Advanced Synthesis Methods for Renewable Energy Integration and Automated Data-Driven Model Adaption for Industrial Systems

by Leopold Prendl

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Vienna, February 2022

Leopold Prendl

Abstract

To keep environmental goals of initiatives like the European Green Deal reachable, joint efforts of the whole society are needed. As a contribution to this cause, this thesis deals with the prominent topic of industrial energy systems process optimization. The first part of this work revolves around the development of a mixed integer linear programming (MILP) optimization approach that allows the simultaneous integration of heat pumps (HP) and storages (ST) into heat exchange network synthesis (HENS). A thorough literature study showed that energy integration and waste heat recovery were extensively researched in the last decades. Contrary, literature about the integration of HP and ST into HENS to enhance heat recovery capabilities and the possible integration of renewable energy sources still shows potential for improvements. Evaluating possible potential and the propper applicability of optimization approaches are gaps that still have to be filled by further developments such as those carried out in this thesis. A case study on a set of example cases based on processes of the energy intensive industry (EII) showed the enormous economic and thermodynamic potential of the proposed novel approach. Since every optimization is highly dependent on their input parameters and underlying models, the second part of this thesis deals with developing methods for the automated data-driven model adaption. Especially the nonlinearity of thermodynamic components of energy systems and common mechanisms like fouling or abrasion that can change physical properties during operation make accurate predictions of their behavior complicated. If component models and thus their predictions are not accurate enough, the savings achieved through optimization may be consumed by process control that has to counteract the incorrect predictions to keep the real process in a feasible state. The developed framework based on OPC UA and other state-of-the-art communication protocols allows a continuous automated adaption of component models to match the current properties of the real physical system. The framework's application on a packed bed thermal energy storage with continuous fouling during operation showed a major improvement of the prediction capabilities of the trained model compared to a model without adjustments.

Kurzfassung

Um die Umweltziele von Initiativen wie dem Europäischen Green Deal erreichbar zu halten, sind gemeinsame Anstrengungen der gesamten Gesellschaft erforderlich. Als Beitrag dazu beschäftigt sich diese Arbeit mit dem prominenten Thema der Prozessoptimierung industrieller Energiesysteme. Der erste Teil dieser Arbeit dreht sich um die Entwicklung eines Optimierungsansatzes der gemischt-ganzzahligen linearen Programmierung, der die gleichzeitige Integration von Wärmepumpen und thermischen Speichern in die Wärmeaustauscher-Netzwerksynthese ermöglicht. Eine fundierte Literaturrecherche hat gezeigt, dass die Energieintegration und die Abwärmenutzung in den letzten Jahrzehnten in zahlreichen Studien ausführlich untersucht wurden. Im Gegensatz dazu zeigt die Literatur über die Integration von HP und ST in HENS zur Verbesserung der Wärmerückgewinnung und die mögliche Integration von erneuerbaren Energiequellen noch Verbesserungspotenzial. Die Bewertung möglicher Potenziale und die bessere Anwendbarkeit von Optimierungsansätzen sind Lücken, die durch Weiterentwicklungen, wie sie in dieser Arbeit durchgeführt wurden, noch geschlossen werden müssen. Eine Fallstudie an einer Reihe von Beispielen, die auf Prozessen der energieintensiven Industrie basieren, zeigte das enorme wirtschaftliche und thermodynamische Potenzial des vorgeschlagenen neuen Ansatzes. Da jede Optimierung in hohem Maße von ihren Eingangsparametern und zugrundeliegenden Modellen abhängig ist, befasst sich der zweite Teil dieser Arbeit mit der Entwicklung von Methoden zur automatisierten datengetriebenen Modellanpassung. Insbesondere die Nichtlinearität der thermodynamischen Komponenten von Energiesystemen und of auftretende Mechanismen wie Verschmutzung oder Abrieb, die die physikalischen Eigenschaften während des Betriebs verändern können, erschweren genaue Vorhersagen ihres Verhaltens. Wenn die Komponentenmodelle und damit ihre Vorhersagen nicht genau genug sind, können die durch die Optimierung erzielten Einsparungen durch die Prozesssteuerung aufgezehrt werden, die den falschen Vorhersagen entgegenwirken muss, um den realen Prozess in einem funktionsfähigen Zustand zu halten. Das entwickelte Framework auf Basis von OPC UA und anderen modernen Kommunikationsprotokollen ermöglicht eine kontinuierliche automatisierte Anpassung von Komponentenmodellen an die aktuellen Eigenschaften ihres physikalischen Gegenstückes. Die Anwendung des Frameworks auf einen Festbett-Wärmespeicher, bei dem kontinuierlicher Verschmutzung während des Betriebs auftritt, zeigte eine deutliche Verbesserung der Vorhersagefähigkeiten des trainierten Modells im Vergleich zu einem Modell ohne Anpassungen.

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I would like to thank all my wonderful colleagues and companions at the TU Wien for making the last few years an extraordinary experience. In particular, I would like to thank Verena and Lukas for their support and their always open ears. They helped me in countless exciting discussions to further develop and improve my ideas when I got stuck, thus contributing significantly to this work's success.

Finally, I would like to thank my family, friends, and especially my wife Lisa for their encouragement, understanding, and unconditional support that gave me the strength and inspiration to walk this path.

Preface

This thesis was enabled trough my participation in the cooperative doctoral school SIC! - Smart Industrial Concept[1]. The overall aim of SIC! is the development of interdisciplinary and holistic approaches to meet the challenges of energy optimal operation of industrial plants through research in the area of digitalization and decarbonization. To be able to combine a scientific approach with industrial know-how, the consortium of SIC! consists of three scientific partners, TU Wien, AIT Austrian Institute of Technology, and Montanuniversität Leoben as well as five industrial partners which are EVN, evon, FunderMax, ILF Consulting Engineers, and OSIsoft. Within this consortium, 8 PhD students conducted research in the area of the four main pillars of SIC! which are depicted in the graphic below. Especially the cooperative work on the overlapping areas of the individual research topics, which is one of the most important possibilities of SIC!, allowed for detailed insights while keeping the big picture in focus.

Main pillars of SIC! ©TU Wien

[1] https://sic.tuwien.ac.at/

My research within SIC! revolved around the pillar optimal design optimization of energy supply with emphasis on the integration of storages and renewable energy sources, dealing mainly with the following topics:

- Extension of computer aided design optimization approaches, especially mixed integer linear programming (MILP) heat exchange network synthesis (HENS), for the integration of heat pumps and storages for cost and emission reduction.
- Development of a framework for automated data-driven model adaption to enable more accurate predictions of real component behaviour for all kind of optimization procedures.

The importance of the topics of SIC! gets underlined by the invitation of the International Energy Agency (IEA) that allowed SIC! to take part in the IAE IETS Annex XVIII. Within this international research project titled "Digitalization, Artificial Intelligence and Related Technologies for Energy Efficiency and GHG Emissions Reduction on Industry", the SIC consortium provided the White Paper "Digitalization in Industry - An Austrian Perspective", which combines the accumulated experience of the different PhD theses.

Contents

List of Figures

Nomenclature

Acronyms

CO_2	Carbon Dioxide
EII	Energy Intensive Industries
GHG	Greenhouse Gas
HI	Heat integration
ICT	Information and Communication Technology
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
MER	Maximum Energy Recovery
MILP	Mixed-Integer-Linear-Programming
MINLP	Mixed-Integer-Nonlinear-Programming
PI	Process Integration
SIC	Smart Industrial Concept
1T ST	One Tank Storage
2T ST	Two Tank Storage
COP	Coefficient of Performance
HEN	Heat Exchange Network
HENS	Heat Exchange Network Synthesis
HEX	Heat Exchanger
HP	Heat Pump

ICT Information and Communication Technologies

OPC UA Open Platform Communications Unified Architecture

PBR Packed Bed Regenerator

PDM Pinch Design Method

ST Storage

TAC Total Annual Cost

Subscripts

cu cold utility

hp heat pump

hu hot utility

hu step fixed costs

$st1T$ one tank stoarage

$st2T$ two tank stoarage

Symbols

β cost exponent for heat exchanger area

ΔT temperature lift of heat pump

Γ big-M coefficient

τ_{ap} annual operation time of period

A heat exchanger area

a linearization coefficients COP

b linearization coefficients P_{el}

F heat flow capacity of process streams

$LMTD$ log. mean temperature difference

N number of binary variables

P_{el}	electrical power demand
Q	heat flow
T	temperature
U	heat transfer coefficient
Z	binary variable for existence of installation
c	cost coefficient
CPS	number of cold process streams
Cs	cold stream
Cu	cold utility
HPS	number of hot process streams
Hs	hot stream
Hu	hot utility
i	index for hot streams
j	index for cold streams
k	index for stages
NOK	number of stages
NOP	number of time period
p	index for time periods
x	index for approximation redions

Superscripts

in	input
out	output

Research summary

The following sections of this chapter intend to shed light on the environment in which the research of this thesis leading to the publications was conducted. Section 1 shows the motivation of this thesis by giving an overview of the current state of GHG emissions and their possible reduction towards climate neutrality with a focus on the share of the industry. Following the introduction, Section 2 provides a general explanation and discussion of the topics addressed in this thesis to place the resulting publications in the context of the existing literature. In Section 3, the objectives of this work and their associated research questions are presented. Following, Section 4 provides an outline and short motivations for each of the publications, as well as the correlations between them. In the last section, Section 5, the results of the research are recapitulated, the research questions are answered, and an outlook for future work is given.

1 Introduction

The modern society stands on the brink of essential decisions that can drastically shape the future living conditions.

The increasing number of natural disasters such as recent floods, droughts, or forest fires that not only happen on the other side of the world, but also right here on our doorstep, should make it impossible for anybody to look away or deny the existence of climate change. Recent publications like the report by the Intergovernmental Panel on Climate Change clearly state that immediate action is required to be able to limit such dramatic effects of man made climate change. Without radical reduction of overall GHG emissions, especially CO_2, the global temperature increase will very likely exceed the 2 °C target initially set by the Paris Agreement (IPCC 2021). This does not mean that nothing has been done about this topic in the past. While the final energy consumption of the EU in 2019 is almost on the same level as back in 1990, the total GHG emissions decreased by almost 25 % to about 3.7 billion tonnes of CO_2 as visible in Figs. 1 and 2. This results from the shift of the energy sources from solid fuels and petroleum products towards biofuels, renewables and electricity. Nevertheless, the direct correlation of final energy consumption and GHG emissions is clearly visible, especially for the transport sector, which is the only GHG source of the EU that increased emissions (by almost 32 %) between 1990 and 2019, and the industrial sector, that reduced its GHG emissions by around 36 % (Eurostat 2021).

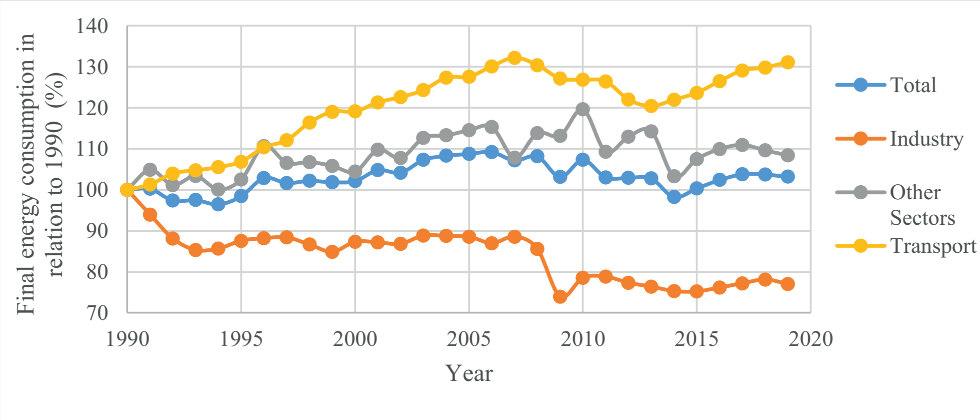

Figure 1: *Final energy consumption of the EU per sector compared to 1990. Adapted from Eurostat 2021*

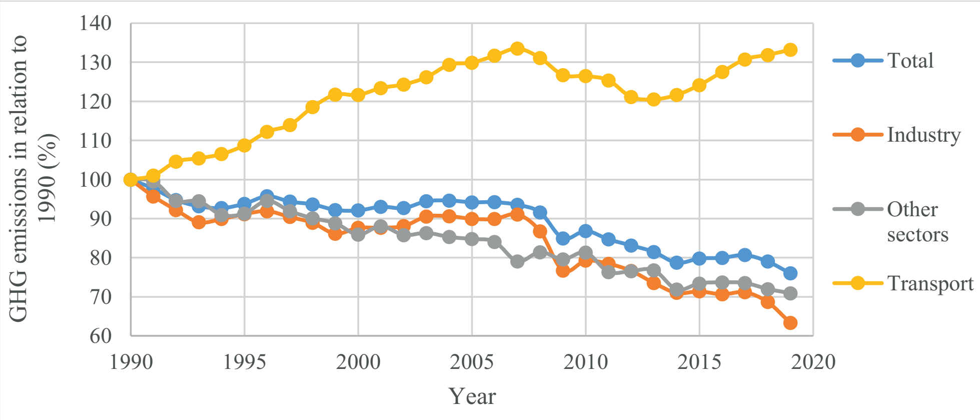

Figure 2: *GHG emissions of the EU per sector compared to 1990. Adapted from Eurostat 2021*

The industrial sector accounts for 25 % of the final energy consumption of the European Union and is thus one of the key areas that have to be dealt with on the way to the target of carbon neutrality (Eurostat 2020). Considering that the average annual reduction of GHG emissions for industry of 1.2 % since 1990 would continue, it would take another 50 years to reach a state of zero emissions.

The energy intensive industries (EII), with its most important branches iron and steel, refineries, cement, petrochemicals, fertilizer, lime and plaster, pulp and paper, aluminum, inorganic chemicals, and hollow glass, are responsible for 85 % of the industries GHG emission within the EU. To reach the EU target of climate neutrality by mid-century given by the European green deal (Eurpean Comission 2019), especially these EII have to deal with drastic changes. According to Bruyn et al. 2020, some of the most promising adaptions to reach this target are:

- Reduction of primary energy demand through efficiency improvements or development of new production methods: Independent on the energy source, if less energy is needed, less GHG emissions, either from the combustion or consumption of fossil fuels or indirect emissions from the generation of electricity, are produced.
- Usage of renewable energy sources or carbon-neutral energy carriers: The direct usage of electricity from carbon neutral sources or the indirect usage with the help of carbon neutral energy carriers like hydrogen or biofuels produced with it have enormous potential for reducing GHG emissions in all sectors.
- Utilization of carbon capture and storage technologies: Especially for processes that produce CO_2 by chemical reactions that are necessary for the process, carbon capture and storage offers a potential solution for climate neutrality.

However, the implementation of these measures faces major obstacles that are mostly of financial nature. Improvement of energy efficiency or development of new production methods is always coupled with considerable cost. Investments for energy efficient or novel alternatives are often more capital-intensive compared to their traditional counterparts. While the usage of electricity from renewable energy sources has considerable potential, the fluctuating nature of PV and wind creates significant challenges for the electrical supply network, which also result in investment costs for energy storage and smart grid management. Carbon capture and storage, the production of hydrogen, and the production of biofuel with captured CO_2 are all technologies that are coupled with massive investment costs for infrastructure and are dependent on the availability of low-cost renewable energy. These short term costs are often used as economic arguments against GHG emission reducing technologies. Because to reduce the risk of investments, often payback times have to be shorter than three to five years to be acceptable options. But this type of thinking is not compatible with the long term task of reducing climate change. Studies on the economic damage of climate change like from Hsiang et al. 2017 estimate that an increase of the global mean temperature by 1 °C results in damages of about 1.2 % of the global gross domestic product, consisting of market and nonmarket damages in sectors like agriculture, health, and natural disasters.

Overall, the question of whether carbon neutrality is reachable is not technological but a social one. There are plenty of technologies, either already available or under development, that have the potential to reduce GHG emissions, improve energy efficiency, and make it possible to reach carbon neutrality. Furthermore, as presented in this thesis, extensive research is conducted worldwide to improve or develop such technologies. The implementation of them is solely dependent on the question if society is able to work together towards this goal. Reaching from consumers' behavior, which needs to shift from buying the cheapest option to buying sustainable options, over governmental decisions like carbon taxes or subsidies for green investments, to company policies that revolve around sustainability and development, everyone has to participate in changing the future.

2 Context

On the way towards a sustainable future, the energy optimization of the industry plays an important role. Numerous technologies that allow reducing the carbon footprint of processes are already available or currently in development for employment in the near future. One of the main obstacles for the introduction of such GHG reducing technologies is that such investments always have to compete with traditional investments like the expansion of production capacities, which often offer a better return over short time horizons (Bruyn et al. 2020). To lower these barriers, developments in the sector of mathematical optimization offer the potential to help with the optimal integration of emission-reducing technologies and thus increase their economic viability. Especially the integration of volatile renewable energy sources and the recovery of waste heat show high potential but also pose major challenges for optimization procedures. Because of this, the integration of heat pumps (HP) and storage (ST) solutions into heat supply systems gained interest over the last years in the field of design optimization.

However, to reduce the energy consumption of processes or increase their efficiency and thus lower their GHG emissions, it is necessary to generate and utilize detailed knowledge about them. The results of every optimization procedure, independent of the type of optimization, are only as accurate as allowed by their input parameters and underlying models. Especially for the refurbishment of existing plants and operational optimization, the current physical properties of assets are essential information needed to apply optimization procedures effectively. Over the last years, the acquisition of process data rapidly gained popularity in what is often referred to as the fourth industrial revolution, which aims to use the rapidly increasing amounts of measurement data for improvement of cost and energy efficiency (Bonilla et al. 2018). Analyzing accumulated process data with the now available computational capabilities offers possibilities for process insight on an unprecedented scale.

Focusing on the two topics of computer-aided design optimization of extended heat exchange networks with HP and ST integration and methods for the automated data-driven model adaption, this thesis aims to improve the design optimization capabilities of industrial processes. The approaches developed during this work shall contribute to the variety of tools needed for the industry's transition towards a GHG emission-free future.

This chapter provides a brief overview of the research areas in this thesis to set the introduced developments in proper context.

2.1 Design Optimization

Optimization is often understood as the improvement of the current state towards a defined target like reduced energy demand or cost reduction. This weakened definition can be seen as a common misunderstanding. The strict definition of optimization is the search for the best possible solution in a defined solution space, often under the consideration of limitations or boundary conditions (Floudas et al. 2009).

The continuously rising complexity of industrial processes made it necessary to develop methods and procedures that help to understand, plan, and operate them. A common distinction is made between the two main application areas of mathematical optimization - design and operational optimization:

Operational optimization shall answer how an existing or already designed process is operated in the best way concerning a defined target.

Design optimization has the target to either find the optimal design in the sense of where specific components in which size have to be placed for new processes or how to replace or integrate components in existing processes for a given operational scenario.

These definitions already show one of the main difficulties in optimizing processes: If the design is optimized after the operational scenario is set, the operational plan is maybe no longer optimal for the resulting design and vice versa. This is caused by the fact that every optimization is only valid within the boundaries of the assumed simplifications and constraints. For the design optimization, the primary constraint is that the operational plan is set beforehand and thus an input parameter. While current developments aim towards combined optimization that allows simultaneous optimization of design and operation, the main focus in this work lies in the design optimization of energy intensive industrial processes. The here developed methods in the area of heat exchange network synthesis with the integration of renewable energies and energy storage intend to strengthen the base of knowledge for future research.

Heat Exchange Network Synthesis

The field of heat exchange network synthesis (HENS) is a part of the broad topic of process system engineering. Since the first introduction of the heat exchange network (HEN) design problem almost 80 years ago by Broeck 1944 and the first formal definition of HENS by Masso et al. 1969, the topic has undergone increasingly extensive research because of its importance for industrial processes (Furman et al. 2002).

Basic HENS after the definition of Masso et al. 1969 is described as follows: A given process is reduced to the process streams that are necessary for its operation, which are hot process streams (Hs) that have to be cooled from their inlet temperatures (T^{in}) to their outlet temperatures (T^{out}), and cold process streams (Cs) that have to be heated from their inlet temperatures (T^{in}) to their outlet temperatures (T^{out}). The flow rates and heat capacities of all process streams have to be known. The available utilities with their temperatures and specific costs and the cost data for heat exchangers (HEX) have to be given. The target of HENS is to find the network of HEX with the minimum total annual costs (TAC) considering the given physical boundaries.

The core idea originates from heat integration (HI), which can be seen as a predecessor to process integration (PI) since heat was the main energy source for early industrial processes. HI is still an important part of PI and stands for two different things. While in the physical world, HI is the actual arrangement of components, equipment, or sections of the process, it also is the name of a specialized area of process synthesis. The latter deals with procedures and methods that have the target to improve the energy efficiency of industrial applications by matching excess heating or cooling demands to reduce external energy demand (Gundersen 2013).

A milestone of HENS was the development of the heat recovery pinch concept in the late 1970s, which was discovered independently by different researchers (Hohmann E.C. 1971, Huang F. et al. 1976, Linnhoff et al. 1978, Umeda T. et al. 1978). As one of the most commonly known HENS concepts, the pinch concept led to a change from the traditional design practice of following the learning curve. Instead of choosing the best result of a number of case studies that depended on the experiences of the individual designer, it made it possible to set performance targets previous to the design phase.

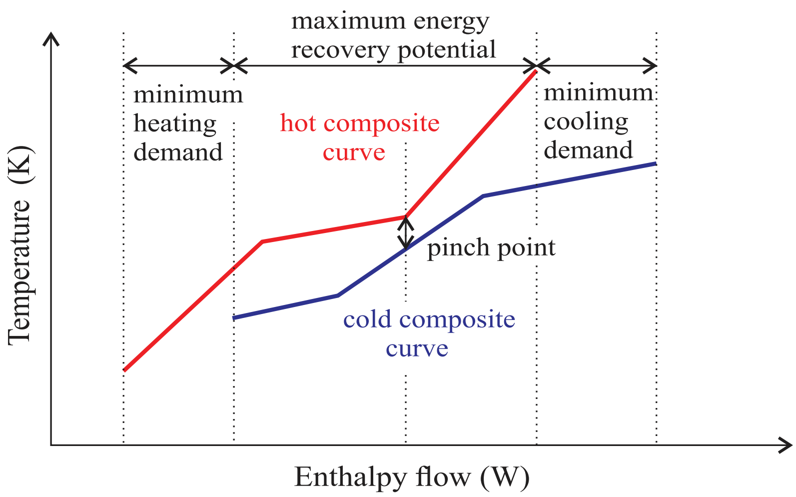

Figure 3: *Schematic temperature-enthalpy diagram with composite curves and pinch point*

The basic principle of the heat recovery pinch concept is the graphical representation of a process's heating and cooling demand to gain information. To achieve this, the cumulative heating and cooling demands of a process are drawn in a temperature-enthalpy diagram as exemplarily depicted in Fig. 3. These two separate curves are commonly called "composite curves". Because heat transfer can only occur from higher to lower temperatures, and heat transfer is dependent on the driving temperature difference, the smallest vertical distance between the demand curves can be seen as the bottleneck of the process. The point of its occurrence is called the pinch point or heat recovery pinch. The heat recovery pinch splits the process into two regions above and below the pinch. Below the pinch, there is a heat surplus, while above the pinch, heating is required. From the diagram, the minimum heating and cooling demands, the maximum energy recovery (MER), and the process pinch can be obtained as shown in Fig. 3. One of the most important insights provided by this graphical representation is that any heat transfer from above the pinch to below the pinch results in higher heating demand and cooling demand and should thus be avoided for the target of a MER HEN. From this base, different step-wise empirical design procedures like the pinch design method (PDM) for the development of HEN with the lowest possible external energy demand were developed (Linnhoff et al. 1983).

These methods aim to achieve cost optimality while only the operational costs for utility demand are considered. Thus, these methods can guarantee to result in HEN with minimum external energy demand. Other costs like step fixed costs for installations or costs for variable HEX sizes can only be considered in additional steps afterward, where parts of the solution of the previous step are the parameters for the following.

Because the different targets are not considered simultaneously, the trade-offs between the targets can not be accounted for. Decisions in earlier steps can have negative impacts on the results of later steps (Escobar et al. 2013).

To overcome this disadvantage approaches like the superstructure for heat integration by Yee et al. 1990b were proposed that allow consideration of different design targets within one optimization step without decomposition of the problem. In Yee et al. 1990a, the approach is formulated in a mixed integer nonlinear programming (MINLP) model where unit costs, area costs, and utility costs are all considered simultaneously to find a network with the lowest possible TAC.

Among other factors, these developments were enabled by the rapidly increasing availability of computing power that is necessary to calculate the solutions in reasonable times. For further understandment, it has to be said that HENS was proven to be a NP-hard problem by Furman et al. 2001. NP-hard means that a problem is especially hard to solve and that it is impossible to create an exact solution algorithm, solving within polynomial time. This is caused by the combinatorial nature of the problem.

So overall, there are two opposing directions of solution approaches for HENS: On the one side, the decomposition of HENS into different parts treated sequentially, like maximum energy recovery, a minimum number of matches, and minimum costs, reduces overall complexity and accuracy. On the other side, the simultaneous consideration of all assumed targets allows considering the trade-offs between them, but with the cost of higher complexity.

These described basic HENS developments are still limited to the integration of HEX between streams and HEX between streams and utilities. The need to improve efficiency to stay competitive and changes in the environmental policies and legislatures led to increasing interest in waste heat recovery, flexibilities in the production, and integration of renewable energy sources. This leads to the need to optimize HEN that consider more than one operational state and additional installations like HP or thermal energy storages, which is even more complex. To be able to deal with this problem, different approaches have been improved or developed over the last years by different researchers.

Becker et al. 2012 proposed a multi-objective optimization algorithm on the base of the heat cascade formulation for HENS that solves the thermodynamic calculations and the energy integration as subproblems in a serial manner. Miah et al. 2015 approached the problem by developing and methodological heat integration framework that divides the problem into different zones that are solved serial to find the optimal location for HP. Stampfli et al. 2019 utilized insight based and nonlinear programming techniques for the sequential integration of ST and HP into multi-period processes with the target of optimal HP operation. The common denominator of all these approaches is that nonlinear optimization in combination with a problem decomposition has been used to solve the problem in multiple steps, leaving a research gap for simultaneous integration approaches for the integration of HP and ST into multi-period HENS.

This chapter is not intended to be an all-encompassing explanation and comparison of the development of different HENS methodologies, since this task has already been fulfilled by various publications like the extensive reviews by Furman et al. 2002 or Escobar et al. 2013. It should be seen as an appetizer for the following description of the development of such methods on the case of a superstructure formulation for HENS, which was extended in the course of this thesis.

2.2 Superstructure Formulation

As already analyzed and stated by Ciric et al. 1991, a simultaneous optimization is superior to sequential targeting optimization procedures because of the uncertainty that is added to the solution in every decomposition step. One popular and widely used approach for HENS without decomposition is the superstructure formulation introduced by Yee et al. (Yee et al. 1990a, Yee et al. 1990b) as graphically represented in Fig. 4.

The starting point of the formulation is the initial definition of HENS as given by Masso et al. 1969. A number of Hs_i (i = 1,...,HPS) that need to be cooled and a number of Cs_j (j = 1,...,CPS) that need to be heated are given with their corresponding inlet temperatures, outlet temperatures, heat capacities and heat transfer coefficients. Hot utilities (Hu_i) and cold utilities (Cu_j) with their temperatures, heat flow capacities, and heat transfer coefficients are also assumed to be known. To make it possible that HEX can be positioned on multiple temperature intervals of one stream, the concept of stages is introduced. Within every stage k (k = 1,...,NOK), HEX between every Hs_i and every

Cs_j can occur. It is assumed, that if more than one HEX is chosen for a stream in one stage, the stream gets split in the beginning of the stage and mixed at the end of the stage. For reasons of simplification, isothermal mixing of the streams is assumed.

