific costs of 104,600 €/MWH^{th} for a RS enhanced with phase-change material layers with a capacity of 70 MWh^{th}. Investment costs for this specific storage are determined within the work of a project focusing on a high-temperature heat storage for a heat collection and distribution station in Austria [48].

Regarding costs for further thermal water tank storages the following data found in literature was considered:

- In a storage technology report elaborated by six working groups in Austria in 2016 [49] 5–7 €/kWh without additional equipment are reported for small scale water storage units (capacity of several kilo-watt-hours). For large scale water storage systems (capacity ⩾20 MWh and several 100,000 m^3) investment costs of 1,300 €/m^3 are stated.
- For the largest sensible heat storage systems in Germany, which are seasonal hot water storage systems with volumes of 5,000 to 10,000 m^3, Sterner and Stadler [50] state specific investment costs of 0.5 to 3 €/kWh.
- Verda et al. [51] assumed investment costs for thermal storages in DH systems with supply temperatures of 120 °C to account for 2,400 €/m^3.
- Wolf [28] presented a correlation in the same form as Eq.(A.1). Linear regressions were derived for investments costs in i) the range 10–100 m^3, see Eq.(A.3) ii) the range 10–600 m^3, see Eq.(A.4). Both ranges had equidistant steps of 10 m^3.

$$C_{invest,ST} = 15,755€ + 760.08€/m^3 \quad (A.3)$$

$$C_{invest,ST} = 45,520€ + 437.67€/m^3 \quad (A.4)$$

Based on these results the following assumptions were made for this work.

- For low-temperature storage units (⩽50 °C): 15,000 € + 400 €/m^3
- For medium-temperature storage units with higher insulation requirements: 30,000 € + 400 €/m^3
- Pressurized water storage unit: 100,000 € + 1500 €/m^3
- Hot water, but not pressurized water storage unit: assumed to account for one third of pressurized water storage costs

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Paper 4

Assessment and conceptualization of industrial energy flexibility supply in mathematical optimization in a competitive and changing environment

published in Energy Conversion and Management in collaboration with René Hofmann.

This work focuses on different aspects of flexibility. Understanding incentives for industrial flexibility is crucial to include them in mathematical optimization. Based on this analysis, this work presents a newly proposed multi-step formulation for flexibility in mathematical optimization adaptable to a broad range of flexibility types. The formulation is tested for an industrial use case related paper production and "energy source flexibility". One optimal steady set of design decision variables shall be derived for different operational scenarios where every energy source carrier shall be reduced as far as possible. The results reveal (i) a significant investment cost increase for more flexible systems and (ii) the first energy carrier that cannot be substituted completely anymore would be natural gas, followed by electricity from the grid. This work highlights challenges for industrial energy supply regarding flexibility and economically feasible decarbonization.

My contribution: Conceptualization, Methodology, Formal Analysis, Writing - Original Draft, Writing - Review & Editing, Visualization

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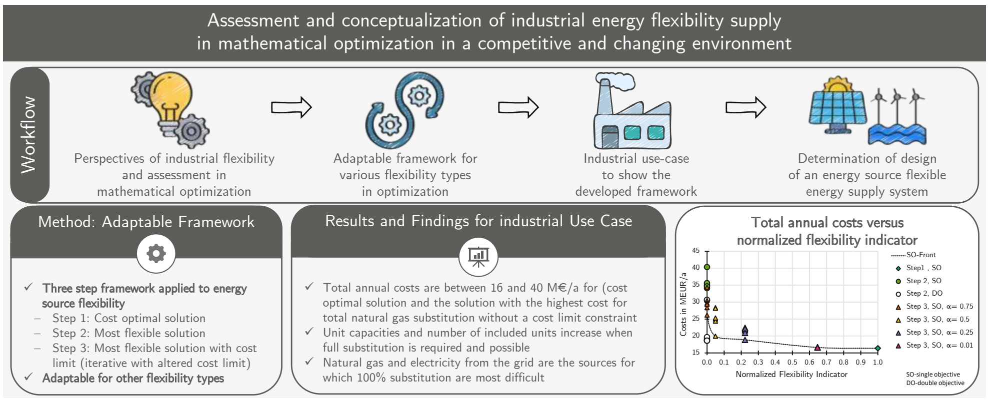

Figure 10: *Graphical Abstract Paper 4*

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Assessment and conceptualization of industrial energy flexibility supply in mathematical optimization in a competitive and changing environment

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ABSTRACT

Competitive and changing frame conditions, such as the need for decarbonization of energy supply or the growing share of renewable electricity generation, are driving the need for flexibility in different systems, e.g., in power supply and industrial production. Flexibility is often included in mathematical optimization applications. However, integrating it in optimization may create conflicting understandings of flexibility due to the properties of relativity and goal orientation. Establishing a common understanding of flexibility in industrial systems among all stakeholders, and a general but adaptable formulation for inclusion in mathematical optimization could better exploit the potential for flexibility in the future and make a greater contribution to energy transition. In this paper, an overview of flexibility, the incentives for it, and its integration into the decision variables, constraints, and objectives of mathematical optimization is provided. This enables the authors to conceptualize industrial flexibility in optimization and provide the basis for the presented approach: a three-step mixed-integer linear programming optimization model for integrating flexibility in the evaluation of cost-optimal energy supply systems.

The presented approach is generally suitable for various flexibility types but is applied in this study to assess energy-source flexibility and elaborate its cost implications in a use case from the industry. For the identified energy supply systems with full energy carrier flexibility, the total annual costs increased by 62 to 112% compared to the cost-optimal solution with all available energy carriers, of which a relevant share was due to the investment cost increase by a factor of up to four. The two main conclusions are that (i) the results of the presented use case reveal the order of magnitude in cost increase for energy-source flexible supply systems, and (ii) the presented approach should be further used and developed to evaluate different types of industrial flexibility e.g., analysis of cost increase for robust energy systems in a changing environment, a potential contribution of flexibility for energy markets or power grids, or the flexibility to allow production changes.

1. Introduction

Over the last few decades, flexibility has become an indispensable component in maintaining and restoring stability in systems that must react to anticipated and unanticipated variability. One significant driver of this development has been the increased need for flexibility in power systems. Thus, new opportunities have arisen, such as the exploitation of flexibility at industrial production sites. Providing flexibility in industrial processes yields benefits for both power system operators and industrial actors. Measures to exploit flexibility include flexible consumption from spot markets to provide ancillary services or redispatch and congestion management. For example, the frequency of required congestion management and redispatch in the Austrian electricity transmission system has increased over the last decade, driven by a growing share of fluctuating, renewable electricity provision from the grid [1]. In the past, congestion management measures and a high share of ancillary services were provided by controllable power generation assets, these being mainly hydropower, pumped energy storage, and conventional thermal generation capacities [2]. Thanks to the decarbonization efforts of energy supply companies, decommissioning of conventional, fossil-fired thermal power plants is ongoing and there has been no new commissioning of such equipment since the second half of the decade 2010 to 2020. Thus, finding new assets that can provide the required flexibility will be a crucial task in the next few years. This development is also summarized in the literature as a flexibility gap, visualized in Fig. 1.

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Nomenclature

Acronyms

CEEGEX	Central Eastern European Gas Exchange
DV	Decision variable(s)
IEA	International Energy Agency
IES	Industrial energy system
MILP	Mixed-integer linear programming
PPA	Power-purchase agreement
PV	Photovoltaic
VDI	Verein Deutscher Ingenieure

Sets

$Flex$	Set of all operating scenarios to determine flexibility
$GRID$	Set of all grid connections
$PERIOD$	Set of all considered periods
$SOURCE$	Set of all sources
$TIME$	Set of all time steps
$UNIT$	Set of all supply units

Parameters

α	Adaptive factor to set cost limits (–)
$\Delta\tau$	Time step duration (h)
ΔT	Duration of representative period (h)
CAP	Capacity in (MW or MW h)
c	Specific cost coefficient (€ MW^{-1} or € MW h^{-1})
EM	Emissions (t)
em	Specific emission factor (t MW h^{-1})
n	Number of years for depreciation (–)
r	Interest rate (–)

Subscripts

$energy$	Energy related value (–)
inv	Investment related value (–)
$power$	Power related value (–)
g	Grid connection
limit	Limit
ng	Natural gas
s	Energy source
u	Unit

Superscripts

*	Optimal value
fix	Fixed investment costs
max	Maximum
power	Power related value
spec	Specific investment costs
UB	Upper bound

Variables

CAP	Capacity in (MW or MW h)
ω	Integer indicating weight of representative period (–)
C	Cost (€)
c	Charging power (MW)
d	Discharging power (MW)
E	Energy (MW h)
$ESLI$	Objective value for flexibility integration (–)
f	Fuel power (MW)
f	Operating scenario (–)
i	Binary variable for unit existence (–)
$LCOE$	Levelized cost of electricity (€ MW h^{-1})
$LCOH$	Levelized cost of heat (€ MW h^{-1})
lim	Continuous variable to determine reduction potential (–)
p	Electric power (MW)
p	Representative period (–)
q	Thermal power (MW)
s	Supply power (MW)
t	Timestep (–)
v	Binary variable for start-up of unit (–)
w	Binary variable for shut-down of unit (–)

There are currently both ecological and political reasons for providing more flexibility in energy systems, the latter arising following geopolitical developments in 2022. In the context of the ensuing energy crisis in Europe, the International Energy Agency (IEA) listed flexibility in power systems as one of ten key criteria involved in reducing and overcoming reliance on natural gas [3].

It is, however, not only external factors and political developments that drive the increase in importance of flexibility in industrial systems, but the burgeoning need for flexibility in power systems. Industrial (production) systems, including both manufacturing and energy supply systems, require flexibility to remain competitive and fulfill individual customer wishes and needs in a volatile market.

In considering the above-presented drivers of flexibility over recent decades it must be remembered that understanding, meaning, and interpretation of flexibility strongly depend on the context. In addition, different types of flexibility can be distinguished, and assessment and planning of flexibility and flexible systems, e.g., an energy supply system, can be performed for different life-cycle phases, typically for a system's design or operation mode. Furthermore, various methods can be used to assess flexibility. Frequently applied methods are simulations or mathematical optimization.

It is therefore clear that precise wording of descriptions and definitions is a crucial prerequisite in dealing with the topic of industrial (energy) flexibility.

1.1. Industrial energy flexibility

Flexibility in the context of energy systems in general – and in detail for electric grids and production systems – has been widely discussed in the literature over decades. From an energy (often power system) perspective, flexibility is often understood as one of the key enablers in decarbonizing electricity generation. From the perspective of industrial production sites, it is understood as a competitive advantage; nowadays, it is often already a requirement. Not only can the incentives to incorporate flexibility be various but the types, levels, and strategies for providing flexibility can differ in power and industrial production systems. A significant difference between the industrial and power sectors is the energy vectors considered. The power sector primarily focuses on electricity. Thus, flexible electricity consumers are of particular interest. They can be found in industry but also in the building sector. For industrial sites, flexibility is of significant interest not only for electricity but also for further energy carriers, e.g., hot water or steam. Furthermore, flexibility in the production process, e.g., the product portfolio or production amounts, is a relevant domain in the industry. A short though not comprehensive overview of power

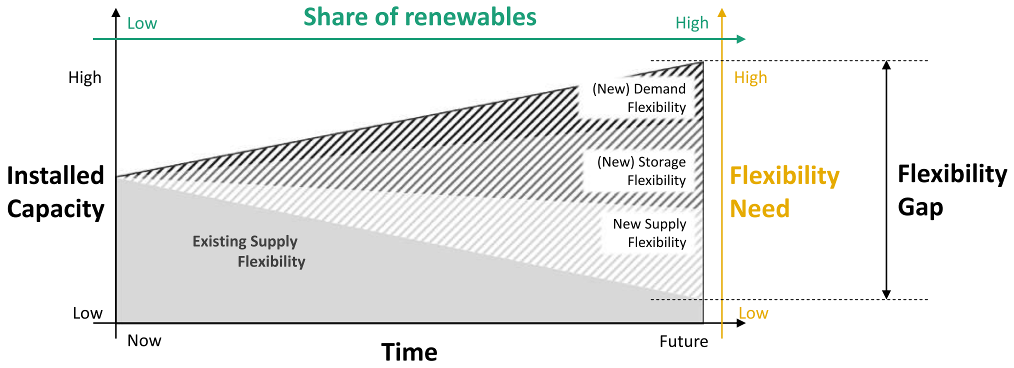


Fig. 1. Simplified visualization of increasing flexibility need and gap from a power system perspective.
Source: Figure adapted from Papaefthymiou et al. [4].

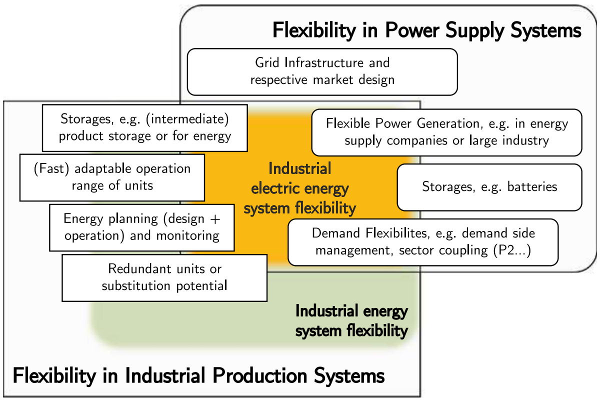


Fig. 2. Visualization of exemplary but not complete measures to increase flexibility in power supply systems (upright) summarized from a study presented by IRENA [5] and Papaefthymiou et al. [4] and measures to increase flexibility in industrial production systems summarized from Pierri et al. [6].

system and industrial flexibility and their intersections and overlaps is given in Fig. 2.

The importance of (industrial) flexibility provision is also emphasized by the fact that in 2019 and 2021, first drafts for two parts of a Verein Deutscher Ingenieure (VDI) standard for *Energy-flexible factories* were published. Part one considers [7] the fundamentals of energy-flexible factories. Part two aims to support the identification and technical assessment of flexibilities [8]. In general, the marketing of energy flexibility in factories should be promoted. The economic performance of factories and the rising volatility in overall electricity supply can benefit from the integration of industrial energy flexibility in markets, ancillary services, or congestion management. [7,8].

The following discusses different interpretations, properties, features, and dimensions of flexibility. Examples are adduced that emphasize the importance of establishing a clear understanding of this term, which has remained a matter of debate.

Interpretation and definition of industrial flexibility. The VDI standard addresses flexibility in industrial factories, focusing on exploiting flexibility in markets and for grid services. However, the definition and interpretation of industrial flexibility can differ. This can be seen by comparing the understanding in the VDI standard described above with, e.g., Luo et al.'s work discussed below. Luo et al. [9] present different types of flexibility in industry. In their conceptual framework, they find at least 17 different flexibility terminologies identified in the literature. Based on these terminologies, they summarize five flexibility types with their respective concept and design strategies. These types are: **Feedstock flexibility** is understood as ability to handle changes in quantities or qualities of inflow materials. This flexibility type and in particular, fuel or energy source flexibility is the focus of the elaborated use case later in this study (see Sections 2 and 3). **Product flexibility** refers to the ability to modify the properties of the produced materials. The ability to vary throughput is understood as **volume flexibility**. **Scheduling flexibility** is the ability to adapt resource allocation to meet the needs of various production cycles. **Production flexibility** allows for switching to another production scheme.

Another challenge that complicates the formulation of one concise definition is raised by Luo et al. [9]: Not only is there a change in the interpretation and meaning of the term flexibility over time but regarding concepts and terms in the thematic field of flexibility, three cases recur in the scientific literature: First, different terms are used for one concept (e.g., fuel and load flexibility for flexibility regarding changes for input and output streams). One specific term is only used for one concept (e.g., scheduling flexibility). Third, the same term is for different concepts (e.g., plant flexibility as summarizing terminology for all types of flexibility in a plant).

There have been recurring attempts to define flexibility in the scientific literature of the last few decades. Such attempts often depend on the perspective, e.g., power system perspective vs. industrial perspective. Among others, the aspect of dimensions of flexibility has been discussed in the past, e.g., level and type of flexibility, measures, and strategies, how flexibility is technically provided, and incentives for flexibility. Despite the many definitions found in the literature, no consistent definition of the term has yet emerged in the energy industry according to the project report by WINDNODE in 2020 [10]. However, upcoming challenges in the transition of energy systems involve different stakeholders. Thus, having a common basis, such as a standard, consistent definition, and understanding, is an indispensable prerequisite to overcoming future challenges [11]. A comprehensive review of the characteristics and dimensions of flexibility with a focus on power supply systems was presented in 2021 by Degefa et al. [11].

Properties, features and dimensions of flexibility. Luo et al. [9] classify flexibility as *relative value*. Usually, one specification is more or less flexible than another one. They recommend comparing flexibility key performance indicators of two or more specifications instead of just evaluating it for one specification exclusively. Compared to flexibility, other system characteristics, e.g., costs, emissions, or primary energy consumption, are absolute parameters, which can also be compared for different specifications but allow interpretation without comparison. Another property of flexibility derived from the literature is that it usually serves a higher purpose. In other words, typically, there are incentives or targets (compare [7]) to increase the flexibility of a specification. One example of a typical incentive is to use flexibility to react to volatile energy prices with the overriding aim of minimizing energy costs. This measure can also be seen as a reactive demand adaption to price fluctuations. Another incentive to use flexibility is to offer energy flexibility externally with the overriding aim of benefiting economically. Either costs can be reduced, or additional incomes can be created. Here, the change in power consumption is proactively offered, either directly or via an aggregator/flexibility service provider [7]. Both relativity and target orientation lead to the conclusion that flexibility is a property having more than one dimension, which in turn leads to multiple definitions.

1.2. Overview of strategies and technical measures to provide flexibility in industrial (energy) systems

The flexibility types and concepts described above, as well as the examples given, indicate that flexibility is the ability of a system to adapt its operation to an internal or external incentive. The following offers a short overview of how this can be realized in industry. Strategies and technical and organizational measures as well as incentives for flexibility, will be explained. Reference is intermittently made to the challenge of inconsistent definitions.

Regarding the hierarchical level of a plant, where flexibility is enabled, examples are given, e.g., by Pierri et al. [12]. Among other hierarchical levels, they distinguish, for instance, management or plant level, operational level, control level, process level, equipment, or technical building service level.

In the literature, the following terms are often introduced when it comes to strategies and measures for flexibility: demand side management, demand (side) response, energy storage, or flexible generation [11]. While demand side management and demand (side) response are partly applied synonymous, some authors also make a clear distinction between these two — often identifying demand response as a sub-group of demand side management [11].

With regard to flexible electricity consumption, the following industrial units and components should be mentioned. On the one hand, flexibility potential arises from sector-specific industrial processes with a high electrical energy demand. The best-known and most relevant of these processes is mostly be characterized by high loads of individual processes and units. Examples identified by Esterl et al. [13] are (1) in the pulp and paper sector: mechanical wood grinders, pulpers, and refiners and, to a smaller extent, also paper machines; (2) in the chemical and petrochemical industry: chlorine electrolysis, air separation, and calcium carbide production; (3) in the iron and steel sector: electric (arc) furnaces; (4) in the non-ferrous metal sector: the primary route for aluminum production — aluminum electrolysis and electric furnaces; and for (5) the non-metallic mineral sector: mills for ceramic products (e.g. cement production), presses for ceramic products or electric glass production.

However, in general, cross-sectoral technologies such as lighting, cooling, compressed air, and energy supply can provide flexibility. Examples of flexible energy supply options are combined heat and power generation assets. Often, the operation of gas turbines, steam turbines, combinations of those, or smaller engines can be adapted and, thus, flexibilized to fulfill the needs of industrial energy supply. Lately, power-to-heat assets, such as electric and electrode boilers and heat pumps, have had increased interest in flexible use. Boldrini et al. [14] find an increase in the contribution of power-to-heat assets in combination with thermal storages in district heating systems for balancing service provision.

The reasons industrial flexibility potentials for power systems are usually not fully exploited are numerous [13]. In general, there are technical, economic, regulatory, and cultural burdens. In particular, small and medium-sized enterprises typically do not have a sufficient knowledge base and the technical and organizational resources necessary for comprehensive flexibility utilization. Furthermore, exploiting flexibility potential can increase the risk of reduced product quality or reduced production. As production is the core competence of industrial sites, this increased risk is often avoided.

The following general, asset-independent distinctions for flexibility strategies have been identified and summarized from the literature [7]. **Load increase** is realized as load increase compared to a reference operation point and typically occurs without a countermeasure to cover losses. Thus, this measure leads to an absolute power and energy consumption change. Examples from industry are, e.g., the reduction of electricity production from a gas turbine or the increase of chlorine production in the chlorine electrolysis process. **Load reduction** is realized as a partial or whole shutdown of load consumption compared to the reference point. As before, usually no countermeasures are necessary, and an absolute change in consumed power and energy can be observed. Typical examples are, e.g., an increase in the electricity production of an engine or the reduced power consumption of an electric boiler. **Load shift** is typically a combination of load increase and reduction compared to the reference operation profile. Depending on the asset, an advance, a delay, or both of the planned load consumption is possible. This most often occurs with countermeasures, e.g., earlier increased operation of an electric boiler. The heat is loaded to thermal storage, which can be discharged later. This discharging and fulfilling of the heat demand by the storage allows a decrease in heat generation of the electric boiler at a later time. Another example of industrial load shifting is moving the production of groundwood to another timestep while using groundwood storage as an intermediate buffer, ensuring a sufficient supply of the downstream processes.

A difference in assessing the **load reduction** strategy can be recognized for the power system and the industrial production site perspective. Degefa et al. [11] see load shedding in power systems, which they also refer to as load reduction, as a drastic measure and not as flexibility. From an industrial perspective, load reduction does not automatically account for disrupting routine operations. A simple example can be found in sector coupling applications. The load consumption of a power-to-heat unit for hot water or steam supply can be reduced without effects on production if units allow a fuel switch, e.g., fuel-fired steam boilers. However, for renewable electricity generation, the load reduction, often also referred to as curtailment of renewables, is, according to Degefa et al. [11], not assessed as readily available flexibility.

Such strategies can be applied as proactive load adjustment, e.g., for price incentives, or as reactive load adjustment, e.g., when external signals trigger the adjustment [7]. Although the above examples again focus on electric load, these concepts can also be applied to thermal energy supply. Also, here, the idea of energy flexibility is important.

The above-described general strategies can often be distinguished regarding their life cycle, i.e., whether they are considered during the design or the operation phase. Further options for differentiating flexibility measures are related to their role in flexibility resource enabling. Enabling flexibility resources can often be related to hierarchical levels such as technical measures vs. operational measures [11]. The latter, operational measures, e.g., the planning for a cost-optimal unit commitment of flexible assets, are often also referred to as organizational measures [15] and take advantage of the technical flexibility inherent in single units.

Technical measures of single assets, e.g., energy conversion units or storages, can be characterized by key performance indicators for technical features and characteristics. Dotzauer et al. [16] identify three crucial dimensions for the flexibility of a single unit in order to provide power in line with fluctuating demand profiles. Positive and negative ramp rates, in Dotzauer et al. also referred to as velocity ramps, describe the ability of a unit to change the produced power from one time step to another. The higher this value is, the more flexible (in terms of adaptability) a unit is. In optimization models, this value is often included as a parameter and in ramping constraints for energy conversion units. The dimension of the power range is characterized, e.g., by the base load ratio. A high base load ratio, i.e., the minimum load versus the rated capacity, allows a wide range of technically feasible operation points. This is also often included in optimization constraints and parameters. The third dimension is the duration of specific load conditions. Units are characterized by their start duration and their maximum duration for the maximum and minimum load. Except for the start duration, compare, e.g., [17] these parameters are not normally included in optimization formulations.

1.3. Decision support and applied optimization approaches including flexibility in industrial energy systems

Combining strategies for flexibility provision, single, technically flexible units and possibly organizational measures such as planning and determination of optimal unit commitment and economic dispatch, increases flexibility potentials. Combination strategies for flexibility, technical, and organizational measures are often well suited for mathematical optimization applications. Some examples are given in Tristan et al. [15], e.g., (re)scheduling of production processes as well as adapting electricity generation and consumption to price profiles or fluctuating renewable generation.