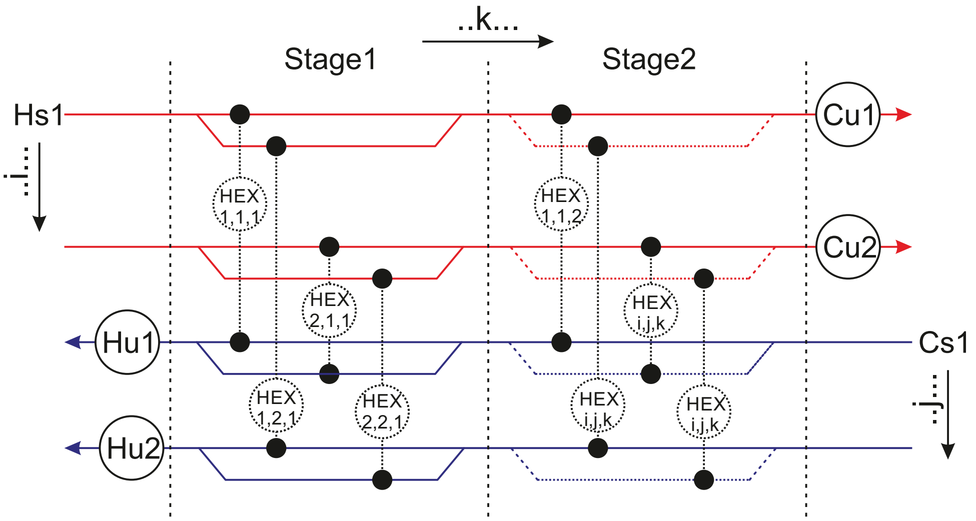

Figure 4: *Graphical representation of the superstrucutre proposed by Yee et al. 1990b*

Cost function and targets To be able to consider the trade-off between energy recovery and thus utility demand reduction, and costs for the installation of heat exchangers, three different kinds of costs are considered with the help of their corresponding cost coefficients in the cost function from Yee et al. 1990b, as simplified given in Equ. 1.:

- **Cost coefficient for step fixed investment costs c_f:** Accumulated investment costs for every installed HEX. These costs are a combination of engineering costs, piping costs, transportation costs, and other fixed costs that can be linked to the additional installation of a single HEX unit.
- **Cost coefficient for variable investment costs c:** Costs that are dependent on the HEX area (A), which are linked to the size dependent on production costs and material costs.
- **Cost coefficients for utilities c_{cu} and c_{hu} :** Costs per unit of external Hu or Cu that is needed to fulfill the physical demands of the process if it is not possible or profitable to meet them with heat recovery.

$$
\begin{aligned}
&\min TAC = \\
&\underbrace{\sum_i \sum_j \sum_k c_f Z_{ijk} + \sum_i c_f Z_{cui} + \sum_j c_f Z_{huj}}_{\text{step fixed investment costs}} \\
&\underbrace{+ \sum_i \sum_j \sum_k c A_{ijk}^{\beta} + \sum_i c A_{cui}^{\beta} + \sum_j c A_{huj}^{\beta}}_{\text{variable investment costs}} \\
&\underbrace{+ \sum_i c_{cu} Q_{cui} + \sum_j c_{hu} Q_{huj}}_{\text{energy costs}} \\
&\forall\, k = 1, ..., NOK, i = 1, ..., HPS,\ j = 1, ..., CPS
\end{aligned}
\tag{1}
$$

In the term of the step fixed investment costs all possible matches between every Hs$_i$ and every Cs$_j$ in every stage k are simultaneously considered with the help of the binary variables Z_{ijk} that indicate if a HEX exists in a given position or not. Also right before the outlet of every stream a possible utility is considered with the binary variables Z_{cui} and Z_{huj}. Simultaneous to these binary variables, the temperatures of the streams after every stage are considered as optimization variables of the type integer. These temperatures are used to calculate the heat flows

$$Q_{i,j,k} = F_i(T_{i,k} - T_{i,k+1}) = F_j(T_{j,k} - T_{j,k+1}) \tag{2}$$

of the HEX between the streams and the utility heat flows Q_{cui} and Q_{huj} analogously, as well as the heat exchanger areas.

$$A_{i,j,k} = Q_{i,j,k}/(U_{i,j,k} LMTD_{i,j,}(T_i, T_j)) \tag{3}$$

While the heat flows are linear functions of the variable stream temperatures, one can see that even when the heat transfer coefficients U are assumed constant over the temperature, Equ. 3 and thus the cost function is nonlinear and non-convex. The constraints of this optimization problem, like the energy balances of the streams or the constraints that account for no physical boundaries to be violated, are linear and thus not discussed here.

Development of the formulation While this mixed integer nonlinear programming (MINLP) approach was found to deliver satisfying results in terms of the minimization of the annual costs, the non-linearity comes with several drawbacks. Nonlinear programming procedures need a feasible initial solution to start the optimization, which is often hard to find even for small problems (Escobar et al. 2013). Also the computational effort is higher compared to linear procedures.

As mentioned before, the solution of HENS problems is difficult to obtain, which is caused by its initial definition. For every possible position for the placement of a HEX, two questions have to be answered for a possible solution. The first question is whether or not a HEX exists at a position, which can only be answered with yes or no, and thus resulting in a binary variable. If a HEX exists at a certain position, the second question is the optimal size the HEX, resulting in an integer variable.

For the formulation by Yee et al. 1990b, the number of binary variables can be calculated with Equ. 4, and the number of integer variables can be calculated with Equ. 5. For a given problem with two Hs (HPS = 2), two Cs (CPS = 2), and two stages (NOK = 2) as displayed in Fig. 4, this results in a total of 12 binary variables and 8 integer variables that have to be optimized. For a problem with only one additional Hs and one additional Cs, these numbers increase to 24 binary variables and 12 integer variables which shows that the complexity increases not linear but exponential with the size of the problem.

$$\text{number of binary variables} = HPS\, CPS\, NOK + CPS + HPS \tag{4}$$

$$\text{number of integer variables} = (HPS + CPS)\, NOK \tag{5}$$

As defined at the beginning of Section 2.1, optimization is the search for the best possible solution within a defined solutions space. Because an analytical solution is rarely possible, numerical mathematical algorithms that consist of rows of mathematical operations are used for this purpose. The increased mathematical complexity of problems consisting of integer variables and binary variables results from the fact that each possible combination of binary variables leads to a different solution space that has to be searched for an optimal solution. For N binary variables, 2^{N} possible combinations and thus solution spaces exist. For the example above, this results in 4096 combinations for 12, and 16.78 million combinations for 24 binary variables. This shows that a reduction of the computational complexity for the search of each possible optimal solution in each of the solution spaces adds up to a considerable reduction of the overall computational effort.

For this purpose, Beck et al. 2018 presented an approach to linearize the superstructure formulation from Yee et al. 1990a. By replacing all nonlinear terms of the cost function with convex linear approximations, a MILP approximation of the original MINLP superstructure was created.

The main advantage of MILP formulations compared to MINLP formulations is that solving linear problems is mathematically easier and requires less mathematical operations than solving nonlinear problems. The computational times are drastically lower, which is very important considering the exponential increase of complexity of the problem with size. Also, the optimization always results in a global optimum without the need for a feasible starting solution. The drawback is that any linearization leads to certain deviations of the results from the actual nonlinear behavior.

While a linearization of the formulation aims to improve and simplify the initial HENS problem, other developments aim to enhance the formulation of HENS towards the integration of additional installations.

For example, Beck et al. 2019 proposed a sequential MINLP approach for the integration of thermal energy storages into HENS. In the first step, the storage size gets optimized, while in the second step, a multi-period extension from Zhang et al. 2006 of the initial MINLP formulation by Yee et al. 1990a gets extended and used to optimize the HEN. This extension to multiple time periods and the possibility of additional HEX from the streams to the storages increase the problem's complexity even further.

Extension Within this Thesis These previous approaches inspired the further development of the superstructure in the course of this thesis. To increase heat recovery capabilities and allow the possibility of integrating renewable energy sources while keeping the mathematical effort as low as possible, we developed an approach for the simultaneous integration of HP and different thermal energy storages into a multi-period MILP HENS superstructure. As can be seen in Fig. 5, the possible number of connections for every stream in every stage in every time period p (p = 1,...,NOP) are increased drastically. Additional to the HEX between every Hs and every Cs, the streams can exchange heat with the different ST and a HP on each possible location.

For calculating the number of variables for this extended problem with Equs. 6 and 7, again, a problem with two Hs (HPS = 2), two Cs (CPS = 2), and two stages (NOK = 2) is assumed. Additionally, now two time periods (NOP = 2), two ST, and possible HP on every location are given. The resulting 72 binary variables and 20 integer variables that have to be optimized result in 4722 trillion ($4.722 * 10^{22}$) possible solution spaces and therefore in an extremely increased mathematical effort.

$$\text{number of binary variables} = (HPS\ CPS\ NOK + (CPS + HPS)(1 + 3NOK))NOP \tag{6}$$

$$\text{number of integer variables} = (HPS + CPS)\ NOK\ NOP + 2NOP \tag{7}$$

This increased complexity can also be seen in the cost function of the extended formulation given in Equ. 8, which is described in detail in Publication **Paper 2**. The additional terms considered in the cost function are step fixed and variable investment costs for ST,

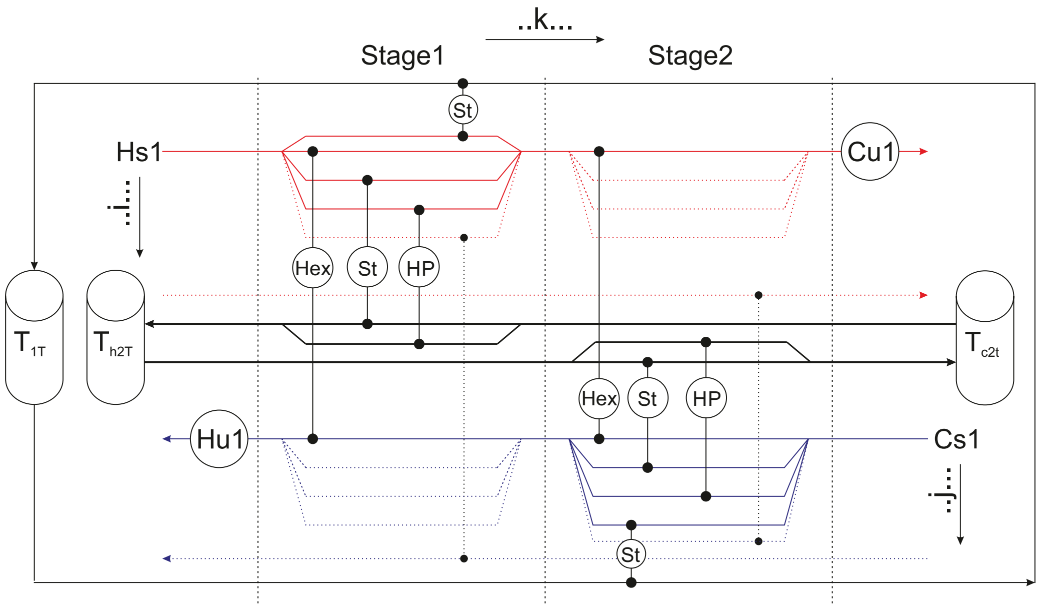

Figure 5: *"Superstructure with possible Stream-Stream Hex (HEX), Stream-Storage Hex (ST) and Heat Pumps (HP)" from Prendl et al. 2021c/CC BY 4.0*

HEX between streams and ST, HP, and energy costs for the electrical energy needed to power the HP.

$$
\begin{aligned}
&\min TAC = \sum_i \sum_j \sum_k c_f Z_{ijk} + \sum_i c_f Z_{cui} \\
&\underbrace{\begin{aligned}
&+ \sum_j c_f Z_{huj} + c_{fst\ 2T} Z_{st\ 2T} + c_{fst\ 1T} Z_{st\ 1T} \\
&+ \sum_i \sum_j \sum_k c_f Z_{2T\ ijk} + \sum_i \sum_j \sum_k c_f Z_{1T\ ijk} \\
&+ \sum_i \sum_j \sum_k c_{hp} Z_{hp\ ijk}
\end{aligned}}_{\text{step fixed investment costs}} \\
&\underbrace{\begin{aligned}
&+ \sum_i \sum_j \sum_k c A^{\beta}_{ijk} + \sum_i c A^{\beta}_{cui} \\
&+ \sum_j c A^{\beta}_{huj} + c_{vst\ 2T} S_{st\ 2T} + \sum_i \sum_j \sum_k c A^{\beta}_{2T\ ijk} \\
&+ \sum_i \sum_j \sum_k c A^{\beta}_{1T\ ijk} + \sum_i \sum_j \sum_k c A^{\beta}_{hp\ ijk}
\end{aligned}}_{\text{variable investment costs}} \\
&\underbrace{\begin{aligned}
&+ \sum_i \sum_p c_{cu} \dot{Q}_{cuip} \tau_{ap} + \sum_j \sum_p c_{hu} \dot{Q}_{hujp} \tau_{ap} \\
&+ \sum_i \sum_j \sum_k \sum_p c_{Pel} Pel_{ijkp} \tau_{ap}
\end{aligned}}_{\text{energy costs}} \\
&\forall\ p = 1, ..., NOP,\ k = 1, ..., NOK, \\
&i = 1, ..., HPS,\ j = 1, ..., CPS
\end{aligned}
\tag{8}
$$

A combination of different measures has been applied within this work to reduce the computational effort drastically. To overcome the before mentioned drawbacks of nonlinear formulations, all nonlinear parts of the cost function got linearized with convex linear approximations inspired by the approach of Beck et al. 2018. Exemplary, the novel linear integration of the HP carried out in multiple steps is described in the following. First, the nonlinear characteristic curve of the relationship between the COP and the temperature lift of the HP was approximated as shown in Fig. 6 and Equ. 9, where a_1 and a_2 are the linearization coefficients.

$$
COP(\Delta T) \approx a_1 + a_2 \Delta T \tag{9}
$$

Because not the COP but the electrical power consumption (P_{el}) of the HP is needed for the integration of the energy costs into the costs function, the next step was to

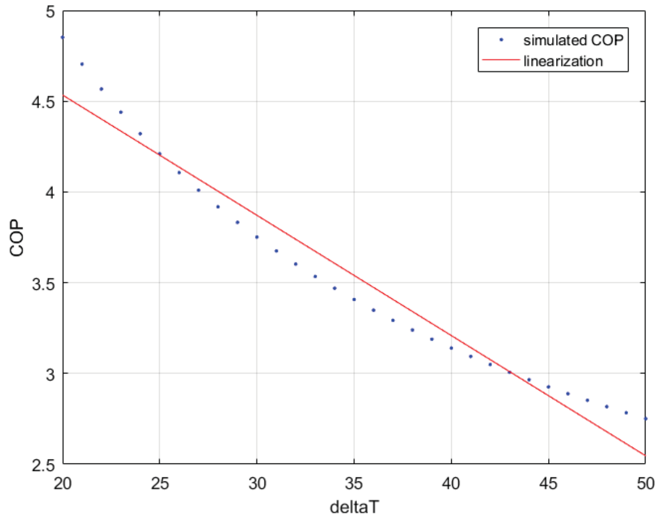

Figure 6: *"Linearized COP over ΔT" from Prendl et al. 2021c/CC BY 4.0*

linearize the nonlinear and nonconvex correlation of the heat flow ($\dot{Q}_{hp}$) and the COP that expresses P_{el} with a convex piecewise linear approximation $CP_{el\,x}$ as given in Eq. 10. For this purpose, the solution space for P_{el} was split into three regions along the ΔT axis with the index x.

$$P_{el} = \dot{Q}_{hp}/COP = P_{el}(\dot{Q}_{hp}, \Delta T) \approx b_{1x} + b_{2x}\dot{Q}_{hp} + b_{3x}\Delta T = CP_{el\,x} \tag{10}$$

Furthermore, a lower boundary for the COP got implemented as a tightening measure. In Fig. 7, where the nonlinear solution space of P_{el} is given with its piecewise linear approximation in grey, the lower boundary for the COP is displayed in red. The area above the red surface gets discarded to reduce possible potentially uneconomical solutions because of their low COP, reducing the computational complexity and improving the accuracy of the approximation within the remaining feasible solution space.

For the linear integration of the approximation into the superstructure formulation, the so-called big-M formulation for the activation or deactivation of constraints was used, as shown in Equ. 11, and described as following: The electrical power consumption $P_{el\,ijkp}$ of the HP on a certain position i, j, k, p of the superstructure is a positive term of the cost function, and thus the solver aims to minimize it. If a HP exists at this position, the binary variable $Z_{hp\,ijkp}$ equals 1, and the approximation $CP_{el\,ijkp}$ is the lower boundary for $P_{el\,ijkp}$. If no HP exists, the binary variable $Z_{hp\,ijkp}$ equals 0, the big-M coefficient Γ_{Pel}, which is a sufficiently large number bigger than the possible maximum of $CP_{el\,ijkp}$, leads to a right side of Equ. 11a smaller than zero, which deactivates the constraint and makes Equ. 11b the active constraint. This makes it possible to consider HP on every possible location in the cost function without the need for nonlinear correlations. The

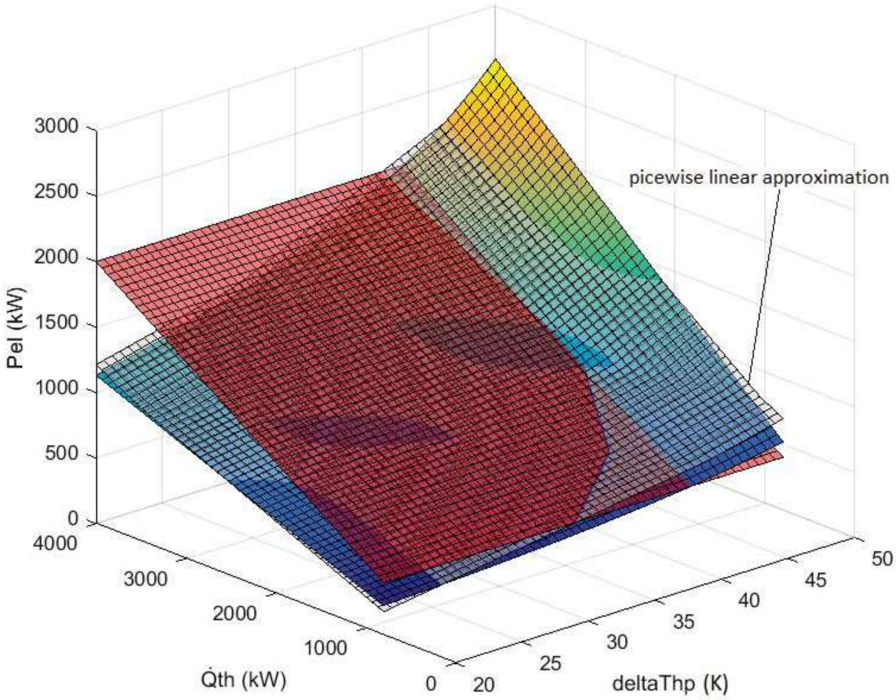

Figure 7: *"Reduced solution space for P_{el}" from Prendl et al. 2021c/CC BY 4.0*

full mathematical formulation with the linearization steps for the remaining parts of the cost function is given in full detail in **Paper 2**.

$$P_{el\,ijkp} \geq CP_{el\,ijkp} - \Gamma_{Pel}(1 - Z_{hp\,ijkp}) \tag{11a}$$

$$P_{el\,ijkp} \geq 0 \tag{11b}$$

As already mentioned in Section 1, the reduction of external energy demand and the integration of renewable energy sources is crucial for the target of a carbon neutral future. Novel optimization procedures like the introduced MILP HENS approach for the simultaneous integration of HP and different ST can improve the process optimization of existing and future industrial applications for this cause. But independent of the type of optimization carried out, the results of the procedures are strongly dependent on the accuracy of the used models and the assumed input parameters. Thus before optimization, suitable component models and process data are needed.

2.3 Model Training Framework

The development of the linear optimization approach in the first part of this thesis inevitably led to the consideration of typical modeling peculiarities that are bound to the nature of mathematical modeling. A mathematical model is a simplified description of a real-world phenomenon for a given target application. Every assumption or simplification made during the model building process can essentially change the model's behavior and thus alter it from reality (Hritonenko et al. 2003). Therefore, it is always crucial that the model used meets the requirements of the application. For example, the HP model in this thesis was linearized to reduce its mathematical complexity to be able to solve the complex problem of HENS with HP and ST integration on the cost of reduced accuracy compared to the real, nonlinear behavior. The solution space had to be tightened to keep the accuracy of the simplified model in an acceptable range. But all such measures only make sense as long as the original model matches the process sufficiently well. Especially the modeling of nonlinear relations of thermal systems pose serious challenges that can get even more complicated when physical properties of components change during operation due to wear or fouling mechanisms. While processes such as design optimization only require a snapshot of the system's current state, process optimization or predictive models need to be continuously adjusted to utilize their full potential for energy and cost savings. To enable both, we developed a framework for the automated data-driven model adaption for industrial energy systems. In the following paragraphs, I will give a short overview of the most important topics necessary for developing the framework.

Condition Monitoring and Digitalization The importance of condition monitoring and process analtytics continuously gained significance over the last decades due to the increase of process complexity and economic pressure. Condition monitoring is generally known as recording the current state of a physical entity using measurement data (Tejado Balsera 2018; Chaulya et al. 2016), and thus can be seen as a base for a lot of measures concerning the operation improvement of processes. Initially, one of the main applications was condition based maintenance, in which maintenance action is taken after a certain parameters exceed given boundaries to prevent failure. But in the last years, the increasing digitalization of the industry has taken place in what is often referred to as the fourth industrial revolution. The development towards the so-called Industry4.0, which refers to the intelligent networking of machines and processes, is driven by the constant evolution of Information and Communication Technologies (ICT) (Parida et al. 2019) and offers enormous potential for increasing the economic sustainability of the industry while also reducing energy consumption (Branca et al. 2020; Kiel et al. 2017; Beier et al. 2017). This potential can be leveraged for example with preventive or predictive maintenance, which is an important paradigm of Industry4.0 and reliant on real-time data analytics to achieve real-time collaboration between physical and computational processes (G. Cheng et al. 2016). In this maintenance strategy, mathematical models of the process are constantly feed with process data to predict and classify possible system faults.

This allows to initiate maintenance when needed with the necessary preparation and planning to extend the lifespan of machinery to reduce cost and end of life waste (Scarf 2007). Some prominent examples are the fault detection for wind turbines (Azevedo et al. 2016), electric motors (Cakir et al. 2021), or general rotary machines (Hasani et al. 2017; Dinardo et al. 2016; Lim et al. 2013). Also, the analysis of anomalies of electrical equipment (Han et al. 2003) or the wear of cutting tools (Čuš et al. 2011) have been the subject of research in this area.

These approaches rely on parameters that are easy to measure, like vibrations, frequencies, or temperatures. They also have the advantage that many similar or same units are in operation, which allows gathering large amounts of data to develop the models and provides a broad field of possible application. Contrary to this, especially in thermal process engineering, the direct measurement of some important process variables can be complicated, unreliable, or impossible. Also, units are often tailor-made for their application, which makes modeling more complex.

Like predictive maintenance, process optimization also relies on accurate mathematical models to predict the future behavior of components and processes. The difference lies in the target application of the model. While mathematical models for predictive maintenance are built to distinguish whether action is required or not, models for operational optimization are needed to accurately simulate the behavior of components or processes to make proper optimization and thus cost and energy saving possible. Therefore the required accuracy for the later models is much higher and makes the development of approaches like the presented framework necessary.

Communication and Data Acquisition While some concepts of Industry4.0 are theoretically ready for use, the implementation in existing industrial processes still poses major difficulties. Most of these concepts need enormous amounts of measurement data of the right quality for proper function. Thus, one important part of the broad topic of Industry 4.0 is the functioning of cross-system communication. The service life of large industrial systems, especially in the EII, is often very long, which traditionally causes communication problems between system parts that are deployed years apart from each other. Over decades communication standards can change, or the software of different suppliers are not compatible with each other anymore.

Because of that, unified open protocol communication standards that enable interoperability gain popularity and thus shares in the industrial communication market (Drahos et al. 2018). This standard allows transporting measurement values and enriching them with semantic data like sensor accuracy, position, control values, or calibration data necessary for ensuring their quality. Overall, functional bidirectional communication between all parts of a process is an essential foundation necessary for all developments in this field, which is often the first barrier for implementation in industrial processes.

Modeling and Automated Model Adaption There are two main types of mathematical models for physical systems. The one type describes the process with the help of physical relations. Because its behavior is solely dependent on the known physical relation and thus relatively comprehensible, this type is also called white-box model. The second type, so-called data-driven, or black-box model, uses input and output data of a system to find a correlation between them without any additional knowledge about the physical behavior of it (Solomatine et al. 2008). A combination of both types that is called grey-box model, that uses physical relations and process data combined, gained research interest in the last years (Halmschlager et al. 2021).

Simplified, the differences between these modeling approaches can be described with the example of a heat exchanger. The input parameters for the model are the inlet temperatures and heat flow capacities of the two streams, while the output parameters are the outlet temperatures of the two streams that pass through the HEX. For this assumption, Equ. 2 and Equ. 3 are a physical model of the HEX. This model needs the heat exchanger area and heat transfer coefficient of the real physical process to deliver accurate results. On the other hand, a black-box model would be trained with a set of corresponding input and output data to find a correlation without the need for physical parameters.

Suppose it is assumed that both models are fitted correctly and accurately. In that case, they have the capability to simulate the real HEX within their given boundaries, as long as the physical behavior of the real HEX doesn't change. But when the physical behavior of the HEX changes due to mechanisms like fouling or wear during operation, the accuracy of the model output will decrease because the models are only fitted to represent one specific physical state. If the difference between the behavior of the model and the physical process gets too big, optimization results based on the models get unreliable. A way to keep such models up-to-date to the physical state of the process is to continuously adapt or retrain them, which comes with many difficulties, as explained again on the HEX example. To keep the white-box model up-to-date, continuous measurement of the HEX area and the heat transfer coefficient would be necessary, which is not possible through direct measurement. But it is possible to indirectly measure a lumped parameter as a combination of these two by measuring the input and output temperatures and then calculate it with the help of Equs. 2 and 3. The black box model can be retrained with current measurements of input and output data, but with the drawback that further coherent physical behavior of the model is not automatically guaranteed.

But independent of the used model, the main difficulty lies in the automation of such processes. The right data in the right quality must be provided in the necessary composition to utilize a training algorithm properly. This means measurement data must be preprocessed, validated, and analyzed beforehand. If incorrect or the wrong data gets feed into the model training, the resulting model also delivers incorrect results. Literature research showed that the field of real time data analysis with capabilities to autonomously act on results of predictive analytics still has a need for further improvements (Peres et al. 2018) and that no such approach for industrial thermal energy systems has been presented so far. This led to development of the presented framework to enable accurate predictions for the optimal utilization of design and operational optimization.

3 Problem Statement

As already mentioned, the way towards a sustainable future depends on the efficient deployment of existing technologies and the development of novel ones. Based on the initial topic of design optimization and dynamic component modeling as well as the consultation of relevant literature, two main research directions in the area of industrial energy systems that serve these purposes developed:

Design Optimization: Because of the importance of the topic, numerous researches in the last decades dealt with design optimization of industrial energy systems, especially with the topic of HENS with many different approaches. While the focus lay on the maximum energy recovery because external energy demand was seen as the main cost, the development of more complex processes and the change of the economy shifted the focus. The need for flexible production to stay competitive, the changing energy market, and the need to integrate fluctuating renewable energy sources made it necessary to develop methods to deal with the increasingly complex problems. Especially the simultaneous integration of HP and ST into HEN poses a considerable challenge that can tap enormous potentials. This discussion leads to the first objective of this thesis with its corresponding sub-questions Q:

Objective 1: *Simultaneous integration of HP and ST into HENS by the utilization of an appropriate mathematical approach*

> ***Q1.1:*** *Is it possible to counteract the increasing mathematical complexity resulting from the problem extension by keeping the formulation linear?*
>
> ***Q1.2:*** *Are the solutions obtained with the help of the developed method consistent and validatable?*
>
> ***Q1.3:*** *What is the economic and thermodynamic potential of the approach for future industrial applications, especially in EII?*

A widely used HENS superstructure formulation that has been adapted in various ways from different researchers as described in Section 2.2 has been chosen as starting point on the way towards the objective because of its proven versatility and clear structure. Because of the lack of publicly available industry data and the low number of suitable test cases from the literature, a set of example cases based on industrial processes from the EII (Hamel et al. 1979) was created to search for the answers of the formulated questions.

Automated Model Adaption: The outcome of optimization procedure, whether design or operational optimization, is strongly dependent on the parameters and models used during the formulation of the problem. The used models are often based on physical equations or relations, making them robust and reliable, given the necessary physical properties are known. This works fine for conceptualizing new plants on the green field but faces difficulties for operational optimization during operation or the refurbishment of long-running equipment. To use the potentials of increasing flexibility and efficiency of industrial processes, the accurate prediction of the behavior of a component is essential. Especially in thermal energy system engineering, nonlinear relations and changing behavior during operation due to fouling, wear, or other effects make it necessary to use real-time process data to keep the digital model of the physical component up to date. To properly utilize the rapidly increasing amount of measurement data for this purpose, the second objective within this thesis emerged:

Objective 2: *Development of a framework for automated data-driven model adaption*

> ***Q2.1:*** *Which communication, data processing and data analysis methods are suitable as the basis of the framework?*
>
> ***Q2.2:*** *Which degree of automation is reasonable considering the trade-off between efficiency and reliability.*
>
> ***Q2.3:*** *Can the functionality of the developed methodology be proven based on a realistic use-case?*

An existing test rig of a thermal energy storage, which has already been the topic of several studies, serves as a use-case for this problem. Said storage is a sensible thermal energy storage that uses gravel as a storage medium and is perfectly suitable for this task for several reasons:

- Different validated models for simulation and optimization of the test rig are available.
- The storage characteristics are nonlinear and dependent on several factors like the heat transfer coefficients or the physical properties of the storage medium, which can change due to processes like fouling or wear during operation.
- Measured and simulated data sets of different operational modes are available.

4 Research Approach

The research conducted during this thesis revolves around the topic of design optimization of industrial processes with a focus on process integration. The core of the first part of this work is the development of an MILP optimization approach that allows the simultaneous integration of HP and ST into HENS by the expansion and improvement of a superstructure formulation of the basic HENS problem. The different stages of the development processes are presented in **Paper 1** and **Paper 2**, while in **Paper 4** the enormous potential of the approach for improvement of processes of the EII is shown. Because accurate optimization is dependent on models that represent the real state of their physical counterpart, the second part of this thesis deals with the creation of a framework for an automated data-driven model adaption for industrial energy systems as indicated in the lower section of Fig. 8. The exemplary implementation of the framework,

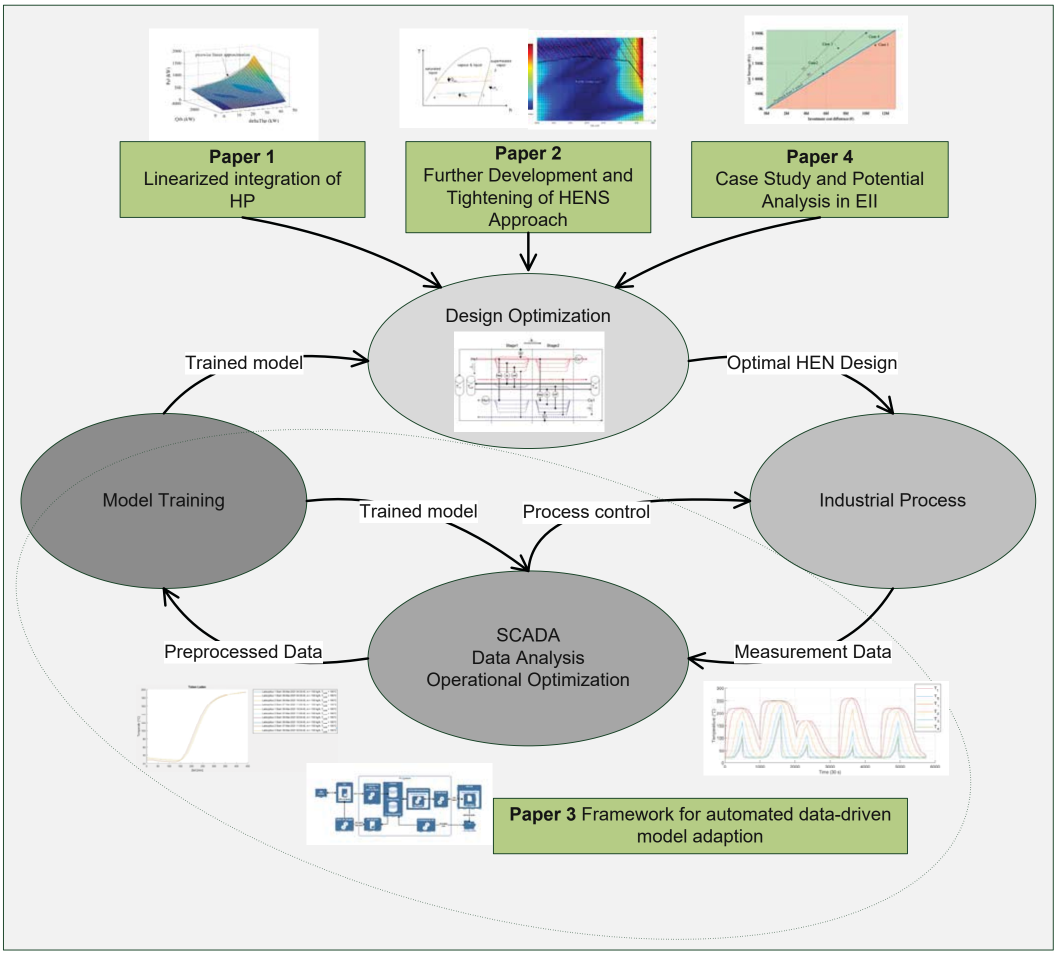

Figure 8: *Overview and placement of the core publications in relation to industrial processes*

which is based on OPC UA and other state of the art communication protocols, is presented in **Paper 3**. Figure 8 places the core publications of this thesis in relation to the industrial process.

4.1 Design Optimization

Originating from the overall target of this thesis to improve the optimal design of energy supply systems defined in the context of SIC! Smart Industrial Concept, the extension of HENS for the integration of renewable energy sources and storage technologies crystallized as the main focus of this work. The topic of HENS is not a new one. Due to its importance for improving efficiency and the continuously increasing complexity of processes and their operation boundaries, extensive research to improve heat recovery has been carried out in the last decades. The thorough consultation of the relevant literature showed that research concerning the integration of HP and ST into HENS for improvement of heat recovery capabilities and the possible integration of renewable energy sources gains interest and still has potential for further improvement. One remaining gap is the simultaneous consideration of HP and ST without decomposition of the problem to allow to consider all possible trade-offs. To fill this gap and overcome difficulties from the occurring nonlinearities, the creation of a linear approach for this purpose has been decided.

The formulation proposed in this thesis is based on a prominent MINLP superstructure formulation of the basic HENS problem that has proven to be adaptable for different purposes. To allow a linear integration into the cost function, the energy consumption of HP in dependency of the thermal energy flow and the temperature lift was approximated by a convex linearization. This concept is first presented in **Paper 1** on a small test case with four streams, one possible ST, and an assumed HP characteristic curve of the COP. The optimization results already delivered two essential insights. Firstly, the integration of HP and ST led to more complex HEN but was able to drastically reduce external energy demand and TAC and thus fulfilled its purpose. The second important finding was, that the resulting HEN as well as the computational times are strongly dependent on the chosen coefficients and physical parameters, which is caused by the combinatorial nature of mixed integer programming.

With the basic functions of the concept proven to work, the further development and refinement of the formulation was the logical next step. Based on the results of the initial concept, we identified several areas for potential improvement towards better applicability. For a linear formulation, the size and temperature of a storage can not be optimized simultaneously, which reduces the capabilities for optimal integration. Thus, we extended the superstructure to allow simultaneous integration of different types of ST. While the 1T ST has a fixed mass and variable temperature, the 2T ST operates at two preset temperature levels, but its size is variable and part of the optimization. The fixed temperatures of the 2T ST are needed for the linear integration of the HP, while the variable initial temperature of the 1T ST allows its integration on the economic optimal temperature interval. To improve the accuracy of the HP approximation while also reducing the computational effort, we introduced tightening measures for the solution space of the COP. To obtain a realistic HP characteristic curve and thus realistic HP behavior, a simulation of a vapor compression HP was deployed. In **Paper 2**, we published the complete mathematical formulation of this tightened multi-period MILP HENS approach together with a test case used to validate its behavior. Compared to a HEN without HP and ST options, the application of the approach reduced the TAC by 61.2 % and the total external energy demand by 58.4 %, respectively. In combination with the resulting HEN structures and ST charging curves, these results underlined the functionality and applicability of the method while also keeping the computational effort reasonably low.

Finally, to show the economic and thermodynamic potential for industrial applications and to comprehensibly test the robustness of the approach, we performed a case study. Because literature research showed that only a very limited number of example cases with suitable temperature ranges for the integration of HP exist for multi-period HENS, a set of four example cases based on representative processes of the EII was created. The cases come from the sectors pulp and paper, refineries and petrochemical, and inorganic chemicals. Accounting for around 33 % of the industrial CO_2 emissions in the EU, these sectors are especially important for the transition towards carbon neutrality (Bruyn et al. 2020). In **Paper 4**, the results of the study are presented. The integration of HP an ST led to a reduction of the TAC between 29.39 % and 55.43 % compared to the basic HEN solutions. The different heat recovery potentials led to a wide variation of resulting external energy demands. While for three cases the external energy demand got reduced between 12.52 % and 87.10 %, the external energy demand of the fourth case increased by 13.31 %. This behavior is caused by the structure of the formulation and the specific cost coefficients. Because even if the external energy demand increased, the annual energy costs, in this case, got reduced by $2,003,480$ €y^{-1}. Under the simplifying assumption that the electrical energy demand is satisfied through and GHG neutral sources and that the Hu are the only GHG source during the operation of the processes, the extended HEN solutions yield a theoretical potential for the drastic reduction of GHG emissions between 52.3 % and 100 % in this study. The payback times of the cases were calculated with an assumed lifespan of 25 years to analyze the economic viability of the extended HEN results. Three of the cases lay within the realistic set limit of 5 years for the profitability of the investment with 4.9 years, 3.6, and 4 years of payback time, while one case with 5.2 years payback time is not profitable according to the given limit. Overall, the results obtained in the study show the enormous potential of heat integration in the EII and that the set of test cases is perfectly suitable for the validation of multi-period HENS procedures under realistic conditions.

4.2 Automated Model Adaption

The topic of the second part of this work emerged during the evaluation of the developed optimization approach. Process optimization aims to reduce cost or energy demand, which gets more and more important due to economic pressure and the need to reduce GHG emissions. But every optimization procedure optimizes the process as depicted by the models and information used as input for them. Because the real operation of the process is bound to its physical behavior, theoretical savings from inaccurate optimization results can be consumed by process control that is needed to keep the process in a physically feasible state. This gets even more problematic when the physical behavior changes during operation. Especially industrial thermodynamic machinery has to deal with mechanisms like fouling or wear that are hard to monitor during operation and directly impact important physical properties like heat transfer coefficients or surface properties. To deal with this problem and to allow to utilize the full potential of optimization procedures, we decided to develop a framework for a continuous automated data-driven model adaption for industrial thermal energy systems as presented in **Paper 3**.

Literature research showed that most developments in the direction of automated model adaption revolve around the topic of fault detection in the context of condition monitoring, where models are continuously trained to predict and classify possible damages and determine if a process is in a normal or abnormal state. The classification in these cases for rotary equipment (Azevedo et al. 2016; Cakir et al. 2021), cutting tools (Čuš et al. 2011), or electrical components (Han et al. 2003) is used to classify well-known and distinguishable phenomena with the help of easy-to-measure properties like frequencies, forces, or temperatures. In contrast, the approach developed in this work allows up-to-date prediction of future behavior of thermodynamic components to enable operation adaptions for maximum efficiency.

The proposed framework is based on the OPC UA communication protocol, allowing maximum flexibility and changeability of the used components. It was developed on the use-case of an existing packed bed regenerator (PBR) thermal energy storage test rig in a TU Wien laboratory, an ideal example of the heterogeneous structure of technologies typically found in industries with long service life.

The concept of the framework is shown in Fig. 8 and can be described with the help of the use-case: Measurement data of the PBR is provided by an OPC UA server hosted on the programmable logic controller of the PBR in real-time and stored in a data processing server of the OSIsoft® PI System. The stored time series data gets preprocessed, analyzed, and grouped into individual states like charging or discharging of the storage for further usage in model training. The preprocessed and sorted data is transferred to MATLAB® where the actual model training takes place. The now retrained model is used to predict the response of the PBR for the planned future operation, which is then transferred back to the PI System and to the process control, which directly allows the consideration of the actual system behavior for further operation.

The framework was tested with the help of two existing models of the PBR. A validated finite-difference model based on the modeling approach by Walter et al. 2018 was used to generate training and test data sets to train a grey-box model presented by Halmschlager et al. 2021. For simulated pollution of the PBR during operation, the heat transfer coefficient between the storage medium and heat transfer fluid was reduced continuously for a given repeating load cycle. For comparison, one model was only trained with the initial not polluted simulated measurements, and the appliance of the framework continuously updated a second model. The comparison of the predictions of the two models showed that the framework's application reduced the prediction error up to 70 % compared to the static model within the given boundaries. This accuracy improvement shows that the framework allowed the model to learn the changed behavior and thus proves the concept's capabilities.

5 Conclusion and Outlook

The research of this thesis focuses on the improvement of process optimization of industrial systems. During the first part of this work, a multi-period mixed integer linear programming optimization approach for the simultaneous integration of heat pumps and storages into heat exchange network synthesis was developed and tested in a case study. In the second part of this thesis, a framework for the automated data-driven model adaption for industrial energy systems was developed. The improvement of energy recovery capabilities and the integration of renewable energies as achievable with optimization procedures like the developed MILP HENS approach, on the base of accurate component models as provided by the introduced framework, are essential steps on the way towards a sustainable and carbon neutral future.

The extended MILP HENS superstructure formulation is based on the linearization of a prominent MINLP superstructure formulation for the basic HENS problem. To keep the complexity of the extended problem and thus the needed computational effort low, we aimed for a linear integration of HP and ST into the formulation. First, to allow the integration of HP into the cost function of the formulation, the energy consumption of HP as a function of the thermal energy flow and the temperature lift was approximated by a convex linearization. Further, different storage types were integrated to enhance the capabilities to exploit heat recovery potentials. In summary, the presented approach allows finding an optimal global solution for the simultaneous integration of HP and ST into HEN without decomposition of the problem within one optimization step while considering all possible trade-offs between the possible installations.

For a comprehensible test of the robustness and capabilities of the approach, while also showing the thermodynamic and economic potential for industrial applications, the developed optimization procedure was applied on a set of example cases based on representative processes of the EII. The most important findings of this case study, where the solutions of the here presented novel approach are compared with basic HENS solutions without the possibility of HP and ST integration, are given in the following:

- The integration of HP and ST led to considerable possible reductions of the external energy demand of up to 87.1 % and possible reductions of the total annual costs of up to 55.43 % for the examined cases under the given boundary conditions.
- The computational effort necessary for solving the optimization problem as well as the resulting HEN configurations are very sensitive to changes of the input parameters like cost coefficients or physical parameters, which is related to the combinatorial nature of HENS and MILP.
- An economic analysis of the optimization outcomes resulted in payback times between 3.6 and 5.2 years for the different cases, which underlines the potential of energy integration with the help of design optimization for the reduction of CO_2 emissions while improving the cost efficiency of industrial processes.

During the development of the here presented approach, possible starting points for future work on this topic have been derived: The utilized mathematical formulation has a clear structure and can be easily adapted to integrate additional considerations. Examples for such adaptions could be the consideration of specific energy cost coefficients for each time period to include the dynamic behavior of the energy market or the restriction of specific installations to incorporate additional requirements of real processes. Also, integrating more detailed storage characteristics may improve the significance of possible HEN solutions. For the application of the approach for the refurbishment of existing processes, it could be useful to consider preexisting HEX to incorporate their possible re-utilization into the HEN solution directly. Furthermore, a comprehensive parameter sensitivity analysis on the optimization approach's input parameters may provide additional insights on how to reduce the mathematical complexity further and thus reduce the computational effort. This excerpt of possible future work shows that research in this area is far from exhausted. Even if individual methods such as the developed MILP HENS optimization procedure already provide satisfactory results within their boundaries and assumptions, only continuous research and development will allow us to keep up with the increasingly complex tasks of the ongoing energy transition.

Finally, the following conclusion can be drawn concerning the objective and research questions formulated in Section 3: The developed multi-period MILP HENS approach allows the simultaneous integration of HP and ST for the improvement of heat recovery capabilities and the possible integration of renewable energies into HEN. The linearization of the energy consumption of HP as a function of the temperature lift and the thermal energy flow allowed to keep the mathematical formulation linear, which reduces the mathematical complexity, and thus the computational effort as well as the computational time needed for optimization. Also, the linearity of the formulation causes that the optimization always results in a globally optimal solution within the given boundary conditions. Initially, a small test case has been optimized with a variation of different cost coefficients to verify the fundamental behavior of the procedure. As expected, increasing electrical power costs or decreasing utility costs led to a reduction of the size and number of HP until all HP options get discarded from the solution, while increasing costs for storage material led to decreasing storage sizes until no more additional storage is considered in the solution. Further comprehensive testing of the approach on a set of example cases also showed a consistent and traceable behavior conforming to the mathematical structure of the formulation and the used cost coefficients. The case study on these representative cases based on representative processes of the EII shows enormous potential for the reduction of the external energy demand of up to 87.1 % and the total annual cost of up to 55.43 % by the integration of HP and ST in comparison to basic HEN solution without HP and ST options. With payback times between 3.6 and 5.2 years, these obtained results prove the economic and thermodynamic potential of the approach for industrial applications, especially in the EII.

The second part of this thesis deals with the development of a framework for the automated data-driven model adaption to satisfy the need for accurate component models that represent the current state of a physical entity, even if changes of the behavior during operation occur. Such models are essential for the appropriate utilization of process optimization measures and other smart services emerging from the developments towards Industry4.0. Especially industrial thermal energy systems show considerable potential for energy and cost optimization, but are also commonly prone to changes of the physical behaviour during operation due to mechanisms like wear or fouling that make the utilization of real-time process data necessary to keep digital models up to date. The framework is based on open protocol bidirectional live communication with OPC UA and other state of the art communication protocols to enable the proper communication between the broad range of different technical systems that traditionally occur in grown industrial systems.

The application of the developed framework to a packed bed thermal energy storage that is operated under conditions that lead to continuous fouling to prove the functionality of the concept led to the following revelations:

- The comparison of a static model that is only trained once with data from the unpolluted test rig and a model continuously adapted during the simulated operation of the test rig with the help of the proposed framework showed the capabilities and enormous potential of the framework. The learning of the changing physical behavior improved the accuracy of the continuously updated models prediction by up to 70 % compared to the prediction of the static model within the given assumptions.
- The proper application of the framework is highly dependent on the used component model and the data preprocessing implemented. Automated data-driven model adaption can only work if the data is filtered, analyzed, and validated according to the requirements of the particular model, which requires high effort in error-proofing when no human interaction is intended. Also, the used model has to be robust and suitable for the given purpose. As for every data-driven model training, only the combination of a suitable model and suitable data can lead to successive results.
- The structure of the framework makes it highly adaptable for different thermal energy systems. Because it is based on open protocol live communication utilizing the broadly recognized OPC UA standard, the framework is not bound to the software components used in the proof of concept. It can easily be fitted to the given digital infrastructure of possible industrial applications, which considerably increases the possible range of applications.

In the ongoing development of methodologies for the usage of the continuously increasing amounts of process data, the proposed framework can be seen as an addition to the foundation necessary for live condition monitoring, fault prediction, predictive maintenance, and other smart services. Future work should include the further evaluation of the framework with the help of real measurement data including physical changes of processes during operation. For this purpose, our research unit has already started a research project concerning the enhancement of the PBR test rig used for the proof of concept that allows the contamination of the heat transfer fluid with pollutants. Also, the real-time usage of the framework on a model utilized by an operational optimization procedure could be considered as the logical next step in the development towards Industry4.0.

In summary, the objective formulated in Section 3 was achieved by the development of a framework for automated data-driven model adaption that relies on open protocol bidirectional communication. The framework features real-time analyzes and feedback based on the current physical properties of the system and can fast and easily be modified for different models or applications. Following, the associated research questions from Section 3 are addressed: The utilization of a unified open communication protocol as the base for the formulation allows the real-time communication necessary to extract data from different processes or systems. Simultaneously, the enrichment of measurement data with semantic information like sensor accuracy, measurement position, control values, or calibration data enables the detailed analyses necessary to extract further information. Dependent on the requirements of the model, the data has to be validated, filtered and analyzed to allow a proper automated model adaption. The difficulty lies in the fact that the automated treatment of the raw data has to include analyzes like plausibility checks that verify if the behavior of the measurement data is consistent with the real physical process to guarantee proper model training. If incorrect or the wrong training data is fed to the model training procedure, the resulting model becomes useless. For manual model training, such tasks are often undertaken by the operator. The automated process lacks the human experience and pattern recognition capabilities if they are not explicitly integrated, which is often complex and time-consuming. Thus, depending on the application, it is necessary to decide if human interaction or the automation of an analysis task is more efficient or reliant. The application of the framework on the use-case of a thermal energy storage showed that the continuous training of a model during the operation of a process with changing physical properties improves its capabilities for accurate predictions considerably and thus proves the framework's effectiveness.

Overall, the developed MILP HENS approach for the simultaneous integration of HP and ST and the proposed framework for automated data-driven model adaption could satisfactory prove their functionality and potential within their given boundaries and assumptions. Future work could include further adaptions of the HENS optimization procedure that considers more detailed component models or boundaries that include additional process requirements to improve its potential. Combining the framework with an application that utilizes the predictions of a model continuously adapted by it could be the next step towards Industry4.0. In summary, the approaches developed in this thesis can contribute to the overall goal of a clean energy future. Nevertheless, the achievability of carbon neutrality depends not only on the availability of the technology but also on the willingness of each individual to take responsibility and act accordingly.

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Publications

This chapter contains all relevant publications that have been produced in the course of this thesis. As core publications three journal papers as well as one conference paper are presented. Further publications and scientific contributions are given for completeness in the end of this chapter. The core publications, which consist of the knowledge generated during this work, are included in their published format. Additional short descriptions, my contribution to the publications in the form of CRediT author statements[5], and the complete references are given for them.

Core Publications

Further Publications

[5]According to the Elsevier CRediT author statement: https://www.elsevier.com/authors/policies-and-guidelines/credit-author-statement

Paper 1

An Extended Approach for the Integration of Heat Pumps into HENS Multi-Period MILP Superstructure Formulation for Industrial Applications

Presentation at ESCAPE 30 Conference 2020 and published by Elsevier in collaboration with René Hofmann

This publication, which was the first in the course of this thesis, deals with the proposed extension of the linearized superstructure formulation for heat exchange network synthesis. A linearization of the energy consumption of heat pumps as a function of the temperature lift and the thermal energy flow allows for a linear extension of the cost function that takes the size and energy consumption of heat pumps into account. For the proof of concept, an existing process and a predetermined heat pump characteristic are assumed. A comparison of the optimization results with and without utilizing the extended approach showed a considerable possible reduction of the total annual costs and the external energy demand.

My contribution: Conceptualization, Methodology, Validation, Investigation, Formal Analysis, Writing – Original Draft, Visualization

L. Prendl and R. Hofmann (2020). "An Extended Approach for the Integration of Heat Pumps into HENS Multi-Period MILP Superstructure Formulation for Industrial Applications". In: 30th European Symposium on Computer Aided Process Engineering. *Vol. 48. Computer Aided Chemical Engineering. Elsevier, pp. 1351–1356. ISBN: 9780128233771.*

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An Extended Approach for the Integration of Heat Pumps into HENS Multi-Period MILP Superstructure Formulation for Industrial Applications

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Abstract

This paper deals with the extension of the linearized superstructure formulation for heat exchange network synthesis (HENS) proposed by Beck and Hofmann (2018a). The energy consumption of heat pumps as a function of the temperature lift and the thermal energy flow is approximated by a convex linearization to enable the integration into a linear cost function. This allows for a linear extension of the cost function that takes the size and the energy consumption of heat pumps into account. As given problem an existing process and a predetermined heat pump characteristic is assumed. A test case consisting of two hot and two cold process streams has been constructed to investigate the proposed optimization method. The test case has been optimized with and without the extended approach for comparable results. The HEN resulting from the newly developed approach has 16.1 % lower total annual costs (TAC) and a 48.1 % lower external energy demand than the network resulting from the HENS without storages or heat pumps. This improvements come with the drawback of a more complex HEN with 15 installations compared to the simple HEN with 7 installations.

Keywords: Mathematical Programming, Linearization, Heat Recovery, Heat Pump, HENS

1. Introduction

The recovery of thermal energy is becoming more and more important, taking into account the overall objective of the reduction of primary energy consumption and thus reduction of greenhouse gas emissions. One way towards achieving this goal is the enhancement of energy exchange and conversion networks. Heat exchange network synthesis (HENS) was broadly investigated and approached with many different approaches over the last decades as recapitulated by Escobar and Trierweiler (2013). The integration of heat pumps into non continuous processes has also been the subject to a number of scientific publications as, for example, by Stampfli et al. (2019). Nonetheless, the integration of heat pumps into HENS for the economic optimization of batch processes with multiple time steps was not being thoroughly investigated. An existing paper from Becker and Maréchal (2012) uses the heat cascade formulation as approach. In contrast to this, a superstructure formulation was used as starting point for this work.

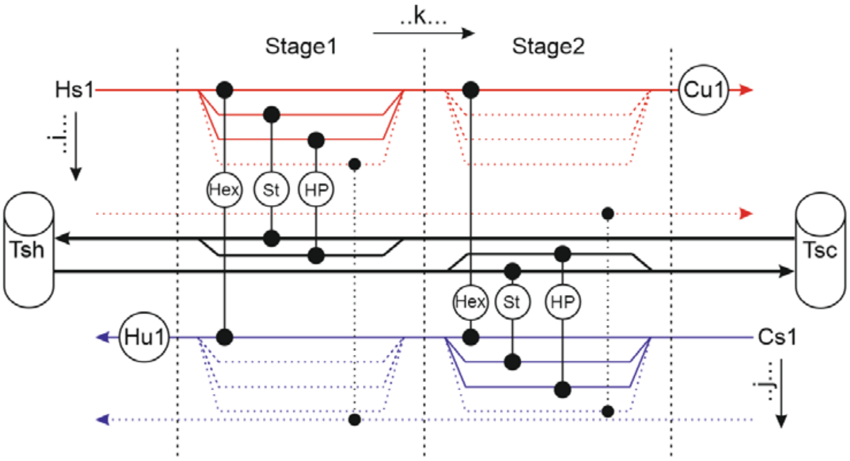

Figure 1: Extended Superstructure with possible Stream-Stream Hex (Hex), Stream-Storage Hex (St) and Heat Pumps (HP).