Mathematical optimization for industrial applications can cover various areas. Typical industrial optimization applications are heat exchanger network synthesis (design or retrofit), which aims to find the best trade-off between heat recovery and external utilities providing process heating and cooling; design optimization aimed at finding the best supply and/ or production system; operation optimization, which seeks the best trajectories for operation profiles in a given energy supply system and scheduling, which aims to determine the best order of tasks in production processes.

Including flexibility in optimization applications is a challenge and often leads to modeling, formulation, and numerical resolution difficulties. However, various concepts covering flexibility and optimization together have been applied in the past.

Often **single step and single-objective optimization models** are set up, e.g., aiming at cost optimality, with (at least in the short-term) a-priori known costs. Here, the incentives leading to flexible operation or design are implicitly included in the model. Examples of this are, e.g., analysis of the optimal operation and the impact of thermal storage integration of industrial combined heat and power systems with a rolling time horizon for fluctuating electricity costs in a mixed-integer linear programming (MILP) model in Panuschka and Hofmann [18]. Also, Takeshite et al. introduce a linear cost-optimal model to assess the potential of different business customers (no industry) with combined heat and power plants to provide grid flexibility [19].

Optimal operation and integration of new units in a pulp and paper factory focusing on integrating high shares of fluctuating renewables is presented as a MILP model in Puschnigg et al. [20]. In these examples, typically, technical flexibilities are modeled, and overall costs are evaluated. Sometimes, further performance indicators are assessed, which reveal condensed information about the technical flexibility of a system in the parametrized configuration. Examples might include the average operation state, number of starts, or statistical indicators of all operation states of a component.

Other approaches include multi-step (and sometimes multi-objective) optimization. Here, flexibility is typically included by a parameter variation and iterative calculation. Montastruc et al. [21] state that determining optimal design without considering flexibility does not lead to flexible solutions. They propose an iterative optimization calculation for an eco-industrial park with three sub-companies by deriving a Pareto front and comparing feasible solutions. Boix et al. [22] investigate how to derive an optimal network that can withstand deviations in demand. The aim is to develop a generic approach capable to evaluate the cost of the flexibility to serve at the decision stage. They consider different formulations, one leading to oversized capacities and, thus, (too) high costs. Another results in a considerably long computational time. They compare their two-step approach for an eco-industrial park with 15 companies to results found with an integrated procedure, including more combinations of parameter deviations. They consider flexibility as a feature of the whole system when single parameters, e.g., demands, deviate from the assumed basic state. Another multi-stage approach is proposed by Ahmadi et al. who develop a framework to determine optimization-based long-term energy system resilience [23]. The incentive for long-term energy system resilience in their study considers climate change disruptive events with high impacts but low probability. On a technological basis, they found a shift from coal and hydropower to PV when resilience should be maximized. Similar to flexibility, the concept of resilience continues to invites different understandings, interpretations, and definitions.

A third approach to considering flexibility is using **a-posteri performance indicators** that are derived from a previous optimization. Here, many iterative optimization runs may be required. Key performance indicators already proposed in the 80ies are, for instance, the Swaney and Grossman Flexibility Index, which evaluates the smallest maximum deviation that fluctuating parameters can still deal with. Here, the number of deviations that need to be considered are 2^n for n considered parameters. Furthermore, Saboo et al. [24] introduced the Resilience Index, which defines the measure of how a system can adapt to unforeseen changes or events. Here, $2n$ variations need to be considered to derive this indicator.

A scenario-based optimization approach including flexibility is presented by Aguilar et al. [25]. They optimize operation and design and consider flexibility based on a scenario variation. More recently, the concept of performance indicators for flexibility in industrial systems has also been set in the context of resilience. Valenzuelas-Venegas et al. suggested an indicator for the resilience of eco-industrial parks [26]. This indicator considers the possible interfaces between participants in the park and the ability of each flow to change in case of dropped-out suppliers in the park. This was later enhanced with a multi-objective optimization formulation, including minimal costs, minimal environmental impact, and maximum flexibility [27].

Given the challenges in defining flexibility, it can generally be understood as a system's ability to adapt. In further consequence, flexible systems can offer alternatives to conventional operating states, designs, etc. In the last decade, the concept of *modeling to generate alternatives* to expand our thinking on energy futures [28] gained interest. An example of the application of *modeling to generate alternatives* is presented in Pickering et al. who show the diversity of options to eliminate fossil fuels and reach carbon neutrality across the entire European energy system [29]. This concept is also relevant for the integration of flexibility in mathematical optimization. Such methods can be supported by the multi-step and multi-objective approach elaborated in this study.

In Table 1, the authors present a comprehensive overview of various incentives for flexibility and their corresponding objective functions. The table also includes examples of how to incorporate different types of flexibility into various industrial optimization applications such as operation optimization, design optimization, process scheduling and heat exchanger network synthesis.

1.4. Contribution

In the present study, the authors identify a gap in existing studies and work on how to include industrial flexibility in mathematical optimization. The following need for further research was derived based on the presented understanding of industrial flexibility and concepts of including flexibility in optimization. Thus, the authors aim to contribute to the field of industrial flexibility in the following ways:

- Analyze definitions, dimensions, and understanding of flexibility, as well as measures and operational concepts providing industrial flexibility, which should provide a clear picture of challenges in analyzing industrial energy flexibility.
- Provide an overview of the requirements to include various levels of energy flexibility in mathematical optimization.

Table 1
Selection of requirements that need to be fulfilled if different types of flexibility need to be considered.

Flexibility type	Typical objective function	Selection of requirement to integration flexibility types for			
		Operation optimization	Design optimization	Scheduling	Heat recovery network synthesis
Fuel flexibility (Feedstock flexibility)	No explicit obj. function, often: Min cost	Often not expressed explicitly but implicit by parametrization of available technical unit flexibility: ramping or minimum on- and off-line time of units	Often not expressed explicitly but implicit by parametrization of available technical unit flexibility: ramping or minimum on- and off-line time of units	Hardly considered	Hardly considered
Market flexibility	Min cost	Forecasts (prices, demands, self-production), Realize rolling horizon optimization	Forecasts (prices, demands, self-production)	Forecasts (prices, orders)	Forecasts (Prices)
Grid support e.g. balancingor redispatch (product flexibility)	Min cost Max profit	Typically needs a two-step approach. Step 1: determine baseline without support Step 2: determine support possibilities	Often only with probabilities due to lower temporal resolution	Hardly considered	Hardly considered
Planning with fluctuating sources (e.g. renewables or batch demands) (feedstock or volume flexibility)	Min cost, Max self-sufficiency	Forecasts, technical flexibility expressed in model (e.g. ramping)	Limited computational resources require typ. periods, technical flexibility expressed in model	Include temporal profile of availabilities/prices which is included as parameter	Use multi-period stream table
Adaption to unforeseen changes (volume flexibility)	Min cost or Max product	Realize rolling horizon, iterative calculation, fast solving times, Eventually stochastic optimization or storage operation constraints	Often integrated by calculation for a scenario set where possible ranges are considered	Realize rolling horizon, iterative calculation, fast solving times, Eventually stochastic optimization or storage operation constraints	Often found with parametrization and integrated by calculation for a scenario set
Adaption to customer wishes product(ion) flexibility	Max profit	Hardly considered	Hardly considered	Important incentive to set-up this type of optimization,	Hardly considered

- And last but not least, develop a formulation to include different incentives and aspects of flexibility in a framework of a mathematical optimization model.
- This method is applied to an industrial use case. Feedstock flexibility's economic and ecologic impact, particularly energy source flexibility in industrial energy system (IES), are evaluated and assessed.

The contribution of this study goes beyond the state of the art as, to the best knowledge of the authors, no approach has thus far been presented where different incentives for flexibility, optimization applications, objective functions, constraints, and strategies to consider flexibility in the optimization are presented together, see Table 1. Also, as far as the authors know, general and modularized adaption steps of optimization models allowing the integration of a wide range of flexibility types into design and operational optimization have not been previously presented. Thus, as flexibility is becoming more and more important, adaptable and reusable concepts for mathematical optimization and flexibility form an important contribution.

2. Method

In this work, an adaption of an MILP optimization problem for the design and operation optimization of industrial energy supply systems is presented. This adaption aims to facilitate the integration of different flexibility types in mathematical optimization. First, the concept and hierarchy of the developed and applied approaches are shown. Next, the underlying general formulation for MILP design and operation optimization is presented in Section 2.1. The summary of proposed changes in constraints and objective functions in order to cover different flexibility applications is discussed in Section 2.2. These proposed, new, and innovative adaptions of the basic formulation are applied for the operational optimization of an exemplary IES, which is presented in Section 2.4.

In general, the following approach is suitable for both exclusive operation optimization as well as combined design and operation optimization. The proposed formulation can answer the question of how flexible a system is for different flexibility types, e.g., regarding the availability of one specific energy carrier. For the remainder of this study (use case, results, and conclusion), the example of energy carrier flexibility will be the focus. At the same time, the developed approach shows high potential for application to other flexibility types, e.g., the availability of machines, sudden changes in demand or supply, etc.

As introduced earlier, there are usually overriding aims at industrial production sites to which flexibility should contribute. These aims are usually optimization objectives, e.g., minimizing costs. Thus, typical cost-optimal formulations are the starting point and basis for the formulation proposed in the present study.

The developed approach, also shown in Fig. 3, can be summarized as follows. A multi-step approach is set up and applied to consider energy sources' flexibility in an industrial energy supply system. However, other flexibility types could also be considered.

The following steps are part of the proposed approach:

Step 1: A typical MILP optimization problem is solved. Cost-optimal design and operation of an industrial energy supply system are determined for given profiles of energy source availability and demand. A

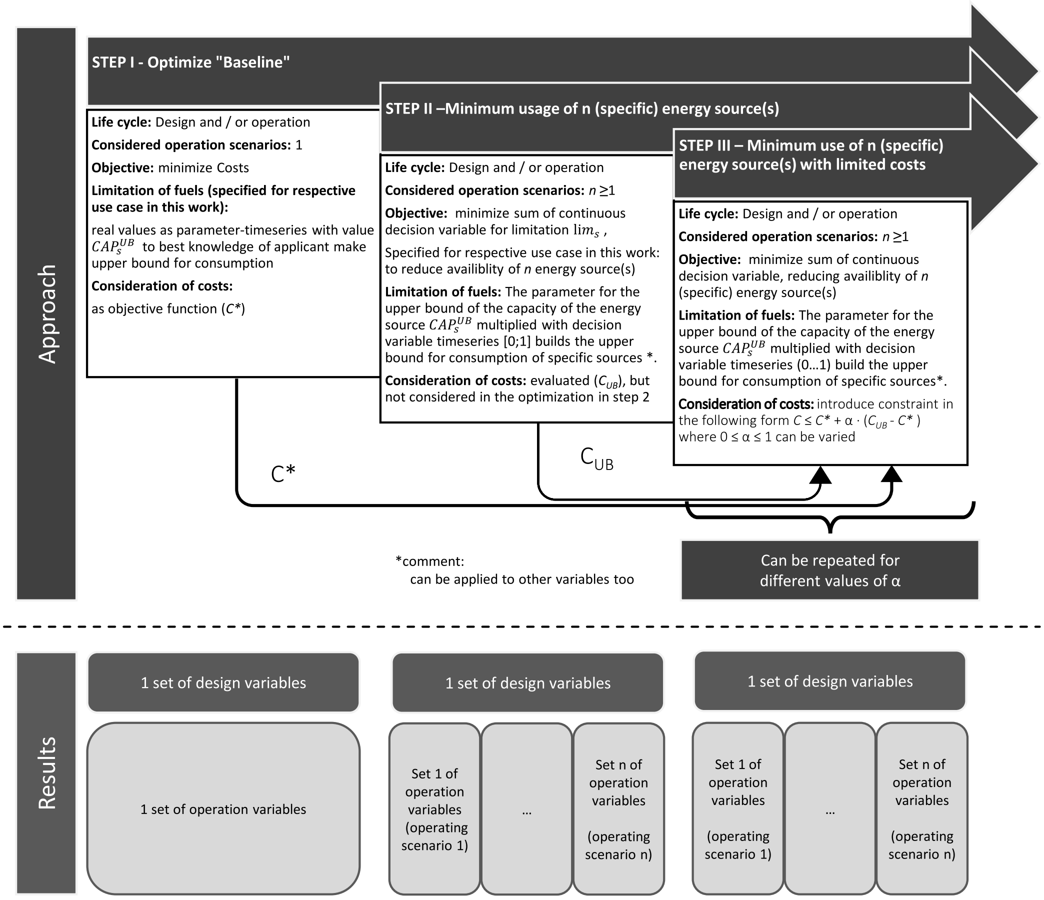


Fig. 3. Visualization of workflow to integrate different types of flexibility into industrial optimization problems.

new component is introduced in the optimization model. For the actual use case of energy carrier flexibility, this new component represents an upper bound for energy source consumption. In this first step, it is realized as a time series of parameters and not decision variable (DV). The optimal design and operation for the superstructure are determined with the objective of minimizing costs.

Step 2: A solution for the design is calculated where different operating scenarios are considered with the goal of finding a system that is flexible regarding the availability of all energy carriers. These operating scenarios are distinguished sequentially by reducing each energy source in turn. For example, in the first scenario natural gas is reduced as much as possible, in the second scenario on-site produced biogas, in the third biomass, and in the fourth electricity consumed from the electric grid, etc. For each scenario one of the newly introduced parameter time series is multiplied with a time series of DV. These are defined as positive continuous DV with values between 0 and 1. The new objective is to minimize the sum of all these continuous DV. This approach should identify feasible design solutions that are found to match the lowest possible contributions of all energy carriers. Consequently, there will be more than one possible operation solution. Thus, in this second step, the total costs are evaluated as parameters, furnishing important information for the third step.

Step 3: The problem from step two is solved again, but now the total costs are not allowed to exceed defined bounds. These bounds can be derived from the cost-optimal solution from step one and the costs determined in step two. This third step can be repeated several times, e.g., first for the objective minimal costs +50% of the difference between minimal costs from step 1 and the costs for the energy carrier flexible system from step 2.

Derived results from every calculation run are, e.g., unit capacities and total annual costs for n sets of operation variables. This enables us to determine the interaction between total costs for the different operating scenarios of every step and the ability of the configuration to completely renounce an energy source. These two criteria are plotted against each other. This visualization is the Pareto curve showing the trade-offs between cost efficiency and energy carrier flexibility.

The benefits of this approach are, first the concept can also be applied to an exclusive operation optimization. Second, the concept can also be applied to find flexibility only for specific energy carriers, e.g., electricity, and for defined periods, e.g., peak load hours in the mornings and evenings. And, last but not least, the concept can also be applied to the availability of units or to demands. For the latter, additional evaluation of performance indicators, e.g., losses, is considered an important addition to the approach.

2.1. Basic formulation of design and operation optimization

The basic formulation provides the foundation for all performed optimization runs, including the baseline calculation in step one, but also further flexibility formulations in steps two and three. It proceeds as follows:

For a given set of energy conversion units a MILP, power-based operational optimization is formulated based on presented formulations for tight and compact unit commitment problems amongst others, e.g., by Gentile et al. [30] and Morales-España et al. [31]. Adaptions of their unit commitment (only operational optimization) based formulations for design optimization are presented, e.g., by Hofmann et al. [32] and Halmschlager et al. [33].

To best represent the distinctive characteristics of renewable energy sources, an additional feature has been integrated into the optimization model. Each supply component in the system now incorporates a time series that accurately indicates the maximum availability of that specific source. This attribute has been incorporated into both the basic and revised versions of the model. Such time series can have constant values, e.g., upper bounds for biomass as well as for gas or electricity consumption via grid connection but also profiles, e.g., for renewable energy carriers.

The problem is set up with the following features and characteristics. The temporal resolution is equidistant time steps of $\Delta\tau = 1$ h. Operational and design DV are defined. Examples for operational DV are e.g., continuous variables for fuel consumption $f_u(t)$, heat supply $q_u(t)$, power supply $p_u(t)$, supply from source $s_s(t)$, charging $c_u(t)$, discharging $d_u(t)$, state-of-charge $soc_u(t)$, etc. Examples for design DV are binary variables for the existence of unit i_u and continuous for capacity of unit CAP_u). Here, subscript u indicates a unit in the set $UNIT$, and subscript s indicates a source in the set $SOURCE$. Regarding investment costs, two factors are considered for new units: fixed costs (scaled with i_u) and specific investment costs (scaled with CAP_u). For all continuous DV (design and operation), lower and upper bounds are applied, e.g., CAP_u^{UB} is the parameter for the upper bound (UB) of the capacity of unit u. In case the unit's minimum part-load is >0 an additional binary DV $u_{unit}(t)$ indicating on- and offline state is required and included for this unit. Ramping constraints are included for all energy conversion units, e.g., turbines or boilers. These constraints ensure that the change of one load point to another in two consecutive time steps is limited according to the unit's technical characteristics. For minimum up- and down times of units >0 additional constraints and additional DV, being able to take the value 0 or 1 are introduced, indicating start $v_{unit}(t)$ or shut-down $w_{unit}(t)$ of a unit. The same additional DV are required to realize a maximum generation >0 right after start-up or before shut-down for unit's with minimum part-load operation >0. The corresponding constraints are also modeled with $v_{unit}(t)$ and $w_{unit}(t)$. All units are assumed to have constant conversion efficiencies over the operation range.

Furthermore, the objective function of minimizing total annual costs (TAC) is defined for the optimization problem in step 1 of the presented approach (compare Fig. 3).

$$\min TAC = C^* = C_{energy} + C_{power} + C_{inv} \tag{1}$$

In general, fixed and variable operational costs as well as start-up or shut-down costs can also be considered in the TAC. In this example, the focus was laid on energy costs C_{energy}, costs for maximum power consumption from a grid-bound energy carrier, e.g., electricity or natural gas, C_{power} and investment costs C_{inv}. How these costs are calculated is presented in Eq. (2), (3), and (4). The sum of these cost factors yields the lowest cost C^* further used in step 3 of the presented approach (Fig. 3).

$$C_{energy} = \sum_{s \in SOURCE} \sum_{p \in PERIOD} \omega(p) \cdot \frac{8760}{\Delta T} \sum_{t=1}^{\Delta T \cdot \Delta\tau} s_s(p,t) \cdot c_s(p,t) \cdot \Delta\tau \tag{2}$$

where $SOURCE$, $PERIOD$ and $TIME = [1, \Delta T_p \cdot \Delta\tau]$ are sets for (1) different sources, (2) different periods considered in the optimization, e.g., typical days or typical weeks used to simplify the optimization of a longer duration (e.g., one year) with their corresponding weights ω_p and duration of each period of ΔT in hours and (3) the time steps t in each of these typical periods with a time step length of $\Delta\tau$. The DV for supply in MW of a specific source in each period and time step $s_s(p,t)$ are multiplied for each time step with the specific costs of this source, $c_s(p,t)$.

$$C_{power} = \sum_{g \in GRID} CAP_g \cdot c_g^{max,power} \tag{3}$$

where $GRID$ is a set including all grid connections and $c_g^{max,power}$ are the power-related share of fees for grid-bound energy carriers given in €/(kW·a) or €/(MW·a).

$$C_{inv} = \frac{(1+r)^n \cdot i}{(1+r)^n - 1} \cdot \Big(\sum_{s \in SOURCE} (CAP_s \cdot c_s^{spec} + i_s \cdot c_s^{fix}) + \sum_{u \in UNIT} (CAP_u \cdot c_u^{spec} + i_u \cdot c_u^{fix}) \Big) \tag{4}$$

where r is the interest rate and n is the depreciation period and $UNIT$ is a set including energy conversion and storage units. For the investment costs two parameters are introduced - a fixed investment factor $c_{s/u}^{fix}$ as soon as the unit (or source - e.g. PV) is considered and a specific factor leading to higher costs for higher capacities $c_{s/u}^{spec}$.

2.2. Integration of flexibility

To integrate flexibility as presented for steps two and three in Fig. 3 several adaptations need to be made.

Increase dimension of operational decision variables. First, another set needs to be introduced. In Section 2.1 sets for components (e.g., $SOURCE$ and $UNIT$) were introduced along with sets for the temporal resolution of operational DV in the optimization problem: $TIME$ and $PERIOD$. For the latter, the operational DV, a third set (dimension) is introduced. For instance, the operational DV for the supply of source s is altered from $s_s(p,t)$ to $s_s(f,p,t)$ with $f \in FLEX$.

The set $FLEX$ introduces F different operating scenarios for sources and units, with $F = |FLEX|$, for a subsystem with only one solution set for the design variables, i and CAP of the considered components. In the use case presented here, such an operating scenario is introduced for every consumed energy source. The aim of these operating scenarios is to reduce the usage of the corresponding energy source as far as (technically) possible. Thus, one can conclude that for F both of the following relations are valid: $F = |SOURCE|$ as well as $F = |FLEX|$.

Introduce new decision variables and constraints. In the following, new DV $\lim_s(f,p,t)$ are introduced for all sources to be minimized in different scenarios represented by the set $FLEX$. As an example, if three different sources should be minimized in subsequent operating scenarios, the set $FLEX$ has the length three as well. The DV $\lim_s(f,p,t)$ can take in general any value in the range [0, 1].

These DV are used to limit the supply of a specific source as far as technically feasible in the respective scenario where this specific energy source should be reduced, see Eq. (5). Here, the supply of source s is limited by the newly introduced DV $\lim_s$ and the parameter for the upper bound of the capacity of energy source s (=maximum possible consumption). To allow the usage of that specific energy source in all other operating scenarios, another constraint needs to be introduced. Eq. (6) ensures that values of this DV for one specific energy source take the value 1 for all scenarios, where the specific energy source does not need to be minimized.

$$s_s(f,p,t) \le \lim_s(f,p,t) \cdot CAP_s^{UB} \quad \forall \quad f \in FUEL, p \in PERIOD, t \in TIME \tag{5}$$

$$\lim_{s_i}(k,p,t) = 1 \quad \forall \quad k \neq i \in FUEL, p \in PERIOD, t \in TIME \tag{6}$$

where s_i is the ith element of set $SOURCE$.

As a consequence, for the ith energy source, the level of limitation $\lim_{s_i}(i,p,t)$ can only take any value between the upper (1) and lower bound (0) in the scenario i.

By the definition of the objective function, the DV $\lim_{s_i}(i,p,t)$ are forced to take values as low as technically feasible. Thus, the consumption of all considered energy sources is reduced as far as possible in subsequent operating scenarios. This subsequent minimization of all energy sources, while the other sources are fully available, is applied to determine a resilient and energy-source flexible energy system.

New objective function. Instead of costs, as in step 1 of the presented approach, for steps 2 and step 3, the sum of the limitation factors which are not previously set to the value one (Eq. (6) is minimized. Thus the objective function is defined as presented in Eq. (7).

$$ESLI = \sum_{i \in FLEX} \sum_{p \in PERIOD} \omega(p) \cdot \frac{8760}{\Delta T} \sum_{t=1}^{\Delta T \cdot \Delta\tau} \lim_{s_i}(i,p,t) \quad (7)$$

In the remainder of this study, this objective is also referred to as *energy source limitation indicator* ($ESLI$). Due to the introduction of Eq. (6), the values of all scenarios where a specific source is not required to be minimized would just add an offset to the objective. Thus, these values are not included in the objective value, as the integration of this offset has no impact on the result of the optimization.

Also, C_i^{max}, the costs (for energy, grid, and investment) for each operating scenario i and the design for the maximal possible limitation of all energy sources are determined. The costs are calculated according to Eq. (1). The maximum of these values, C^{max} will be further used in step 3.

Additional constraints for step 3. In step 3 of the presented approach, the optimization problem of step 2 is solved repeatedly but with an additional constraint, limiting the overall costs. Thus, the constraint including and limiting the costs for each operating scenario i determined with Eq. (1) is introduced as presented in Eq. (8).

$$C_i^{\alpha} \leq C^* + \alpha \cdot (C^{max} - C^*) \quad with \quad 0 \leq \alpha \leq 1 \quad (8)$$

where C^{max} are the highest costs obtained with the optimization model in step 2, and C^* are the lowest optimal cost obtained with the optimization model in step 1.

2.3. Additional remarks on modeling

Two additional remarks need to be considered. By choosing the values for CAP_s^{UB}, the value of the *energy source limitation indicator* is influenced and, thus, also the value of the objective function. Replacing the value of CAP_s^{UB} was discussed. Alternatives, e.g., using the operation profile from step 1, lead to other drawbacks. In this special case, a value of zero for a specific time step and energy source in step 1 cannot be replaced anymore. Other alternatives would make higher upper bounds than 1 necessary for the variable $\lim_{s_i}$. Thus, the proposed formulation was further used. This parameter is recommended to include domain knowledge and stick to technical boundaries. In Section 2.4, an exemplary industrial use case is introduced with realistic boundaries, based on historic values, sector-specific characteristics, and technology or fuel-specific values.

A second remark is that for step 2 of the proposed approach, choosing the maximum possible conversion or storage unit capacity (upper bound) by the solver is no disadvantage in terms of worsening the objective value. Thus, the applicant needs to be careful, especially for units with no minimum part-load operation range, e.g., electric boilers. Here, the maximum capacity can occur as part of the solution, although this is not necessary and might lead to ambiguous solutions. Measures to avoid this can be (1) setting the minimum part-load range to 0.01 instead of zero or (2) adding a small percentage of the cost to the sum of limitation in Eq. (7). For the presented use case both measures are taken. Thus, in the Results section below, the findings for step 2 are presented for two objective modes, referred to as single and double objective. The objective function for step 2 (single objective - SO) is equivalent to Eq. (7). For the calculation run in step 2 (double objective - DO), the following objective function is applied:

$$ESLI_{do} = ESLI + 0.00001 \cdot TAC \quad (9)$$

2.4. Use case definition and implementation

The main contribution of the present study is to develop adaptions of existing optimization formulations to derive energy source flexible solutions for industrial energy supply. A simple, but realistic use case is introduced to demonstrate the benefits of the proposed concept to find an energy source flexible IES. The optimization model for this use case was set up in Python using the optimization module Pyomo [34,35]. The class of MILP optimization models was applied for the following reasons. First, in this class, convergence towards a global optimum is guaranteed while the solution accuracy can be determined with the indicator *optimality gap* for a current solution [36]. Furthermore, efficient solvers are available for MILP formulations and have greatly improved over recent decades [37]. In this study, an efficient MILP solver – CPLEX [38] – was used.

For this use case, green-field planning of industrial energy supply in an energy-intensive industrial production plant was assumed. Examples for energy-intensive production plants are, e.g., paper mills or steel mills but also large chemical or food sector sites. No existing components are part of the superstructure for a greenfield planning approach. In addition, an interest rate of 5% and a depreciation period of 10 years is assumed for all investments for newly integrated units.

In the remainder of this study, a paper factory was assumed. Thus, realistic demand values are derived and presented in the following for a generic paper mill. To fulfill a given energy demand of the production process, energy conversion, and storage units from a given superstructure can be chosen in the optimization process by the solver, see Fig. 4. The choice of technologies integrated into the superstructure was based on an assessment of current technologies in today's pulp and paper factories as described by Suhr et al. [39]. Furthermore, also on-going developments have been considered. Trends towards more electrification of industrial energy supply [40] but also to include high-temperature heat pumps [41], e.g., in the pulp and paper production process, can be observed.

Besides their design variables (binary variable i_u for a unit's existence and the continuous variable CAP_u for a unit's capacity), time series for their operation, e.g., fuel consumption $f_u(f,p,t)$ or heat generation $q_u(f,p,t)$, as well as time series for the consumption of proposed energy carriers $s_s(f,p,t)$ are also optimized. The temporal resolution of the presented use case is a set of four days. These days (D1, D2, D3, and D4) represent one winter, spring, summer, and autumn day. They are up-scaled to one year with adaptable (here equal) weights of 25% for each day. Each of the calculated days is considered in hourly periods. This results in a total of $N = 96$ periods. As high annual production hours were assumed, no significant changes in energy demand over the different days (such as on-off states or seasonal differences) were considered.

The following Sections 2.4.1–2.4.3 give an overview of the considered energy demand, the IES and assumed parameters and times series.

2.4.1. Energy demand

On the demand side, the use case includes slightly fluctuating demands of electricity and steam at a middle-pressure level (150 °C, 4.5 bars absolute). Moreover, industrial excess heat with thermal power of about one-third of the production process steam demand between 20 and 30 °C was assumed, e.g., heat recovery from typical excess heat sources such as humid air streams from drying processes, waste water, or excess heat of cooling processes. The average thermal demand accounted for approx. 43 MW. This figure was derived from 300,000 tons of paper with a steam demand of 1.15 MWh_{steam}/t_{paper} and 8000 load hours per year - compare values to benchmarks in "Best available technologies/Best reference" document [39]. The electricity demand of approx. 12 MW accounted for 20%–30% of the thermal demand.

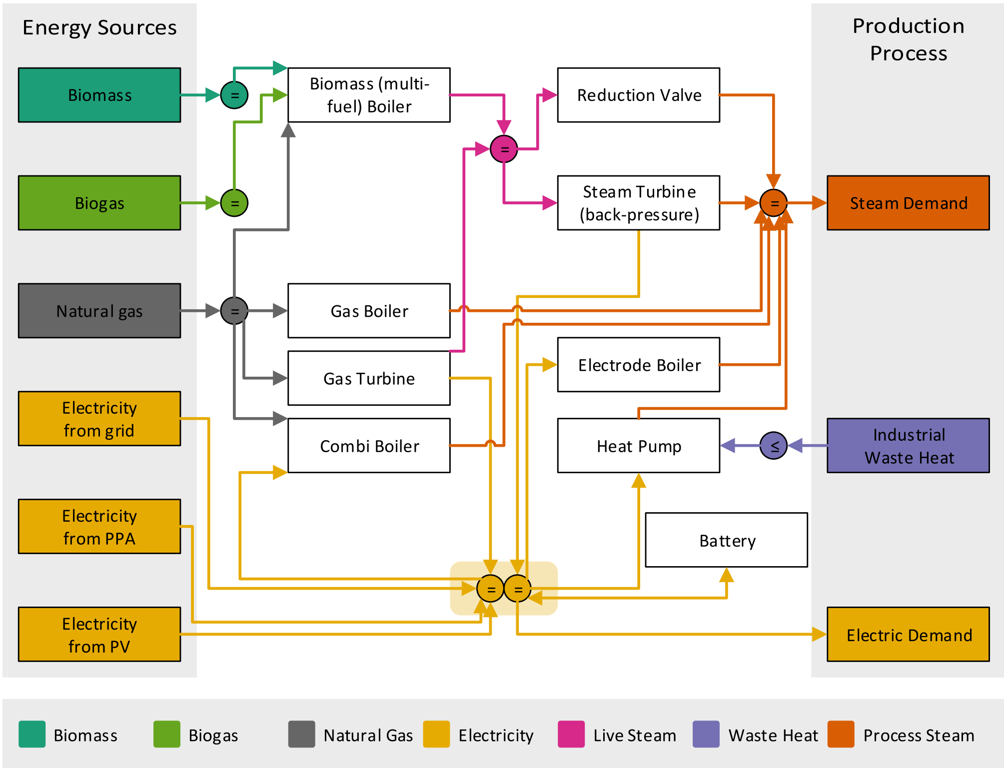


Fig. 4. Visualization of the modeled superstructure in the optimization model, where each energy carrier is always shown in a specific color - balancing nodes are symbolized by colored circles and the corresponding relation between the left (incoming) and right (outgoing) side of the balancing equation (options: $=$, $\leq$ or $\geq$). Remark: In this use case, biogas (CH_4 + CO_2) differs chemically from natural gas (CH_4) and, thus, cannot be used in the gas turbine.

2.4.2. Industrial energy system

The optimization model consists of (1) energy sources, (2) energy conversion units, (3) energy storages, (4) energy demands (explained above), and (5) balancing nodes, where ports of the formerly mentioned components are connected and related to each other. The superstructure, shown in Fig. 4 of the IES considered six different energy sources (fuels and electricity from different sources). The usage of each of these six energy sources is to be minimized in a sequential calculation (which is the main contribution of the enhanced optimization model presented in the present study). Furthermore, two grid connections were integrated, one for natural gas and one for electricity sources consumed via the public grid. The proposed system is based on current energy supply options and conversion technologies [39], as well as potential new energy supply options such as those presented in a lifecycle assessment study for the pulp and paper sector in Puschnigg et al. [20].

Energy supply. Regarding the energy supply, the following sources were considered: *Natural gas* This energy carrier is considered with a maximum consumption of 50 MW per time step. Such limited grid connections for industrial sites typically result for technical or regulatory reasons. Considered cost components are purchase costs from energy market costs, grid fees related to both energy (in €/MWh) and power (in €/MW), and costs for CO_2 certificates. Here, a specific emission factor of 0.21 tons CO_2 per MWh of natural gas is applied in the model. *Biogas* This is considered an on-site residual energy stream with a maximum of 2 MW per time step. As this source is an on-site by-product, no costs occur for the usage. *Biomass* Solid fuels, in this case biomass, are also considered purchase options with a maximum consumption of 30 MW. In reality, limitations for solid fuel usage often occur due to logistics or space limitations. This energy source is considered in the model with energy costs. *Electricity* This supply is bought on markets or from usual suppliers. The present study considers day-ahead spot market costs and grid fees for energy (in €/MWh) and power (in €/MW). *PV PPA* This represents electricity that is physically consumed via the electric grid. The billing and the purchase quantities and profiles are based on bilateral contracts where energy costs are decoupled from the fluctuating price on spot markets. As for electricity bought on the market, fees need to be considered. PPA is becoming a supply option of interest in the sector of pulp and paper production. This is shown, e.g., in a flexibility and life cycle assessment for a German paper mill by Puschnigg et al. [20]. *PV on-site* Electricity produced on-site is also a considered energy source. As is the case for real PV installations in the pulp and paper sector, the available areas and thus the possible peak power is limited compared to the overall electricity needs, in this case to 3 MW_{el}. For this source, only investment costs (i.e., no energy costs or fees) are considered.

Energy conversion and storage units. Furthermore, several energy conversion units and one energy storage unit, a battery for decoupling electricity supply and demand, were considered. The following energy conversion units are part of the superstructure in the optimization model (see 4). A biomass boiler (max. 100% of fuel biomass) with the possibility of additional firing with other fuels (max. 20% biogas and max. 20% natural gas) provides live and process steam with a fixed ratio of 60:40. Also, a gas boiler, fired by natural gas, provides process steam. Additionally, a gas turbine (incl. a waste heat recovery boiler not explicitly shown in the visualization) is included to supply live steam and electricity fired by natural gas. A back-pressure steam turbine consumes live steam and provides process steam and electricity. Also, a steam pressure reduction valve is part of the superstructure to provide an alternative of converting live steam into process steam. A

Table 2
Summary of modeled nodes.

Node	In Fig. 4	Left side	Relation	Right side
Biomass	Yes	Supply of source biomass	==	Consumption of biomass boiler
Biogas	Yes	Supply of source	==	Consumption of biomass boiler
Natural gas	Yes	Supply of source natural gas	==	Consumption of gas boiler, gas turbine and combi boiler
Electricity	Yes	Supply of electricity, power-purchase agreement (PPA), PV, the electric production of gas and steam turbine as well as battery discharging	==	(electric) consumption of combi boiler, heat pump, electrode boiler, electric demand, and battery charging
Process steam	Yes	Supply of biomass boiler (partial), combi boiler, gas boiler, electrode boiler, heat pump, and steam turbine	==	Thermal process demand
Live steam	Yes	Supply of gas turbine and biomass boiler (partial)	>=	Consumption of steam turbine, and consumption of reduction valve
Waste heat	Yes	Industrial excess heat	>=	Heat source of heat pump
Electric grid	No	Consumption via electric grid	==	Supply of electricity and PPA
Gas grid	No	Consumption via gas grid	==	Supply of natural gas

Table 3
Overview of upper bounds for energy source consumption and energy costs, fees, and investment costs considered in the optimization model, derived from [42–46].

Energy source	Upper bound	Energy cost	Fees	Investment
Natural gas	50 MW_{fuel}	c_{ng}, see Eq. (10)	2 €/MWh, 3 k€/MW.a	–
Biogas (on-site residue)	2 MW_{fuel}	–	–	–
Biomass	20 MW_{fuel}	33.9 €/MWh	–	–
Electricity (via grid)	50 MW_{el}	EPEX spot	10 €/MWh, 30 k€/MW.a	–
PV PPA (via grid)	20 MW_{el}	40 €/MWh	10 €/MWh, 30 k€/MW.a	–
PV (on-site)	3 MW_{el}	–	–	5 k€ + 914 €/kW_{peak}

combi boiler is also included. It is modeled as a gas boiler with an electric heating element fired by max. 60% natural gas or max. 40% electricity and provides process steam. Two more units are integrated to increase the power-to-heat potential in the superstructure. On the one hand, an electrode boiler can provide process steam. On the other hand, a high-temperature heat pump is included, using industrial excess heat as a source and electric energy for working fluid compression to provide process steam. A realization of the heat pump would include a cascading steam-providing heat pump system and a mechanical vapor compression unit to increase steam pressure and temperature. As two to three single units would be involved in this concept, high specific investment costs for the considered system occur in the superstructure.

Nodes. Balances for fuel, heat, and electric power supply and consumption are part of the optimization model. The following nodes, of which the majority are shown in Fig. 4, are considered and described in Table 2.

2.4.3. Parameters and time series

In this section, assumed technical and economic parameters are presented, as well as the considered time series for demands, costs, and irradiation. For the considered use case, price data from 2019 was assumed for the following reasons: Recent developments, e.g., the pandemic and energy crisis, led to fast-changing frame conditions for energy markets and thus also to extreme developments (high and low) in energy prices between 2020 and 2022. Consequently, assuming prices, e.g., from 2021 with an extreme incline in costs for natural gas, CO_2, or electricity over the year, could complicate the interpretation of results. However, in the discussion and analysis of the developed method, a typical year with no extreme events, and thus no extreme changes in energy markets, was assumed.

Parameters required to represent energy sources in the model are summarized in Table 3

$$c_{ng}(d) = c_{ng}^{CEEGEX}(d) + 0.21 * c_{CO_2}^{ETS}(d) \quad (10)$$

where c_{ng} are specific costs for natural gas for one of the considered days $d \in [D1, D2, D3, D4]$, including the specific average costs on the day ahead market of Central Eastern European Gas Exchange (CEEGEX) for the corresponding season of day d and the specific average CO_2 costs from the ETS trading in the corresponding season of day d. Table 4 summarizes values used for days one to four. The natural gas price was derived from CEEGEX, the Hungarian gas trading platform, as data there are, first, publicly available and, second, comparable to Austrian prices from the Central European Gas Hub.

Table 4
Assumed costs for natural gas and CO_2 certificates. Values based on data for 2019.

Considered day	Natural gas cost	CO_2 cost
D1	24.14 €/MWh	22.99 €/t
D2	17.83 €/MWh	25.25 €/t
D3	13.45 €/MWh	28.05 €/t
D4	11.99 €/MWh	24.56 €/t

The following technical parameters have been used for the parametrization of the optimization model. For all energy conversion units, minimum up- and down times were set to 1 h. Maximum generation after shut-up and before shut-down was assumed as 100% load. Also, ramping abilities of 100% of the maximum capacity within one hour were assumed. Start and fixed operational costs were not considered in this use case.

Differing cost and technical parameters applied for the energy conversion units and the battery are presented in Table 5. For efficiencies in Table 5, the following remarks need to be considered: The multi-fuel boilers' efficiencies were related to the corresponding inputs — if not stated otherwise, one value for all fuels or a specific value for each indicated input. For the heat pump, the efficiency η corresponded to the second law efficiency, which is the ratio between the Carnot coefficient of performance and the actual coefficient of performance. For the battery, the efficiency value was applied for charging, discharging, and state-of-charge, indicating which share of the stored energy is still available after one hour. The battery's maximum charging and discharging power is equal to the upper bound of the capacity.

The assumed time series are visualized in Figs. 5 and 6.

2.5. Further analysis

To better understand the results and the impact of economic parameters on the technology choices in the use case of this study, a short analysis of the levelized costs of energy is performed. Based on a simplified formula applied, e.g., in Tegen et al. [48], the levelized costs of heat $LCOH$ and electricity $LCOE$ are derived. In general, they are calculated as the ratio between the annualized costs of the technology divided by the annual energy production of the respective technology u. The annual costs are the sum of the annualized investment costs, the energy costs of source s for technology u, and the power-related (grid) costs of source s for technology u.

$$LCOH_u = \frac{C_{inv,u} + C_{energy,s,u} + C_{power,s,u}}{E_u} \quad (11)$$

Eq. (11) is applied to the technologies of the gas boiler, the electrode boiler, the heat pump, the biomass (multifuel) boiler, and the combi boiler. For the comparison, a total heat generation capacity of 10MW is assumed for all analyzed units. The efficiencies are assumed as shown in Table 5. The coefficient of performance of the heat pump results to be 1.54 derived from the temperatures of the excess heat and process heat, the assumed second law efficiency, and temperature differences between the refrigerant and the source and sink outlet of 5K. Furthermore, the respective source is consumed from either fuels or electricity from the grid. The maximum generation is 10MW for all variations shown. Varied parameters are the (i) depreciation period taking values of 3, 5, 10, and 15 years, (ii) the full load hours taking values of 4000, 6000, and 8000 h/a, and (iii) the level of the average electricity energy cost taking values of 100% of the cost in the presented use case, 75%, and 50%.

The LCOE is evaluated for the consumption from electricity markets via the grid, electricity provision from the gas turbine, and the steam turbine. However, as the two latter are combined heat and power plants, additional assumptions need to be drawn to consider the heat production of these technologies. In the first step, the levelized costs for electricity are calculated according to Eq. (11) with the produced electricity as annual energy production. Then, the corresponding amount of heat for each part of the electricity is determined. Thus, overall efficiencies of 98% (electricity + thermal production) are assumed. The produced heat is multiplied by the levelized costs of the gas boiler as reference technology, which is then subtracted from the value derived with Eq. (11). For the steam turbine, no fuel costs but levelized costs of heat (live steam) from the biomass boiler are assumed. In addition, the levelized costs of on-site PV plants are evaluated. For this technology, the full-load hours are varied for 1000, 750, and 500 h/a. Also, here, Eq. (11) is applicable. However, only investment is required for the PV plant, and no energy or power costs are accounted for. To finalize this cost calculation description — no investment costs occur for the energy source *electricity from the grid*.

However, applying only the method of levelized energy costs has several drawbacks that come together with its significant advantages of simplicity and a high level of comprehensibility. Therefore, the method of levelized energy costs (heat or electricity) is understood as an addition to the mathematical optimization for technology option analysis in this study. The advantages of this addition lie in the simple evaluation of the influences of, for example, depreciation periods, operating hours, or energy source costs. The increasing complexity in multi-technology systems, such as time variable price and demand profiles, brings up new challenges for the method of levelized energy costs. For example, electricity required for electrode boiler and heat pump integration could be provided by, e.g., gas or steam turbines or on-site PV plants. Thus, for complex systems such as industrial energy supply systems, not only levelized costs of energy but also further economic assessment indicators such as the defined objective function of total energy system costs show higher potential for analysis and interpretation [49].

2.6. Further variations of use case parameters

Two more scenarios for the use case calculation in the presented framework are performed to assess the impact of varying frame conditions.

First, a calculation is performed for the requirement of fossil decarbonization. Thus, the following adaptions of the presented optimization model are necessary. A new constraint is included to limit the emissions of the fossil energy source natural gas (ng) with the specific emission factor $em_{ng} = 0.21$. The total emissions must be below a defined limit $EM_{limit} = 0$. For the other use cases this constraint is deactivated.

$$em_{ng} \cdot \sum_{p \in PERIOD} \omega(p) \cdot \frac{8760}{\Delta T} \sum_{t=1}^{\Delta T \cdot \Delta\tau} s_{ng}(p,t) \cdot \Delta\tau \le EM_{limit} \quad (12)$$

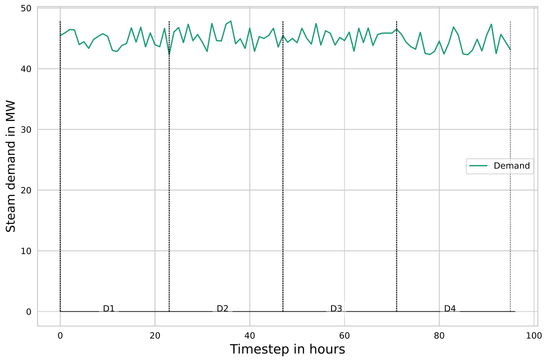
Second, the temperature of the process demand is lowered from 150 to 130 °C while the available excess heat is assumed to be between 40 and 60 °C instead of 20 to 40 °C. These temperature changes impact the coefficient of performance of the heat pump. Thus, the feasibility of heat pump integration can be increased. Adaptations such as checking and adjusting the temperature requirements or adapting heat recovery schemes can be possible.

3. Results

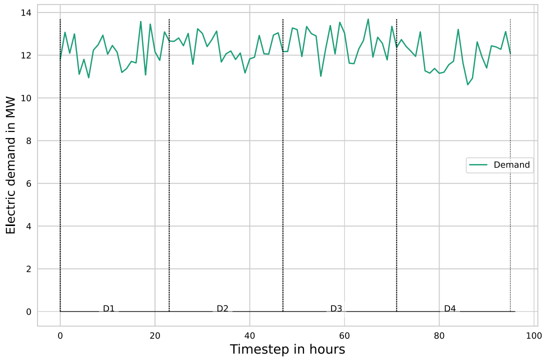
This section discusses a greenfield, energy source flexible IES for the proposed use case of an energy-intensive paper production site. The energy source flexible design and operation are optimized through a multi-step approach first presented in this study. In analogy to the structure of the method section this section is organized as follows. First, a comprehensive overall summary with the aim of emphasizing the approach presented in this study of the results regarding the determined unit sizes in step 1, step 2, and step 3 with different values for α are presented together with total costs and annualized investments. These overall results are discussed in Section 3.1. Next, in greater detail, the cost-optimal solution (step 1 of the introduced approach) is presented in Section 3.2 which is based on the formulation presented in Section 2.1. All following detailed results in this section are based on the new formulation introduced in this study which is described in Section 2.2. Based on the cost-optimal solution, all cases where the design allows full substitution of every specific energy source are explained and compared in Section 3.3. This occurs for the calculations in step 2 and the calculation in step 3 with a high value for α =

Table 5
Techno-economical parameters in the optimization model.