2. Extended Mathematical Model

The superstructure is based on the formulation by Beck and Hofmann (2018a), which is a linearization of the superstructure proposed by Yee and Grossmann (1990). The objective function as shown in Eq. (1) is extended by considering a two tank liquid thermal storage, heat exchangers between the streams and the storage and heat pumps between the streams and the storage. The possible connections for every stream in every stage are exemplarily represented in Figure 1. The two tank storage is modelled according to Beck and Hofmann (2018b). The multiple time periods during the cyclic process are realized by using the time slice model for cutting the process into different time slices in which the process parameters are constant. Isothermal mixing after every stream split is assumed. If heat exchangers occur at the same spot in different time periods p, the largest heat exchanger area A is taken into account for the calculation. In the other time steps the isothermal mixing is assured by bypasses. Furthermore, as a simplification to keep the problem linear, the heat transfer coefficients are assumed to be constant.

$$
\begin{aligned}
\min\ TAC = & \sum_i\sum_j\sum_k c_f Z_{ijk} + \sum_i c_f Zcu_i + \sum_j c_f Zhu_j + \sum_i\sum_j\sum_k cA_{ijk}{}^{\beta} \\
& + \sum_i cA_{cu\,i}{}^{\beta} + \sum_j cAhu_j{}^{\beta} + \sum_i\sum_p c_{cu} qcu_{ip}\tau_p + \sum_j\sum_p c_{hu} qhu_{jp}\tau_p \\
& + C_{fixst} + C_{varst} Size_{st} + \sum_i\sum_j\sum_k c_f Zst_{ijk} + \sum_i\sum_j\sum_k cAst_{ijk}{}^{\beta} \\
& + \sum_i\sum_j\sum_k c_{hp} Zhp_{ijk} + \sum_i\sum_j\sum_k cAhp_{ijk}{}^{\beta} + \sum_i\sum_j\sum_k\sum_p c_{Pel} Pel_{ijkp}\tau_p
\end{aligned}
\tag{1}
$$

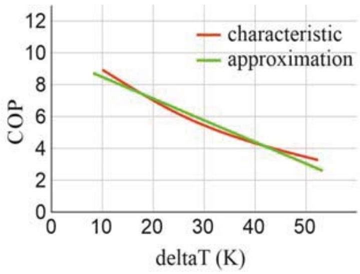

Figure 2: Linearized COP over deltaT

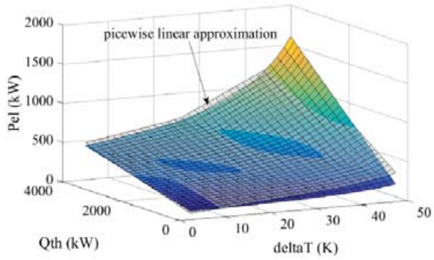

Figure 3: Linear Approximation of P_{el}

3. Linearization

For the integration of heat pumps into the MILP superstructure several linearizations are necessary. In the following chapter the chosen approach is explained in detail.
The coefficient of performance (COP) of heat pumps is defined in Eq. (2) as the ratio of useful heat supplied by the heat pump (Q_{th}) to the required work (P_{el}).

$$COP = \frac{Q_{th}}{P_{el}} \tag{2}$$

In this work it is assumed that the heat pump characteristic curve of the COP over the temperature lift of the heat pump (deltaT) is known. For the linearization this characteristic curve is approximated by a polynomial of first order. In Figure 2 an example for a characteristic curve with its associated linear approximation is shown. From Eq. (2) it is visible that P_{el} can be calculated as the ratio of Q_{th} to COP. This nonlinear relation is linearized with an approach inspired by the linearization of the heat exchange area by Beck and Hofmann (2018a). The nonconvex, nonlinear feasible solution space is split into three regions. Each of these regions is then approximated by a linear equation which is fitted with least squares methods. This piecewise linear approximation is shown in Figure 3 with the underlying solution space. The linear approximations are used as constraints for P_{el} with the help of big-M formulations. In these constraints Γ is a sufficient large number to activate or deactivate Eq. (3) dependent on whether a Heat Pump exists on this position or not.

$$P_{el} \geq P_{el,approx} - (1 - Zhp_{ijk})\Gamma \tag{3}$$

The heat exchanger area between the streams and heat pumps is approximated with the same procedure as for the heat exchangers between the streams. As measurement to keep the objective function linear, the heat pump approach temperature gets set to a fixed value. Due to the preset storage temperatures it is possible to linearize the reduced heat exchange area between storage and heat pump as function of the heat flow Q_{hpst} as shown in Eq. (4) because the denominator remains constant.

$$A_{hpst}^{\ \beta} = \left(\frac{Q_{hpst}}{U\ LMTD_{hpst}} \right)^{\beta} \longrightarrow A_{hpst}^{\ \beta} \approx c_{A1} + c_{A2} Q_{hpst} \tag{4}$$

4. Test Case

Table 1: Stream data and cost coefficients

Stream	Tin (°C)	Tout (°C)	CP (kW/K) period 1	CP (kW/K) period 2	CP (kW/K) period 3	h (kW/m^{2}K)
H1	120	40	18	50	9	0.5
H2	90	30	22	22	1	0.5
C1	20	100	20	10	10	0.5
C2	50	90	50	40	70	0.5
UT h	150	150	-	-	-	1
UT c	5	10	-	-	-	1

exchanger cost = 4000+500[A(m^2)]$^\beta$ €y^{-1}, storage cost = 7000+0.15[kg] €y^{-1}, hot utility cost = 0.07 €kW^{-1}h^{-1}, cold utility cost = 0.007 €kW^{-1}h^{-1}, β = 0.83, electrical power costs = 0.06 €kW^{-1}h^{-1}, dTmin = 5 °C, Heat Pump cost = 11000 €y^{-1}

As test case an example which consists of two hot and two cold process streams was investigated. The assumed cyclic process has a duration of three hours and is split into three periods of one hour each. It is assumed that the process is operated annually for 8600 h. The superstructure model was set up with two stages. The cost coefficients and stream data used are given in Table 1. A two tank storage which operates at 70 °C and 100 °C with thermo-oil as storage medium with an specific heat capacity of cp_{oil} = 2 kJkg^{-1}K^{-1} and an heat transfer coefficient of h_{oil} = 0.5 kWm^{-2}K^{-1} was chosen. The assumed heat pump has a power consumption range from 400 kW to 2000 kW and a given approach temperature of $T_{hpaproach}$ = 5 K. The linearized COP characteristic is given as COP = 10 – 0.15 K^{-1} deltaT and the heat transfer coefficient as h_{hp} = 5 kWm^{-2}K^{-1}. A lower boundary of the COP of COPmin = 1 was set as constraint. As solver for the MILP Gurobi 8.1.0 was used.

The plausibility of the optimization was tested with the variation of different cost coefficients. With increasing costs for electrical power or decreasing costs for utilities, the size and number of heat pumps gets reduced until no more heat pumps get chosen for the system. Similarly increasing costs for storage material lead to smaller storage sizes and finally the exclusion of solutions containing storages. This behavior matches the results expected from the structure of the used cost function.

5. Results

The test case was optimized in two different configurations. In the first configuration the HEN was optimized without heat pumps or storages in order to be able to obtain comparable results. In the second configuration the test case was optimized with the extended approach including a storage and heat pumps.

5.1. Configuration 1: Test case without heat pumps and storage

For this setup, the solver found a solution after 0.02 s with total annual costs of TAC = 1,120,500 €y^{-1}. The obtained heat exchange network which is shown in Figure 4 consists of three stream – stream heat exchangers and four utility heat exchangers. The obtained heat flows for the different time periods are given in Table 2. The high amount of needed cold utility in period 2 and needed hot utility in period 3 shows potential for temporal energy shifting. The total utility energy demand adds up to 20.869 GWh y^{-1}.

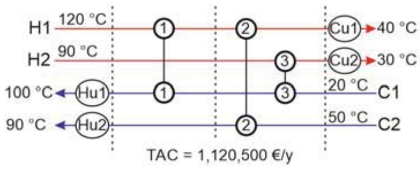

Figure 4: Hen obtained without Heat Pump

Table 2: Heat Flows without Heat Pump (kW)

	p1	p2	p3
1	294.3	150.00	720.00
2	875.70	1600.00	-
3	1300.00	650.00	-
Hu1	5.72	-	80
Hu2	1124.3	-	2800.00
Cu1	270.00	2250.00	-
Cu2	20.00	670.00	60.00

5.2. Configuration 2: Test case with integrated heat pumps and storage

For the extended case a solution was found after 54.12 s with total annual costs of TAC = 940,260 €y^{-1}. The extended heat exchange network which is shown in Figure 6 consists of five stream – stream heat exchangers, two stream – storage heat exchangers, four utility heat exchangers, two heat pumps and a storage tank with 192334 kg of thermo-oil which has a storage capacity of 3.206 MWh. The obtained heat flows and the electrical power demands for the different time periods are given in Table 3. The total utility energy demand is 6.074 GWh y^{-1} and the electrical energy demand for the heat pumps is 4.755 GWh y^{-1}. This adds up to a total external energy demand of 10.829 GWh y^{-1}. The charging state of the storage over the cycle time is given in Figure 5. The storage has a variable storage charge at the beginning of the cycle which has to be reached again at the end of the cycle. This is ensured by suitable boundary conditions.

5.3. Comparison:

The TAC of the extend network are 16.1 % lower compared to the simple network and the total external energy demand of the obtained extended structure is only 51.9 % of the total energy demand of configuration 1. From Table 2 and Table 3 it is visible that the utilities are significantly smaller for configuration 2 and that a big part of the energy is supplied by the heat pumps instead. Although configuration 2 has lower TAC and energy demand it has to be noticed that it is much more complex with 15 installations and a storage compared to the simple configuration 1 with 7 installations.

6. Conclusion

An extension for the integration of heat pumps into HENS for multi-period MILP superstructures by linearizing the energy consumption of heat pumps has been developed. A test case consisting of two hot and two cold process streams with varying mass flows for different time steps has been constructed to demonstrate the proposed method. This test case was optimized with and without the possibility of including a storage and heat pumps to compare the gained results. The obtained extended HEN has 16.1 % lower TAC and 48.1 % lower external energy demand compared to the conventional HEN which comes with the drawback of a higher complexity of the network. The test case was chosen rather small because the target was to check if the optimization results are plausible which is hardly possible for bigger problems. From the results of the optimization without storage and heat pumps it can be concluded that a storage device that shifts energy between the time periods is able to reduce the TAC if the costs of the storage, the heat pumps and the electrical energy are low enough compared to the utility costs. This is consistent with the results of the second configuration. When comparing results it has to be taken into account that the results of these optimizations are strongly dependent on the

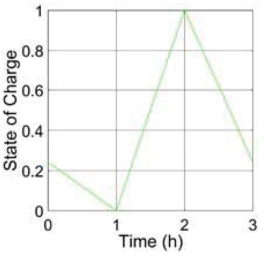

Figure 5: Storage Charging State over Cycle Time

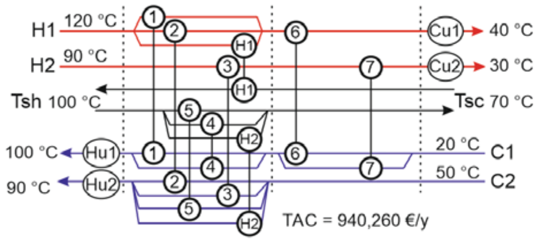

Figure 6: Hen obtained with Heat Pumps and Storage

Table 3: Heat Flows and P_{el} results with Heat Pump (kW)

	p1	p2	p3		p1	p2	p3
1	549.38	456.93	216.24	Hu1	100.00	-	50.00
2	577.21	630.00	368.76	Hu2	250.00	200.00	-
3	770.00	770.00	-	Cu1	47.84	622.29	-
4	373.64	-	398.76	Cu2	238.59	550.00	60.00
5	402.79	-	262.44	Hp1	-	1947.70	-
6	265.58	343.07	135.00	Hp2	-	-	2168.80
7	311.41	-	-	Pel Hp1	-	1257.80	-
				Pel Hp2	-	-	400.90

chosen coefficients. Small changes of cost coefficients or physical parameters can result in very different network solutions because of the nature of mixed integer programming.

7. Acknowledgment

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Paper 2

Simultaneous integration of heat pumps and different thermal energy storages into a tightened multi-period MILP HENS superstructure formulation for industrial applications

Published in Computers and Chemical Engineering in collaboration with Karl Schenzel and René Hofmann

In this paper, the approach presented in **Paper 1** was developed into the direction of applicability for real industrial applications. The improved multi-period MILP HENS superstructure formulation allows simultaneous integration of heat pumps and different thermal storages. Furthermore, measures for tightening the solution space of the COP are introduced, improving the accuracy of the HP approximation while simultaneously reducing the computational effort. Additionally, a simulation of a vapor compression HP with a chosen refrigerant was deployed to obtain realistic HP characteristic curves. Applying the proposed method on a test case resulted in the reduction of cost of 61.2 % and a reduction of the external energy demand of 58.4 %. These significant results underline the capability of computer aided design optimization.

My contribution: Conceptualization, Methodology, Validation, Investigation, Formal Analysis, Writing – Original Draft, Visualization

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Simultaneous integration of heat pumps and different thermal energy storages into a tightened multi-period MILP HENS superstructure formulation for industrial applications

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ABSTRACT

Design optimization of industrial installations with help of mathematical programs offers high potential for energy savings and cost reduction, which steadily gains importance. Heat exchange network synthesis (HENS) is one of the commonly used and promising methods. This paper deals with simultaneous integration of heat pumps and two different storage types into mixed integer linear programming (MILP) HENS by extending a multi-period superstructure formulation proposed by Beck and Hofmann (2018c). Further measures for tightening the solution space for the coefficient of performance (COP) are introduced. This improves the accuracy of the heat pump (HP) approximation, reduces computational effort and prevents solutions with uneconomical low COP. The obtained approach allows to design cost efficient heat recovery systems with storages (ST) and HP for the improvement of the energy recovery capabilities. A constructed test case was used to analyze the performance of the method and to show its possible potential.

1. Introduction

In the last decades extensive research in the area of waste heat recovery has been carried out and it still gains scientific popularity. This is caused by the complexity of the topic and the considerable potential for energy savings which provides economic benefits with short payback times (Eichhammer and Rohde, 2016). The problem gets even more complex by extending classical HENS by additional installations like HP or ST. Simplified approaches are needed to find suitable solutions with acceptable computational effort. The complexity is caused by the nature of the mathematical formulation of HENS. It is proven to be an NP-hard problem, which means there is no possibility for the existence of a polynomial exact solution algorithm for the problem (Furman and Sahinidis, 2001). The advantage of linear programming approaches is that they always deliver global optimal solutions without the need for initial feasible solutions. Even for small problems suitable initial solutions are often hard to find (Escobar and Trierweiler, 2013). As proposed by Nemet et al. (2019) for basic HENS without HP, solutions obtained by MILP approaches could also be used as near optimum starting solutions for a mixed integer nonlinear programming (MINLP) optimization. As already stated by Ciric and Floudas (1991), the simultaneous optimization with a minimum cost target is superior to sequential performed targeting, because every decomposition adds an element of uncertainty to the solution. Other researchers already approached the problem of integrating HP into heat exchange networks. For example Stampfli et al. (2019) used the principle of heat recovery loops to integrate ST and HP into non-continuous processes by utilizing insight based and nonlinear programming techniques sequential with the target of optimal HP operation. Miah et al. (2015) developed an methodological framework for heat integration which consists of several analysis steps that divide the problem into different zones to decide where HP have to be located. Becker and Maréchal (2012) utilize heat cascade formulations and calculate the optimal solution by setting up an multi objective optimization algorithm that solves the thermodynamic calculations and the energy integration serial as sub problems. In contrast, this work is based on the linearization of the widely used superstructure formulation initially introduced by Yee and Grossmann (1990), which was proposed by Beck and Hofmann (2018c).

Differing from the sequential approach for integration of multiple thermal ST used by Beck and Hofmann (2019), here an simultaneous optimization that considers different thermal ST and HP in one step was developed. The linear integration of the HP and ST

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Nomenclature

Acronyms

HENS	heat exchanger network synthesis
MINLP	mixed integer nonlinear programming
MILP	mixed integer linear programming
LP	linear programming
HEX	heat exchanger
HP	heat pump
ST	storage
Hu	hot utility
Cu	cold utility
Hs	hot stream
Cs	cold stream

Parameters

a_1, a_2	linearization coefficients COP (-)
b	linearization coefficients Pel (-)
COP	coefficient of performance (-)
Q_{st}	storable heat (kJ)
β	cost exponent (-)
U	heat transfer coefficient (kW m−2 K−1)
F	flow capacity of process streams (kW/K)
c	cost coefficient for heat exchanger area (€ $m^{-2\beta}$)
c_f	step-fixed cost coefficient (€)
c_p	specific heat capacity (kJ kg−1 K−1)
m	mass (kg)
$\dot{m}$	massflow (kgs^{-1})
c_{fst}	step-fixed storage cost coefficient (€)
c_{vst}	variable storage cost coefficient (€ kg^{-1})
c_{hp}	step-fixed HP cost coefficient (€)
c_{hu}	cost coefficient hot utility (€ kWh^{-1})
c_{cu}	cost coefficient cold utility (€ kWh^{-1})
c_{Pel}	cost coefficient electricity (€ kWh^{-1})
Ω	upper bound for heat exchange (kW)
$\Delta T_{\min}$	minimum approach temperature (°C)
Γ_T	temperature big-M coefficients (°C)
Γ_A	area big-M coefficients (m^2)
Γ_{Pel}	electircal power big-M coefficients (kW)
NOK	number of stages (-)
NOP	number of time periods (-)
HPS	number of hot process streams (-)
CPS	number of cold process streams (-)
τ	duration of time interval (h)
τ_a	annual duration of time interval (h)

Subscripts

shift	shift variable
ap	approach
st	storage
hp	heat pump
2T	two tank storage
1T	one tank storage
i	index hot stream
j	index cold stream
x	index approximation region
k	index temperature stage
p	index time period
min	minimum value
max	maximum value
hu	hot utility
cu	cold utility
h	hot tank temperature
c	cold tank temperature

Superscripts

in	inlet
out	outlet
2T	two tank storage
1T	one tank storage
hp	heat pump

Variables

A	heat exchanger area (m^2)
CA	constraint heat exchanger area (m^2)
$\dot{Q}$	heat flow (kW)
$LMTD$	logarythmic mean temperature difference (°C)
$CLMTD$	constraint logarythmic mean temperature difference (°C)
Z	binary variable for existence of HEX (-)
S_{st}	storage size (kg)
Z_{st}	binary variable for existence of storage (-)
Z_{hp}	binary variable for existence of heat pump (-)
$LMTD$	logarithmic mean temperature difference (°C)
T	temperature (°C)
ΔT	temperature difference (°C)
TAC	total annual costs (€)
Pel	electrical power (kW)
$CPel$	constraint electrical power (kW)
CH	storage charge state (%)

allows to find a global optimal solution for the given parameters without the need for initial feasible solutions. All adaptions that have been made compared to previous superstructure approaches are shown in the following Chapter 2.

2. Proposed extension of the HENS superstructure

A previous publication Prendl and Hofmann (2020) extended the linearized superstructure proposed by Beck and Hofmann (2018c) to consider the integration of HP. In continuation of this work a further extension has been made by introducing additional storage possibilities to enhance the capability of shifting energy on different temperature levels over time periods. A real vapor compression HP was modeled and simulated to obtain a realistic HP characteristic as explained in Chapter 4. Also the solution space for the COP has been tightened to improve the accuracy of the approximation and to reduce the computational effort. As can be seen in Fig. 1, possible installations are a one tank ST (1T ST), a two tank ST (2T ST), heat pumps between streams and the 2T ST, HEX between streams, HEX between streams and ST as well as hot and cold utilities. The 1T ST has a preset fixed mass and variable temperature. Because the initial temperature of the 1T ST is also an optimization parameter the storage gets integrated on the economically optimal temperature interval. The 2T ST operates at two preset temperature levels. The size of the ST gets optimized simultaneously with the solution of the superstructure. For both ST the heat transfer fluid is used as storage medium so no HEX inside the ST are needed. The simultaneous integration of ST with fixed mass and variable temperature as described by Beck and Hofmann (2019) and ST with fixed temperatures and variable mass allows to utilize the benefits of both types simultaneously (Walmsley et al., 2014). The course of the charging states of the different thermal energy storages over the operation periods resulting from the solving of the optimization problem allows to gain better insights into the system behavior. HEX, HP and ST are possible in every stage, while utilities are only possible before the first and after the last stage. The utilities provide the energy needed to fulfill the temperature boundaries of the streams if it is not possible to satisfy them within the stages.

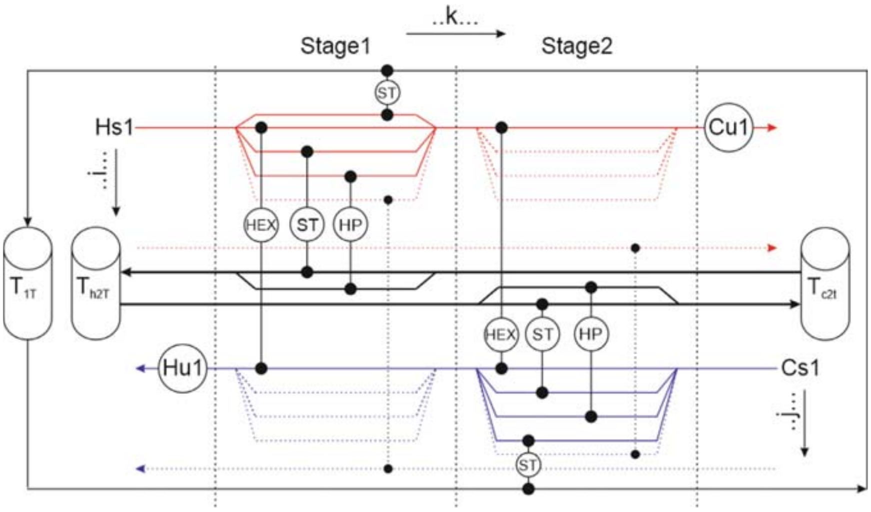

Fig. 1. Extended Superstructure with possible Stream-Stream HEX (HEX), Stream-Storage HEX (ST) and Heat Pumps (HP).

3. Mathematical model

The objective for the extended stagewise superstructure shown in Fig. 1 is a minimization of the total annual costs (TAC) to provide the needed energy to change the temperatures of the streams to match the given process parameters. The cost function (Eq. (1)) consists of three different types of costs:

- Step fixed investment costs for the installation of stream-stream HEX, hot- and cold utilities (Hu,Cu), Storages (ST), stream-storage HEX and heat pumps (HP).
- Variable investment costs for the surface area and thus the size of all HEX as well as variable costs for the size of the two tank storage.
- Energy costs for the external energy demand of the obtained solution which consists of the costs for the hot and cold utilities and the costs for the electrical energy consumed by the HP.

$$\begin{aligned}
&\min TAC = \underbrace{\textstyle\sum_i \sum_j \sum_k c_f Z_{ijk} + \sum_i c_f Z_{cui} + \sum_j c_f Z_{huj} + c_{fst\,2T} Z_{st\,2T} + c_{fst\,1T} Z_{st\,1T} + \sum_i \sum_j \sum_k c_f Z_{2T\,ijk} + \sum_i \sum_j \sum_k c_f Z_{1T\,ijk} + \sum_i \sum_j \sum_k c_{hp} Z_{hp\,ijk}}_{\text{step fixed investment costs}} \\
&\underbrace{\textstyle + \sum_i \sum_j \sum_k cA^{\beta}_{ijk} + \sum_i cA^{\beta}_{cui} + \sum_j cA^{\beta}_{huj} + c_{vst\,2T} S_{st\,2T} + \sum_i \sum_j \sum_k cA^{\beta}_{2T\,ijk} + \sum_i \sum_j \sum_k cA^{\beta}_{1T\,ijk} + \sum_i \sum_j \sum_k cA^{\beta}_{hp\,ijk}}_{\text{variable investment costs}} \\
&\underbrace{\textstyle + \sum_i \sum_p c_{cu} \dot{Q}_{cuip} \tau_{ap} + \sum_j \sum_p c_{hu} \dot{Q}_{hujp} \tau_{ap} + \sum_i \sum_j \sum_k \sum_p c_{Pel} Pel_{ijkp} \tau_{ap}}_{\text{energy costs}} \\
&\forall\ p = 1, \ldots, NOP,\ k = 1, \ldots, NOK, \\
&i = 1, \ldots, HPS,\ j = 1, \ldots, CPS
\end{aligned} \tag{1}$$

3.1. Energy balances

In the following (Eq. (2)), the energy balances for all process streams are given with the extensions necessary for considering the heat flows to the storages and heat pumps.

$$\begin{aligned}
&\sum_j \sum_k \dot{Q}_{ijkp} + \sum_k (\dot{Q}_{2T\,ikp} + \dot{Q}_{1T\,ikp} + \dot{Q}_{hp\,ikp}) \\
&+\dot{Q}_{cuip} = \dot{m}_{ip} cp_{ip} (T^{in}_{ip} - T^{out}_{ip}) = \dot{Q}_{ip} \\
&\sum_i \sum_k \dot{Q}_{ijkp} + \sum_k (\dot{Q}_{2T\,jkp} + \dot{Q}_{1T\,jkp} + \dot{Q}_{hp\,jkp}) \\
&+\dot{Q}_{hujp} = \dot{m}_{jp} cp_{jp} (T^{out}_{jp} - T^{in}_{jp}) = \dot{Q}_{jp} \\
&\forall\ p = 1, \ldots, NOP,\ k = 1, \ldots, NOK, \\
&i \in HPS,\ j \in CPS
\end{aligned} \tag{2}$$

T^{in} and T^{out}, the inlet and outlet temperatures of the streams, where i are the hot streams and j are the cold streams, with their heat capacities cp_{ip} and cp_{jp} as well as their massflows $\dot{m}_{ip}$ and $\dot{m}_{jp}$ are the physical requirements that have to be fulfilled for a given problem. The balances for every stage k in every time period p which are given in the following Eq. (3) show that isothermal mixing is assumed after every stage. If more than one installation occurs at one one position $ijkp$, the stream is split up and they are arranged in parallel configuration.

$$\begin{aligned}
&\sum_j \dot{Q}_{ijkp} + \dot{Q}_{2T\,ikp} + \dot{Q}_{1T\,ikp} + \dot{Q}_{hp\,ikp} \\
&= \dot{m}_{ip} cp_{ip} (T_{ik} - T_{i,k+1}) \\
&\sum_i \dot{Q}_{ijkp} + \dot{Q}_{2T\,jkp} + \dot{Q}_{1T\,ijkp} + \dot{Q}_{hp\,jkp} \\
&= \dot{m}_{ip} cp_{jp} (T_{jk} - T_{j,k+1}) \\
&i \in HPS,\ j \in CPS \\
&T_{i,k=1} = T^{in}_i,\ T_{j,k=NOK} = T^{in}_j
\end{aligned} \tag{3}$$

For simplification of the formulation, utilities are only allowed directly before the outlet of streams as in the basic superstructure proposed by Yee and Grossmann (1990). The utility heat loads in Eq. (4) are calculated as the heat flows that are needed to change the temperatures of the streams to the demanded output temperatures required by the given processes. In the proposed superstructure, utilities are modeled as streams with fixed input and output temperatures that are provided in the needed quantities. They have corresponding HEX to interact with the hotstreams and coldstreams.

$$\dot{Q}cu_{ip} = \dot{m}_{ip}cp_{ip}(T_{i,k=NOK+1,p} - T^{out}_{ip})$$
$$\dot{Q}hu_{jp} = \dot{m}_{jp}cp_{jp}(T^{out}_{jp} - T_{j,k=1,p}) \tag{4}$$

For the 1T ST, the accumulated energy content is calculated through the temperature change of the storage medium (Eq. (5)), where a perfect mixing inside the storage tank is assumed. The temperature differences for the heat transfers (Eq. (11)) are calculated with the temperatures at the start and end of the time periods according to the formulation by Beck and Hofmann (2018a). For taking the periodic operation into account, the temperature at the start of the first time period has to be the same as the temperature at the end of the last time period and is defined as T_{shift}. To consider the physical constraint of thermal stability of the storage medium, a maximum storage temperature $T_{\max_{1T}}$ is defined. The requirement to keep the program linear prevents a simultaneous optimization of the temperature and sizing of the one tank storage. However, the resulting temperature curve of the storage can be used to gain information of the system and to adapt the storage size or material.

$$m_{1T}cp_{1T}(T_{1T\ p+1} - T_{1T\ p}) =$$
$$\left(\sum_i\sum_k \dot{Q}_{1T\ ikp} - \sum_j\sum_k \dot{Q}_{1T\ jkp}\right)\tau_p$$
$$T_{1T\ p=1} = T_{shift} = T_{1T\ p=NOP}$$
$$0 \le T_{1T} \le T_{\max_{1T}} \tag{5}$$

The 2T ST operates at fixed temperatures and the masses in the two tanks change. The energy balance of the ST (Eq. (6)) is an adaption of the storage model by Beck and Hofmann (2018a). The constant temperatures are one of the enablers for the linear integration of heat pumps. This storage can be charged or discharged either directly over HEX from the streams or over heat pumps.