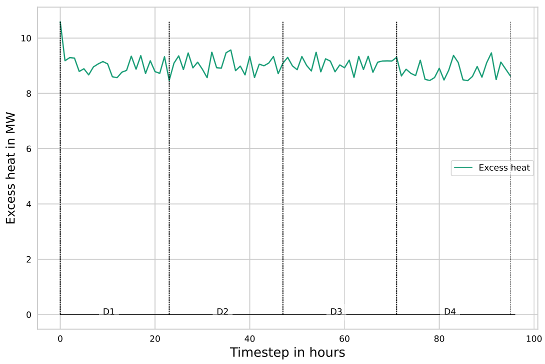
Unit u (Reference)	CAP_u^{UB}	Min. load	Efficiency	Investment cost
Biomass boiler [45]	100 MW_{th}	20%	η_{th} = 88%	50 k€ + 0.746 M€/MW_{th}
Gas boiler [47]	100 MW_{th}	15%	η_{th} = 92%	50 k€ + 0.055 M€/MW_{th}
Gas turbine [45]	25 MW_{el}	25%	η_{el} = 35%	50 k€ + 0.767 M€/MW_{el}
Steam turbine [45]	10 MW_{el}	40%	η_{el} = 14.75 (calc.)%	50 k€ + 0.5 M€/MW_{el} (as.)
Reduction valve	30 MW_{th}	1% (as.)%	–	50 k€
Combi boiler [47]	100 MW_{th}	15%	η_{th} = 92% (NG), 99% (E)	50 k€ + 0.10 M€/MW_{th} (as.)
Electrode boiler [47]	100 MW_{th}	2%	η_{th} = 99%	50 k€ + 0.12 M€/MW_{th}
Heat pump [47]	25 MW_{th}	75% (as.)	η_{carnot} = 50%	50 k€ + 1.643 M€/MW_{th}
Battery	50 MWh_{el}	–	η_{el} = 99	50 k€ + 0.55 M€/MWh_{el}



(a) Thermal demand on considered days, modeled/calculated

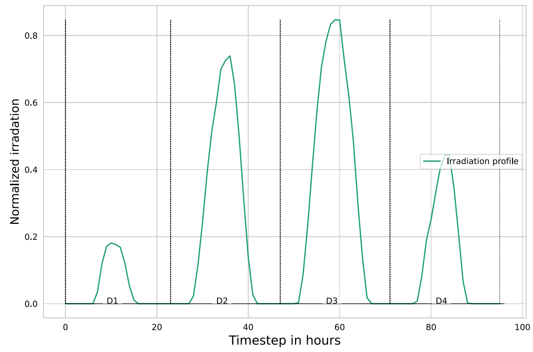


(b) Electric demand on considered days, modeled/calculated

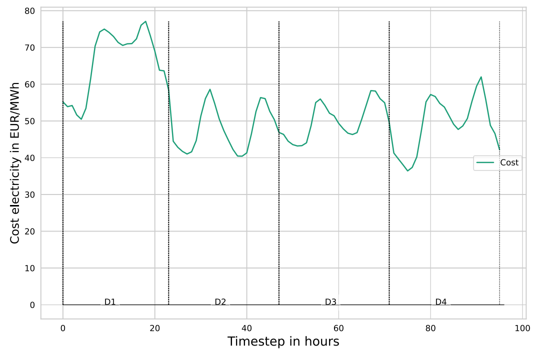


(c) Available excess heat on considered days, modeled/calculated

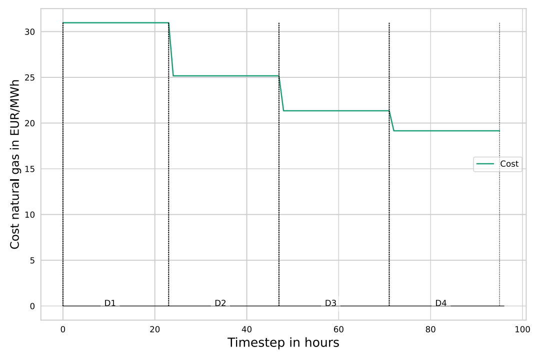
Fig. 5. Assumed time series for electric and steam demand, and excess heat for the assumed days (D1 - D4) in the optimization model.



(a) Average hourly solar irradiation related to the maximum annual value (Source: 2019 data for one Austrian measuring point from GeoSphere Austria - https://data.hub.zamg.ac.at)



(b) Average electricity prices in respective season (Source: 2019 day-ahead data + 100 kV grid fees for one Austrian province (42))



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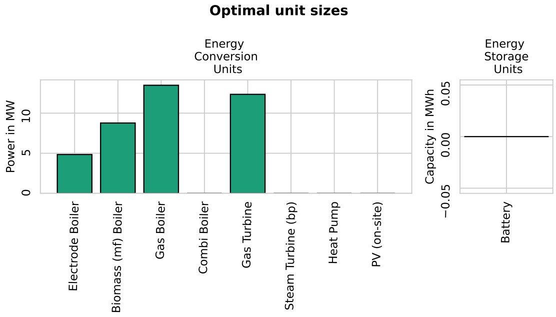
(c) Average natural gas and certificate costs, derived for 2019 from CEEGEX day-ahead data (43) and Emission Auctions (44)

Fig. 6. Assumed time series for prices for electricity and natural gas (incl. energy-related grid fees) as well as irradiation for the assumed days (D1 - D4) in the optimization model.

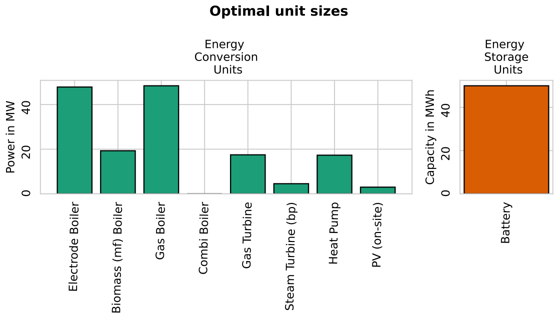
0.75. Lastly, those solutions where no full substitution is possible are presented in Section 3.4. These solutions result from calculations in step 3 with values for $\alpha < 0.75$. In addition, as introduced in Section 2.3, a comparison is made between different approaches for considering multiple objectives to assess the suitability of the proposed approach (Section 3.5). In this study, the following two specific objective criteria are considered: *cost* and *energy source flexibility*. Finally, in Section 3.6 this study presents a summarized analysis of the economic and ecological aspects of the energy source flexibility in the evaluated use case introduced in Section 2.4.

3.1. Overall results

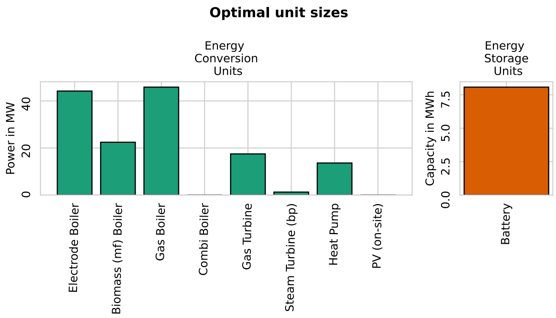
Figs. 7 and 8 show the determined unit sizes in step 1, step 2, and step 3 with different values for α. Furthermore, the corresponding annualized investments are presented in Fig. 9. The underlying aim was



(a) Unit sizes determined in step 1

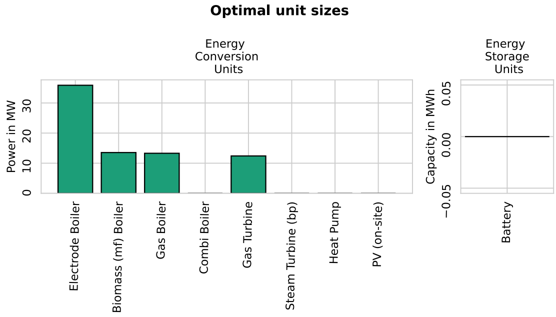


(b) Unit sizes determined in step 2

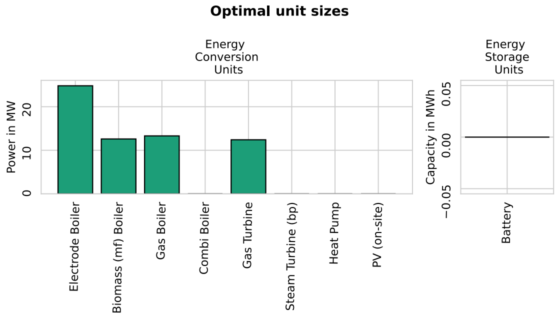


(c) Unit sizes determined in step 3, with α=0.75

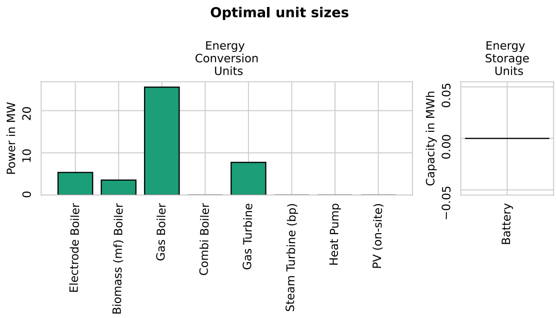
Fig. 7. Unit sizes determined in steps 1–3 (here only single objective calculation runs are shown) with α = 0.75 in step 3. Capacities for boilers and the heat pump are given in MW_{th}, while capacities for turbines, PV and the battery are given in MW_{el} and MWh_{el}, respectively.



(a) Unit sizes determined in step 3, with α=0.5



(b) Unit sizes determined in step 3, with α=0.25



(c) Unit sizes determined in step 3, with α=0.01

Fig. 8. Unit sizes determined in step 3 with different values of α. Capacities for boilers and the heat pump are given in MW_{th}, while capacities for turbines, PV and the battery are given in MW_{el} and MWh_{el}, respectively.

to identify system configurations that are flexible toward the availability of energy sources. Thus, for every step of the presented approach, only one set of design variables for all units was determined. It is evident from Fig. 9 that the systems configurations with a large battery capacity of approximately 7.7 and 48 MWh (Fig. 7) receive the highest annual investments, amounting to 8 and 12 MEUR/a, respectively. The corresponding calculations are step 2 with single objective and step 3 with α = 0.75, which have full substitution potential for all energy sources. These two calculations also include heat pumps in addition to other less expensive solutions.

Furthermore, overviews of total costs, including annualized investments and energy costs, are presented in Fig. 10. In contrast to the design variables, here a set of different values results for steps 2 and 3. For step 1, only one value for total costs results from the optimization. For every calculation in steps 2 and 3, six different cost values are evaluated, resulting from six different operating scenarios (see Fig. 10). Here, each total cost value for an operating scenario represents the case that the energy system would be operated without or with a minimal amount of one specific energy source for a whole year. Fig. 10 displays the range of total annual costs resulting from calculations in steps 1 to 3 with single and double objective functions and different values for α as well as the different operating scenarios in every step. The resulting costs account for 16.39 MEUR/a for the cost optimal solution up to 40.34 when natural gas is replaced in step 2.

A detailed summary of all values can be found in the Appendix, Table A.6.

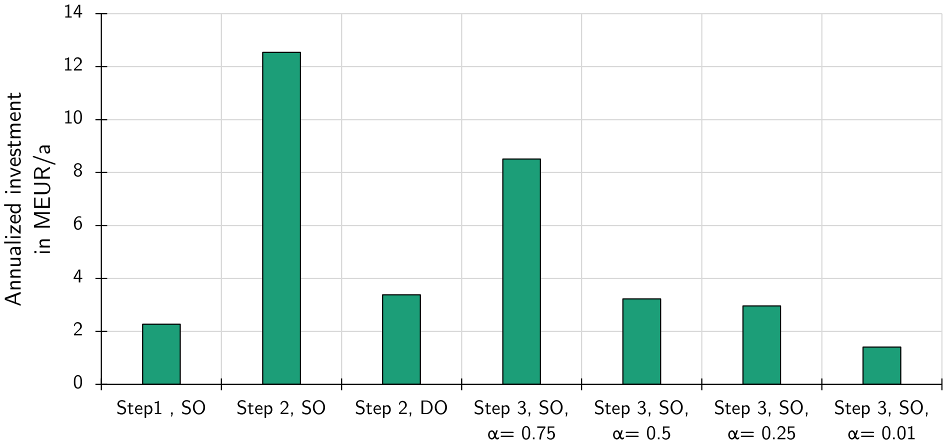


Fig. 9. Overview of annualized investment for steps 1–3. SO indicates calculations with only one objective criterion at a time — either cost on the y-axis or flexibility on the x-axis. DO indicates calculation with a sum of two weighted optimization criteria at a time.

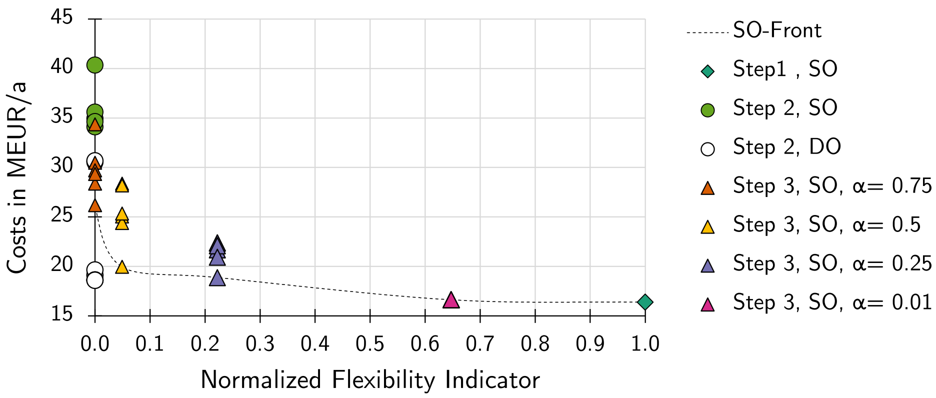


Fig. 10. Overview of costs and normalized flexibility indicator for steps 1–3. Each operating scenario in steps 2 and 3 aims at reducing one specific energy source as far as possible for one year. SO indicates calculations with only one objective criterion at a time — either cost on the y-axis or flexibility on the x-axis. DO indicates calculation with a sum of two weighted optimization criteria at a time. The single objective front connects the lowest values of all single objective calculation runs.

3.2. *Cost optimal solution - Step 1*

For step 1, the balancing of the nodes for process steam, electricity, natural gas, biogas, biomass, and live steam is shown in Fig. 11. It can be seen that in a cost-optimal solution, live steam is produced by the gas turbine and, to a lesser extent, by the multifuel biomass boiler, which is supplied by biomass and biogas. The live steam is converted to process steam through the reduction valve. To cover the process steam demand as well, the gas boiler is used. The electrode boiler also supplies a small share of the process steam. Another factor that affects electricity consumption is the electricity demand of processes. Electricity is mainly supplied by the gas turbine and to a lesser extent by the electric grid. Regarding the natural gas balance, one important finding is that the most significant consumer is the gas turbine. The gas boiler consumes a smaller share. Furthermore, the consumed natural gas corresponds to the upper consumption limit of 50 MW for the entire optimization duration. The cost-optimized IES consists of an electrode boiler with 4.8 MW_{th}, a biomass boiler with 8.8 MW_{th}, a gas boiler with 13.7 MW_{th} and a gas turbine with 12.2 MW_{el} (see Fig. 7). All values were rounded to one decimal place.

A further quantitative analysis of the results (see also the Appendix, Table A.6) reveals a value for total annual costs of 16.39 M€/a. Of this, 2.27 M€/a comes from annualized investments. Due to the high natural gas consumption, emissions are 91.98 kt/a. Ranking the energy amounts of the possible energy sources from high to low results in energy provided by natural gas (full potential used) > energy provided by biomass > energy provided by electricity > energy provided by biogas (full potential used) > energy provided by PV and PPA (both not used).

3.3. *Solutions with full substitution of all sources*

For some calculation runs in steps 2 and 3, all energy sources could be fully substituted in the corresponding operating scenarios with the IES determined in the calculation run. The feature of full energy source substitution corresponds to a value of zero for the optimization objective in steps 2 and 3 - the *energy source limitation indicator*. For the presented use case (Section 2.4), the following calculation runs can be considered as flexible in terms of the complete substitution of all considered energy sources.

Step 2: Minimizing the energy source limitation indicator as a single objective. The main results for this calculation run are, on the one hand, a cost increase for energy and investment compared to step 1. On the other hand, emissions reduced by up to 100% in the best and 1%–2% in the worst case. Detailed operation profiles of the energy conversion and storage units for all six operating scenarios are shown in the Appendix (Figs. A.20–A.23).

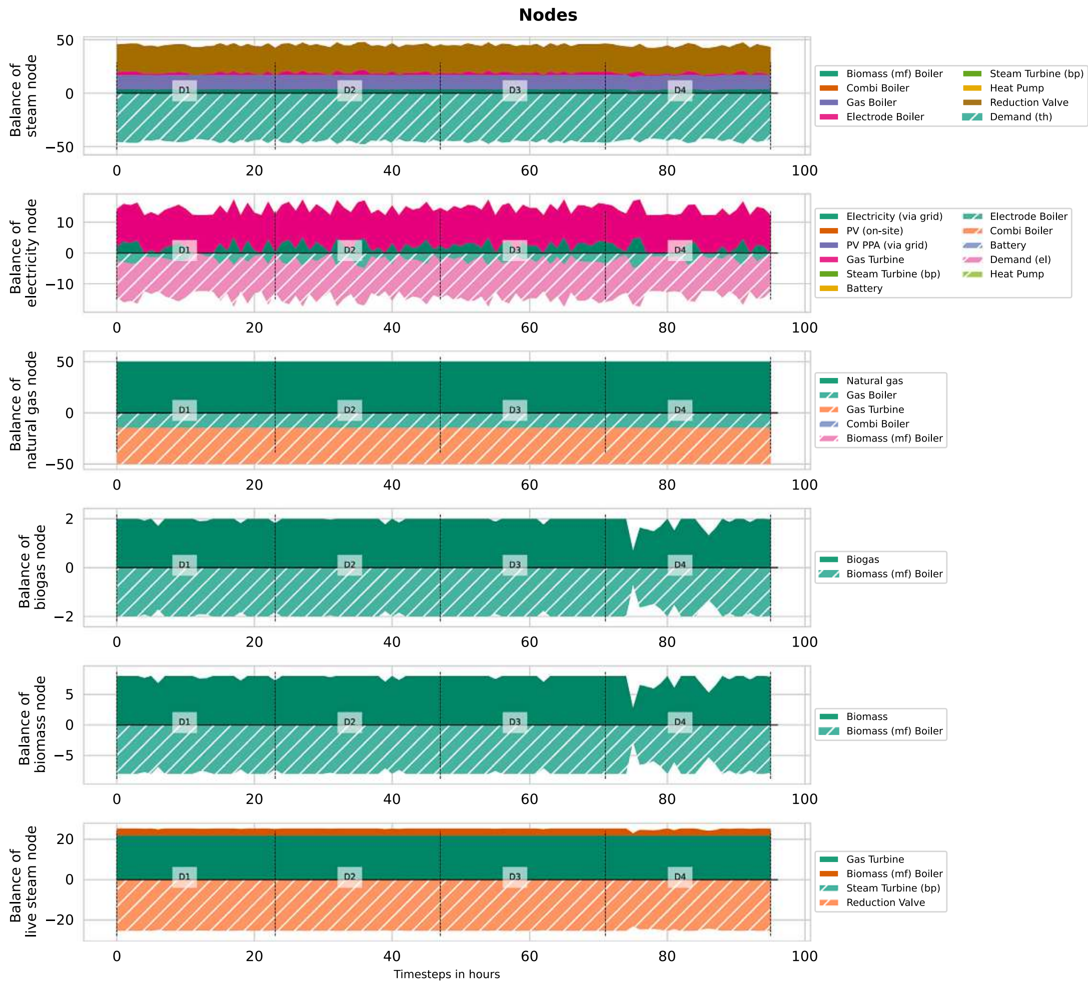


Fig. 11. Overview of balancing nodes for step 1.

The increase of total annual costs compared to the solution in step 1 accounted for 86.15–146.07% depending on the operation scenario and on which energy carrier should be reduced as far as possible. When electricity consumption from the grid is wholly substituted, compensated by higher biomass, PV and PPA usage, the lowest increase in total annual costs compared to the cost-optimized solution from step 1 was found. The highest increase in total annual costs was found for substituting natural gas, mostly with electricity. The increase in annualized investment accounts for 10.27 M€/a compared to step 1. This corresponds to a factor of 5.53 compared to the annualized investment in the cost-optimized solution from step 1. The system configuration for this calculation run includes all possible conversion and storage units except the combi-boiler. Compared to step 1, all unit sizes are significantly increased, including a 50 MWh battery used in all operating scenarios. For step 2, the emissions range between 0 and 90.9 kt/a for the different operating scenarios compared to 91.98 in step 1. When natural gas is substituted, the emissions result in 0 kt/a. The second lowest value is 47.2 kt/a from the operating scenario where PV is substituted. The reduced natural gas consumption compared to step 1 results from the significantly reduced operation of the gas turbine while the heat pump is included in heat provision.

Step 2: Minimizing the energy source limitation indicator and a small share of the total costs as a double objective. This calculation run differs from the aforementioned calculation run by the defined objective function. While for the single objective run only the criterion of the *energy source limitation factor* forms the objective function, two criteria were considered in the double objective run. In addition to the *energy source limitation factor* 0.00001 · total annual costs, which is the objective in step 1, are considered in the objective too. The primary motivation for including this calculation step was to compare different approaches to evaluation multi-criteria optimization.

The increase in total annual costs compared to the solution in step 1 accounted for 13.48–87.08%, depending on the operation scenario. When PPA consumption is completely substituted, the lowest increase in total annual costs was found. For reducing PV and electricity from the grid, similar values for cost increase (<14%) were found. The highest increase in total annual costs was found for substituting natural gas, primarily by electricity. The increase in annualized investment accounts for 1.11 M€/a, corresponding to a factor of 1.49. The solution for this calculation run includes the same set of units as step 1 and a small PPA. Compared to step 1, the size of the electrode boiler increased (37.8 instead of 4.8 MW) while the gas boiler capacity decreased (10.4

instead of 13.8 MW). The capacity of the other included units slightly increased. Except for operating scenario 1, when natural gas is reduced, emissions are equal to the value in step 1 of 91.98 kt.

Step 3: Minimizing the energy source limitation indicator for limited costs and $\alpha = 0.75$. The increase in total annual costs compared to the solution in step 1 accounted for 59.71–109.55%, depending on the operation scenario. This is a higher increase than the previously described calculation step 2 with a double objective. In general, the qualitative system setup and, thus, the included units are similar to step 2 (single objective). When electricity consumption is completely substituted, the lowest increase in total annual costs was found. The highest increase in total annual costs was found for substituting natural gas, mostly with electricity. The increase in annualized investment accounts for 6.24 M€/a, corresponding to a factor of 3.75 compared to step 1. The lower cost increase compared to step 2 (single objective) results from smaller capacities than in step 2. Smaller capacities occur for the electrode boiler, the gas boiler, the steam turbine, and the heat pump. The decrease of those capacities is in the range of 3–4 MW. A capacity of 8.1 MWh instead of 50 MWh is found for the battery. The same capacities are determined for the gas turbine, the PPA and PV. A higher capacity is found for the biomass boiler, with an increase of 3.2 MW. Emissions are within the range of step 2 (single objective), accounting for 48.6–85.4 kt/a and 0 kt/a when natural gas is substituted.

Further reduction of α. For the further reduction of α *energy source limiting indicators* ≥ 0 are found. Thus, no complete substitution of all six sources is possible anymore. However, similar values for total annual costs and investments are found when step 2 (double objective) is compared to step 3 with $\alpha = 0.5$. This leads to the conclusion that full substitution potential could be found even for values of α below 0.75 and close to 0.5. However, in our study, only four values of α were evaluated.

3.4. Solutions with partial energy source substitution

The further calculation runs include operating scenarios leading to values of the *energy source limitation indicator* greater than zero. This is because the complete substitution of the required energy source is not entirely possible in specific operating scenarios. When costs and the *energy source limitation indicator* are compared, these results are found when the constraint for total annual cost limitation (Eq. (8)) poses more challenging limits for energy source substitution. Detailed values are summarized in Table A.6 in Appendix.

For $\alpha = 0.5$, electricity and natural gas can no longer be fully substituted. The lowest electricity consumption from the grid is 1.26 GWh compared to 228.6–331.8 GWh in the other operating scenarios. For natural gas, 50.4 GWh is compared to 195.5–412.6 GWh. The increase in total annual costs compared to step 1 is between 22 and 73% (electricity and natural gas substitution). The annualized investments account for 3.23 M€/a and thus are 0.96 M€/a higher than in step 1.

For $\alpha = 0.25$, the lowest value of natural gas consumption overall operating scenarios is already 231.5 GWh, while the lowest possible electricity consumption accounts for 1.72 GWh. The increase in total annual costs compared to step 1 is between 15 and 37%. The annualized investments are 2.96 M€/a and thus 0.69 M€/a higher than in step 1.

For both of the above-described calculation runs, the same set of energy conversion and storage units are found in step 1. However, their capacities differ from step 1. Generally, the electrode and biomass boiler capacities are higher, while gas boiler and gas turbine capacities do not change significantly.

For $\alpha = 0.01$, lower annualized investment costs but higher total annual costs of approx. 1% are found. The gas boiler capacity is significantly increased, while the biomass boiler and gas turbine capacities are reduced.

3.5. Suitability of approach to consider multiple objective criteria including flexibility

In general, the presented approach is a suitable procedure for integrating flexibility into mathematical optimization. Some practical aspects are analyzed in the following.

When analyzing the solutions with full substitution potential, three combinations of considering costs and the *energy source limitation indicator* were tested in this study. First, in calculation run step 2 (single objective), only the *energy source limitation indicator* was minimized without any consideration of the costs. This led to a significant cost increase. As a consequence, this setting alone, without further calculations, cannot be recommended to determine (cost-)efficient and flexible solutions. Considering an objective function with two criteria and specific weights as in the calculation run step 2 (double objective) resulted in fewer and smaller over-capacities and a good estimate of investment and energy costs for energy source flexible systems. Nevertheless, this second, double objective approach has a significant drawback compared to the iterative approach included in step 3 and by the variation of α. By performing only one optimization run, a general statement about the interaction of flexibility and costs or an interpretation of these criteria's correlation is impossible. By varying α and generating a set of results close to cost optimality a more detailed interpretation of the systems's flexibility is possible.