The variable CH_{2T} represents the charging state of the ST and has the physical limitation to be between zero (empty) and one (full charged). Similar to the 1T ST, CH_{shift} gets used to ensure that the ST has the same state of charge at the beginning and end of the cycle. The storage size $S_{st\ 2T}$ gets calculated by multiplying the available storage mass m_{2T} with the maximum charging difference that occurs during one cycle. It is assumed as a linear component of the cost function (Eq. (1)).

$$Q_{st\ 2T} = m_{2T}cp_{2T}(T_{h2T} - T_{c2T})$$
$$CH_{2T,p+1} = CH_{2T,p} + \frac{\tau_p}{Q_{st\ 2T}}$$
$$\left[\sum_i\sum_k(\dot{Q}_{2T\ ikp} + \dot{Q}_{hpst\ ikp})\right.$$
$$\left.-\sum_j\sum_k(\dot{Q}_{2T\ jkp} + \dot{Q}_{hp\ st\ jkp})\right]$$
$$CH_{2T,p=1} = CH_{shift} = CH_{2T,p=NOP}$$
$$S_{st\ 2T} = m_{2T}(\max(CH_{2T}) - \min(CH_{2T}))$$
$$0 \le CH_{2T} \le 1 \tag{6}$$

The heat pumps are formulated as power to heat device without losses. In Eq. (7) it can be seen that HP that charge the ST can only occur between hot streams and ST. HP that discharge the ST are only possible between cold stream and ST.

$$\dot{Q}_{hpst\ ikp} = \dot{Q}_{hp\ ikp} + P_{el\ ikp}$$
$$\dot{Q}_{hpst\ jkp} = \dot{Q}_{hp\ jkp} - P_{el\ jkp} \tag{7}$$

3.2. Additional constraints

The constraints given in the following Eq. (8) make sure that the binary variables for the existence of installations are only non zero when the corresponding heat flows lie within their boundaries and thus establish the needed connection between them. For the stream - stream HEX and the stream - storage HEX, the minimum heat flow $\dot{Q}_{\min}$ has the aim of tightening the solution space for the HEX area. Thus the accuracy of the linear approximations can be improved and the computational time can be reduced (Beck and Hofmann, 2018b).

$$Z_{ijkp}\dot{Q}_{\min} \le \dot{Q}_{ijkp} \le Z_{ijkp}\dot{Q}_{\max\ ijkp}$$
$$\dot{Q}_{\max\ ijkp} = \min(\dot{Q}_{ip}, \dot{Q}_{jp})$$

$$Z_{2T\ ijkp}\dot{Q}_{\min\ st} \le \dot{Q}_{2T\ ijkp} \le Z_{2T\ ijkp}\dot{Q}_{ijkp}$$
$$Z_{1T\ ijkp}\dot{Q}_{\min\ st} \le \dot{Q}_{1T\ ijkp} \le Z_{1T\ ijkp}\dot{Q}_{ijkp} \tag{8}$$

$$Z_{cu\ ip} \le \dot{Q}_{cu\ ip} \le Z_{cu\ ip}\dot{Q}_{ip}$$
$$Z_{hu\ jp} \le \dot{Q}_{hu\ jp} \le Z_{cu\ jp}\dot{Q}_{jp}$$

The constraints for the temperature differences for all heat exchanges in the system (Eq. (11)) are set up by using BIG-M formulations, where Γ is a sufficient large number to deactivate the constraint if no installation exists at a given position. Additional, a lower boundary for all temperature differences is set as a tightening measure (Eq. (9)).

$$\Delta T \ge \Delta T_{\min} \tag{9}$$

With decreasing logarithmic mean temperature difference (LMTD) values, the heat exchange areas and thus the variable costs increase, which causes that the optimization wants to maximize the temperature differences in HEX. Thus it is possible to formulate the constraints for the LMTD as given in Eq. (10). *CLMTD* are the piecewise linear approximated solution spaces for the logarithmic mean temperature difference as introduced by Beck and Hofmann (2018c). This approach benefits from the strict convexity of the LMTD that is proven in Mistry and Misener (2016).

$$LMTD_{ijkp} \le CLMTD_{ijkp}(\Delta T_{ijkp}, \Delta T_{ij,k+1,p})$$
$$LMTD_{2T\ ijkp} \le CLMTD_{2T\ ijkp}(\Delta T^{2T,1}_{ijkp}, \Delta T^{2T,2}_{ijkp})$$
$$LMTD_{1T\ ijkp} \le CLMTD_{1T\ ijkp}(\Delta T^{1T,1}_{ijkp}, \Delta T^{1T,2}_{ijkp})$$
$$LMTD_{hp\ ijkp} \le CLMTD_{hp\ ijkp}(\Delta T^{hp,1}_{ijkp}, \Delta T^{hp,2}_{ijkp}) \tag{10}$$

$$\Delta T_{ijkp} \le T_{ikp} - T_{jkp} + \Gamma_T(1 - Z_{ijkp})$$
$$\Delta T_{ij,k+1,p} \le T_{i,k+1,p} - T_{j,k+1,p} + \Gamma_T(1 - Z_{ijkp})$$

$$\Delta T^{2T,1}_{ikp} \le T_{ikp} - T_{h\ 2T} + \Gamma^{2T}_T(1 - Z_{2T\ ikp})$$
$$\Delta T^{2T,1}_{jkp} \le T_{h\ 2T} - T_{j,k+1,p} + \Gamma^{2T}_T(1 - Z_{2T\ jkp})$$
$$\Delta T^{2T,2}_{ikp} \le T_{i,k+1,p} - T_{c\ 2T} + \Gamma^{2T}_T(1 - Z_{2T\ ikp})$$
$$\Delta T^{2T,2}_{jkp} \le T_{c\ 2T} - T_{j,k+2,p} + \Gamma^{2T}_T(1 - Z_{2T\ jkp})$$

$$\Delta T^{1T,1}_{ikp} \le T_{ikp} - T_{1T\ p} + \Gamma^{1T}_T(1 - Z_{1T\ ikp})$$
$$\Delta T^{1T,1}_{jkp} \le T_{1T\ p} - T_{j,k+1,p} + \Gamma^{1T}_T(1 - Z_{1T\ jkp})$$
$$\Delta T^{1T,2}_{ikp} \le T_{i,k+1,p} - T_{1T\ p+1} + \Gamma^{1T}_T(1 - Z_{1T\ ikp})$$
$$\Delta T^{1T,2}_{jkp} \le T_{1T\ p+1} - T_{j,k+2,p} + \Gamma^{1T}_T(1 - Z_{1T\ jkp}) \tag{11}$$

$$\Delta T^{hp,1}_{ikp} \le T_{ikp} - T_{i,k+1,p} + T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ ikp})$$
$$\Delta T^{hp,1}_{jkp} \le T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ jkp})$$
$$\Delta T^{hp,2}_{ikp} \le T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ ikp})$$
$$\Delta T^{hp,2}_{jkp} \le T_{j,k+1,p} - T_{j,k+2,p} + T_{hp\ ap}$$
$$+\Gamma_T(1 - Z_{hp\ jkp})$$

As physical constraints Eq. (12) are given which prevent that the heat flows or the HEX areas get negative.

$$A^{\beta} \ge 0, \quad \dot{Q} \ge 0 \tag{12}$$

The lower boundary for the HEX area is necessary because in the constraints for the heat exchange areas (Eq. (13)), the BIG-M coefficient Γ_A has to be big enough to make the right side of the equation smaller than zero to deactivate the constraint (Beck and Hofmann, 2018c). The boundary for the heat flows enforces the monotonic temperature decrease over the stages.

$$\begin{aligned} &A^{\beta}_{ijkp} \geq CA^{\beta}_{ijkp} - \Gamma_A(1 - Z_{ijkp}) \\ &CA^{\beta}_{ijkp} = CA^{\beta}_{ijkp}(LMTD_{ijkp}, \dot{Q}_{ijkp}) \\ &A^{\beta}_{2T\ ijkp} \geq CA^{\beta}_{2T\ ijkp} - \Gamma_A(1 - Z_{2T\ ijkp}) \\ &A^{\beta}_{1T\ ijkp} \geq CA^{\beta}_{1T\ ijkp} - \Gamma_A(1 - Z_{1T\ ijkp}) \\ &A^{\beta}_{hp\ ijkp} \geq (CA^{\beta}_{hp\ ijkp} + CA^{\beta}_{hpst\ ijkp}) \\ &\quad -\Gamma_A(1 - Z_{hp\ ijkp}) \end{aligned} \tag{13}$$

The decision whether a storage is introduced or not is derived from the existence of installations that connect streams to them as given in the following Eq. (14).

$$\begin{aligned} &Z_{st\ 2T} \geq Z_{2T\ ijkp}, \quad Z_{st\ 2T} \geq Z_{hp\ ijkp} \\ &Z_{st\ 1T} \geq Z_{1T\ ijkp} \end{aligned} \tag{14}$$

For the proposed formulation it is assumed, that if a HEX, HP or utility exits at one position in more than one time step p, the biggest heat exchange area gets installed and at the other time steps bypasses balance out the differences (Eq. (15)).

$$A^{\beta}_{ijk} \geq A^{\beta}_{ijkp}, \quad Z_{ijk} \geq Z_{ijkp} \tag{15}$$

The following Eq. (16) formulate the tightening of the solution space for the COP which is described in Chapter 4 and Eq. (17) are the HP formulations derived from Eqs. (8) and (13) for the HEX.

$$\begin{aligned} &\dot{Q}_{hp\ st\ ikp}/P_{el\ ikp} \geq COP_{\min} \\ &\dot{Q}_{hp\ jkp}/P_{el\ ikp} \geq COP_{\min} \\ &\Delta T_{hp\ ijkp} \leq \Delta T_{hp\ \max} + \Gamma_T(1 - Z_{hp\ ijkp}) \\ &\Delta T_{hp\ ijkp} \geq \Delta T_{hp\ \min} - \Gamma_T(1 - Z_{hp\ ijkp}) \end{aligned} \tag{16}$$

$$\begin{aligned} &Z_{hp\ ijkp} Pel\ \min \leq P_{el\ ijkp} \leq Z_{hp\ ijkp} P_{el\ \max} \\ &Z_{hp\ ijkp} \dot{Q}_{\min\ hp} \leq \dot{Q}_{hp\ ijkp} \leq Z_{hp\ ijkp} \dot{Q}_{ijkp} \\ &P_{el\ ijkp} \geq CP_{el\ ijkp} - \Gamma_{Pel}(1 - Z_{hp\ ijkp}) \end{aligned} \tag{17}$$

4. Linearized HP model

Due to the nonlinearities of the process-specific thermodynamic relations as well as material properties, the heat pump characteristics between Pel, $\dot{Q}$ and ΔT are of nonlinear nature. As stated in Prendl and Hofmann (2020), it is necessary to linearize this characteristics for a linear integration of heatpumps into the superstructure. The approach explained in the following is based on the linearization of the nonlinear relationship between COP and ΔT. While in the previous publication (Prendl and Hofmann, 2020), a typical heat pump characteristic was assumed, now a real vapor compression HP was modeled and simulated with a given refrigerant and given temperature ranges to obtain the corresponding HP characteristic.

The T-h-diagram in Fig. 2 shows the thermodynamic cycle of the refrigerant (yellow) in a heat pump. This cycle consists of compression of the superheated vapor (1-2), condensation and subcooling (2-3), expansion (3-4) and the vaporization (4-1). In the HP model these single processes were modeled according to their corresponding thermodynamic relations and connected to a closed thermodynamic cycle. As stated in Eq. (7) any external losses were neglected. The refrigerant R1234 ZE was chosen in the model. With the assumption of exact saturation of vapor and condensation a characteristic for the relationship between COP and temperature difference was obtained. In Fig. 3 this characteristic is shown

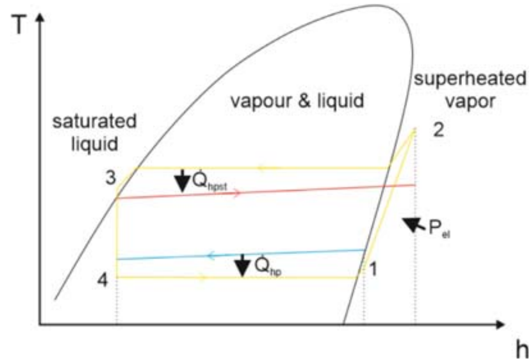

Fig. 2. T-h-Diagram of the HP model.

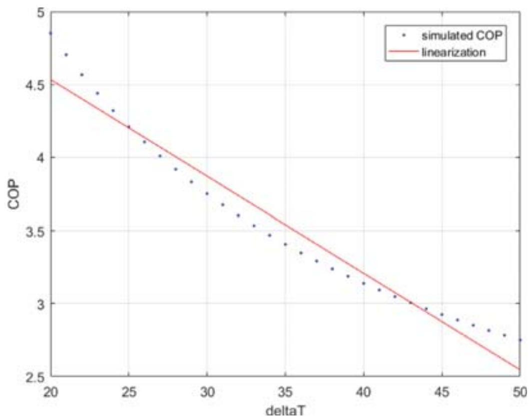

Fig. 3. Linearized COP over ΔT.

alongside with its linear approximation given in Eq. (18). The maximum deviation between the calculated COP values and the approximation for this case lies at 7.5%.

$$COP(\Delta T) \approx a_1 + a_2 \Delta T \tag{18}$$

With this relation the electrical power consumption can be expressed as a function of the supplied heat flow (in this case Q_{hpst}) and the temperature lift (Eq. (19)).

$$Pel = \dot{Q}_{hpst}/COP = Pel(\dot{Q}_{hpst}, \Delta T) \tag{19}$$

Due to the similarity of the nonlinear equation of Pel to the calculation of the heat exchanger area, a similar linearization approach as Beck and Hofmann (2018c) proposed was used. The nonlinear and nonconvex solution space for Pel gets split up into three regions along the ΔT_{hp} axis according to Eq. (20) with the index x. In this regions Pel as formulated in Eq. (19) gets approximated with linear polynomials as expressed in Eq. (21) with least squares procedure. The maximum of the obtained planes (Eq. (22)), which are shown in Fig. 4, is then used as piecewise linear and convex Constraint $CPel$ in Eq. (17) with means of BIG-M formulations.

$$\begin{aligned} &\Delta T_{hp\,1} = \Delta T_{hp\ \min} + 0.3(\Delta T_{hp\ \max} - \Delta T_{hp\ \min}) \\ &\Delta T_{hp\,2} = \Delta T_{hp\ \min} + 0.7(\Delta T_{hp\ \max} - \Delta T_{hp\ \min}) \\ &\Delta T_{hp\ \min} \geq \Delta T_{hp} > \Delta T_{hp\,1} \rightarrow x = 1 \\ &\Delta T_{hp\,1} \geq \Delta T_{hp} > \Delta T_{hp\,2} \rightarrow x = 2 \\ &\Delta T_{hp\,2} \geq \Delta T_{hp} > \Delta T_{hp\ \max 1} \rightarrow x = 3 \end{aligned} \tag{20}$$

$$Pel_x(\dot{Q}_{hpst}, \Delta T_{hp}) \approx b_{1x} + b_{2x}\dot{Q}_{hpst} + b_{3x}\Delta T_{hp} = CPel_x(\dot{Q}_{hpst}, \Delta T_{hp}) \tag{21}$$

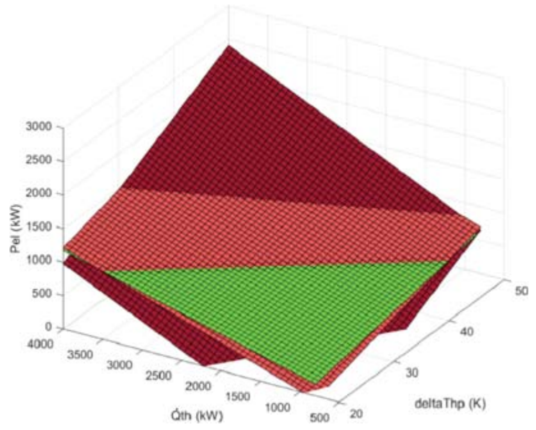

Fig. 4. Linear approximation of P_{el}.

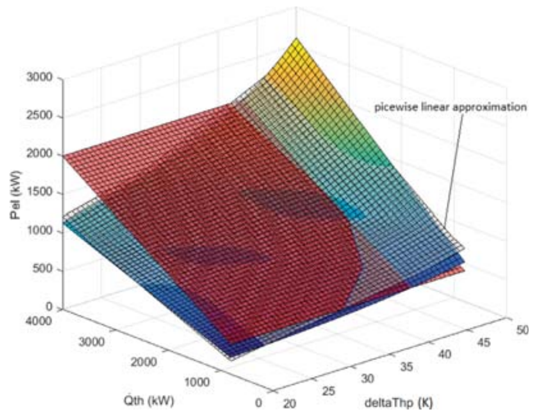

Fig. 5. Reduced solution space for *Pel*.

$$CPel(\dot{Q}_{hpst}, \Delta T_{hp}) = \max(CPel_x(\dot{Q}_{hpst}, \Delta T_{hp}) \quad x = 1, 2, 3 \tag{22}$$

Fixed boundaries for parameters of the HP, a minimum and maximum power consumption ($Pel_{\min} = 400\ kw$, $Pel_{\max} = 2000\ kw$) as well as boundaries for the temperature lift $\Delta T_{hp\ \min} = 20\ K$ and $\Delta T_{hp\ \max} = 50K$ were used. Also the HP approach temperature gets set to fixed value ($T_{hp\ ap} = 5\ K$). As further tightening measure, a lower boundary for the COP is chosen ($COP_{\min} = 3$), which cuts of the solution space as displayed in Fig. 5. The solution space above the red surface gets discarded which reduces the possible solutions and thus the computational effort considerably. The limitation of the range for the COP is justified by the fact, that heat pumps are often only considered as an economically reasonable option over an certain COP. Also the accuracy of the approximation improves and the computational times sink if the approximation domain gets tightened.

In Fig. 6 it is visible, that the percentual deviation of the approximation lies well under 10% in broad areas of the solution space. It can also be seen that the tightening cuts off areas with higher deviations, which are caused by the type and shape of the approximation surface. The lower boundary of the power consumption of the heat pump cuts of areas where even small absolute deviations cause high relative deviations where the calculated power consumption approaches zero.

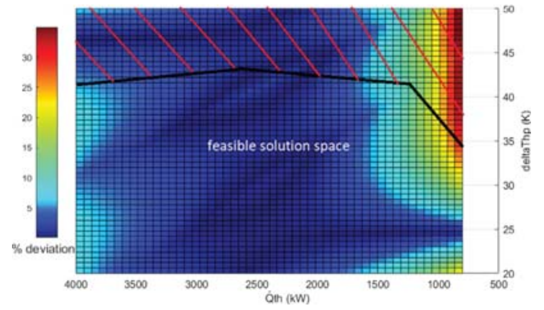

Fig. 6. Deviation of the approximation for P_{el}.

5. Test case

For the evaluation of the proposed method, a previous used test case from Prendl and Hofmann (2020) has been extended. The assumed process has a cycle time of four hours and is split into four operational periods of one hour each. It consists of three hot and three cold process streams which have varying mass flows in the different time slices. The annual operation time of the process is assumed as 8600 h. The extended superstructure model was set up with two stages with the stream data and cost coefficients given in Table 1. The two storages operate with thermo-oil as storage medium, where both oils have a heat transfer coefficient of $h_{oil} = 0.5kWm^{-2}K^{-1}$, the oil for the one tank ST has a heat capacity of $cp_{oil1T} = 1.5kJkg^{-1}K^{-1}$ and the oil for the two tank ST has a heat capacity of $cp_{oil2T} = 2kJkg^{-1}K^{-1}$. The fixed size of the one tank ST is 100000 kg and the two tank ST operates at 70 °C and 100 °C. The parameters and boundaries of the chosen HP are given in Chapter 4 except the assumed heat transfer coefficient of $h_{hp} = 5kWm^{-2}K^{-1}$. Gurobi 8.1.0 was used as solver for the MILP. The test case was chosen rather small to keep the results more traceable and the computational effort low. It has to be mentioned that even in the linear cost function, small changes of the coefficients can have huge impacts on the solution of the system. For example a modification of the variable HEX costs has an effect on all installation options and the changes in the results are hard to trace because of the complexity of the problem. Some parameters have been varied to test the behavior of the optimization for plausibility. When the electrical power costs increase, the system tends to chose HP that operate at points with higher COP, until the costs surpass a critical point where no more HP get chosen for the system. The same behavior is obtained for sinking utility costs. Also when the costs for the two tank ST increase, at some point the ST and also the HP are not chosen anymore because of the connection between them. These reactions are expected from the optimization, and are only traceable for small problems.

6. Results

The test case described in Chapter 5 was optimized in two different setups with the same parameters. First the optimization was done without the option for ST or HP to be chosen in the HEN to be able to compare the new method to traditional HENS. Then the proposed integration of HP and ST was applied to the problem.

6.1. Test case optimized without HP and ST

The optimized HEN without options for HP or ST is shown in Fig. 7 and has total annual costs of $TAC = 3,132,700$ € y^{-1}. It consists of seven stream - stream HEX and six utility HEX and the heat flows of the installations for each time period are given in Table 2. The total utility energy demand adds up 25.413 GWh y^{-1}.

Table 1
Stream data and cost coefficient of the test case.

Stream	T_{in} (C°)	T_{out} (C°)	CP (kW/K) period 1	CP (kW/K) period 2	CP (kW/K) period 3	CP (kW/K) period 4	h ($kW/m[2]K$)
Hs1	120	40	18	50	9	6	0.5
Hs2	90	30	22	22	1	2	0.5
Hs3	190	120	50	-	-	-	0.5
Cs1	20	100	20	10	10	15	0.5
Cs2	50	90	50	40	70	30	0.5
Cs3	120	150	-	-	25	25	0.5
Hu	200	200	-	-	-	-	1
Cu	10	15	-	-	-	-	1

HEX cost = 4000+500 $[A(m^2)]^{\beta}$ € y^{-1}, ST cost 1T = 28000 € y^{-1}, ST cost 2T = 7000+0.15 $[kg]$ € y^{-1}, hot utility cost = 0.2 € $kW^{-1}h^{-1}$, cold utility cost = 0.02 € $kW^{-1}h^{-1}$, $\beta = 0.83$, $dT_{\min} = 5\,^{\circ}$C electrical power costs = 0.03 € $kW^{-1}h^{-1}$, HP cost = 11000 € y^{-1}

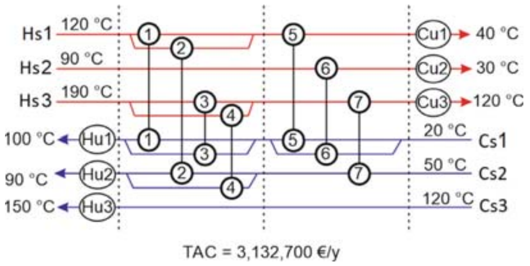

Fig. 7. HEN obtained without HP and ST.

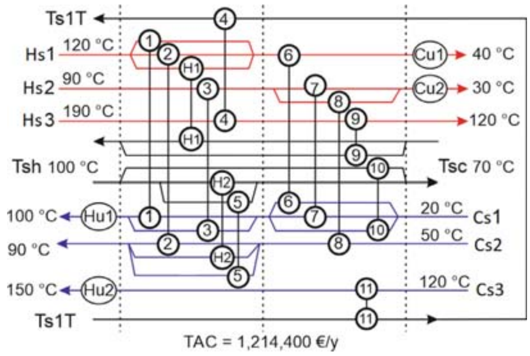

Fig. 8. HEN obtained with HP and ST.

Table 2
Heat Flows without HP and ST (kW).

	p1	p2	p3	p4
1	279.90	361.10	-	480.00
2	656.40	1600.0	585.00	-
3	914.80	-	-	-
4	694.50	-	-	-
5	186.00	297.70	135.00	
6	219.30	141.30	-	120.00
7	649.10	-	-	-
Cu1	317.70	1741.3	-	-
Cu2	1100.7	1178.7	60.000	-
Cu3	1241.7	-	-	-
Hu1	-	-	665.00	600.00
Hu2	-	-	2215.0	1200.0
Hu3	-	-	750.00	750.00

Table 3
Heat Flows and P_{el} results with HP and ST (kW).

	p1	p2	p3	p4
1	608.92	-	134.29	180.00
2	-	-	120.00	-
3	-	228.50	-	-
4	1193.2	-	-	-
5	-	1058.5	744.00	1200.0
6	737.10	421.50	465.71	300.00
7	253.99	-	-	120.00
8	516.01	541.50	-	-
9	2306.8	-	-	-
10	-	-	200.00	555.00
11	-	-	724.40	468.80
Cu1	93.990	936.01	-	-
Cu2	550.00	550.00	60.000	-
Hu1	-	150.00	-	45.000
Hu2	-	-	25.582	281.24
HP1	-	2642.5	-	-
HP2	1484.0	-	1936.0	-
Pel HP1	-	1321.2	-	-
Pel HP2	400.00	-	506.90	-

6.2. Test case optimized with integrated HP and ST

The obtained extended HEN after the application of the proposed method is shown in Fig. 8 and has total annual costs of $TAC = 1,214,400$ € y^{-1}. The network consists of six stream - stream HEX, five stream - ST HEX, four utility HEX, two HP, one 1T ST and one 2T ST and its calculated heat flows and electrical power demands are given in Table 3. For the extended HEN the total utility energy demand is 5.7873 GWh y^{-1} and the electrical energy demands for powering the heat pumps is 4.7904 GWh y^{-1} which adds up to a total external energy demand of 10.578 GWh y^{-1}. The optimized storage size for the 2T ST is $m_{St} = 247684\ kg$ thermo-oil with a storage capacity of 4.1280 MWh. Its charging state displayed over the cycle time is given in Fig. 9. The 1T ST operates between 132 °C and 161 °C and its temperature profile over the cycle time is given in Fig. 10.

6.3. Comparison

The TAC of the HEN obtained with the proposed extended approach are 61.2% lower than the TAC for the network optimized without HP and ST. The total external energy demand is 58.4% lower compared to the total external energy demand of the basic HEN which can also be seen from the values in Tables 2 and 3. Much less energy is needed because the storages allow to shift the energy over the time periods as visible in Figs. 9 and 10. The 2T ST gets charged in the first and second period and discharged at the third and fourth period. Similar the 1T ST gets charged during the first time period and discharged in the third and fourth.

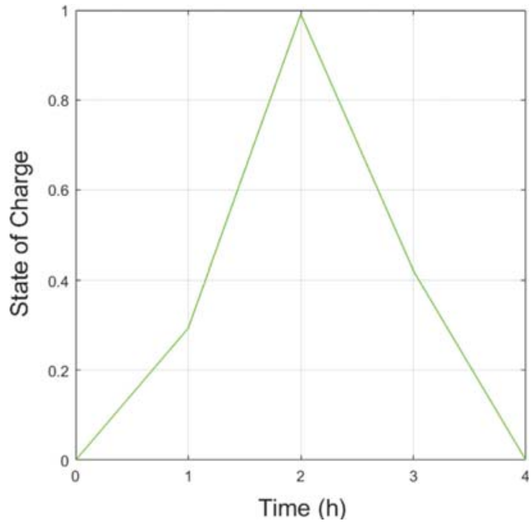

Fig. 9. Storage charging state 2T ST over cycle time.

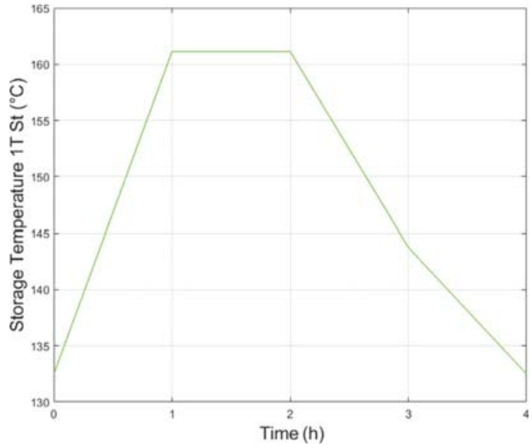

Fig. 10. Storage temperature 1T ST over cycle time.

7. Conclusion

A multi period MILP HENS approach that allows the integration of HP has been extended for the option to integrate ST with variable mass and fixed temperatures as well as ST with fixed mass and variable temperatures. In order to get more realistic HP characteristic curves, a simulation of a vapor compression HP with a chosen refrigerant was deployed. Further tightening of the COP solution space is used to improve the accuracy of the approximation and to reduce the computational effort. An previously used test case has been adapted to demonstrate the proposed method and to verify its behavior. The HEN resulting from the optimization with the new approach was able to reduced the TAC by 61.2% and the total external energy demand by 58.4% compared to the classic HEN obtained without HP and ST options. It was found that the computational times of the optimization are very sensitive to changes of physical parameters or cost coefficients. This sensitivity can also be seen in the very different network solutions that result when parameters are varied, which is caused by the nature of mixed integer programming. For comparisons with real applications, additional factors have to be considered. Costs like piping or instrumentation of installations are not included and the costs coefficients are highly dependent on specific geographical and economical factors. Although, the high reduction of cost and energy demand of the used test case is not directly comparable with real applications, even after inclusion of additional costs considerable savings can be expected trough the utilization of the developed mathematical approach.

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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Paper 3

Framework for automated data-driven model adaption for the application in industrial energy systems

Published in IEEE Access in collaboration with Lukas Kasper, Markus Holzegger and René Hofmann

In this paper, the development of a framework for automated data-driven model adaption based on open protocol bidirectional live communication between the physical and the digital system is presented. The capability of the framework to autonomously collect measurement data, train a model, predict an asset's future behavior, and analyze the current system behavior is shown on the example of an existing packed bed thermal energy storage test rig situated in a TU Wien laboratory. This use-case was chosen because of the availability of different mathematical models provided by several scientific publications that dealt with various aspects of it. The automated model adaption is applied on an assumed cyclical storage operation where continuous pollution reduces the heat transfer between HTF and SM over time. The predictions of the model that was able to learn the changed behavior of the PBR due to the developed framework provide an accurate forecast. They show considerable improvements in accuracy compared to a static model. Furthermore, the presented framework is perfectly suitable and an essential foundation for live condition monitoring, fault prediction, predictive maintenance, and operation optimization.

My contribution: Conceptualization, Methodology, Validation, Investigation, Formal Analysis, Writing – Original Draft, Visualization

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Framework for Automated Data-Driven Model Adaption for the Application in Industrial Energy Systems

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ABSTRACT Increasing flexibility and efficiency of energy-intensive industrial processes is generally seen as a big lever towards a decarbonized energy system of the future. However, to leverage these potentials, the accurate prediction of unit behavior is essential to be able to close the gap between supply and demand. Not only pose nonlinear relations a serious challenge in thermal systems engineering and optimization but real-world unit behavior furthermore changes during operation due to wear, fouling and other effects. In the present work, a novel framework for automated data-driven model adaption is presented which is capable of automating fast and accurate predictions of current system behavior. The framework is based on open protocol bidirectional live communication and mechanistic grey box modeling. While especially thermal energy storage is considered a solution to increase flexibility, it is very challenging for operation optimization. A packed bed thermal energy storage operated under severe conditions leading to continuous fouling acts as proof of concept of the proposed framework. The obtained results indicate major improvement for storage output prediction with the novel framework compared to a conventional approach without readjustment. Furthermore, the presented framework is perfectly suitable and an essential foundation for live condition monitoring, fault prediction, predictive maintenance, and operation optimization.

INDEX TERMS Automated model adaption, data-driven modeling, industrial energy systems, OPC UA.

ABBREVIATIONS AND SYMBOLS

$\dot{m}$	Mass Flow of the Heat Transfer Fluid.
l_i	Vertical Distances between the Measurement Layers.
T_{1-4}	Inner Temperatures of the Test rig.
T_b	Temperature on the bottom of the Test rig.
T_{in}	Input Temperature of the Test rig.
T_{out}	Output Temperature of the Test rig.
T_t	Temperature on the top of the Test rig.
V_i	Partial Volumes of the Test rig.
PBR	Packed Bed Regenerator.
PI AF	PI Automation Framework.
PI DA	PI Data Archive.
PLC	Programmable Logic Controller.
RMSE	Root Mean Square Error.
SCADA	Supervisory Control and Data Acquisition.
SM	Storage Medium.
TES	Thermal Energy Storage.

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I. INTRODUCTION

This Introduction presents a short motivation for the present work and a brief history and summary of related work that can be found in current literature, followed by highlighting the main contributions and the remaining structure of this paper.

A. MOTIVATION

Decarbonization efforts are a driving force for the energy-intensive industries to drastically increase energy efficiency. At the same time, we are in the middle of what is often referred to as the fourth industrial revolution or Industry4.0, driven by evolving Information and Communication Technologies [1]. Industry4.0 and the sustainable energy transition share important characteristics and can mutually benefit from each other [2], both being highly influenced by technological innovations [3]. Most researchers agree on the huge potential of digitalization for reducing energy consumption and for increasing economic sustainability [4]–[7]. As another paradigm of Industry4.0, Predictive Maintenance, achieved by real-time monitoring, can also positively affect the environment [3]. Preventive and predictive maintenance promoted by data analytics extends the lifespan of machinery, thus minimizing end of life waste [8].

The key foundation for Predictive Maintenance, as well as energy optimization is automated real-time data analytics, therefore achieving collaborative and real-time interaction between computational and physical processes [9]. Especially in thermal process engineering, so called *soft sensors* provide essential insights into the state of process operations especially in cases where the direct measurement of key process variables is very difficult, impossible or unreliable [10]–[12]. Such soft sensors have thus been developed to estimate key quality variables that are difficult to measure by constructing mathematical prediction models using the easy-to-measure process variables [13]–[15]. Predictive data, i.e. probable future values or states forecasted based on accurate models representing a given process, are therefore essential for numerous applications [16].

B. STATE OF THE ART

In the last decades, process analytics and condition monitoring have gained significant importance due to the increasing complexity of plants and machinery and vigorous economic competition. Condition monitoring can be described as "the assessment of the current condition of a physical entity by employing measurement data" [17], [18]. By preprocessing the raw data (normalization, PCA, Feature Extraction, sensor fusion, soft sensors, . . .), valuable information about the current state of the physical entity is gathered and further utilized in several condition monitoring related services like fault detection, predictive maintenance, and operation optimization. Condition monitoring approaches have relied on specific measurements during plant and machinery operation (e.g. vibration analysis, strain measurement, and thermography) [18], [19]. Current developments in sensors and signal processing systems, big data management machine learning, and improvements in computational capabilities have opened up opportunities for integrated and in-depth condition monitoring analytics [19]. Latest concepts like cyber-physical systems [20] and digital twins [21] aim to take automation to the next level and achieve collaborative and real-time interaction between the real world and the digital world [22]. The foundation for this is the bidirectional connection between the real and the digital world [21] and, therefore, virtual model synchronization.

Automated model adaption in the context of condition monitoring is primarily applied to classify and detect system faults. Prominent examples are bearing fault detection for electric motors [23], fault detection for wind turbines [24], or general rotary machines [25]–[27]. Also, condition monitoring for electrical equipment like transformers [28], or the wear of cutting tools [29] has been the topic of machine learning studies where models have been trained for classification purposes.

In general, the goal of condition monitoring applications is to detect states of damage early or to initiate maintenance before actual damage occurs, based on learned characteristics [30]. So basically, the output of the beforehand trained analysis tools is a decision if the process is in a normal or abnormal state by determining if parameters (e.g. vibration signatures, forces or temperatures) exceed defined or learned borders. This is possible because the damage mechanisms behind the phenomena to classify are often well known and distinguishable.

Contrary to this, the automated data-driven model adaption approach presented in this work allows up-to-date prediction of the future behavior of the thermodynamic component, which extends the range of possible enhancements. Common mechanisms like fouling or abrasion within industrial thermodynamic machinery bear the challenge that they are often hard to monitor during operation and are likely to impact performance and change important physical properties like heat transfer. If these changes are not critical for the lifespan of a machine, the successive task is to adapt it's operation for maximum efficiency. Accurate predictions of the asset's performance gain importance for operational optimization, since the margins of energy and resource savings are shrinking. In case of inaccurate optimization results based on non up-to-date asset models, the forecasted savings are consumed by process control, needed to keep the real process in a physically feasible state [31]. To be able to meet the need for accurate predictions mentioned above, the aim of this study was to create an innovative framework for automated data-driven model adaption for industrial thermal energy systems.

Industrial thermal energy systems are often designed for long-time service life, which traditionally comes with communication problems between systems that become deployed decades apart from each other. Either the software of the suppliers is not compatible or even the communication standard has changed. To tackle this problem, the use of unified open protocol standards continuously gains shares in the industrial communications market [32]. The OPC UA standard is widely recognized in various industries to enable interoperability and communication in all operational layers. Because the hardware and software available during the research were compatible, and the free availability of the communication standard that enables barrier-free research, OPC UA was chosen as the base of the proposed framework.

C. MAIN CONTRIBUTIONS

Peres *et al.* [16] state that there is still a clear need to further combine real-time and historical data at both the resource and system levels, as well as closing the loop to autonomously act on the results of the predictive analytics. Furthermore, solutions should be highly adaptable, being capable of changing even after deployment by learning from newly generated knowledge [33].

To the best of the authors' knowledge, no automated data-driven model adaption framework for industrial thermal energy systems has been presented so far. We therefore consider our main contribution in presenting an automated continuous model adaption framework for the application on industrial energy systems that

- relies on open protocol live communication for maximum flexibility,
- features real-time analyzes and feedback considering the current physical properties of the system and,
- is fast and easily modified on models and systems for similar applications.

Compared to systems that rely on manufacturer-specific communication standards, the presented framework can be used with a wide range of devices or programs from different sources, as long as they support the open source OPC UA standard. Because the framework allows a continuous and automated adaption of prediction models to match the properties of the real physical system, less human intervention is needed compared to traditional condition monitoring systems.

D. PAPER STRUCTURE

The remainder of this paper is structured as follows: In Section II, the proposed automation framework is described. In the following Section III, the use case subject to the proof of concept is given. The results of the exemplary framework application are then discussed in Section IV, followed by Section V, where the conclusion and an outlook on future research is given.

II. AUTOMATION FRAMEWORK

The way measurement data is recorded has undergone a long series of changes and improvements. Starting from written recordings, the emerging of new information processing technologies led to new paradigms. As data storage became cheap and practicable enough, the storage of considerable amounts of raw measurement data started. Nowadays, it is clear that the simple storage of measured data without proper procession is not sufficient for detailed analyzes that are needed for improvements of efficiency or resource demand. The raw measurement data has to be enriched with semantic data like the accuracy of the used sensors, measurement position, calibration data, or control values. A framework for automatic data acquisition and model training for industrial energy systems based on OPC UA and other modern communication protocols has been implemented exemplary on an existing test rig to meet the requirements above.

A programmable logic controller (PLC) from hardware manufacturer B&R Industrial Automation GmbH provides the operational data of the test rig via an OPC UA server hosted on the PLC itself. The test rig is controlled via the XAMControl SCADA system from evon GmbH, whereas the data handling and storage are performed by the OSIsoft® PI System.

A complete illustration of the digital infrastructure of this framework is given in Fig. 1. The test rig is located in a laboratory of TU Wien. It is connected via the university network to the control and data processing server, located in a central server room in a different physical location.

The digital and analog sensor data of the test rig (on the left-hand side of Fig. 1) gets processed in the PLC and passed on to the OPC UA server, which supplies the data to possible clients in the same network. Along with every measured value of a data point, the timestamp of the measurement and the quality of the data are transmitted.

The so-called "PI Connector for OPC UA" of the PI system acts as an OPC UA client that requests the time-series data with all its associated information from the PLC in defined intervals. This information is then copied into a specific subsystem of the PI server, the PI Data Archive (PI DA), where it is stored as a PI point. The PI DA retrieves data and serves it in real-time to all components of the PI system. The PI Asset Framework (PI AF), which is the second part of the PI server, allows an object-orientated, consistent grouping of the measurements of assets. Within the PI AF, the first analyses with low complexity are performed. For example, suppose redundant temperature measurements on the same measurement position are compared, and the difference is higher than expected by known uncertainties. In that case, a warning will be generated that initializes external intervention or even emergency procedures if necessary. So-called event frames allow the classification of states like charging or discharging, making it easier to compare the behavior of an asset for recurring operation conditions. Another connector of the PI System, the PI SQL Data Access Server, is used as a gateway to pass time series data via SQL queries to MATLAB® (on the right-hand side of Fig. 1), where the actual model training and simulation takes place.

In the given use case, the query requests a defined amount of recently completed charging and discharging events to train the model with the current state of the test rig. The trained model is then used to predict the response of the PBR and thus its temperature curves for planned future operation. The resulting prediction is then transferred back into the PI system with the help of a universal file loading interface that reads the data points from a defined output file of the MATLAB® model and copies them into the PI DA (bottom right in Fig. 1).

The predicted values of the temperature measurements are stored as future control values, which can be seen as additional attributes of the measurements, allowing for a real-time comparison of the measured values and their prediction, taking the test rig's real condition into account. Decisions resulting from the analyses or comparisons are then sent back to the PLC and thus to the SCADA system via a custom programmed Python™ Wrapper that acts as connector between OPC and OPC UA, allowing the system to react to them directly.

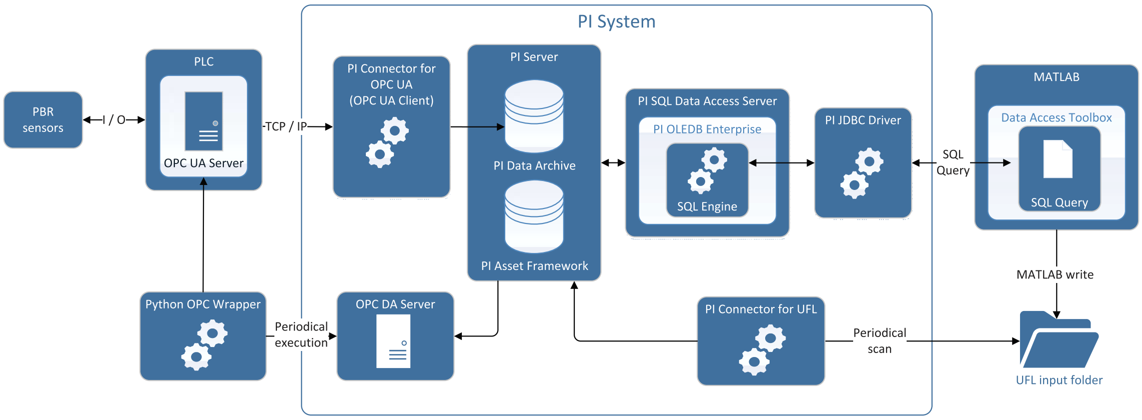

FIGURE 1. **Digital infrastructure of the presented framework.**

III. SELECTED USE CASE

Industrial energy systems typically consist of energy supplying components, energy storages, energy conversion components like heat pumps, and energy demanding components as exemplary depicted in Fig. 2. Therein, two processes, a fractionating column and a particle dryer, are fed with thermal energy by an energy supply component. Without the possibility of storage or conversion of energy, the energy supply has to satisfy the demands regardless of efficiency concerns to keep the processes running. As addressed in earlier work of Prendl *et al.* [34], energy demand and excess energy in industrial processes are often offset in time. Hence, heat recovery in combination with energy storage allows to reduce the external energy demand and, thus, the use of resources and the emission of CO_2. Furthermore, since different temperature levels often occur in energy-intensive processes and not only one temperature level like in Fig. 2, the integration and operational optimization of several different storage units is a common problem. Economic operation of such industrial energy systems is even more complicated by the increasing share of renewable energy sources and the resulting highly volatile energy prices. Therefore, increasing focus is laid on process control with optimized storage management, which is dependent on accurate predictions of component behaviour. In the following, this paper deals with the storage as central component.

A. PBR TEST RIG

As exemplary use case, an existing packed bed regenerator (PBR) thermal energy storage (TES) test rig situated in a TU Wien laboratory is used. It consists of an insulated conical metal container filled with gravel as a storage medium (SM) that is equipped with temperature measurement sensors in several layers as shown in Fig. 3. The PBR is charged by electrically heated air acting as heat transfer fluid (HTF) from top to bottom and discharged with ambient air from bottom to top. A detailed description of the PBR can be found in several scientific publications that dealt with different aspects of the storage and already provided insights on it's properties and behavior [35]–[39]. Also, different models for simulation [36], [37], [40] and optimization [31], [38] for the test rig have been created and validated in the past.

However, in real operation, deviations from ideal laboratory conditions can influence the behavior of machinery. Processes such as fouling or wear that occur over time are often hard to measure or quantify, especially in the running operation. In case of the PBR for example, deposition can occur if the HTF is polluted with particles smaller than the bed material. The passable cross section can change, flow channels can form, or the heat transfer to the bed material can be influenced. Further, the particle size of the bed material can change because of thermal degradation or abrasion. These or similar effects can occur during real plant operation and change the heat transfer inside the PBR. Thus, to maintain optimum operational capability, models used to predict the future behavior of assets must be kept up to date.

B. GREY BOX MODEL

Amongst the simulation models mentioned above, especially the mechanistic grey box model developed by Halmschlager *et al.* [40] is capable of fast and easy adaption to changed properties and is robust at the same time. This modelling approach is therefore used and adapted for the proof of concept of our framework and described in the following paragraph. For a detailed mathematical description of the applied modelling approach, we refer to the chapter "Extended Grey Box Model 2" in the original publication [40].

The mechanistic grey box model consists of physical relations/equations and uses measurement data to optimize specific parameters of these equations. While only a small number of equations needs to be solved for model training, the model shows excellent prediction performance and stands out compared to data-driven and physical models by its high accuracy, low computational effort and high robustness [40]. An illustration of the test rig and the vertical position of the measurement layers is given on the left hand side of Fig. 3. The model uses the inlet temperature T_{in} and the mass

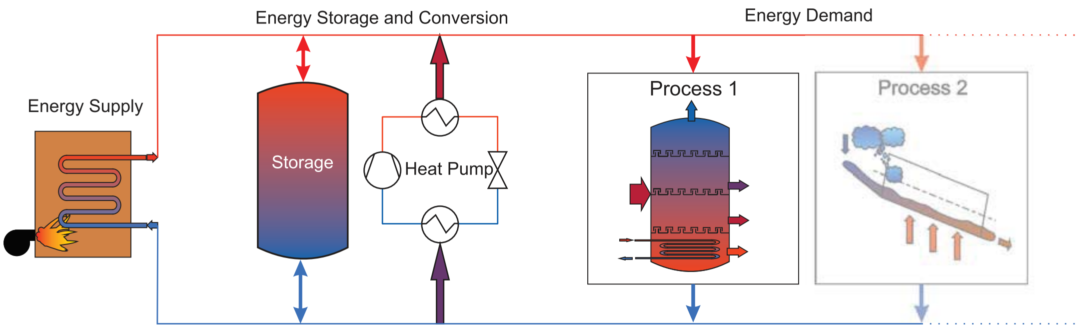

FIGURE 2. Exemplary industrial energy system, consisting of energy supplying components, energy storage components, energy conversion components, and energy demanding components.

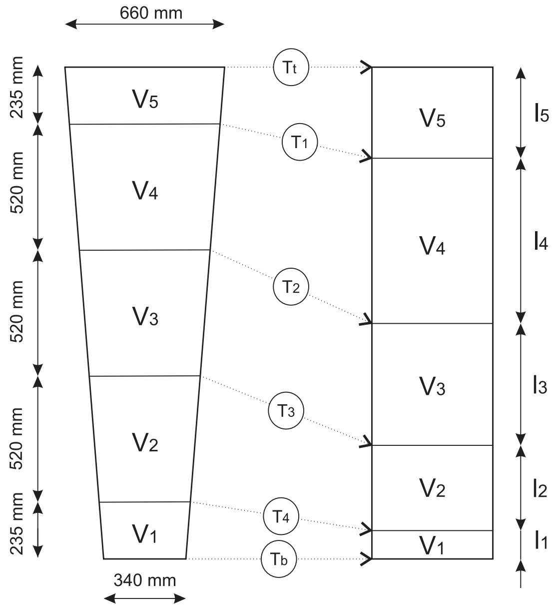

FIGURE 3. Actual conical shape of the PBR with the vertical position of the measurement layers in comparison to the cylindrical simplification of the grey box model.

flow $\dot{m}$ of the HTF to calculate the corresponding output temperature T_{out} of the PBR. During charging, T_{in} equals the temperature at the top of the PBR T_t and the T_{out} equals the temperature at the bottom of the PBR T_b. During discharging, T_{in} equals T_b and T_{out} equals T_t, since the direction of flow is reversed, as explained above.

If the model's target is to predict the output temperature, the cost function to be minimized consists of the root mean squared error (RMSE) of the model output temperature compared to the training data output temperature. In [40], existing measurement data of the PBR is used for the training and validation of the model. While predictions of T_{out} showed high accuracy, predictions of internal temperature values T_1 to T_4, which were not part of the optimization target, showed significant deviations. This is due to the fact that the conical vessel shape of the PBR was approximated to a cylindrical shape.

In case not only the output temperature of the PBR, but also its internal condition is of interest, the prediction of the internal behavior gains importance. In order to improve the prediction, the vector of the measurement positions is corrected in this work, in a way that the ratios of the volumes and thus the ratio of the masses between the measurement layers match the ratio of the volumes of the real conical shape. This transformation is depicted in Fig. 3. Because the heat capacity of the SM, the HTF, and the wall are included in the factors that are fitted during training, only the ratio of the volumes (V_i) and not the absolute values of them is of importance for the accurate prediction of the internal temperatures T_1 to T_4. The assumption of a cylindrical vessel causes the ratios of the distances (l_i) between the measurement positions to equal the volume ratio as expressed in (1). The correction introduced here has no significant impact on the prediction of T_{out} but results in a vast improvement of the prediction of the internal temperatures, which can be seen in Fig. 4. In the upper part of Fig. 4, a time series of simulated temperature measurements of the PBR compared with the predictions of the uncorrected model (dotted lines) and the new corrected model (dashed line) is shown. In combination with the prediction error plot below, it is visible that drastic improvement could be achieved. This shows the importance of choosing the right assumptions and simplifications for the development of models or correlations to meet specific demands.

$$\begin{aligned} V1 : V2 : V3 : V4 : V5 \\ = l1 : l2 : l3 : l4 : l5 \\ = 0.117 : 0.352 : 0.503 : 0.682 : 0.375 \end{aligned} \tag{1}$$

IV. EVALUATION AND RESULTS

For a comprehensive testing of the framework, a validated one-dimensional finite difference model of the PBR based on the modelling approach introduced by [39] is used to generate training and test data sets. The assumed load cycle as given in Fig. 5 is used as an exemplary measurement data. The charging temperatures vary between 170 °C and 260 °C whereas the discharging temperature is constant at a 22 °C ambient temperature. The HTF mass flow $\dot{m}$ is assumed constant at a value of 150 kg/h.

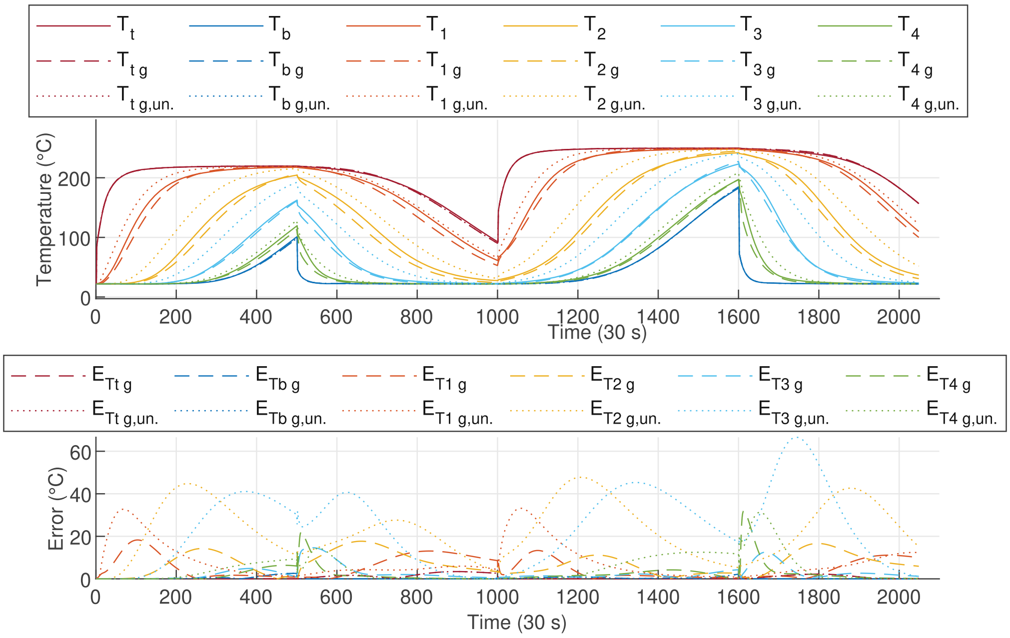

FIGURE 4. Comparison of simulated inner temperatures with the uncorrected model ($T_{i\ g.un}$) and the corrected grey box model ($T_{i\ g}$) and their respective error compared to the measurement values (T_i).

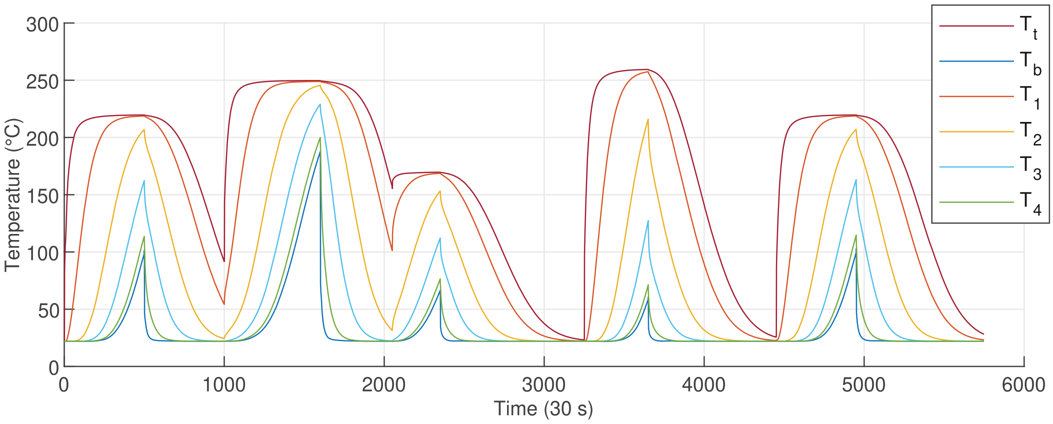

FIGURE 5. Time series of temperature values of the assumed test data set.

For the simulation of pollution or fouling, it is assumed that the given load cycle is repeated in a cyclical manner while the heat transfer coefficient between HTF and SM is gradually decreasing over time. Naturally, real pollution processes not only cause a reduction of the heat transfer coefficient. A variety of mechanisms lead to changes in the behavior of the PBR or the flow conditions of the HTF. However, in this work, the change of the heat transfer coefficient was chosen as pollution indicator, because of the clear impact and traceability of the simulated behavior change.

The temperature response of the PBR is simulated for 8 example cycles while the heat transfer coefficient between the HTF and the SM is reduced by 10 % in every cycle. The resulting temperature curves are then stored on the PLC and supplied to the framework as would be the case when using real sensor data.

Two different model training scenarios are assumed for evaluation of the proposed framework on real operation conditions. Firstly, a traditional model training approach is applied, where the model is trained only once with the initial data without reduced heat transfer coefficient. Secondly, a model is initially trained with the same data but is retrained after every full cycle with the measurements from the previous cycle in order to adapt to changes in the physical behavior caused by pollution. The predictions of the temperatures for the subsequent cycles of the only once trained model (in the following denoted as $T_{i\ g}$) and the continuously trained model (in the following denoted as $T_{i\ gtrain}$) are then compared to the simulated measurement data.