A second significant finding is that the chosen value for the parameter upper bound of the capacity of the energy source (CAP_s^{UB}) has an impact on the *energy source limitation indicator*. As the energy source is the component in the model that shall be flexible, the choice of its upper bound also has an impact on the objective function and the result in steps 2 and 3. This underlines the fact that two aspects are essential in setting up optimization models as proposed above. First, domain knowledge is essential in setting up and parametrizing the optimization model. Second, technological boundaries often limit the potential in actual use cases and must be considered.

3.6. Techno-economic analysis of energy source flexible industrial energy systems

These findings can be interpreted in the following way: With common price structures and relations between energy source prices, both in 2019 and still today in 2023, comparably low natural gas prices typically impact the chosen technologies in cost-optimal solutions for IES. This occurs especially when renewable fuels are limited, such as the on-site residue biogas in this use case.

A compact explanation for the choice of technologies used in the optimization model is provided, for example, by evaluating the electricity and heat generation costs of the technologies used. These are often also referred to as levelized electricity and heat costs, respectively. Evaluating these levelized costs for different technical and economic parameters is presented below. Due to the dependencies and interactions of the optimized system design(s), it is not straightforward to derive levelized energy costs for the technologies in the actual configuration of the use case as presented in Eq. (11). One example of these complex interactions found in the presented use case results is that the electric demand and the electrode boiler are partly supplied by the electricity provided by the gas turbine and electricity from the grid. A direct assignment of energy sources to energy conversion technologies is possible in the optimization model but beyond the scope of this study and the presented use case. However, in this section, the main focus lies in analyzing and interpreting the techno-economic performance of the single technologies. Consequently, their performance also impacts the system's performance. To support the assessment of levelized costs without the drawback of complex interactions, the levelized heat and electricity costs were calculated for a normalized set of units and sources. Units and sources with a capacity of 10 MW were assumed for this purpose. The depreciation period, the full load hours, and the

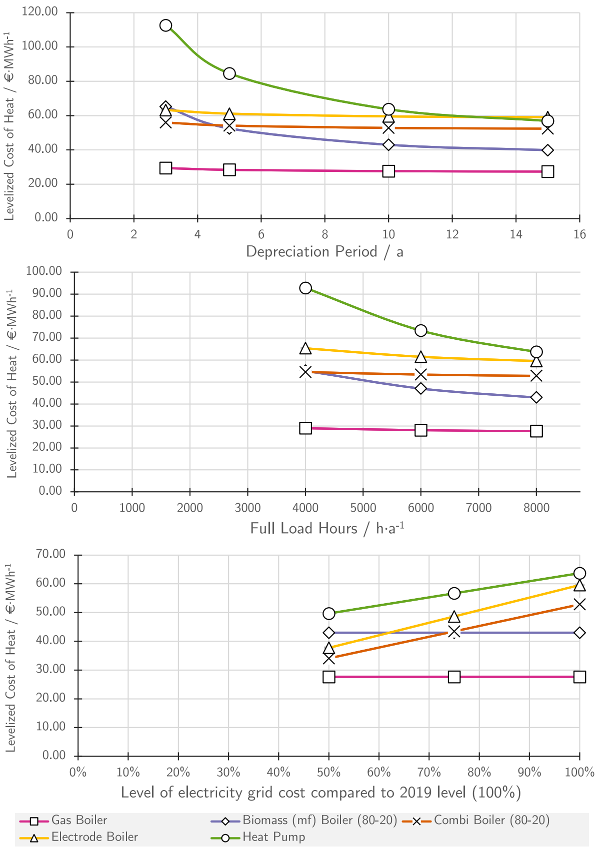


Fig. 12. Overview of levelized cost of heat from different technologies for the variation of units' depreciation periods, units' full load hours, and level of the market electricity costs (without fees) for electricity consumed via the electric grid. In the use case calculation of this work, a depreciation period of 10 years is assumed, and the electricity cost level is set to 100%. The actual full load hours for each technology result from the optimization calculations.

level of electricity prices (share of energy costs) were varied for these. In Figs. 12 and 14, the results for levelized heat and electricity costs are shown, respectively.

For the given frame conditions and all performed variations, the significantly lowest costs are found for the gas boiler. The biomass boiler has the second lowest costs for an appropriately high depreciation period of approximately five years and full load hours above 4100 h per year. Here, an operation with 80% biomass and 20% cost-free biogas is assumed, indicated in the legend by 80–20. Due to its high specific investment costs, compare Table 5 and Fig. 13, for low depreciation periods or full load hours, this technology option is disadvantageous compared to alternatives such as (partially) electrified heat supply. Only for significantly reduced electricity market costs, the combi boiler (80–20) with 80% natural gas and 20% electricity and the electrode boiler might become cheaper than the biomass boiler. For all performed variations, the highest levelized costs of heat are derived for the heat pump. Even for significantly lowered electricity costs, they remain higher than the levelized costs of heat from the biomass boiler. This can be explained by the high share of the investment costs of the heat pump; see Table 5 and Fig. 13.

For the given frame conditions and all performed variations, the significantly lowest levelized electricity costs are found for the gas turbine. Here, the levelized costs for combined heat and power technologies are determined by deducting the product of heat generated and the lowest leveled heat costs of the given technologies, the gas boiler, in this study. Only for significantly low depreciation periods of approximately three years and significantly lowered electricity market costs does electricity from the grid represent a competitive alternative. However, from Fig. 15, one can see that for a depreciation period of 10 years and assumed full load hours of 8000 h per year, the investment costs still contribute to approximately 15% for the levelized costs of electricity. Significantly higher investment costs of gas turbines will, therefore, lead to higher levelized electricity costs of this technology, making electricity consumption via the grid more advantageous.

Both the on-site PV plant and the steam turbine have significantly higher levelized costs of electricity. Thus, the steam turbine is not included in the optimal system of the previously presented use case. The PV plant only becomes part of the solution in configurations with significantly higher overall costs if other limitations are imposed on the system, such as the need for energy source flexibility, as in this study.

Furthermore, from the applied method for finding energy source flexible IES and the derived results, findings regarding the decarbonization potential in this use case can be concluded. Not only are flexibilization and independence on fossil fuels (resilience) increasingly important, but decarbonization of IES is becoming a major challenge. In the above-presented use case, solutions for the IES being capable of supplying the required energy without natural gas (operating scenarios 1 for steps 2 and 3) are found in step 2 for single and double objective calculation runs as well as for step 3 with a value of 0.75 for α. Total annual costs for these solutions range from 30.67–40.34 M€/a.

Thus, additional calculations were performed. If step 1 is re-calculated with the additional assumption of reducing fossil CO_2 emissions to zero, a system including the electrode and biomass boiler with total annual costs of 28.96 M€/a is found. High-temperature heat pumps become part of the solution for higher depreciation periods (15 years instead of 10). Thus, one can conclude that at least for this use case, the cost increase for decarbonizing total fossil scope 1 emission is almost as high as finding systems able to continue supplying energy even if one of the available energy carriers needs to be substituted.

3.7. Impact of further frame conditions of flexibility

Two further use case evaluations are performed to show how the flexibility potential and the economic performance of the system change. The main results are summarized in the following. Here, deviations in the overall conditions triggered by current developments are assumed. The first variation - Case 2 - represents the need to decarbonize energy supply. The second variation - Case 3 - assumes improved process requirements due to higher needs for efficiency. For this case, the process improvement is realized as lower process temperature requirements and increased heat recovery temperatures.

3.7.1. Case 2: Fossil decarbonization of energy supply required

For this scenario, also called case 2, it is assumed that the energy supply needs to be decarbonized. Fossil scope 1 emissions are not allowed anymore. The results of this use case are shown below. Three significant findings are (i) that feasible solutions are found for all steps and thus the remaining set of permissible energy sources is sufficient to fulfill the plant's energy demand, (ii) the new optimal cost level is considerably higher, and (iii) with the remaining energy supply options, no solutions can be found anymore, which allows complete replacement of all remaining energy sources. The second and third findings are visualized in Fig. 16. Compared to the initial use case, the cost-optimal solution (step 1) for this second use case shows a cost increase of 76.67%. This gives an example of the economic side effects of decarbonization at a microeconomic level and from the perspective of manufacturing companies. The effects of decarbonization on the macroeconomic level, e.g., the effects on social, ecological, and economic indicators, are beyond the scope of this study and not assessed here. Analyzing the change in the highest costs for the single-objective calculation in step 2 shows that these only increase by two percent.

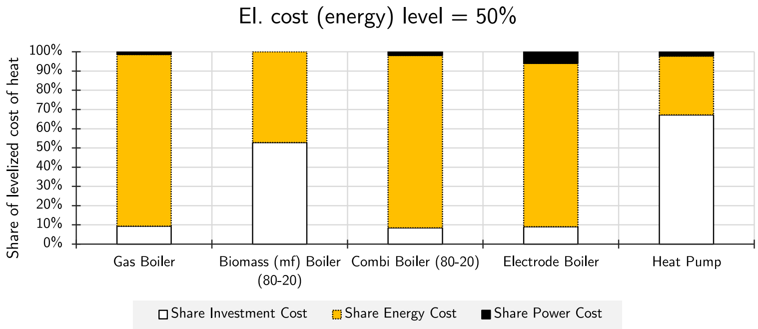


Fig. 13. Relative contributions to the levelized costs of heat from investment, energy, and power costs according to the definition of those costs in Section 2 for reduced electricity cost compared to the elaborated use case. This variation is performed for a depreciation period of 10 years and assumed 8000 full load hours.

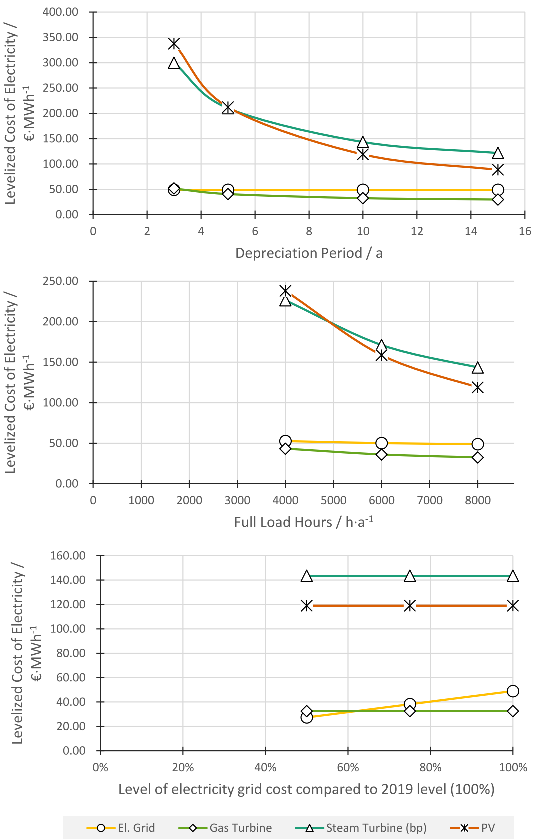


Fig. 14. Overview of levelized cost of electricity from different technologies for the variation of units' depreciation periods, units' full load hours, and the level of the market electricity costs consumed via the grid. In the use case calculation of this study, a depreciation period of 10 years is assumed, and the electricity cost level is set to 100%. The actual full load hours for each technology result from the optimization calculations.

Already in the initial use case, several decarbonized solutions could be found. Thus, the similarly sized total costs for such decarbonized solutions are explainable and comprehensible.

In addition to the disadvantage of higher costs, the total substitution potential is no longer possible compared to the initial use case. No solution was found with a normalized energy source limiting indicator below 0.22. For the initial use case, steps 2 and 3 with an α of 0.75 found solutions for substituting all energy sources. The importance of other energy sources will rise to keep complete flexibility in future energy systems. Examples are further renewable fuels and electricity sources, e.g., more biogenous fuels such as biomass biogas, other fuels such as green hydrogen, or PPA from other sources such as wind power. Furthermore, the importance of storage systems may also rise. When comparing the capacities of all units for all steps in case 2 from Fig. 17 with the capacities from the initial use case, one can find the battery as part of the optimal solution for all steps except step 1 and step 3 with $\alpha = 0.01$. The initial use case included the battery as part of the optimal solution only for the single objective calculations in step 2 and step 3 with $\alpha = 0.75$, see Figs. 7 and 8.

3.7.2. Case 3: Process improvements

For this scenario, also called case 3, it was assumed that the production process requirements were adopted. On the one hand, the process temperature and pressure could be reduced from 150 to 130 °C and 4.5 to 2.5 bar, respectively. Furthermore, improved waste heat recovery led to a heat source outlet temperature of 40 instead of 20 °C. These measures change the coefficient of performance of the heat pump to approx. 2 compared to 1.54 before.

Details are shown in Figs. 18 and 19. From Fig. 18, one can see that, again, as for the initial use case, complete substitution for all energy sources is possible. With increasingly restrictive requirements on total costs, full substitutability decreases, as in the intrinsic use case.

Compared to the initial use case, the total annual costs in step 1 (cost-optimal solution) could be reduced by 1.43%. One significant difference, also shown in Fig. 19 is that the heat pump integration is already in the cost-optimal system. Other than in the initial use case, the heat pump remains part of the optimal solution for all further steps — only the capacity changes. While in step 1, a capacity of 10.28 MW was derived, larger capacities for the heat pump (11.94–17 MW) were found in all subsequent steps.

While the heat pump remained the technology with the highest levelized heat costs in the variations above, the change in the heat pump's operation point (temperature) led to a coefficient of performance ≥ 2. This results in a competitive range of levelized heat costs compared to gas or biomass boilers.

In the initial and decarbonization use cases, the heat pump only became part of the solution when energy source flexibility was requested. The highest costs and the system design for the single-objective calculation in step 2 are comparable to the initial use case. Also, for the further steps, the overall costs and system configurations are mainly comparable to the initial use case. Slight deviations can be found for the PPA integration. Due to the higher relevance of the heat pump and thus electrification in this use case, the renewable generation from the PV PPA is also integrated in later steps of the applied approach with more restrictive constraints on the costs.

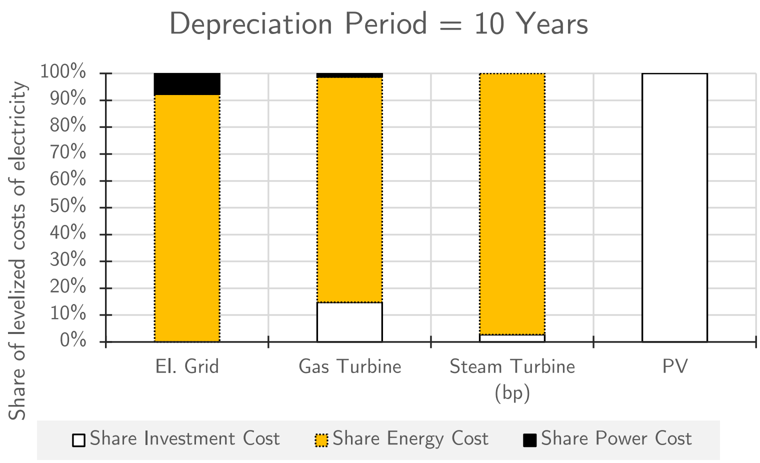


Fig. 15. Relative contributions to the levelized costs of electricity from investment, energy, and power costs according to the definition of those costs in Section 2 for a ten year depreciation period, 8000 full load hours, and the same electricity cost level as assumed for the use case.

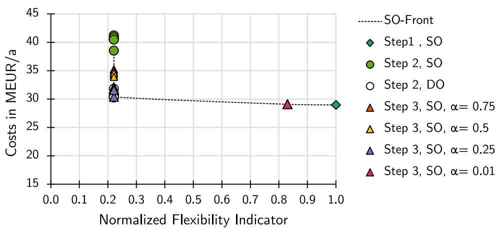


Fig. 16. Overview of costs and normalized flexibility indicator for steps 1–3 in the second case. Each operating scenario in steps 2 and 3 aims to reduce one specific energy source as far as possible for one year. SO indicates calculations with only one objective criterion at a time — either cost on the *y*-axis or flexibility on the *x*-axis. DO indicates calculation with a sum of two weighted optimization criteria at a time. The single objective front connects the lowest values of all single objective calculation runs.

4. Conclusion and outlook

This study provides an overview of existing applications for mathematical optimization for industrial energy supply systems considering flexibility as well as an overview of different perspectives and types of industrial flexibility. As Pareto-curves are rarely applied in considering aspects of flexibility our study suggests a promising new approach for future mathematical optimization models in different industrial sectors and applications.

In this section, first, the main conclusions are presented, followed by a short analysis of the rollout potential and an assessment of the adaptability of the presented approach. Finally, an outlook for further development options for as well as limitations of the presented approach, are given. The main conclusions of this study are:

Pareto-inspired adaptable approach: The first conclusion is that using a Pareto-curve-inspired approach is an effective measure to include various types of flexibility. As its main contribution, this study presents a general and adaptable framework, including a new layer of decision variable time series, capable of incorporating different types of flexibility in optimization in industry. A discussion about the rollout potential of this approach shows examples for the adaptability of the presented approach to other flexibility types. Furthermore, multi-step optimization approaches also gained interest in deriving optimal systems while uncertainty is considered. Pickering et al. [29] use a multi-step optimization with a high number of variations to design a self-sufficient, carbon-neutral European energy system that lies within 10% of optimal costs.

Multi-criteria objectives: The second conclusion considers approaches for multi-criteria optimization. Step 2 of the study involved testing two different objective functions. The initial strategy involved minimizing the second objective criterion – a defined *energy source limitation indicator*. This resulted in an annual cost increase of between 86 and 146% for the initial use case. Additionally, the CAPEX increased by a factor of 5.52 for the initial use case. Based on these results, a second strategy was included, mainly for comparison reasons. In this step, the single objective was exchanged by an objective function with two criteria and specific weights. Still, a solution could be found with the full substitution potential of all energy carriers. The total annual costs increased by only 13 to 87 percent, with CAPEX up by a factor of 1.49 for the initial use case. It can be concluded that weighted multi-criteria objective functions can also contribute to Pareto-curve-inspired approaches. This strategy appears promising, particularly for objective criteria involving relative features like flexibility.

Feedstock flexibility, new technologies and concepts: A third conclusion can be drawn from the use case. For the elaborated use cases, it was shown that the combination of innovative and new concepts for industrial energy can be included in industrial energy supply systems. However, in the initial use case an analysis of the economic performance compared to the typical status quo derived as cost optimal result from step 1 reveals the drawbacks of the innovative systems designs. The solution with the lowest cost for full substitution potential of all energy carriers was the aforementioned double objective calculation in step 2. Still, a solution could be found with the full substitution potential of all energy carriers. The total annual costs increased by only 13 to 87 percent, with CAPEX up by a factor of 1.49. In step 3 the calculation with $\alpha = 0.75$ also had full substitution potential. The cost increase there was between 60 and 100% with a CAPEX increase of 3.75 in the initial use case. For $\alpha = 0.5$ no full substitution could be achieved anymore in the initial use case. However, the economic indicators for that case are in a comparable range of the double objective calculation. Cost increase was between 22 an 73% with a CAPEX increase of 1.42. To fully integrate new technologies as high-temperature heat pumps but also new concepts such as PPA drivers beyond profitability are necessary. A slightly different picture was found for the decarbonization use case. Here, the overall cost-optimal solution resulted to have already 76% higher costs than the cost-optimal solution from the initial use case. By requesting energy source flexibility the cost increase was not as high anymore as for the initial use case. However, no full substitution of all remaining energy sources was possible anymore. By adapting process requirements, as in

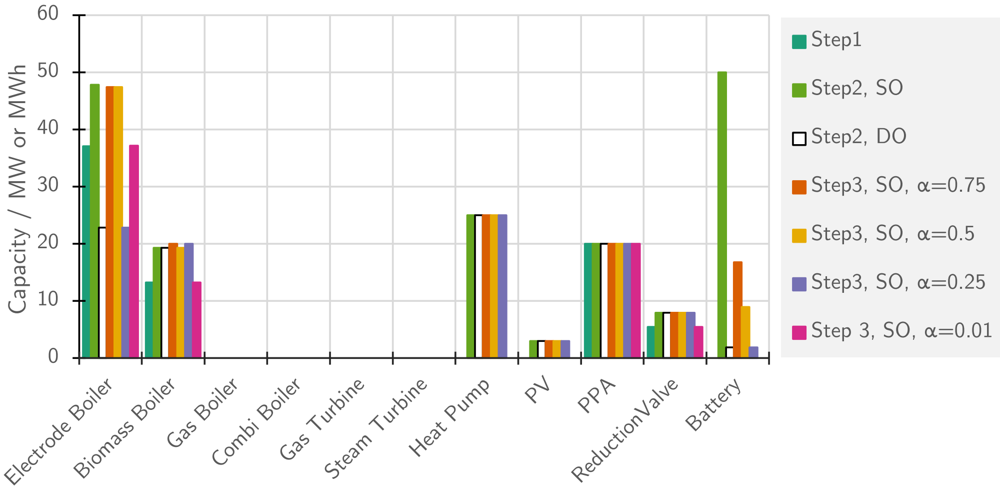


Fig. 17. Overview of units' capacities for steps 1–3 in the 2[nd] case. SO indicates calculations with only one objective criterion at a time — either cost or flexibility.

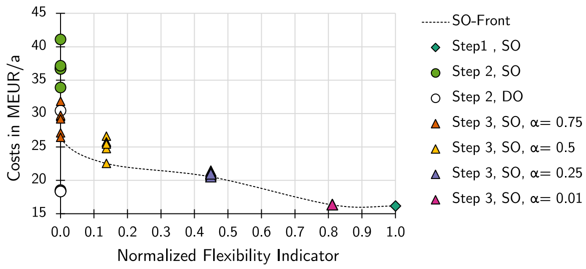


Fig. 18. Overview of costs and normalized flexibility indicator for steps 1–3 in the third case. Each operating scenario in steps 2 and 3 aims to reduce one specific energy source as far as possible for one year. SO indicates calculations with only one objective criterion at a time — either cost on the y-axis or flexibility on the x-axis. DO indicates calculation with a sum of two weighted optimization criteria at a time. The single objective front connects the lowest values of all single objective calculation runs.

case three, the feasibility and competitiveness of new technologies such as high-temperature heat pumps, can be significantly increased.

Challenges for decarbonization: A fourth conclusion can also be drawn from the presented use cases. Current price levels and ratios of typical industrial energy sources lead to significant cost increases when solutions are required where all sources can be fully substituted. The highest cost increase in the initial use case is observed when natural gas needs to be substituted. Thus, one can conclude that for the analyzed price levels decarbonization and independence from fossil fuels is economically challenging. However, as the price level in the use case was assumed from 2019 one could argue that the situation changed in 2023. Nevertheless, it has to be mentioned here, that the relative price levels of the single energy carriers to each other are still comparable to the situation of 2023. Thus, this conclusion is also valid for prices in 2023. The subsequent analysis of a decarbonized use case evaluation also showed, that decarbonization comes along with high increases in total system costs. Also the need for new energy sources and storage technologies might increase.

It can be concluded that this study proposes an approach that can consider different types of flexibility with only a few adjustments of modularized optimization formulations. The use case demonstrates how Pareto curves help analyze trade-offs between costs, optimization criteria, and flexibility. The results for the chosen use case highlight challenges in energy flexibilization and decarbonization.

4.1. Rollout potential of the approach presented

The application cases and potential of the presented approach are comprehensive and reach beyond the scope of the presented use case. The main advantage is that this approach can be applied to different meanings and contexts of flexibility in industrial optimization models. It can be used for both design and operation optimization. While the limitation of energy sources was assumed, this can be extended to the availability of single units or the energy demands that need to be fulfilled. Thus, different flexibility types but also flexibility on different hierarchical factory levels (e.g., technical building service, process level, or plant level) can be considered in independent calculations or simultaneously. Simultaneous consideration of flexibility aspects in optimization avoids pitfalls such as higher costs. Where the considered type of flexibility Eq. (5) is changed, the presented approach would need to be adapted. However, the general approach of considering iterative and different operation scenarios is an essential and repeatable key element for other flexibility types. Explicit adaption measures of the proposed approach are integrating the new layer for all (operating) decision variables, and the general approach for formulating different objective functions.

Types of flexibility relevant for the pulp and paper sector this approach shows potential to be applied to, which are beyond the border of the use case presented here, include, for instance, the following. The first type would be finding the flexibility of an existing system for (reducing) energy consumption from a specific source, e.g., the grid. This is often referred to as positive flexibility for the power grid, e.g., for ancillary services, for specific time steps. Compared to the definition in Luo et al. [9] one could also consider this a special form of **feedstock flexibility**. Here, operating scenarios as introduced in step 2, could be the variation of periods for which flexibility needs to be assessed over the day. The second type would be determining flexible systems that can react to unforeseen events while avoiding excess energy that cannot be used. In Luo et al. [9] it is also described as **production flexibility**. In the case of paper production, a common example would be the sheet break in the drying section of a paper machine. This can occur e.g., daily, several times a day, or several times a week. Here, one option for step 2 of the presented approach is to define operating scenarios for minimizing the demand in different time steps without energy losses. With such a model, it is possible to determine how far the energy demand could be reduced (with or without storage) before losses occur. Also, storage capacities can be evaluated with such an approach. A third type of flexibility that could be elaborated in the presented approach considers scheduling

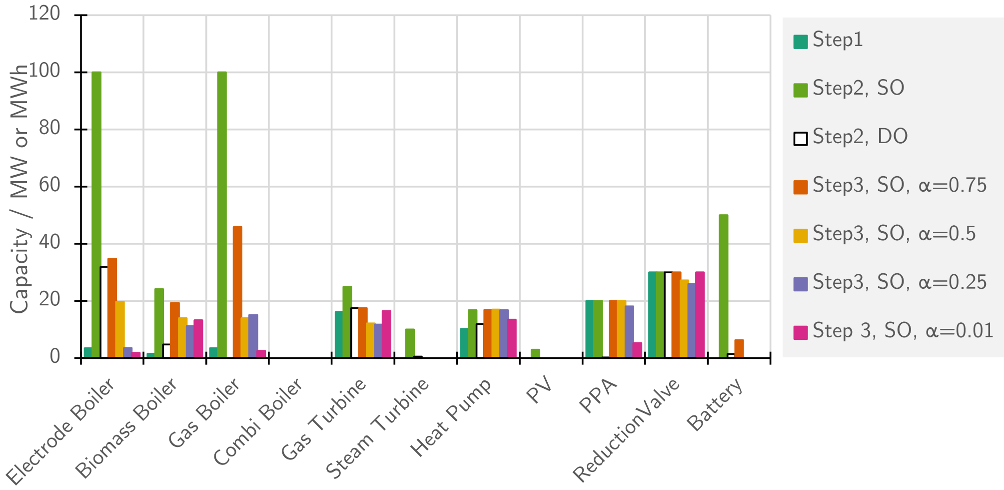


Fig. 19. Overview of units' capacities for steps 1–3 in the 3^{rd} case. SO indicates calculations with only one objective criterion at a time — either cost or flexibility.

of products. **Scheduling flexibility** is, according to Luo et al. [9], the ability to adjust resource allocation for different production cycles. In general it seems promising to adapt the presented approach also to scheduling. However, the main prerequisite for this adaptation would be an extension of the modeled system. Actual production and products would have to be represented by DV and constraints and integrated into the model. For such a model, extensive cooperation with logistics is required. After these changes, possible operating scenarios for step 2 to determine the plant's scheduling flexibility could integrate different order portfolios to create different operating scenarios.

The proposed concept is also suitable for application to optimization models for other industrial sectors and applications. District heating and residential and commercial supply could be implemented, for instance. However, the quantitative results, such as changes in total costs or increases in capacities, might vary from a medium to greater extent.

4.2. Outlook and limitations of the presented approach

In terms of outlook, possible next steps, besides the above-presented adaptations of the use case, could be developing this approach to include a rolling time horizon. In general, a high level of automation and advanced control concepts, such as model-predictive controllers, support realizing flexibility's advantages. As mentioned above, integrating order and production scheduling into the presented approach poses an interesting challenge, which raises new questions in terms of considering logistics and overall planning over the complete value chain in the industry.

The critical aspects and potential pitfalls of our approach were identified and discussed in Section 2. On the one hand, the parametrization of the optimization model is important. To fully exploit a plant's flexibility potential, having a profound knowledge base about the plant and all relevant interfaces to external stakeholders is indispensable. A second critical aspect is (potentially) oversized unit capacities for calculation runs without cost limitations. Here, a recommendation for modeling is given, and an additional optimization approach combining costs and flexibility with specific weights in the objective function is presented.

CRediT authorship contribution statement

Sophie Knöttner: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **René Hofmann:** Supervision, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

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

Data availability

Data will be made available on request.

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Appendix

A.1. Detailed results

In Table A.6 for all calculations and all different operating scenarios, the total annual costs (TAC), annualized investment (CAPEX), operating cost (OPEX), emissions, the value for the objective term in step 2 and 3 (energy source limitation indicator - ESLI) and its normalized value as well as consumed energy for the six energy sources in GWh/a are shown.

A.2. Detailed operation - Use case step 2, single objective

In the following, operation profiles for step 2 (single objective) for included units and for the assumed days (D1 - D4) are divided into two sets of units and shown for all six operating scenarios. For these operation profiles, visualizations are shown. Always minimizing the usage of fuels is shown together in a plot as well as minimizing electricity sources.

A.3. Detailed operation - Use case step 3, single objective, $\alpha = 0.75$

In the following, balancing nodes for step 3 (single objective) for the assumed days (D1 - D4) are visualized for all six operating scenarios. Always minimizing the usage of fuels is shown together in a plot as well as minimizing electricity sources (see Figs. A.24 and A.25).

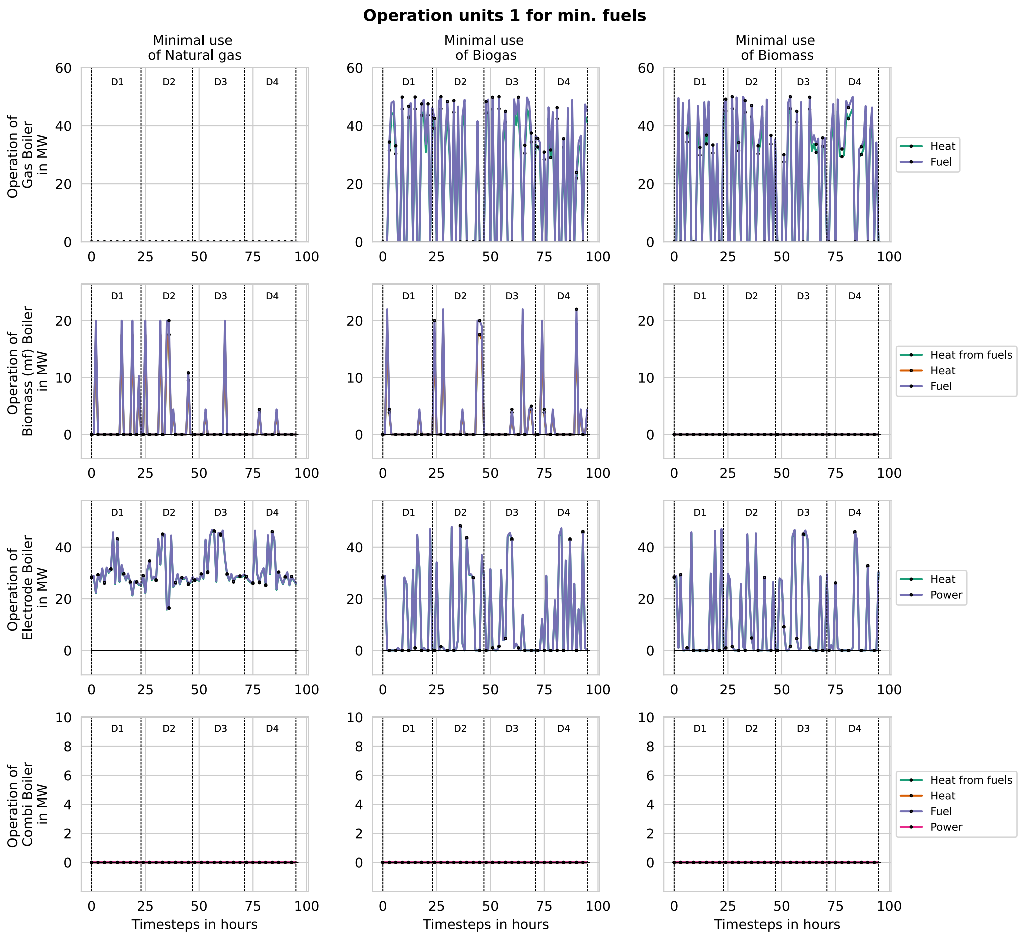

Fig. A.20. Operation of Gas Boiler, Biomass Boiler, Electrode Boiler, and Combi boiler (shown in rows) for minimizing fuels (shown in columns) for the single objective calculation in Step 2.

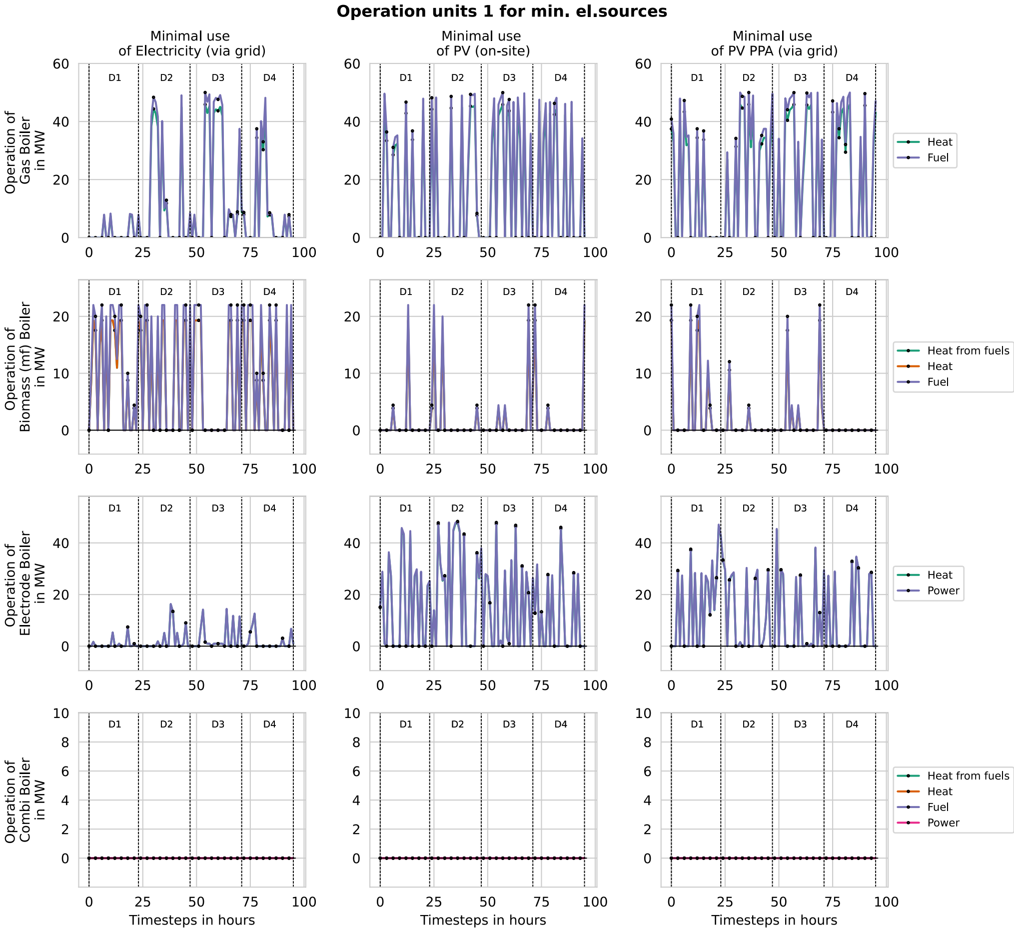

Fig. A.21. Operation of Gas Boiler, Biomass Boiler, Electrode Boiler, and Combi boiler (shown in rows) for minimizing electricity (shown in columns) for the single objective calculation in Step 2.

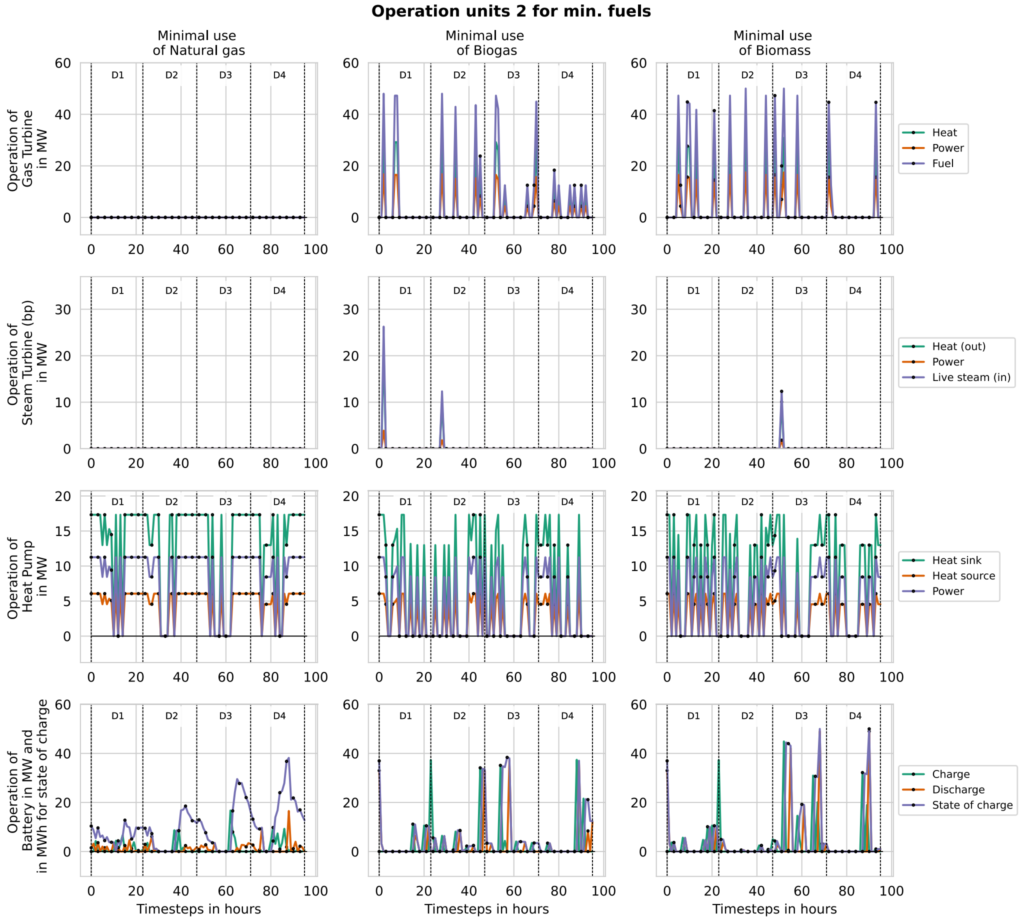

Fig. A.22. Operation of Gas Turbine, Steam Turbine, Heat Pump and Battery (shown in rows) for minimizing fuels (shown in columns) for the single objective calculation in Step 2.

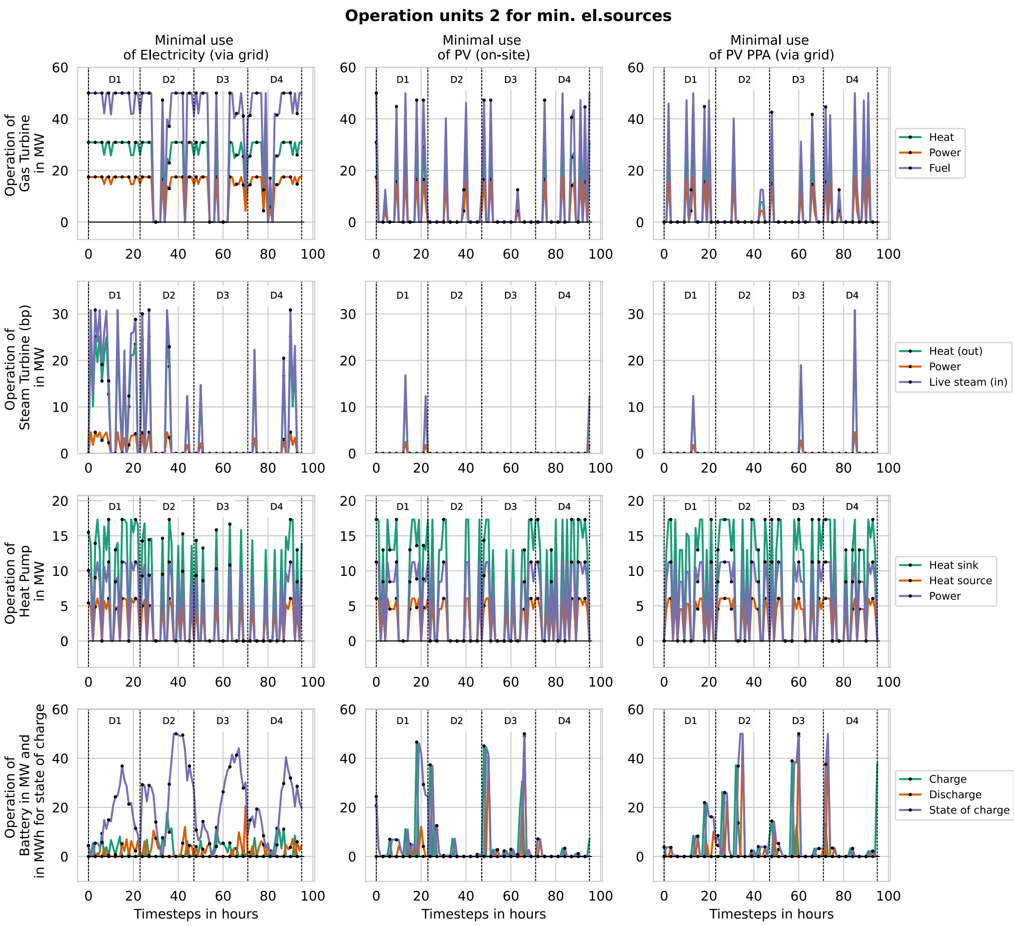

Fig. A.23. Operation of Gas Turbine, Steam Turbine, Heat Pump and Battery (shown in rows) for minimizing electricity (shown in columns) for the single objective calculation in Step 2.

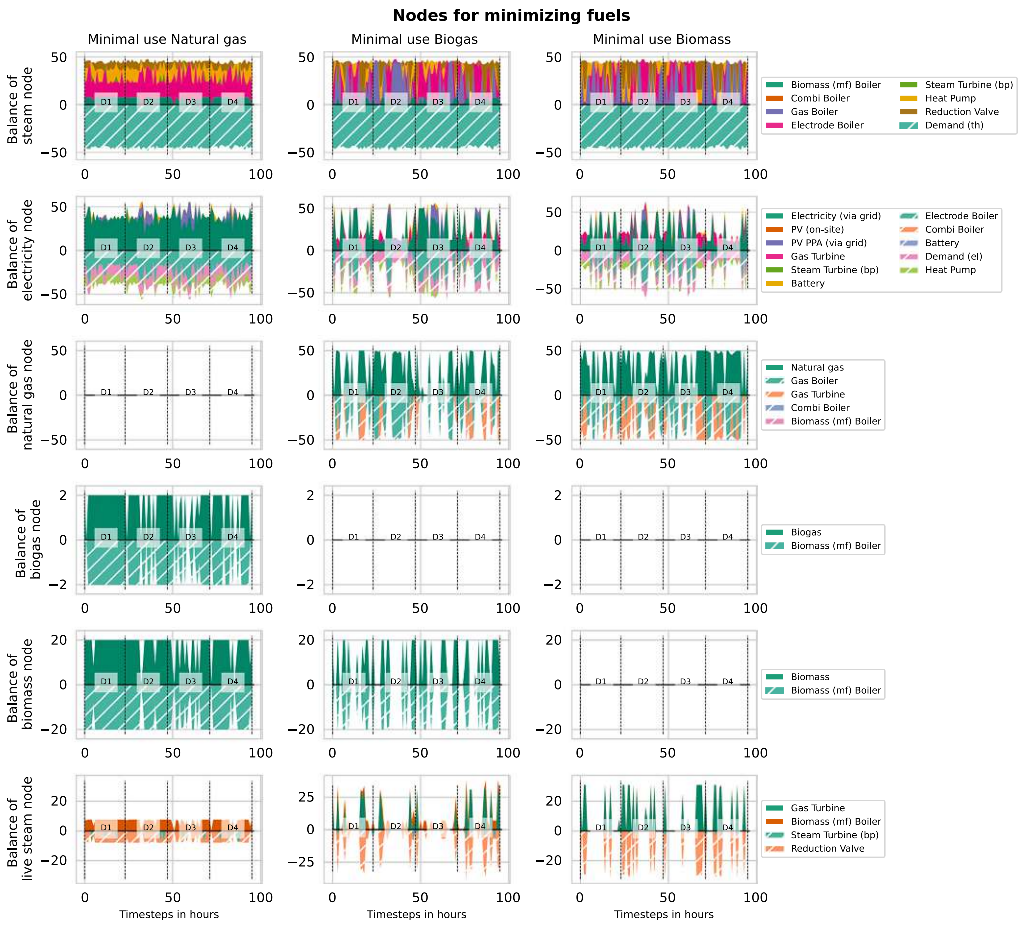

Fig. A.24. Balancing nodes (shown in rows) for minimizing fuels (shown in columns) for the single objective calculation in Step 3 with $\alpha = 0.75$.

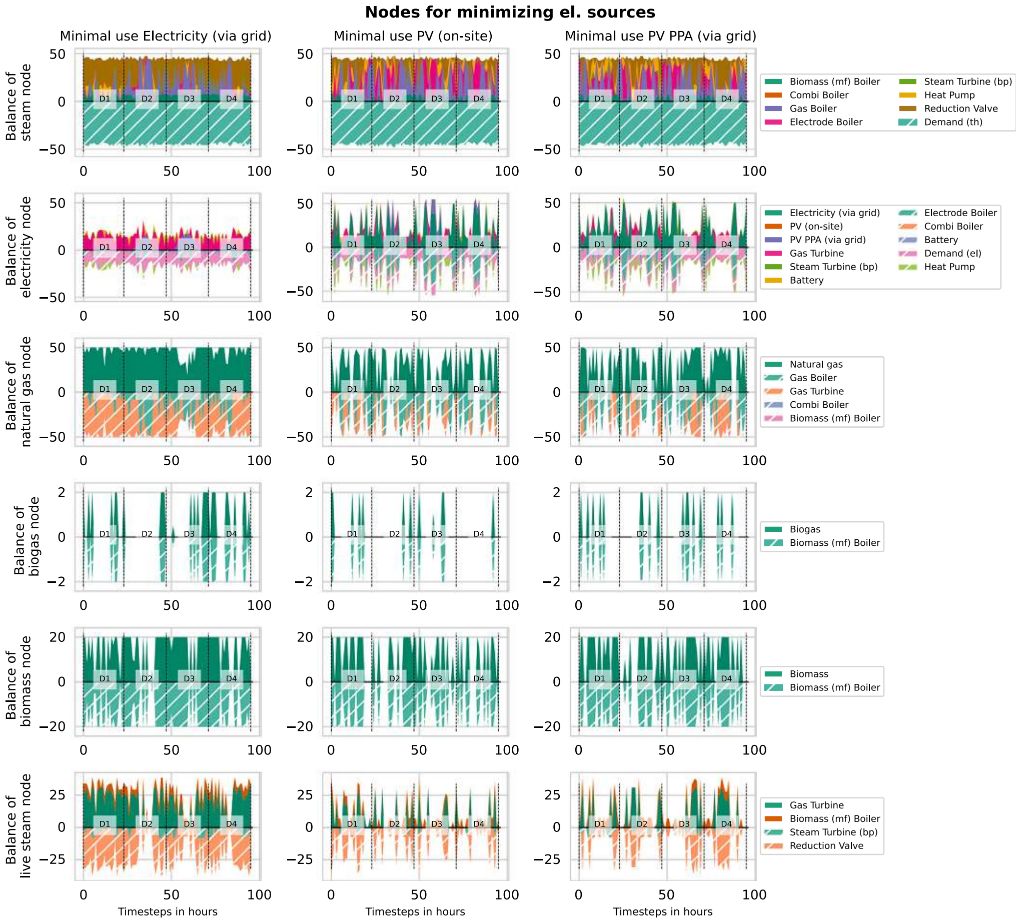

Fig. A.25. Balancing nodes (shown in rows) for minimizing electricity (shown in columns) for the single objective calculation in Step 3 with α = 0.75.