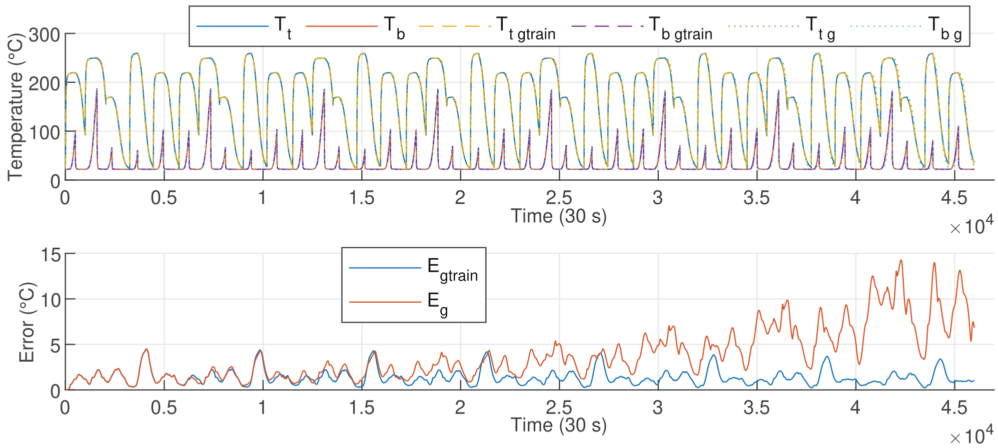

FIGURE 6. Comparison of simulation results for the input and output temperatures of the cyclical trained model ($T_{i\ gtrain}$) and the only initial trained model ($T_{i\ g}$) over the continuous sinking heat transfer between HTF and SM and their errors (E_i) compared to the generated measurements (T_i).

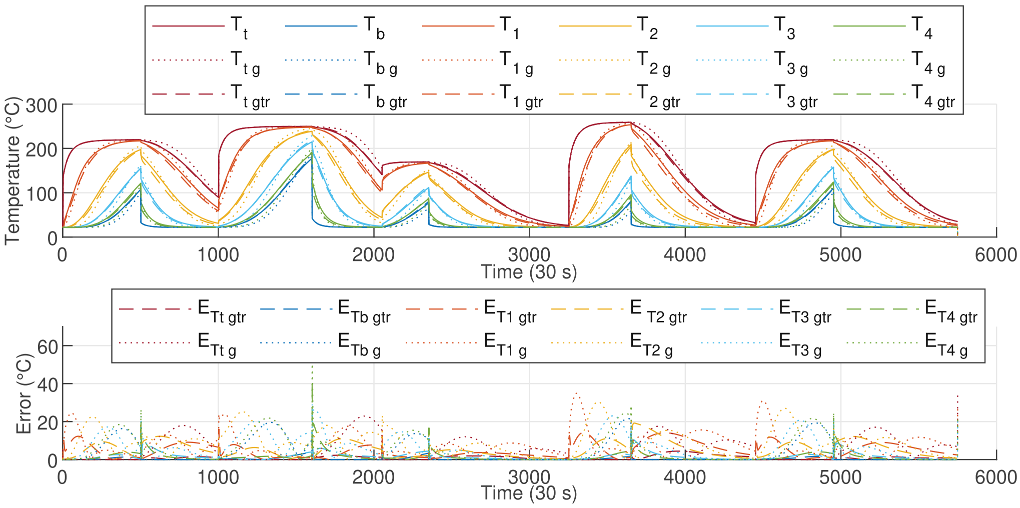

FIGURE 7. Simulation results of the cyclical trained model ($T_{i\ gtrain}$) and the only initial trained model ($T_{i\ g}$) for the cycle with the maximum pollution and their respective errors (E_i) compared to the generated measurement values (T_i).

In Fig. 6 the input and output temperature curves are given with their respective prediction results and the absolute errors between them. The values for the static model $T_{i\ g}$ are dotted, and the values of the adapted model $T_{i\ gtrain}$ are dashed. It is clearly visible here, that the absolute error of the once trained model is steadily increasing over time while the error of the continuously trained model stays in the same range. The error for $T_{i\ gtrain}$ even slightly decreases over time, which might be a consequence of more data that is available for model training.

For the sake of better visibility, the inner temperatures predictions are not shown in Fig. 6. However, to visualize the vast improvement the last test cycle with maximum pollution is given in detail with all inner temperatures in Fig. 7. One can see that the predictions of the static model (dotted lines) clearly differ from the measurements, while the predictions of the continuously trained model are hardly visible because of the small error. This also shows in the lower part of Fig. 7, where the errors of the predictions are displayed.

For quantitative analysis, the total RMSE (Root Mean Square Error) for all temperature predictions of the cycle with the highest pollution, given in Fig. 7, is calculated. For the untrained model, a RMSE of 9.10 °C was obtained whereas the retrained model featured a RMSE of 4.05 °C. This improvement in accuracy requires additional computational time of only a few seconds for retraining of the model, whereas measurement intervals for the PBR sensors of one minute are considered sufficient. Even this seemingly small difference of a few degrees in the model output can significantly change the optimum solution of optimization procedures like the heat exchange network synthesis (HENS) [34] or scheduling [31], resulting in deviating planning and control strategies.

V. CONCLUSION

A novel framework for the automated data-driven model adaption for industrial energy systems is presented. The framework's capability to autonomously collect measurement data, train a model, predict an asset's future behavior, and analyze the current system behavior is shown with the help of a PBR TES as a use case.

The automated model adaption is applied on an assumed cyclical operation of the storage where continuous pollution reduces the heat transfer between HTF and SM over time. The predictions of the model that was able to learn the changed behavior of the PBR due to the developed framework provide an accurate forecast and show considerable improvements in accuracy compared to a static model. The maximum absolute error of the static model was up to 14.2 °C whereas the maximum error of the learning model was only 4.3 °C. This means the prediction error could be reduced up to 70 % within the given boundaries. Considering that even small potential efficiency improvements add up to large monetary savings for the energy-intensive industry, improvements like this are gaining importance as the crucial factor in economic operation.

However, it is important to consider that automated model adaption comes with all its advantages and disadvantages. As long as a robust and suitable model is used, the automation reduces the operator's workload. However, if incorrect measurement data is not detected and then used for the model training, the resulting model and it's predictions are also incorrect. Thus, accurate and up-to-date predictions are needed to monitor the measurements and initialize immediate system response or external intervention if necessary.

The implemented framework can be seen as a foundation for real-time condition monitoring, fault prediction, predictive maintenance, and operation optimization, all of which rely on advanced communication.

The presented automation framework yields the potential to characterize similar TES with small adaptions and only little training data from initial measurements.

Furthermore, our framework is applicable for variable industrial energy systems, provided appropriate system models are used. For further evaluation of this topic, a research project concerning the enhancement of the test rig that allows for the contamination of the HTF with pollutants is already in the development state within the author's research unit. The real measurement data obtained by this enhancement of the test rig will allow for comprehensive comparisons of different prediction approaches for this problem and further evaluation of the framework presented in this work.

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Paper 4

Case Study of Multi-Period MILP HENS with Heat Pump and Storage Options for the Application in Energy Intensive Industries

Published in Energies in collaboration with René Hofmann

Due to the lack of suitable publicly available industry data and literature use-cases, this paper introduces four industry-orientated use-cases from different energy-intensive industries (EII) sectors for multi-period HENS with heat pump and storage options. The cases are based on the popular energy analyses of industrial processes by Hamel et al. (1979). The application of the approach developed in **Paper 1** and **Paper 2** resulted in a reduction of the total annual costs up to 55.43 % and a reduction of total external energy demand up to 87.1 % compared to the basic HEN without heat pumps and storages. In combination with their solutions, the introduced cases and their underlying open-accessible mathematical formulation of the optimization procedure contribute valuable information to the literature in the field of HENS.

My contribution: Conceptualization, Methodology, Validation, Investigation, Formal Analysis, Writing – Original Draft, Visualization

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Article

Case Study of Multi-Period MILP HENS with Heat Pump and Storage Options for the Application in Energy Intensive Industries

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Abstract: The environmental goals of initiatives such as the European Green Deal, which aims to achieve climate neutrality for the EU by 2050, increase the importance of improving and optimizing industrial processes. Mathematical optimization methods like heat exchange network synthesis (HENS) are crucial tools in enabling industry to identify potential energy savings and cost reductions. The lack of publicly available industry data suitable for comprehensive testing of novel optimization procedures is often a major obstacle in development and research. To tackle this problem for extended HENS with potential heat pump and storage integration and show the potential of energy integration in energy-intensive industries (EII), the authors introduce a set of four use-cases based on representative industrial processes from the EII. The application of a previously presented a HENS approach for the integration of heat pumps and storage on these cases resulted in a potential reduction of total annual costs up to 55.43% and total external energy demand up to 87.1%. The presented cases, their solutions, and the open-access mathematical formulation of the optimization procedure make a valuable contribution to the literature and future research in the field of HENS.

Keywords: mixed integer linear programming; heat recovery; heat pump; thermal energy storage; design optimization; case study

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1. Introduction

With a share of around 25% of the final energy consumption in the European Union, the industrial sector plays an essential role in the ongoing transition necessary to reach the target of carbon neutrality [1]. A certain part of the industry, the energy-intensive industries (EII), which mainly consist of the sectors iron and steel, refineries, cement, petrochemicals, fertilizer, lime and plaster, pulp and paper, aluminum, inorganic chemicals, and hollow glass, account for 85% of Europe's industrial greenhouse gas (GHG) emissions. Especially for these EII, the planned climate neutrality by mid-century is coupled with drastic changes in production. The most promising adaption options are reducing energy demand through efficiency improvement, using clean energy sources in the form of renewable electricity or carbon-neutral energy carriers, and utilizing carbon capture and storage technologies. Major obstacles for these measures are that over short time horizons, traditional investments like capacity expansion often offer a better return, and the lower costs of comparable fossil technologies [2]. To lower these barriers as much as possible, the optimal integration of emission-reducing technologies, and thus research in mathematical optimization of processes, plays a crucial role in the energy transition. Independent of the type of optimization, extensive tests with example data sets are needed to evaluate and verify the capabilities of novel approaches. Often industrial data in the right quality or amount are not available, or existing data from the literature are insufficient or unsuitable. This problem was also encountered during previous work on the development of an approach for multi-period

mixed integer linear programming (MILP) heat exchange network synthesis (HENS) with simultaneous integration of storage (ST) and heat pumps (HP) presented in [3].

In this approach, the introduction of HP and ST to HENS represents the before mentioned measures of improving energy efficiency by the possibility of shifting thermal energy over time and usage of renewable electricity through HP. Since suitable multi-period example data for proof of concept was not available in the literature, a previously used test case was extended to multiple time periods to show how the approach is able to properly integrate HP and ST into heat exchange networks.

HENS is an extensively researched and prominent topic which shows in the high number of recently published studies. They deal with the different aspects of HENS, for example, with cost-optimal HENS [4], practical retrofitting of HEN [5], or the consideration of different types of heat exchangers (HEX) in HENS [6]. Case studies for different HENS procedures show some difficulties, as explained in the following. For basic single period HENS, the results of different solvers are generally comparable. An example is a case study comparison by Escobar and Trierweiler [7], where some of the most cited example cases, such as the stream data introduced in [8] or [9] are analyzed. Because these cases only deal with continuous operation in one thermodynamic state and only basic HEN solutions with HEX and utilities are considered, solutions of different optimization approaches are reasonably comparable. In contrast to this, the solutions of multi-period HENS solvers are often not directly comparable, which is due to the different approaches that are used. Further extended multi-period HENS solutions that integrate HP and ST options are even more specific because of the possible placement of installations or the cost coefficients used in the different approaches.

For multi-period HENS, only a tiny number of examples can be found in the literature, like the stream data presented in [10] or [11]. The cases used or introduced in these studies are given for several time periods, but their operational temperatures lay mostly out of the physical boundaries of HP and are therefore not suitable for usage in this work. Other multi-period stream data are used with wholly different approaches like the heat recovery loop approach by Stampfli et al. [12]. This approach focuses more on selecting the optimum HP technology than the optimized integration of given components by using wholly different optimization targets and specific cost coefficients.

As already stated in [3], mixed-integer programming optimizations solutions are sensitive to changes of parameters in the cost function, on account of its combinatorial nature. This means those cost coefficients that have to be assumed because they are not available for given problems, like for HP or ST cost, strongly impact the specific solutions. Because of this, a meaningful comparison of the resulting networks or the total annual cost (TAC) with solutions of cases dealt with in the literature is nearly impossible. We therefore limit ourselves in this paper to comparing the solutions without ST and HP with the solutions with possible HP and ST installations obtained using the described optimization program.

For a more comprehensive evaluation of the approach presented in [3], to show the potential of HP and ST integration for EII, and to augment the existing literature, it was decided to generate a set of example problems, which are described in Section 2 below. These cases are based on information from the detailed energy analyses of a wide variety of processes provided by Hamel et al. [13], which provide flowcharts and energy balances of 108 prominent industrial processes. In combination with the optimization results obtained with the application of the approach explained in Section 1.2, these example problems are intended to extend the possibility of evaluating future multi-period HENS approaches, with an emphasis on the integration of renewable energy sources and contributing to the existing literature.

1.1. Objectives, Novelty and Contribution

As elaborated above, the development and verification of optimization approaches relies on the availability of suitable data. Contrary to HENS studies like the case study by Escobar et al. [7], the analyses by Floudas et al. [10], or the case study by Zhang et al. [11], where only the integration of HEX between the streams and utility HEX are considered, the possible integration of HP and ST has stricter thermodynamicall requirements for suitability of stream data. Because no cases found, either from industry or the literature, satisfyingly fulfill these requirements, this work aimed to provide suitable cases for further research in the area of HENS with HP and ST integration and to show the potential of energy integration for energy integration in EII. Therefore we consider our main contribution in the introduction of four use-cases for HENS that

- Are based on the thermal requirements of representative real industrial processes from different sectors of the EII;
- Have varying potentials for energy shifting and the integration of renewable energy sources;
- Lay within the operational temperature range of HP.

On the one hand, analysis of the presented cases in described in Section 1.2 shows the potential of HP and ST integration for reducing energy demand and costs for different sectors of the EII. On the other hand, the introduced cases with their corresponding solutions and the fully given and open-access mathematical formulation of the optimization procedure are a valuable base for future research in the area.

1.2. Applied MILP HENS Optimization Tool

As mentioned in the Introduction, the implementation of new example cases presented in this paper results from the need for data to support extended testing of the multi-period MILP HENS with simultaneous integration of ST and HP approach presented in [3].

The setup of the stage-wise superstructure of this approach is shown in Figure 1 with all its possible connections and installations. A set of hot streams (Hs) and cold streams (Cs) that have to reach a defined target temperature represent the demands of a given process. The possible installations for each stage in each timestep are heat exchangers (HEX) between every Hs and every Cs, HEX between the streams and the storages, and HP between a two tank storage and the streams. If more than one installation is chosen for one stream in a stage, the stream is split at the beginning of the stage and mixed isothermally at the end of the stage. Utilities are only permitted after the last and before the first stage. If the same HEX location is selected in more than one timestep, the largest HEX surface area is chosen, and bypasses are assumed for the other timesteps. The cost function given in Equation (A1) of Appendix A consists of step fixed investment costs and variable investment costs for all installations, and energy costs for external energy demand. The optimization finds the best combination of the possible installations to minimize the cost function while assuring that all streams reach their required target temperature. The simplifications necessary for the linearization of the problem formulation come with the introduction of uncertainties in the calculations. This negative aspect is canceled out by the multiple advantages, like the reduction of the mathematical complexity, which reduces the calculation effort and thus processing time. The linearity of the approach eliminates the need for an initial solution, which is often difficult to find for mixed-integer problems. Moreover, the linear and convex optimization procedure always results in a globally optimal solution under the consideration of all given boundaries. These improvements allow for quick and easy analysis of a wide range of problems.

For reasons of completeness, the full mathematical formulation of the applied MILP HENS from Prendl et al. [3] is given in Appendix A in Equations (A1)–(A13).

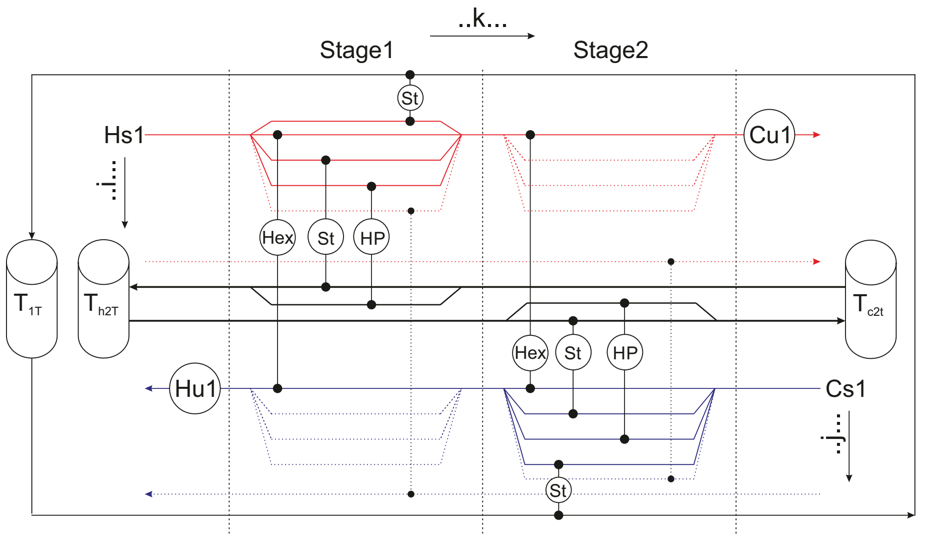

Figure 1. "Superstructure with possible Stream-Stream Hex (HEX), Stream-Storage Hex (ST) and Heat Pumps (HP)" from Prendl et al. [3]/CC BY 4.0.

2. Test Cases

Four processes representative for the EII described in Section 1 have been chosen to analyze the potential improvement by introducing HP and ST with the help of the optimization approach described in Section 1.2. The processes are a weaving mill for human-made fiber (case 1), a pulp mill (case 2), an alkalies and chlorine process (case 3), and a PVC-suspension process (case 4). As explained earlier in Section 1, the data given by the literature are often not suitable for specific approaches without additional assumptions caused by the lack of essential information. The process data from [13], which are used as the base case, are only given for continuous operation in one particular state as energy balances of the different process steps. To generate suitable use-cases, the processes are analyzed to extract streams that have properties suitable for heat exchange between streams. The extracted inlet temperatures and outlet temperatures of this streams are given in the stream data Tables 1–4. Because the energy balances in [13] are scaled down to energy demand per produced unit, the heat capacities are scaled to plant sizes suitable for the optimization procedure, while the ratios of the heat capacities of the streams are kept constant for the first operational period p. The stream data are extended for multiple periods, assuming that parts of the processes change over time depending on the product or startup or shutdown processes, to generate suitable example cases for heat pump and storage integration. Cases 1-3 are extended to four, and case 4 to three time periods. The cases are assumed to repeat cyclically over the annual operation time of 8600 h. Care was taken to ensure that timely mismatch of excess energy and energy demand occurs to generate possible opportunities for storages. Often, multi-period test cases in the literature consist of equal time periods for reasons of simplification as in [14], where stream data from [10] are used and adapted to be usable for the applied method. To test the optimization procedure on its ability to deal with a broader range of applications, the duration of the periods is varied for two of the cases.

The same hot utilities (Hu) and cold utilities (Cu) are given for all processes. Furthermore, the possible ST and HP options are the same for all examined cases.

As utilities, steam with an inlet and outlet temperature of 200 °C and hot utility costs of $c_{hu} = 0.2$ €kWh^{-1}, and cold water with an inlet temperature of 10 °C and an outlet temperature of 15 °C with cold utility costs of $c_{cu} = 0.02$ €kWh^{-1} are given. As HP option, the linearized HP in [3] is used with the following boundaries: The power consumption of the HP lies in the range from $Pel_{min} = 400$ kW to $Pel_{max} = 2000$ kW while the possible temperature lift of the HP ranges from $\Delta T_{hp\ min} = 20$ K to $\Delta T_{hp\ max} = 50$ K. The maximum condensation temperature of the HP is 115 °C. The lower boundary of the COP is set to $COP_{min} = 3$, and the HP approach temperature is chosen as $T_{hp\ ap} = 5$ K. The heat transfer coefficient of the HP is assumed with $h_{hp} = 5$ kWm^{-2}K^{-1}.

The one tank ST uses thermo-oil as storage medium with a heat capacity of $cp_{oil1T} = 1.5$ kJkg^{-1}K^{-1} and a heat transfer coefficient of $h_{oil} = 0.5$ kWm^{-2}K^{-1}. The thermo-oil used by the two tank St has the same heat transfer coefficient but a higher heat capacity of $cp_{oil2T} = 2$ kJkg^{-1}K^{-1}. The one tank storage has a fixed size of 100,000 kg while its operational temperature is optimized during the HENS. The two tank storage has a variable size, but the temperatures of the two tanks, 70 °C and 100 °C, are preset. The remaining cost coefficients used for all cases are given at the bottom of Table 1. In the following subsections, the individual cases are described in detail:

2.1. Case 1

According to the analyses by Shen et al. [15], comparing human-made fiber production around the world, the processes involved have considerable potential for energy optimization. The growing customer demand for environmentally friendly products has increased the industry's willingness to invest in measures to tap this potential. The streams suitable for HENS within the process include pulp slurry that needs to be heated (Cs1) or cooled (Hs2), process water for mixing (Cs2) or cooling (Hs3), process air (Hs3, Hs4), and flue gases (Hs1). As shown in Table 1, where the stream data for case 1 are given, the streams operate in a range from 25 °C to 200 °C. The overlapping temperature intervals of the Hs and the Cs show potential for heat exchange between the streams. The accumulated heat flows of the individual streams range from 350 kW to 7500 kW. Without the possibility of energy transfer between the time periods and assuming no thermodynamic restrictions exist, the minimum heat surplus or demand can be simplified estimated by adding the heat flows of the Hs and subtracting the heat flows of the Cs for each time period. This minimum is in reality only reachable, if the heating and cooling demands fulfill all thermodynamic requirements for heat transfer and is thus only used for a first estimation. For case 1, this results in a theoretical heat surplus of 100 kw in period 1 and a heat surplus of 3200 kW in period 2, while period 3 and 4 have a heat demand of 4400 kW and 1800 kW, respectively. The timely mismatch of energy surplus and demand on the given temperature levels offers potential for the integration of HP and ST to significantly reduce the external energy demand.

Table 1. Stream data and cost coefficients for case 1.

Stream	T_{in} (°C)	T_{out} (°C)	CP (kW/K) Period 1	CP (kW/K) Period 2	CP (kW/K) Period 3	CP (kW/K) Period 4	h (kW/m^{2}K)
Hs1	200	100	20	40	10	40	0.5
Hs2	190	90	20	20	20	20	0.5
Hs3	60	30	100	20	100	20	0.5
Hs4	70	30	35	25	35	25	0.5
Hs5	120	80	40	40	40	40	0.5
Cs1	25	150	14	20	14	60	0.5
Cs2	25	70	150	70	150	70	0.5
Cs3	95	130	40	10	140	10	0.5
Hu	200	200	-	-	-	-	1
Cu	10	15	-	-	-	-	1

HEX cost = (4000 + 500[A(m^2)]^{fi}) €y^{-1}, ST cost 1T = 28,000 €y^{-1}, ST cost 2T = (7000 + 0.15[kg]) €y^{-1}, hot utility cost = 0.2 €kW^{-1}h^{-1}, cold utility cost = 0.02 €kW^{-1}h^{-1}, $\beta = 0.83$, $dTmin = 5$ °C electrical power costs = 0.03 €kW^{-1}h^{-1}, HP cost = 11,000 €y^{-1} period durations: $\tau_1 = 2$ h, $\tau_2 = 3$ h, $\tau_3 = 2$ h, $\tau_4 = 1$ h.

2.2. Case 2

The pulp and paper industry is constantly growing, driven by the need for environmentally friendly packaging and other factors, but faces a challenge in increasing cost efficiency to stay competitive while reducing their environmental impact because of regulations. From the pulp mill process different streams of pulp solutions with cooling demand (Hs1, Hs2) or heating demand (Cs1, Cs3) as well as process water (Hs3, Cs2) have been found potential candidates for HENS. The stream data for these extracted streams are given in Table 2. The temperature intervals of the streams lay between 20 °C and 170 °C and the heat flows of the streams reach from 300 kW to 2610 kW. In period 1 and 4 a theoretical minimal heat demand of 1405 kW and 2490 kW can be calculated, while period 2 has a theoretical heat surplus of 500kW and period 3 has a theoretical heat surplus of 2640 kW, while on the one side the overall utility demand can be potentially reduced by the introduction of ST to shift energy from periods 2 and 3 to periods 1 and 4, especially the streams Hs2, Cs2, and Cs3 seem suitable for installations of HP to replace utility demand with renewable energy sources because of their temperatures.

Table 2. Stream data for case 2.

Stream	T_{in} (°C)	T_{out} (°C)	CP (kW/K) Period 1	CP (kW/K) Period 2	CP (kW/K) Period 3	CP (kW/K) Period 4	h (kW/m^{2}K)
Hs1	170	20	9	9	12	9	0.5
Hs2	110	60	16	32	40	16	0.5
Hs3	60	40	26	26	70	26	0.5
Cs1	25	170	15	6	8	18	0.5
Cs2	55	100	20	40	20	30	0.5
Cs3	30	80	20	6	10	24	0.5
Hu	200	200	-	-	-	-	1
Cu	10	15	-	-	-	-	1

period durations: $\tau_1 = 1$ h, $\tau_2 = 1$ h, $\tau_3 = 1$ h, $\tau_4 = 1$ h.

2.3. Case 3

Chlorine production is an energy-intensive process, where a direct supply of electricity is needed for the electrolysis necessary to produce it. Thus, energy savings are only possible through the reduction of the auxiliary energy demand according to the economic analyses of the chlor-alkali industry by Herrero et al. [16], which is achievable through HENS. From the base process in [13], heating and cooling of brine (Cs1, Cs2, Hs1), process water heating (Cs3), NaOH solution heating (Cs4), as well as hydrogen (Hs2), chlorine gas (Hs3) and caustic liquid cooling (Hs4) were identified as possible streams for this purpose. In Table 3, the stream data for all operational periods are given. The heat flows of the streams reach from 75 kW to 11250 kW and the operational temperature reaches from 25 °C to 110 °C. Theoretically, periods 1 and 2 have a heat surplus of 600 kW and 3900 kW, respectively, while period 4 has an heat demand of 6175 kW. In Period 3, theoretically no external energy is needed if all surplus heat from the Hs is transferable to the Cs. The temperatures of the streams and the timely mismatch of surplus heat and heat demand offer potentials for HEX, HP and ST introduction to reduce the external energy demand.

Table 3. Stream data for case 3.

Stream	T_{in} (°C)	T_{out} (°C)	CP (kW/K) Period 1	CP (kW/K) Period 2	CP (kW/K) Period 3	CP (kW/K) Period 4	h (kW/m^{2}K)
Hs1	80	60	50	50	20	50	0.5
Hs2	110	35	110	150	110	160	0.5
Hs3	110	35	60	60	60	60	0.5
Hs4	100	40	40	40	40	40	0.5
Cs1	25	80	120	120	120	120	0.5
Cs2	60	100	130	70	130	60	0.5
Cs3	25	95	40	70	40	60	0.5
Cs4	40	85	30	30	30	30	0.5
Hu	200	200	-	-	-	-	1
Cu	10	15	-	-	-	-	1

period durations: $\tau_1 = 2$ h, $\tau_2 = 1$ h, $\tau_3 = 2$ h, $\tau_4 = 1$ h.

2.4. Case 4

The energy-intensive production of PVC, which is the main application of chlorine in the EU, shows energy recovery potential on temperature levels suitable for HP and St integration [16]. This is also shown by the stream data extracted from the PVC-suspension process given in Table 4. The process operates on temperatures between 25 °C and 180 °C and the heat flows of the streams range from 680 kW to 9300 kW. The theoretical heat demands of period 1 and 3 are 1740 kW and 6830 kW, while period 2 has a heat surplus of 2860 kW. The relatively high heat demand at the given temperature levels offers opportunities for integration of renewable energies with the help of HP to reduce the hot utility demand.