Table A.6
Overview of results with the following abbreviations: ESLI (energy source limitation indicator) = objective function in step 2 and step 3, OS (Operating Scenario), NG (natural gas), BG (biogas), BM (biomass), E (electricity), SO (single objective), DO (double objective).

	OS	TAC M€/a	CAPEX M€/a	OPEX M€/a	Emissions kt/a	Cost incr. compared to step1	ESLI	Normalized ESLI	NG GWh	BG GWh	BM GWh	E GWh	PV GWh	PPA GWh
Step 1, SO		16.39	2.27	14.12	91.98	–	20,947.03	1.00	438.00	16.89	67.57	18.13	0.00	0.00
Step 2, SO	min NG	40.34	12.54	27.79	0.00	1.46	0.00	0.00	0.00	0.26	17.87	418.57	4.68	31.18
	min BG	34.92	12.54	22.38	55.27	1.13	0.00	0.00	263.19	0.00	19.92	195.11	4.68	31.18
	min BM	34.11	12.54	21.56	56.02	1.08	0.00	0.00	266.77	0.00	0.00	194.06	4.68	31.18
	min E	30.51	12.54	17.97	90.85	0.86	0.00	0.00	432.64	6.57	78.30	0.00	4.68	31.18
	min PV	35.59	12.54	23.05	47.20	1.17	0.00	0.00	224.77	1.12	12.29	232.15	0.00	31.18
	min PPA	34.62	12.54	22.08	51.88	1.11	0.00	0.00	247.05	1.07	13.74	234.08	4.68	0.00
Step 3, SO, $\alpha = 0.75$	min NG	34.35	8.51	25.84	0.00	1.10	0.00	0.00	0.00	13.77	152.60	326.03	0.00	31.18
	min BG	30.48	8.51	21.97	48.59	0.86	0.00	0.00	231.39	0.00	75.13	194.05	0.00	31.18
	min BM	28.37	8.51	19.86	63.98	0.73	0.00	0.00	304.66	0.00	0.00	170.47	0.00	31.18
	min E	26.18	8.51	17.67	85.36	0.60	0.00	0.00	406.47	4.81	131.05	0.00	0.00	31.18
	min PV	29.72	8.51	21.21	51.25	0.81	0.00	0.00	244.03	2.10	90.46	167.49	0.00	31.18
	min PPA	29.33	8.51	20.82	55.27	0.79	0.00	0.00	263.17	3.10	101.78	176.01	0.00	0.00
Step 3, SO, $\alpha = 0.5$	min NG	28.36	3.23	25.14	10.58	0.73	1033.20	0.05	50.40	17.52	110.09	331.78	0.00	31.18
	min BG	25.04	3.23	21.81	48.63	0.53	1033.20	0.05	231.59	0.00	12.96	235.79	0.00	31.18
	min BM	24.39	3.23	21.16	52.65	0.49	1033.20	0.05	250.69	0.00	0.00	228.56	0.00	31.18
	min E	19.95	3.23	16.73	86.64	0.22	1033.20	0.05	412.58	0.00	103.60	1.26	0.00	31.18
	min PV	28.19	3.23	24.97	41.06	0.72	1033.20	0.05	195.51	0.24	70.30	275.29	0.00	31.18
	min PPA	25.34	3.23	22.11	48.47	0.55	1033.20	0.05	230.79	0.00	1.41	278.09	0.00	0.00
Step 3, SO, $\alpha = 0.25$	min NG	22.38	2.96	19.41	48.61	0.37	4664.39	0.22	231.50	17.52	108.28	155.03	0.00	31.18
	min BG	22.38	2.96	19.41	67.46	0.37	4664.39	0.22	321.26	0.00	45.69	140.69	0.00	31.18
	min BM	21.68	2.96	18.71	74.60	0.32	4664.39	0.22	355.23	0.00	0.00	140.87	0.00	31.18
	min E	18.88	2.96	15.91	89.50	0.15	4664.39	0.22	426.19	0.00	84.11	1.72	0.00	31.18
	min PV	22.09	2.96	19.13	68.65	0.35	4664.39	0.22	326.88	0.00	19.63	152.59	0.00	31.18
	min PPA	20.93	2.96	17.96	71.08	0.28	4664.39	0.22	338.50	0.00	17.35	161.89	0.00	0.00
Step 2, DO	min NG	30.67	3.38	27.28	0.00	0.87	0.00	0.00	0.00	17.52	102.63	417.59	0.00	0.53
	min BG	19.10	3.38	15.72	91.98	0.17	0.00	0.00	438.00	0.00	71.28	25.09	0.00	0.53
	min BM	19.65	3.38	16.27	91.98	0.20	0.00	0.00	438.00	0.00	0.00	76.32	0.00	0.53
	min E	18.63	3.38	15.25	91.98	0.14	0.00	0.00	438.00	17.27	88.97	0.00	0.00	0.53
	min PV	18.60	3.38	15.22	91.98	0.13	0.00	0.00	438.00	16.91	79.97	6.71	0.00	0.53
	min PPA	18.60	3.38	15.22	91.98	0.13	0.00	0.00	438.00	16.91	80.49	6.86	0.00	0.00
Step 3, SO, $\alpha = 0.01$	min NG	16.63	1.41	15.22	91.69	0.01	13.56	0.65	436.65	6.76	27.04	46.83	0.00	16.18
	min BG	16.63	1.41	15.22	91.98	0.01	13.56	0.65	438.00	5.59	22.37	49.77	0.00	16.18
	min BM	16.63	1.41	15.22	91.98	0.01	13.56	0.65	438.00	5.59	22.37	49.77	0.00	16.18
	min E	16.63	1.41	15.22	91.97	0.01	13.56	0.65	437.97	6.59	27.71	45.42	0.00	16.18
	min PV	16.63	1.41	15.22	91.98	0.01	13.56	0.65	438.00	6.12	24.37	48.09	0.00	16.18
	min PPA	16.63	1.41	15.22	91.98	0.01	13.56	0.65	438.00	6.96	27.85	61.04	0.00	0.00

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Further publications as co-author

In this section, thesis-relevant further publications within the course of this thesis in the period from 2017 to 2022 are summarized.

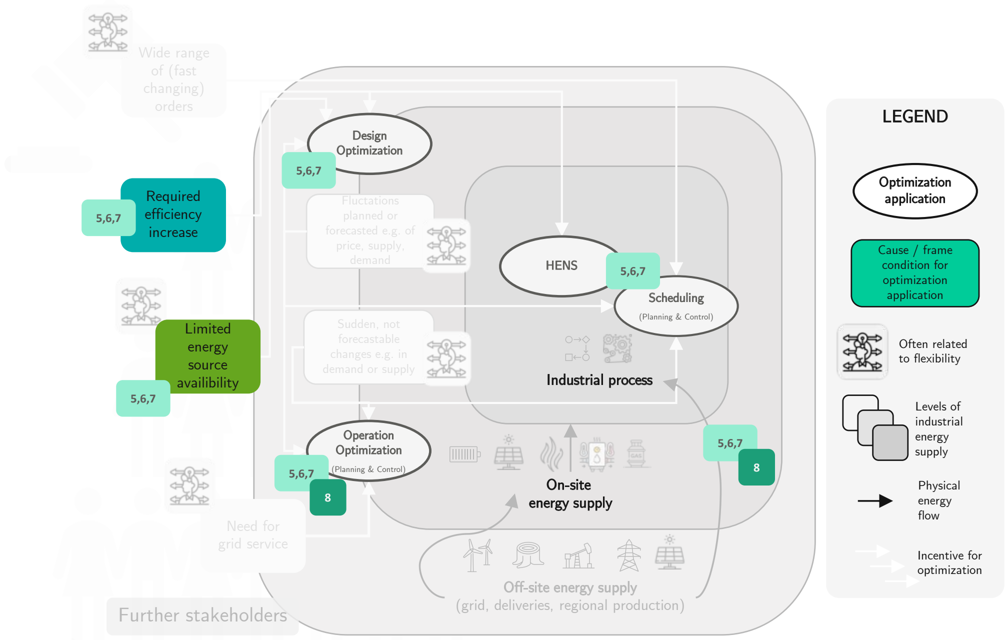

Figure 11: *Adapted stratified visualization for industrial energy supply and consumption levels, incentives, reasons to provide flexibility, and different industrial optimization applications. Some of the further publications of this thesis are classified in this visualization by the numbers 5-8 in small, green rounded rectangles.*

Similarly to the representation of the core publications' contributions in the context of *flexibility, industrial energy supply, and mathematical optimization* in Figure 7, some of the further publications of this work are classified. In Figure 11, the numbers 5-8 in the green rounded rectangles indicate several of the further publications contributing to this work.

Paper 5 A simultaneous optimization approach for efficiency measures regarding design and operation of industrial energy systems

by René Hofmann, Sophie Knöttner and Anton Beck; published in Computers and Chemical Engineering.

For the first time, we combined heat exchanger network synthesis and operational optimization. By comparing sequential and simultaneous solutions, we aimed to identify and quantify the benefits of combined optimization approaches. For a simple industrial test case, the results revealed that a cost and energy-optimal solution would not fully exploit the advantages of both individual applications due to technical limitations typically considered in only one of the two optimization models. In exclusive and sequential approaches, it could even be found that countermeasures occurred, leading to dismissed goals for energy efficiency and cost-optimal operation. Based on this work, a research project proposal focusing on combining industrial optimization applications was successfully submitted. This project led to further publications, e.g., **Paper 6 & Paper 7** of the "Further Publications" in this thesis.

My contribution to parts in the paper: Conceptualization, Methodology, Writing - Original Draft, Writing - Review & Editing, Visualization

Hofmann, René; Knöttner, Sophie & Beck, Anton (2019). A simultaneous optimization approach for efficiency measures regarding design and operation of industrial energy systems. Computers and Chemical Engineering, 128, 246-260. `https://doi.org/10.1016/j.compchemeng.2019.06.007`

Abstract: Sustainability in industrial energy systems has to be increased to achieve climate goals. However, the share of batch processes in industry and changes of the product portfolio have increased. This makes it more difficult to establish sustainable and yet flexible energy supply systems. Current optimization methods for the synthesis of process heat supply systems do not consider all essential aspects. In this paper, optimization of internal heat recovery with heat exchanger networks and storage integration are carried out simultaneously considering operational constraints of the existing supply infrastructure. Furthermore, within this approach storage units can be considered for both heat recovery and load shifting of steam generator units. Necessary interfaces for coupling of operational constraints and design optimization were identified and the complexity of the combined problem was reduced by simplifications. The combined approach was compared to sequential implementation and proved to yield both economical improvements and more sustainable energy use.

Paper 6 Combined optimization for retrofitting of heat recovery and thermal energy supply in industrial systems

by Daniel Halmschlager, Anton Beck, Sophie Knöttner, René Hofmann, Martin Koller: published in Applied Energy.

Based on the initial work in **Paper 5**, the authors enhanced the combined optimization model in this work with two further optimization applications. Design optimization and scheduling of an industrial use case derived from the literature were integrated. A focus was laid on the retrofit formulation of both the heat exchanger network and the existing energy supply systems. The results showed that combining the optimization applications led to more efficient energy use and increased the share of renewable energy in the system. Thus, the discussed method in this work shows big potential to support decision-makers in industrial transition processes toward a more sustainable energy supply.

My contribution to parts in the paper: Conceptualization, Writing - Original Draft, Writing - Review & Editing, Funding acquisition

Halmschlager, Daniel; Beck, Anton; Knöttner, Sophie; Hofmann, René; Koller, Martin (2021). Combined optimization for retrofitting of heat recovery and thermal energy supply in industrial systems. Applied Energy, 305(305), 1-20. `https://doi.org/10.1016/j.apenergy.2021.117820`

Abstract: Predicting the outcome of possible changes in interlinked industrial energy systems is hard, especially in retrofit scenarios. This leads to severe uncertainties when making investment decisions. In this paper, a new combined optimization approach is presented that aims to support decision-making in these cases. Our approach links models for the optimal design of supply systems and heat recovery systems with operational constraints and is specifically designed for retrofit applications. It is formulated as a single combined mixed-integer linear programming (MILP) problem. The approach is applied in a case study representing a typical industrial process, where the supply system and the heat recovery are adapted. The optimal solution shows a cost-effective way for a transition to more efficient use of energy and an increased share of renewable sources.

Paper 7 An Integrated Optimization Model for Industrial Energy System Retrofit with Process Scheduling, Heat Recovery, and Energy Supply System Synthesis

by Anton Beck, Sophie Knöttner, Daniel Halmschlager, Julian Unterluggauer and René Hofmann: published in Processes.

Encouraged by the findings in **Paper 6**, the authors applied the developed method to a real industrial use case from the brewing sector. Cost-optimal solutions for various degrees of decarbonization could be derived and revealed that a relevant share of energy-supply-related emissions could be avoided without increasing the annualized costs.

My contribution to parts in the paper: Conceptualization, Writing - Original Draft, Writing - Review & Editing, Funding acquisition

Beck, Anton; Knöttner, Sophie; Unterluggauer, Julian; Halmschlager, Daniel; & Hofmann, René (2022). An Integrated Optimization Model for Industrial Energy System Retrofit with Process Scheduling, Heat Recovery, and Energy Supply System Synthesis. Processes, 3(10). `https://www.mdpi.com/2227-9717/10/3/572`

Abstract: The urgent need for CO_2 reduction is calling upon the industry to contribute. However, changes within local energy supply systems including efficiency enhancement are bound to several economical and technical constraints, which results in interfering trade-offs that make it difficult to find the optimal investment option for CO2 mitigation. In this article, a new optimization model is presented that allows to optimize the design and operation of a supply and heat recovery system and production scheduling simultaneously. The model was used for retrofitting of a small brewery's local energy system to identify decarbonization measures for eight potential future scenarios with different technical, economical and ecological boundary conditions. The results show that the proposed cost-optimized changes to the current energy system only slightly reduce carbon emissions if decarbonization is not enforced since the optimal solutions prioritize integration of photo voltaic (PV) modules that mainly substitute electricity purchase from grid, which is already assumed to be carbon free. However, enforcing decarbonization rates of 50% for the assumed future boundary conditions still results in cost savings compared to the current energy system. These systems contain heat pumps, thermal energy storages, electric boilers, and PV. Battery storages are only part of the optimal system configuration if low to moderate decarbonization rates below 50% are enforced. An analysis of marginal costs for units not considered in the optimal solutions shows that solar thermal collectors only require small decreases in collector cost to be selected by the solver.

Short Paper

Paper 8 Modeling of Non-Linear Part Load Operation of Combined Cycle Units

by Sophie Knöttner and Réne Hofmann; oral presentation and short paper at the 11^{th} IFAC Symposium on Nonlinear Control Systems (NOLCOS 2019).

Summary: To support achieving ambitious climate goals the accountability of the energy-intensive process industry has to be increased. Recently, the application of optimization methods gained attractiveness to overcome burdens by reducing financial

risks and ensuring process quality for the transition to more sustainable systems. From the modeling perspective, a decisive factor is to enable a tight and compact, accurate modeling of flexible energy supply units. Therefore, a mixed-integer linear programming modeling approach considering varying part-load efficiency industrial energy units was developed. In this contribution, a specific focus was laid on combined cycle units.

Knöttner, Sophie; & Hofmann, René (2019). Modeling of Non-Linear Part Load Operation of Combined Cycle Units. in IFAC Papers online (S. 1334-1335)

S. Panuschka and R. Hofmann (2018). "Modelling of Industrial Energy Systems for Flexibility Increase via Operation Optimization with Mixed-Integer Linear Programming". English. In: Proceedings of the 3rd South East European Conference on Sustainable Development of Energy, Water and Environment Systems*. SEE.SDEWES2018 - 3rd South East European Conference on Sustainable Development of Energy, Water and Environment Systems ; Conference date: 30-06-2018 Through 04-07-2018.*

Scientific Studies and White Papers

Renewables for Industry Within the Research & Development service *Renewables 4 Industry* for the Austrian *Klima- und Energiefonds*, I participated in elaborating a *Discussion Paper* (E) about the coordination of the energy demand of industrial plants and the energy supply from fluctuating renewables, the *Strategic Research Agenda* (F) and a report on *fundamental statements and (technology) policy recommendations* (G).

Moser, Simon; Goers, Sebastian; de Bruyn, Kathrin; Steinmüller, Horst; Hofmann, René; Panuschka, Sophie; Kienberger, Thomas; Sejkora, Christoph; Haider, Markus; Werner, Andreas; Brunner, Christoph; Fluch, Jürgen; Grubbauer, Anna . "Renewables4Industry - Abstimmung des Energiebedarfs von industriellen Anlagen und der Energieversorgung aus fluktuierenden Erneuerbaren. Endberichtsteil 2 von 3 - Diskussionspapier zum Projekt Renwables4Industry". 2018. Last accessed: 16.7.2023. Online available: `Renewables4Industry-DiscussionPaper`

Moser, Simon; Leitner, Karl-Heinz; Steinmüller, Horst. In collaboration with: Brunner, Christoph; Fluch, Jürgen; Gahleitner, Bernhard; Haider, Markus, Hörlesberger, Marianne; Kienberger, Thomas; Königshofer, Petra; Kubeczko, Klaus; Mayrhofer, Julia; Panuschka, Sophie; Rhomberg, Wolfram; Schwarz, Markus; Sejkora, Christoph; Wepner, Beatrix. "Renewables4Industry - Abstimmung des Energiebedarfs von industriellen Anlagen und der Energieversorgung aus fluktuierenden Erneuerbaren. Endberichtsteil 2 von 3 - Strategische Forschungsagenda". 2017. Last accessed: 14.1.2024. Online available: `Renewables4Industry-StrategicResearchAgenda`

Moser, Simon; Steinmüller, Horst; Leitner, Karl-Heinz; Hofmann, René; Panuschka, Sophie; Kienberger, Thomas; Sejkora, Christoph; Haider, Markus; Werner, Andreas; Brunner, Christoph; Fluch, Jürgen; Grubbauer, Anna. "Renewables4Industry - Abstimmung des Energiebedarfs von industriellen Anlagen und der Energieversorgung aus fluktuierenden Erneuerbaren. Endberichtsteil 3 von 3 - Grundlegende Aussagen und (technologie-)politische Empfehlungen". 2018. Last accessed: 14.1.2024. Online available: `Renewables4Industry-FundamentalStatements`

IndustRiES Within the Research & Development service *IndustRiES* for the Austrian *Klima- und Energiefonds*, I participated in elaborating the project results and report *Final Report* (H) about the Energy infrastructure for 100% renewable energy in industry.

Geyer, Roman; Knöttner, Sophie; Diendorfer, Christian; Drexler-Schmid, Gerwin. "IndustRiES - Energieinfrastruktur für 100% Erneuerbare Energie in der Industrie ". 2019. Last accessed: 14.1.2024. Online available: `IndustRiES-Study`

IEA IETS Annex XVIII Within the framework of the IEA IETS Task 18 - Digitalization, Artificial Intelligence, and Related Technologies for Energy Efficiency and GHG Emissions Reduction in Industry - I contributed to a whitepaper elaborated by the Austrian consortium.

Hofmann, René; Halmschlager, Verena; Knöttner, Sophie; Leitner, Benedikt; Pernsteiner, Dominik; Prendl, Leopold; Sejkora, Christoph; Steindl, Gernot; Traupmann, Anna. "Digitalization in Industry - An Austrian Perspective". 2020. Last accessed: 21.5.2023. Online available: `IEA-IETS-Task18-WhitePaper`

RHC SRIA I participated in the Horizontal Working Group *100% Renewable Energy Industries* of the *European Technology and Innovation Platform on Renewable Heating and Cooling*. As part of this collaboration, I contributed to the Strategic Research and Innovation Agenda for Climate-Neutral Heating And Cooling In Europe (J), first published in 2020.

Andreu, Angel; Berberich, Magdalena; Birk, Wolfgang; Brunner, Christoph; Calderoni, Marco; Carvalho, Maria João; Cioni, Guglielmo; Coelho, Luis; Denarie, Alice; Doczekal, Christian; Dragostin, Catalin; Hafner, Bernd; Henzler, Tobias Michael; Höftberger, Ernst; Jaunzems, Dzintars; Ionel, Iona; Kilkis, Birol; Knöttner, Sophie; Kujbus, Attila; Madani, Hatef; , Nikolaos, Margaritis; McKenna, Russell; Mugnier, Daniel; Nielsen, Per Sieverts; Noll, Thomas; Nordman, Roger; Novosel, Tomislav; Pearson, David; Puttke, Bernhard; Repetto, Maurizio; San Román, Marta; Rutz, Dominik; Scoccia, Rossano; Schmidt, Ralf-Roman; Simeoni, Ugo; Skreiberg, Øyving; Haglund Stignor, Caroline; Stryi-Hipp, Gerhard; Urchueguía, Javier;, van Helden, Wim; Weiss, Werner & Willis, Morgan. "Strategic Research And Innovation Agenda For Climate-Neutral Heating And Cooling In Europe - Updated Version". 2022. Last accessed: 14.1.2024. Online available: `RenewableHeatingAndCooling-SRIA`

Presentations

In the course of the work on this thesis, the following presentations were created and given in collaboration with my colleagues as part of various events:

Hofmann, René; Prendl, Leopold; Halmschlager, Verena; Knöttner, Sophie; Knöttner, Alexander; Triebnig, Jörg: Smart Industrial Concept - Holistic Approach with Digitalization of Industrial Processes and Applications for 2050 and beyond.

Event: *Blickpunkt Forschung: Klimaschutz konkret @ TU Wien.* 23.10.2019. Vienna, Austria

Hofmann, René; Halmschlager, Verena; Knöttner, Sophie: Digitalisierung, Künstliche Intelligenz und verwandte Technologien - Annex XVIII.

Event: *Digitalisierung in der Industrie - Workshop im Rahmen des IEA IETS Task XVIII.* 14.11.2019. Vienna, Austria

Knöttner, Sophie; Beck, Anton; Halmschlager, Daniel; Hofmann, René: Betriebsoptimierung + Wie gekoppelte Optimierungsansätze Flexibilität aufzeigen & Effizienzpotentiale nutzbar machen.

Event: *Webinar "Dekarbonisierung der Industrie": Betriebsoptimierung neu gedacht! - Nutzung sämtlicher Abwärmepotentiale und Flexibilitäten.* 20.11.2020. Online webinar

Supervised Thesis

In the course of this work, I have supervised one master's thesis:

Etzl, Klaus: Integrationskonzepte innovativer Technologien in industriellen Energiesystemen; Betreuer:innen: René Hofmann und Sophie Knöttner; E302 Institute für Energietechnik und Thermodynamik; 2019

Appendices

A Industrial Units

The following examples include mostly technologies, which are also considered in the papers belonging to this thesis.

Grid connection and fuel delivery These supply options are fundamentally relevant for the industrial energy system. To increase flexibility and, moreover, reliability, connections to the electric grid can be conducted twice, whereby energy can only be obtained via one reference point at a time.

Direct heat consumption Hot water or steam is consumed from an external provider via local or district heating grids. Here, the energy conversion (fuel to final energy) and the release of scope 1 emissions are outsourced. Also, this energy supply opportunity reduces the possibility of reacting to changing circumstances, such as prices and the availability of energy carriers. Typically, feedstock (fuel) flexibility is not given anymore, or at least it is significantly reduced with this consumption option. Flexibility regarding load change rates can be limited within the delivery contracts.

Boilers These typically fuel-fired units provide a heat transfer medium such as hot water, steam, or thermal oil. The latter is often used to supply process temperatures above $200°C$. Boilers can be designed and built for a wide set of fuels. Common realizations are gas or oil-fired boilers, which typically have high ramping speeds and quick (warm) start types. Boilers for liquid and gaseous fuels often have low investment costs. Thus, this technology group is frequently used to ensure reliability. Often, auxiliary or backup boilers can be found in industrial energy systems.

Steam Turbines (and Steam Boilers) Steam, often called live steam, with high pressure and temperature, is relaxed in multiple turbine stages. The mechanical work is converted into electricity with a generator. The ratio between provided steam and electricity depends on the type of steam turbine and the efficiency of the respective system. There are four different types of steam turbines with different flexibility, with typically a decrease in the relative share of electricity production compared to the heat inlet of the turbine from (i) to (iv):

i condensation steam turbines with only electricity and no process heat supply. The operation of this technology can be quickly adapted to the needs of, e.g., processes or electricity markets.

ii extraction condensation steam turbines with process heat supply at an intermediate steam pressure level and condensation of a mass fraction $\leq 100\%$ of the initial steam flow. This configuration has a high degree of freedom as the electricity generation is not completely independent from heat generation but, to a wide extent, is independent of it.

iii back pressure steam where 100% usage of the initial mass flow is used as process steam at one pressure level without a condensing end of the turbine and. In contrast to condensation steam turbines, less flexibility is possible in changing operation points here. Production flexibility can be realized for energy systems with a steam turbine bypass (e.g., a reduction valve).

iv an extraction back pressure steam turbine where process steam at two different pressure levels is used. For this configuration, the assessment of flexibility is comparable with the former configuration **iii**.

In detail, the idealized back-laying thermodynamic cycle for a combination of boiler and condensing steam turbine is the (Clausius-)Rankine cycle. This clockwise, idealized thermodynamic cycle consists of four steps. First, an (idealized) isentropic compression occurs when the working fluid's pressure increases, e.g., in the feedwater pump. Second, heat is supplied, e.g., by a boiler, and the temperature of the working fluid is increased while its pressure remains at the same level (isobaric). Third, in an (idealized) isentropic expansion, the temperature and pressure of the working fluid are reduced, and mechanical work is extracted and converted to electric energy. In the fourth step, an isobaric heat dissipation is realized in the condenser.

Gas Turbines (and Heat Recovery Boilers) Gas turbine technology provides electricity with an electric efficiency range of 30%- 40%, depending on the operating point, the outside temperatures, and when the system was installed. Due to ongoing developments, newer systems may have higher efficiencies than older systems. Often, not only natural gas but also liquid fuels are possible, which can be summarized as feedstock (fuel) flexibility. Upcoming trends are, for instance, the (partwise) usage of hydrogen as a fuel.

The idealized thermodynamic cycle of a gas turbine is the Brayton cycle, also referred to as the Joule cycle. In contrast to the Rankine cycle, the working fluid in the Brayton cycle is air or gas. This clockwise idealized cycle consists of the following steps. First, an idealized isentropic compression of the ambient air occurs. In the second step, an isobaric combustion of added fuel leads to a temperature increase of the compressed air-flue gas mix. Third, temperature and pressure are reduced in the idealized isentropic expansion, and mechanical work is provided. In the last step, considered isobaric heat dissipation, the hot/warm air stream is released — typically in a subsequent heat recovery boiler.

Usually, gas turbines are not operated as stand-alone technologies in industrial energy systems. However, as stand-alone technologies and in electricity-controlled operation, gas turbines can be characterized by fast ramping speeds, which allows for volume flexibility in electricity production. Nevertheless, in industrial applications, they are often equipped with subsequent heat recovery boilers that can be operated exclusively or with the gas turbine. The air-flue gas mix is cooled down in the heat recovery boilers, and steam is provided. These heat recovery boilers are often equipped with auxiliary firing, which allows more freedom regarding the electricity and heat-produced ratio.

Combined Heat and Power Units with Engines These units are often realized as combinations of the above-presented technologies.

i boilers and steam turbines. This was already referred to in the description of the steam turbines.

ii gas turbines with heat recovery boilers. This was already referred to in the description of the gas turbines.

iii gas turbines with heat recovery boilers and steam turbines, often also referred to as combined cycle power plants. Here, by combined cycle, the Brayton cycle (gas turbine) and Rankine cycle (steam turbine) are indicated.

Another realization also found in smaller industrial supply systems are (e.g., gas-fired) engines with a heat recovery system. Such units often provide electricity, hot water, and even steam. Another application of such generators is the functionality of auxiliary or emergency power generators. These units are usually not realized as combined power to heat units and have little operation hours. In times of grid failures and power outages, they can provide electricity, e.g. for (cooling) processes that require an uninterruptible power supply

Hydropower Plants Depending on the geographic circumstances, small on-site or "close-to-on-site" hydropower plants have also been realized in industrial energy supply systems. These systems have often been built decades ago. Common capacities range between 100 kW and up to several MW. From a technical perspective, volume flexibility can be realized in hydropower plants. However, especially in very small or older plants, the adaptability of the operation point is often not possible while its impact would also be small.

Biogas Plants Several industrial production processes have side streams or residues that can be converted to biogas in anaerobic digestion processes. Typical examples are waste streams from the food sector or wastewater of e.g. plants for paper recycling. The two main components of biogas are carbon dioxide and methane. Depending on the type of residues, the composition and ratio of CH_4 and CO_2 of the biogas change. Necessary treatment steps after the biogas plant need to be done depending on the intended use. With storages for the product *biogas*, such biogas production units can contribute to fuel and scheduling flexibility in an energy system with different supply technologies.

Storages Nowadays, in industrial plants, thermal energy storage or material storages can be found. Common technologies are steam storage, e.g., Ruths steam storage, and water storage, e.g., stratified tanks, intermediate storage tanks, or two-tank systems. Furthermore, cold storages, such as ice storages, are used. In the future, also, storages for electric energy might gain more attractiveness. A common incentive to include energy storage is that it allows the decoupling of supply and production processes. Storages for (intermediate) products allow the decoupling of different production tasks or production and delivery to the customer. In general, this increases efficiency for any case where energy or products would be disposed of without the storage unit. For storages, the increase in efficiency, unlike other technologies in energy supply systems, can go hand in hand with increasing flexibility of resource consumption. Depending on the application, this can contribute to volume, scheduling, and production flexibility.

Refrigeration Units A wide range of production processes also have a cooling demand. Cooling demand typically occurs on different temperature levels for different applications. Space cooling and cooling of production areas, e.g., processing and packaging of food products, is usually set to a temperature of approx. 8°C. Freezing and deep freezing processes have lower temperature requirements down -24°C or even lower for special processes. Sectors with high cooling demands are, for instance, the food sector but also the production of chemical and pharmaceutical products. Beyond industrial applications, the commercial sector also has high cooling demands, e.g., for data centers.

Compression chillers are often, but not exclusively, used to provide cooling. To describe the cooling process, the counter-clockwise Carnot cycle is often used as an idealized thermodynamic cycle. The following steps occur for this process with a refrigerant as working fluid. In the first step, an (isothermic) refrigerant evaporation occurs. The required heat is provided from the medium to be cooled down. Second, isentropic compression occurs, leading to a rise in the refrigerant's pressure and temperature. Usually, electric energy is used to drive the compressor. In step three, the refrigerant's (isothermic) condensation occurs at a higher temperature than the evaporation. Step four consists of an isentropic expansion lowering pressure and temperature, which closes the thermodynamic cycle.

In reality, several losses occur compared to the idealized Carnot cycle. The resulting efficiency (ratio between ideal and real process) is often summarized as *Carnot efficiency* or *second law efficiency*.

Kilns Kilns can usually be found for high-temperature production processes, often with temperature requirements above 1000-1500°C. It is a general term for technologies that are combined units for heat supply and the production process itself. Examples of industrial processes are, for instance, the blast furnace or electric arc furnace for steel production, kilns for firing bricks or other ceramic products, kilns for concrete production, etc. Typical inputs are raw materials or intermediate products and fuels. Various fuels (feedstock flexibility) are possible depending on the product and the kiln type. Substitute fuels such as car tires are also possible in concrete production. Typical outputs are flue gases and intermediate or final products.

Multi-fuel Boilers Especially for industrial sites with high thermal process demands of hot water or steam — approx. in the double-digit megawatt range — boilers for waste streams gained interest. Generally, internal and external residues are used as fuels — often in combination with high-caloric energy carriers such as natural gas or other fossil resources. Small amounts of local residues might also be applicable in such boilers. This application increases feedstock flexibility and often also economic performance. The internal residues used depend on the sector and production process. Examples are, for instance, bark, sludge, reject, and biogas. External residues are, for instance, municipal waste or waste streams from other sectors and sites.

Renewable On-site Electricity While local (on-site or close to on-site) electricity production from hydropower has been enabled as a supply source in the industry for decades, other renewable generation options have also gained relevance lately. The most interesting option here is photovoltaics. Compared to wind power, photovoltaic plants are easier to implement on-site. However, their characteristic generation profiles have several drawbacks, e.g., the reduced generation in typical high-cost periods and the high generation in typical low-cost periods of spot markets. Another limitation of on-site photovoltaics as part of new energy concepts is that the typical space availability for photovoltaic modules is limited. Even the peak power is usually significantly lower than the electric process demand. Compared to several examples above, this energy supply option usually does not contribute to flexibility in a site's energy supply system but requires even more flexibility.

Power Purchase Agreements An alternative to decarbonize the power supply came up as special electricity contracts summarized among the general term *power purchase agreements*. These are typically bilateral contracts between the energy-supplying party and the energy-consuming party. Often the physical generation technologies are close to the actual industrial sites. However, virtual power purchase agreements are also possible. The former bears the additional advantage of balancing generation and consumption on a regional level, thus reducing the challenges for the distribution and transmission of power grids. Usually, these contracts include arrangements about (Deutsche Energie-Agentur 2020):

- the duration of the contract — common run-times can be between even lower than 5 years or even above 9 years
- the price of the product — this can be a fixed price (often below average market prices but above prices in those hours in which the respective technology dominates the power production) or one indexed to markets
- the delivery profile — ranging from *as-produced* (the consumer has to consume the actual amount as it is produced) over minimum delivery, fixed profile to a base-load profile

As indicated above, for on-site generation from renewable energy sources, this energy supply option usually does not contribute to flexibility in a site's energy supply system but requires even more flexibility. Power purchase agreements require a high flexibility increase if large amounts are included as *as-produced* contracts.

Direct and indirect Heat Recovery Direct or indirect heat recovery is often considered a measure for industrial energy supply, driven by the aim of simultaneously increasing economic performance and sustainability. In general, heat recovery can increase the efficiency of energy supply as less primary and final energy is consumed to fulfill the energy demand of the processes. Nevertheless, as presented before, an increase in efficiency can counteract flexibility. Consequently, the emissions can be reduced by fulfilling energy demands. Two main groups of heat recovery measures can be distinguished.

i direct heat recovery utilizing heat exchangers. Heat exchangers can be applied to transfer heat from a hotter working fluid to a colder working fluid. These fluids can be combined in the heat exchanger as cross-flows, counter-flows, or parallel flows. Typical working fluids are either liquid or gaseous. Common design and construction forms are double-pipe, tube-and-shell, or plate heat exchangers.

ii indirect heat recovery employing heat pumps. When indirect heat recovery is applied, excess heat (or a cooling demand) at a lower temperature level is collected (source) and brought to a higher temperature level (sink) by expending technical work. While the working principle is equivalent to chillers, the intended benefit distinguishes it from chillers. The main aim of heat pumps is to supply a heat demand while chillers supply cooling demands. Ideally, the unit combines both advantages and uses the cooling demand as a heat source to supply a heat demand at the sink side of the heat pump. In the past, heat pumps have been applied for domestic or space heating applications. However, lately, their application in industrial energy systems has increased (Biermayr et al. 2022). For industrial applications, the technology of compression heat pumps is often applied. Nevertheless, other technologies, e.g., absorption or adsorption heat pumps, are also possible.

Generally, assessing the economic feasibility of heat recovery measures is a counterplay of additional investment costs while having reduced operational costs.

About the author

Sophie Knöttner has been working for the AIT Austrian Institute of Technology, Center for Energy, since 2017 as a doctoral fellow and since 2020 as a research engineer in Thermal Energy Systems with a focus on efficiency in industrial processes and systems. She has been working on (cost) optimized operation and design of flexible and decarbonized industrial energy supply systems and has become a dedicated "translator" of industrial systems and frameworks into mathematical optimization models in the last few years. She gained extensive experience in application-oriented research for industrial challenges. She built up a profound knowledge base in the fields of energy-related optimization approaches, requirements of industrial production processes, and the energy supply for industrial production processes. She contributed to studies deriving potential future development paths in the Austrian production sector, overcoming challenges of the energy sector transition. At the international level, Sophie has contributed to the "Horizontal Working Group Industry" within the "Renewable Heating and Cooling Platform" on the creation of a new "Strategic Research and Innovation Agenda" and in projects of the Technology Collaboration Program "Industrial Energy-Related Technologies and Systems" of the International Energy Agency. Sophie holds a Master's Degree in Industrial Energy Technology of Montanuniversität Leoben and a Bachelor's Degree in Technical Physics TU Wien.

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SOPHIE KNÖTTNER

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PROFIL

Forscherin im Bereich der mathematischen Optimierung mit Schwerpunkt auf der Auslegung und dem Betrieb industrieller Energieversorgungssysteme und industrieller Flexibilität.

Engagierte Übersetzerin industrieller Systeme und Rahmenbedingungen in Optimierungsmodelle.

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ERFAHRUNG

Austrian Institute of Technology GmbH
SEIT 2020 (RESEARCH ENGINEER)
2017-2020 (PHD-KANDIDATIN)
Mitarbeit & Projektleitung in Forschungsprojekten zu optimiertem Betrieb und Flexibilität für industrielle Energiesysteme, Entwicklungspfade für Digitalisierungs- und Dekarbonisierung, Herausforderungen der Transformation des Energiesystems

Universität für Bodenkultur
03-06/2016 (WISSENSCHAFTLICHE MITARBEITERIN)
03-09/215 (MASTERSTUDENTIN)
Auslegung und ökonomischen Bewertung von Anlagen zur Biokunststoffproduktion

Fröling Heizkessel- & Behälterbau Ges.m.b.H.
02/2015 (PRAKTIKANTIN)
09/2014 (PRAKTIKANTIN)
Leistungsbewertung von Elektrofiltern zur Staubabscheidung bei Hackgutkessel, Recherche zur Rechtslage der Zulassung

Lallemand Inc.
07-09/2010 (LABORASSISTENTIN)
Durchführung von Qualitätstest für Hefe, Fermentationsbetreuung

FÄHIGKEITEN

- **Mathematische Optimierung**
- **Dekarbonisierung & Flexibilität**
  in industriellen Prozessen und Energieversorgung
- **Programmieren**
  Python & Matlab, Grundkenntnisse C & C++
- **Simulationstools**
  Grundkenntnisse in EBSILONProfessional, IPSEpro, KED
- **Sprachen**
  Deutsch, Englisch, Französisch

AUSBILDUNG

TU Wien
SEIT 2017
Doktorat der *Technischen Wissenschaften*

Montanuniversität Leoben
2013-2016
Masterstudium *Industrielle Energietechnik*

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WEITERE QUALIFIKATIONEN

- **Summerschool Data Science**
  Montanuniversität Leoben (07/2022)
- **Female Leadership Development Programme**
  Austrian Institute of Technology GmbH (2021-2022)

PREISE UND STIPENDIEN

- **Young Author Award**
  16. Symposium Energieinnovation 2020 an der TU Graz (2020)
- **2. Platz AIT Posteraward**
  (2019)
- **Top Stipendium**
  NÖ Forschungs & Bildungsges. m.b.H. (NFB) im Bereich „Energie- & Ressourcen-effizienz" für die Masterarbeit (2016)
- **Leistungsstipendium**
  der Fakultät für Physik (2012)

PUBLIKATIONEN

2024	Assessment and conceptualization of industrial energy flexibility supply in mathematical optimization in a competitive and changing environment. In: Energy Conversion and Management. 204. 118205. 30S.	Knöttner, S.; Hofmann, R.
2024	transform.industry Transformationspfade und FTI-Fahrplan für eine Klimaneutrale Industrie 2040 in Österreich: Studie im Auftrag des Klima- und Energiefonds	Schützenhofer, C., Alton, V., Gahleitner, B., Knöttner, S. B., Kubeczko, K., Leitner, K-H., Rhomberg, W., Kienberger, T., Baumann, M. & Böhm, H.
2023	Development of the virtual battery concept in the paper industry: Applying a dynamic life cycle assessment approach. In: Sustainable Production and Consumption, 40, S.438-457, 20S	Puschnigg, S.; Knöttner, S.; Lindorfer, J.; Kienberger, T.
2023	Industrielles Flexibilitätspotenzial zur Bereitstellung von Redispatch, 13. Internationale Energiewirtschaftstagung an der TU Wien: Die Zukunft der Energiemärkte in Europa vor dem Hintergrund neuer geopolitischer Ungleichgewichte. 23 S.	Traninger, M.; Knöttner, S.
2022	Flexibilität durch Wärmepumpenintegration – Analyse eines virtuellen Batteriekonzepts für eine Papierfabrik. Deutsche Kälte- und Klimatagung 2022. 12 S.	Knöttner, S. B., Beck, A., Unterluggauer, J., Helminger, F., Puschnigg, S., Lindorfer, J., Hellkamp, D. & Häring, R.
2022	Perspectives on flexibility in industry - Advantage or Requirement? Vortrag im Rahmen der "Paper and Biorefinery „ Konferenz 2022	Knöttner, S.; Esterl, T.; Hemm, R.
2022	An Integrated Optimization Model for Industrial Energy System Retrofit with Process Scheduling, Heat Recovery, and Energy Supply System Synthesis. 2022, in: Processes. 3. 10S.	Beck, A.; Knöttner, S.; Unterluggauer, J.; Halmschlager, D. & Hofmann, R.,
2022	Impact of recent district heating developments and low-temperature excess heat integration on design of industrial energy systems: An integrated assessment method. In: Energy Conversion and Management. 263, 115612, 17 S.	Knöttner, S.; Leitner, B.; Hofmann, R.
2021	Combined optimization for retrofitting of heat recovery and thermal energy supply in industrial systems. In: Applied Energy, 305 (2021), 305; S. 1 - 20.	Halmschlager, D.; Beck, A.; Knöttner, S.; Koller, M.; Hofmann, R.
2021	100 % erneuerbare Energie für Österreichs Industrie - Ein Ausblick zu alternativen Energieträgern, Prozessen, Infrastrukturanforderungen und Energiebedarfe"; In: Elektrotech. Inftech. (e & i Elektrotechnik und Informationstechnik), 8 (2021), 138; S. 632 - 633.	Knöttner, S.; Geyer, R.; Diendorfer, C.; Drexler-Schmid, G.
2021	100% Renewable Energy for Austria's Industry: Scenarios, Energy Carriers and Infrastructure Requirements. In: Applied Sciences 11 (4), S. 1819. DOI: 10.3390/app11041819.	Geyer, R.; Knöttner, S.; Diendorfer, C.; Drexler-Schmid, G.; Alton, V.
2020	Strategic Research And Innovation Agenda For Climate-Neutral Heating And Cooling In Europe; Herausgegeben von: Andrej Misech - EUREC, BE Lourdes Laín Caviedes - EUREC, BE (creative lead); RHC Platform, Brussels, 2020.	Angel, A.; Berberich, M.; Birk, W.; Brunner, C.; Calderoni, M.; Carvalho, M.; et al.

2020	Betriebsoptimierung + Wie gekoppelte Optimierungsansätze Flexibilität aufzeigen & Effizienzpotentiale nutzbar machen" Vortrag: Webinar "Dekarbonisierung der Industrie": Betriebsoptimierung neu gedacht! - Nutzung sämtlicher Abwärmepotentiale und Flexibilitäten, online	Beck, A.; Halmschlager, D.; Hofmann, R.
2020	Horizontal Working Group Industries", Vortrag: RHC-ETIP Webinar on the Renewable Heating and Cooling Strategic Research and Innovation Agenda, online (eingeladen)	Knöttner, S.
2020	100 % renewable energy for Austria´s industry: alternative energy sources and infrastructure requirements; Vortrag: 16. Symposium Energieinnovation, Stockholm; 14.09.2020 - 17.09.2020; in: "eceee Industrial Summer Study proceedings",	Geyer R., Knöttner S., Diendorfer C., Drexler-Schmid G.
2020	100 % Erneuerbare Energie für Österreichs Industrie Teil 1 – Alternative Energieträger und Prozesse; Vortrag: 16. Symposium Energieinnovation 2020, Graz; 12.02.2020 – 14.02.2020; in: Tagungsband 16. Symposium Energieinnovation 2020.	Knöttner S., Geyer R., Diendorfer C., Drexler-Schmid G.
2020	100 % Erneuerbare Energie für Österreichs Industrie Teil 2 – Infrastrukturanforderungen und Energiebedarfe; Vortrag: 16. Symposium Energieinnovation 2020, Graz; 12.02.2020 – 14.02.2020; in: Tagungsband 16. Symposium Energieinnovation 2020.	Geyer R., Knöttner S., Diendorfer C., Drexler-Schmid G.
2019	IndustRiES - Energieinfrastruktur für 100% Erneuerbare Energie in der Industrie. Klima- und Energiefonds (Hrsg). Wien. 219 S.	Geyer R., Knöttner S., Diendorfer C., Drexler-Schmid G.
2019	Modeling of Non-Linear Part Load Operation of Combined Cycle Units; Vortrag: Joint Mechatronics 2019 & NolCoS 2019, Wien; 04.09.2019 - 06.09.2019; in: "IFAC Papers online", S. 1334 - 1335.	Knöttner S., Hofmann R.
2019	A simultaneous optimization approach for efficiency measures regarding design and operation of industrial energy systems. In: Computers & Chemical Engineering 128, S. 246–260.	Hofmann R., Panuschka S., Beck A.
2019	Photoautotrophic production of poly-hydroxybutyrate – First detailed cost estimations. In: Algal Research 41, S. 101558.	Panuschka S., Drosg B., Ellersdorfer M., Meixner K., Fritz I.
2019	Impact of thermal storage capacity, electricity and emission certificate costs on the optimal operation of an industrial energy system. In: Energy Conversion and Management, 185 (2019), S. 622 - 635.	Hofmann R., Panuschka S.
2018	Modelling of Industrial Energy Systems for Flexibility Increase via Operation Optimization with Mixed-Integer Linear Programming; Vortrag: 3rd South East European Conference on Sustainable Development of Energy, Water and Environment Systems, Novi Sad; 30.06.2018 - 04.07.2018; in: Proceedings of the 3rd South East European Conference on Sustainable Development of Energy, Water and Environment Systems.	Hofmann R., Panuschka S.
2018	Renewables4Industry - Abstimmung des Energiebedarfs von industriellen Anlagen und der Energieversorgung aus fluktuierenden Erneuerbaren: Endberichtsteil 1 von 3 - Strategische Forschungsagenda. 15 S.	Moser, S., Leitner, K-H., Steinmüller, H., Brunner, C., Fluch, J., Gahleitner, B., Haider, M., Hofmann, R., Hörlesberger, M., Kienberger, T., Königshofer, P., Kubeczko, K., Mayrhofer, J., Panuschka, S., Rhomberg, W., Schwarz, M., Sejkora, C. & Wepner, B.
2018	Renewables4Industry - Abstimmung des Energiebedarfs von industriellen Anlagen und der Energieversorgung aus fluktuierenden Erneuerbaren: Endberichtsteil 2 von 3 - Diskussionspapier zum Projekt Renwables4Industry. 144 S.	Moser, S., Goers, S., de Bruyn, K., Hofmann, R., Panuschka, S., Sejkora, C., Kienberger, T., Haider, M., Werner, A., Brunner, C., Fluch, J. & Grubbauer, A.
2018	Renewables4Industry - Abstimmung des Energiebedarfs von industriellen Anlagen und der Energieversorgung aus fluktuierenden Erneuerbaren: Endberichtsteil 3 von 3 - Grundlegende Aussagen und (technologie-) politische Empfehlungen. 12 S.	Moser, S., Steinmüller, H., Leitner, K-H., Hofmann, R., Panuschka, S., Kienberger, T., Sejkora, C., Haider, M., Werner, A., Brunner, C., Fluch, J. & Grubbauer, A
2016	Design einer Demonstrationsanlage zur photoautotrophen PHB-Produktion. Masterarbeit, Wien	Panuschka S.