Table 4. Stream data for case 4

Stream	T_{in} (°C)	T_{out} (°C)	CP (kW/K) Period 1	CP (kW/K) Period 2	CP (kW/K) Period 3	h (kW/m^{2}K)
Hs1	80	25	40	60	40	0.5
Hs2	120	90	90	120	40	0.5
Hs3	180	25	50	60	12	0.5
Cs1	26	60	35	20	50	0.5
Cs2	50	80	60	90	70	0.5
Cs3	50	150	40	40	40	0.5
Cs4	90	180	40	24	16	0.5
Cs5	25	120	40	40	30	0.5
Hu	200	200	-	-	-	1
Cu	10	15	-	-	-	1

period durations: $\tau_1 = 1$ h, $\tau_2 = 1$ h, $\tau_3 = 1$ h.

In summary, the provided set of example cases covers the following aspects:

- Broad variety: The processes come from different energy-intensive industrial sectors to show the potentially wide range of application opportunities for HP and ST.
- Huge potential reduction of external primary energy demand and thus CO_2 emissions: The sectors pulp and paper, refineries and petrochemicals, and inorganic chemicals account for around 33% of the total industrial CO_2 emissions in the EU, and thus even small improvements can have huge impacts [2].
- Temperature range: The processes operate in the range of the physical boundaries of the HP, which is necessary for possible integration and thus usage of renewable energy sources.

3. Results and Discussion

3.1. Results

All test cases presented in Section 2 are optimized in two variations. In the first variation, which in the following is referred to as traditional HEN, only HEX between the streams and utilities are permitted in order to create a basic multi-period HEN in the traditional sense by setting all binary variables for the existence of Z_{hp}) and the existence of ST (Z_{st} (HP) to zero. In the second, the integration of the possible ST and HP options in the extended superstructure formulation given in Appendix A is enabled. The optimization results are described in the following Sections 3.1.1 to 3.1.4 and summarized discussed in Section 3.2.

3.1.1. Results Case 1

In Tables 5 and 6, the heat flows of the HEN solutions for case 1 in Figures 2 and 3 are given. The traditional HEN solution consists of eight stream - stream HEX and four utility HEX and has total annual costs of $TAC = 2{,}999{,}100$ €y^{-1}. The utilities for periods 1 to 4 for this case fit exactly to the minimum utility demand calculated in Section 2.1, which means that within the single periods, the maximum possible energy recovery is obtained.

The extended HEN consists of ten streams, stream HEX, five streams, ST HEX, three utility HEX, and two storages, and has total annual costs of $TAC = 1{,}336{,}700$ €y^{-1}. The chosen 1T ST operates between 100 °C and 183 °C and the 2T ST has a optimized size of $m_{StC1} = 155{,}887$ kg.

Table 5. Heat Flows without HP and ST case 1 (kW).

Installation	p1	p2	p3	p4
1	1005.3	1425.4	-	3340.8
2	994.7	129.2	1000	659.2
3	1400	350	1555.8	350
4	1355.3	1420.8	1350	890.8
5	500	895.5	444.2	1650
6	3000	600	3000	600
7	1400	1000	1400	1000
8	244.7	179.2	250	709.2
Cu1	-	2445.5	-	-
Cu2	100	754.5	-	-
Hu1	-	-	1055.8	1800
Hu2	-	-	3344.2	-

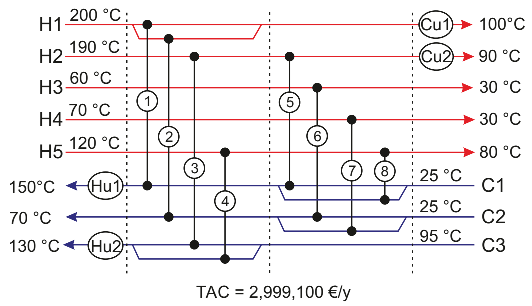

Figure 2. HEN obtained without HP and ST options case 1.

Table 6. Heat Flows and P_{el} results with HP and ST options case 1 (kW).

Installation	p1	p2	p3	p4
1	-	-	-	3150
2	-	-	497.5	250
3	825.1	2000	-	1884.1
4	-	-	488.1	-
5	906.5	1100	906.5	-
6	425.1	350	502.5	100
7	974.9	-	1800	-
8	3000	600	3000	600
9	1400	1000	1400	100
10	693.5	500	205.3	1600
11	920.4	474.4	-	200
12	-	-	1732.1	-
13	1443.5	450	1443.5	1500
14	654.5	3175.6	-	300
15	231.5	-	566.5	865.9
Cu1	200	-	200	115.9
Hu1	-	-	490	-
Hu2	-	-	367.9	-

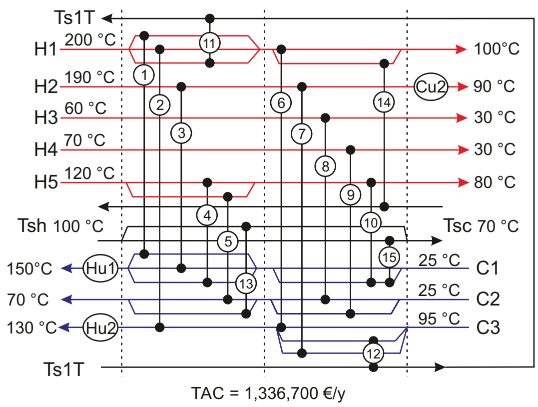

Figure 3. HEN obtained with HP and ST options case 1.

3.1.2. Results Case 2

In Tables 7 and 8, the heat flows of the HEN solutions for case 2 in Figures 4 and 5 are given. The traditional HEN solution consists of five stream - stream HEX and six utility HEX and has total annual costs of $TAC = 2,581,300$ €y^{-1}. That Hu and Cu are necessary within the same time periods show that the theoretical minimum utility demand is not reachable, or at least not financial desirable for this case.

The extended HEN consists of eight stream - stream HEX, two stream—ST HEX, five utility HEX, two HP, and a 2T ST and has total annual costs of $TAC = 1,336,000$ €y^{-1}. The 2T ST has a optimized size of $m_{StC2} = 490,601$ kg and the HP have a maximum electrical power consumption of $P_{elHP1} = 638.3$ kW and $P_{elHP2} = 475.2$ kW, respectively.

Table 7. Heat Flows without HP and ST case 2 (kW).

Installation	p1	p2	p3	p4
1	1260	660	924.4	1260
2	-	180	-	-
3	-	150	250	-
4	800	1600	900	800
5	-	180	195.6	-
Cu1	90	360	625.6	90
Cu2	-	-	1100	-
Cu3	20	190	954.4	-
Hu1	915	30	40	1350
Hu2	100	20	-	550
Hu3	500	-	-	680

Table 8. Heat Flows and P_{el} results with HP and ST options case 2 (kW).

Installation	p1	p2	p3	p4
1	596.3	594.7	700.3	540
2	-	147.4	350.2	-
3	-	150	-	-
4	100	-	350.6	-
5	633.8	245.3	419.7	698.8
6	442.5	-	-	741.2
7	257.5	227.1	199.2	-
8	500	150	250	520
9	500	0	250	680
10	542.5	-	-	-
Cu1	90	212.6	329.8	111.2
Cu2	-	89.2	199.2	58.8
Cu3	20	370	1150	-
Hu1	472.5	30	40	630
Hu2	-	-	-	36.6
HP1	-	1283.7	1251	-
HP2	-	1425.6	-	1313.4
Pel HP1	-	638.3	625.5	-
Pel HP2	-	475.2	-	437.8

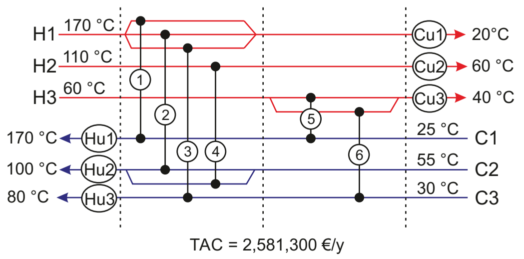

Figure 4. HEN obtained without HP and ST options case 2.

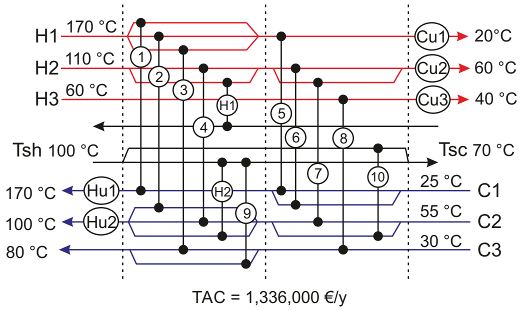

Figure 5. HEN obtained with HP and ST options case 2.

3.1.3. Results Case 3

In Tables 9 and 10, the heat flows of the HEN solutions for case 3 in Figures 6 and 7 are given. The traditional HEN solution consists of eleven stream - stream HEX and seven utility HEX and has total annual costs of $TAC = 3{,}594{,}800$ €y^{-1}. As for case 2, the theoretical minimum utility demand is not reachable, or at least not financial desirable for this case.

The extended HEN consists of nine stream, stream HEX, one stream, ST HEX, three utility HEX, four HP, and a 2T ST and has total annual costs of $TAC = 1{,}880{,}200$ €y^{-1}. The 2T ST has a optimized size of $m_{StC3} = 294{,}312$ kg and the HP have a maximum electrical power consumption of $P_{elHP1} = 665.5$ kW, $P_{elHP2} = 637.8$ kW, $P_{elHP3} = 597.3$ kW, and $P_{elHP4} = 424.6$ kW, respectively.

Table 9. Heat Flows without HP and ST case 3 (kW).

Installation	p1	p2	p3	p4
1	-	-	229.7	518.3
2	4467.8	2259.8	4900	-
3	-	2100	-	-
4	1874	1598.8	2345.5	3398.6
5	556.6	592.8	120.8	373.1
6	2800	2800	2800	2800
7	180.2	209.8	170.3	481.7
8	569.8	540.2	-	-
9	3782.2	3879.8	3350	-
10	763.7	911.7	734.2	728.4
11	705.7	757.2	699.5	-
Cu1	250	250	-	-
Cu2	-	3010.5	-	75
Cu3	600	639.5	600	-
Hu1	-	-	-	1991.4
Hu2	162.3	-	200	2400
Hu3	-	-	-	1400
Hu4	87.7	-	300	458.6

Table 10. Heat Flows and P_{el} results with HP and ST options case 3 (kW).

Installation	p1	p2	p3	p4
1	2728.3	2384.9	3021.5	-
2	-	2100	-	-
3	1605.4	1688.4	1605.4	2519.5
4	587.8	509.8	587.8	765.4
5	2800	2800	2800	2800
6	750	514.1	300	750
7	4050	4494.1	4050	-
8	944.6	417.5	944.6	1215.2
9	762.2	840.2	762.2	-
10	-	-	-	584.6
Cu1	250	584.9	100	250
Cu2	-	895.4	-	75
Cu3	600	1044.1	600	-
HP1	1471.7	1375.6	1178.5	-
HP2	-	-	-	2865.4
HP3	1721.7	-	1878.5	1650
HP4	-	-	-	1400
Pel HP1	665.5	649.3	574.6	-
Pel HP2	-	-	-	637.8
Pel HP3	552.8	-	597.3	532.4
Pel HP4	-	-	-	424.6

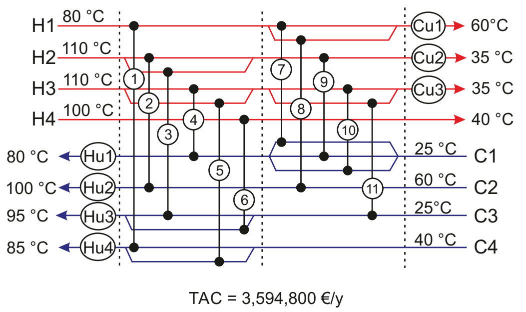

Figure 6. HEN obtained without HP and ST options case 3.

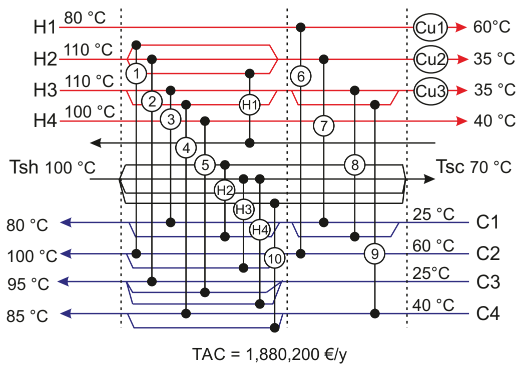

Figure 7. HEN obtained with HP and ST options case 3.

3.1.4. Results Case 4

In Tables 11 and 12, the heat flows of the HEN solutions for case 4 in Figures 8 and 9 are given. The traditional HEN solution consists of ten stream - stream HEX and seven utility HEX and has total annual costs of $TAC = 7,160,800$ €y^{-1}. The large Hu and Cu needed within the same time periods show that the temperature levels and heat capacities of the streams do not allow a heat recovery near the theoretical optimum calculated in Section 2.4.

The extended HEN consists of eight stream, stream HEX, one stream, ST HEX, five utility HEX, four HP, and a 2T ST and has total annual costs of $TAC = 5,056,600$ €y^{-1}. The 2T ST has a optimized size of $m_{StC4} = 199,932$ kg and the HP have a maximum electrical power consumption of $P_{elHP1} = 456.7$ kW, $P_{elHP2} = 739.3$ kW, $P_{elHP3} = 1423.8$ kW, and $P_{elHP4} = 709.6$ kW, respectively.

Table 11. Heat Flows without HP and ST case 4 (kW).

Installation	p1	p2	p3
1	1000	-	1000
2	326.7	1571.1	-
3	1000	822.1	-
4	1805.6	279.32	902.4
5	2444.4	2040	117.6
6	840	371.1	960
7	-	1128.9	-
8	1373.3	1206.8	1200
9	-	308.9	-
10	2600	2777.9	780
Cu1	360	1800	240
Cu2	900	1380	600
Hu1	350	-	740
Hu2	473.3	-	1100
Hu3	821.1	-	1897.6
Hu4	1155.6	120	1322.4
Hu5	200	200	2070

Table 12. Heat Flows and P_{el} results with HP and ST options case 4 (kW).

Installation	p1	p2	p3
1	471.1	-	471.1
2	143.2	1600	-
3	-	1871.1	-
4	3400	2040	1020
5	1190	680	1173.4
6	770	2000	775.7
7	1800	839.7	-
8	-	-	526.6
9	285.7	1160.3	728.9
Cu1	240	620	250.8
Cu2	2088.4	2541.4	313.4
Hu1	1400	-	1400
Hu2	200	120	420
Hu3	668.8	200	576.4
HP1	-	1860.3	2100
HP2	2218	-	1497.8
HP3	2261.6	2847.6	-
HP4	2128.9	2128.9	-
Pel HP1	-	400	456.7
Pel HP2	739.3	-	499.3
Pel HP3	1130.8	1423.8	-
Pel HP4	709.6	709.6	-

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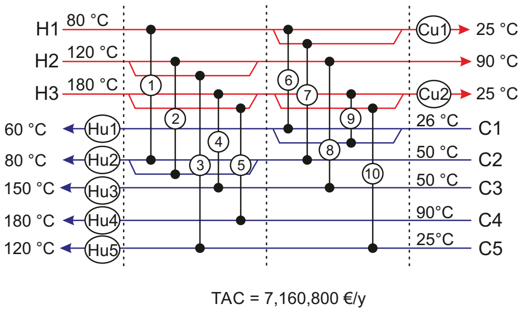

Figure 8. HEN obtained without HP and ST options case 4.

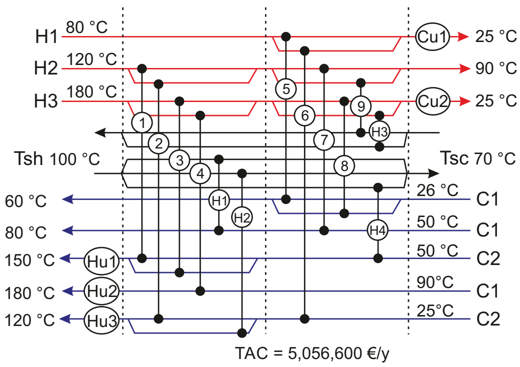

Figure 9. HEN obtained with HP and ST options case 4.

3.2. Discussion

The summarized results of the optimization of the four cases are given in Table 13, where it can be seen that for all cases, the integration of HP and ST into the HEN significantly reduced the TAC. The TAC of case 1 were reduced by $1,662,400$ €y^{-1} or 55.43%, the TAC of case 2 were reduced by $945,300$ €y^{-1} or 41.43%, the TAC of case 3 were reduced by $1,714,600$ €y^{-1} or 47.70% and the TAC of case 4 were reduced by $2,104,200$ €y^{-1} or 29.39%. The total external energy demand for cases 1-3 decreased by 87.10%, 20.95%, and 12.52%, respectively, while the total external energy demand of case 4 increased by 13.31%. Except for case 3, all extended HEN consist of more installations than their basic HEN counterpart.

Table 13. Summary of optimization results.

Case	TAC €y^{-1}	Utilities/Year GWh y^{-1}	Pel/Year GWh y^{-1}	Energy Demand/Year GWh y^{-1}	Installations -	Storage
1	2,999,100	21.93	-	21.93	12	
1 extended	1,336,700	2.829	-	2.829	20	1T, 2T
2	2,281,300	16.37	-	16.37	12	
2 extended	1,336,000	8.256	4.680	12.94	18	2T
3	3,594,800	21.25	-	21.25	18	
3 extended	1,880,200	8.527	10.07	18.59	18	2T
4	7,160,800	45.09	-	45.09	17	
4 extended	5,056,600	31.66	19.43	51.09	19	2T

For case 1, the significant reduction of the utility energy demand is caused by the optimal integration of the two different possible ST options. This is possible because the 1T

ST has a fixed size and the operational temperatures are chosen during the optimization while for the 2T ST the temperature levels of the tanks are fixed and the size gets optimized. Thanks to this combination, the optimized storages allow to shift the heat surplus from period 2 mentioned in Section 2.1 to periods 3 and 4. This reduces the overall Cu energy demand and the overall Hu energy demand for one cycle by 8884.1 kWh, which results in an annual reduction of utility costs of 2, 101, 111 €y^{-1} for the given cost coefficients.

The optimal integration of a 2T ST and two HP in case 2 led to a reduction of the Cu demand per cycle of 799.2 kWh and a reduction of the Hu demand per cycle of 2975.9 kWh. The electrical energy demand of the two HP per cycle is 2176.7 kWh, which shows that Hu demand is shifted towards electrical energy demand, which reduces the annual energy costs by 1, 173, 599 €y^{-1}.

For case 3, the four HP and the 2T ST chosen by the optimization reduced the Cu demand per cycle by 925.6 kWh and led to a solution without Hu, thus decreasing the Hu demand by 7950 kWh. The Hu demand is replaced by the HP, which has an electrical energy demand per cycle of 7024.4 kWh, reducing the annual energy costs by 2, 003, 480 €y^{-1}.

The integration of the 2T ST and the four HP in the resulting extended HEN of case 4 resulted in a higher annual external energy demand than the traditional HEN solution. The Cu demand increased by 774 kWh while the Hu demand was reduced by 5464.8 kWh. The electrical energy demand per cycle of the 4 HP combined adds up to 6778.7 kWh. While it may seem that an increased external energy demand is not an improvement, it must be remembered that the optimization target is the minimization of the TAC and only depends on the specific cost coefficients. Although in this case the external energy demand increased, the annual energy costs for the extended network solution are 2, 003, 480 €y^{-1} lower than for the traditional HEN solution. Even small changes of the cost parameters can result in massive changes in the resulting network solutions. Assuming that the electrical energy demand is satisfied through GHG neutral energy sources and that the Cu only needs electrical energy for transportation of the fluid, the generation of steam for the Hu remains the only GHG source during operation. With this assumption and the given case data and cost coefficients, the extended HEN solutions for cases 1 to 4 yield the theoretical potential for a drastic reduction of GHG emission of 83.8%, 71.1%, 100%, and 52.3% respectively.

As mentioned in the introduction, energy-saving or emission reduction investments have to compete with other measures like capacity improvements. The payback time is often taken as an indicator to determine if a more expensive investment in an environmentally friendly alternative is profitable or not. For the proposed cases, the payback time for an assumed lifespan of 25 years is calculated by dividing the investment cost difference of the extended and the basic HEN results by the annual saving of energy costs. For visualization, the annual cost savings of the cases are given over their investment cost difference in Figure 10. The diagonal line in Figure 10 represents a payback time of five years, which is exemplary set as a realistic limit for the profitability of the investments. Regarding the extended HEN for case 1, a payback time of 5.2 years was obtained, making it not profitable under the assumptions given in Sections 1.2 and 2. The payback times of cases 2–4, that are 4.9 years, 3.6 years, and 4.0 years, respectively, are within the limit and thus profitable investments. The fact that the payback times of the analyzed cases lay close to the profitability limit fits well with reality in the industry. The difficulty of achieving carbon neutrality without the influence of regulations or subsidies is highlighted in the results of case 1, where even an energy demand reduction of 87.10% by the introduced HEN can not be considered profitable from an economic point of view. The obtained results show that the introduced set of test cases with their different optimization potentials are perfectly suitable for extensive tests of multi-period HENS procedures under realistic conditions.

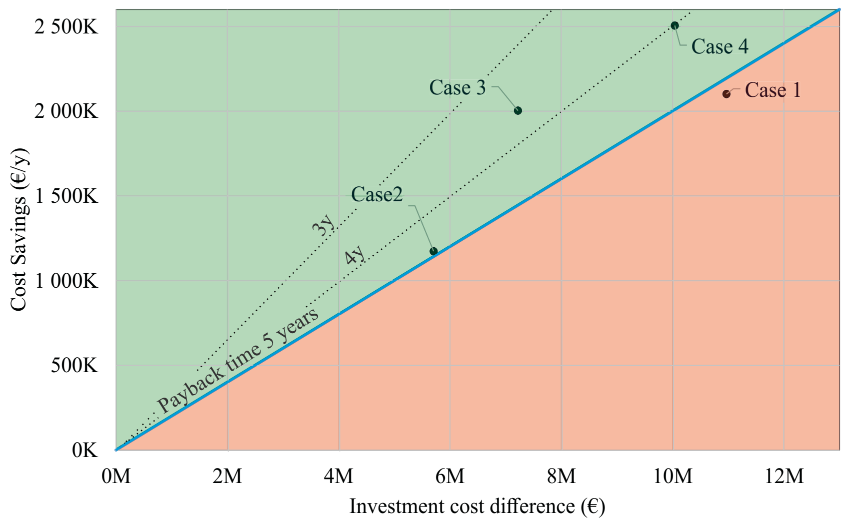

Figure 10. Cost savings per year over investment cost difference between conventional HEN and extended HEN results. In the green area the payback time is shorter than 5 years and in the red area the payback time is longer than 5 years.

4. Conclusions

A set of four example cases suitable for HP and ST integration was created based on industrial processes from the EII to increase the small number of publicly available test cases in the field of multi-period HENS and to show the potential of energy integration in different sectors of the EII. The application of an approach that allows the simultaneous integration of HP and different types of ST presented in earlier work [3] led to a significant reduction of the total annual cost compared to the basic HEN of up to 55.43% for the introduced cases. Moreover, the external energy demand was reduced (up to 87.1%), or shifted towards possible renewable energy sources. These results are perfectly plausible considering the chosen cost coefficients and the structure of the cost function. Within the taken assumptions, three of the four extended HEN results have payback times under five years and are thus potential profitable investments. The results underline the potential of design optimization in the reduction of CO_2 emissions while also improving cost-efficiency, especially in the EII. While it is clear that the optimization of constructed test cases is not directly transferable to real applications, the introduced stream data combined with the results obtained and the fully given mathematical formulation provide a valuable extension to the existing HENS literature and contribute to future research in the field.

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Appendix A. Mathematical Formulation of the Applied Multi-Period MILP HENS Approach

Mathematical formulation as presented in Prendl et al. [3]:
Cost function

$$
\begin{aligned}
\min TAC = {} & \underbrace{\sum_i\sum_j\sum_k c_f Z_{ijk} + \sum_i c_f Z_{cui} + \sum_j c_f Z_{huj} + c_{fst\,2T} Z_{st\,2T} + c_{fst\,1T} Z_{st\,1T} + \sum_i\sum_j\sum_k c_f Z_{2T\,ijk} + \sum_i\sum_j\sum_k c_f Z_{1T\,ijk} + \sum_i\sum_j\sum_k c_{hp} Z_{hp\,ijk}}_{\text{step fixed investment costs}} \\
& \underbrace{+ \sum_i\sum_j\sum_k cA^{\beta}_{ijk} + \sum_i cA^{\beta}_{cui} + \sum_j cA^{\beta}_{huj} + c_{vst\,2T} S_{st\,2T} + \sum_i\sum_j\sum_k cA^{\beta}_{2T\,ijk} + \sum_i\sum_j\sum_k cA^{\beta}_{1T\,ijk} + \sum_i\sum_j\sum_k cA^{\beta}_{hp\,ijk}}_{\text{variable investment costs}} \\
& \underbrace{+ \sum_i\sum_p c_{cu}\dot{Q}_{cuip}\tau_{ap} + \sum_j\sum_p c_{hu}\dot{Q}_{hujp}\tau_{ap} + \sum_i\sum_j\sum_k\sum_p c_{Pel} Pel_{ijkp}\tau_{ap}}_{\text{energy costs}} \\
& \forall\ p = 1,\ldots,NOP,\ k = 1,\ldots,NOK, \\
& i = 1,\ldots,HPS,\ j = 1,\ldots,CPS
\end{aligned}
\tag{A1}
$$

subject to:
stream-wise energy balance

$$
\begin{aligned}
& \sum_j\sum_k \dot{Q}_{ijkp} + \sum_k(\dot{Q}_{2T\,ikp} + \dot{Q}_{1T\,ikp} + \dot{Q}_{hp\,ikp}) \\
& + \dot{Q}_{cuip} = \dot{m}_{ip} cp_{ip}(T^{in}_{ip} - T^{out}_{ip}) = \dot{Q}_{ip} \\
& \sum_i\sum_k \dot{Q}_{ijkp} + \sum_k(\dot{Q}_{2T\,jkp} + \dot{Q}_{1T\,jkp} + \dot{Q}_{hp\,jkp}) \\
& + \dot{Q}_{hujp} = \dot{m}_{jp} cp_{jp}(T^{out}_{jp} - T^{in}_{jp}) = \dot{Q}_{jp} \\
& \forall\ p = 1,\ldots,NOP,\ k = 1,\ldots,NOK, \\
& i \in HPS,\ j \in CPS
\end{aligned}
\tag{A2}
$$

stage-wise energy balance

$$\begin{aligned}
&\sum_j \dot{Q}_{ijkp} + \dot{Q}_{2T\ ikp} + \dot{Q}_{1T\ ikp} + \dot{Q}_{hp\ ikp} \\
&= \dot{m}_{ip} cp_{ip} (T_{ik} - T_{i,k+1}) \\
&\sum_i \dot{Q}_{ijkp} + \dot{Q}_{2T\ jkp} + \dot{Q}_{1T\ ijkp} + \dot{Q}_{hp\ jkp} \\
&= \dot{m}_{ip} cp_{jp} (T_{jk} - T_{j,k+1}) \\
&i \in HPS,\ j \in CPS \\
&T_{i,k=1} = T_i^{in},\ T_{j,k=NOK} = T_j^{in}
\end{aligned} \tag{A3}$$

utility heat loads

$$\begin{aligned}
\dot{Q}cu_{ip} &= \dot{m}_{ip} cp_{ip} (T_{i,k=NOK+1,p} - T_{ip}^{out}) \\
\dot{Q}hu_{jp} &= \dot{m}_{jp} cp_{jp} (T_{jp}^{out} - T_{j,k=1,p})
\end{aligned} \tag{A4}$$

energy balance 1T storage

$$\begin{aligned}
&m_{1T} cp_{1T} (T_{1T\ p+1} - T_{1T\ p}) = \\
&\Big(\sum_i \sum_k \dot{Q}_{1T\ ikp} - \sum_j \sum_k \dot{Q}_{1T\ jkp}\Big)\tau_p \\
&T_{1T\ p=1} = T_{shift} = T_{1T\ p=NOP} \\
&0 \le T_{1T} \le Tmax_{1T}
\end{aligned} \tag{A5}$$

energy balance 2T storage

$$\begin{aligned}
&Q_{st\ 2T} = m_{2T} cp_{2T} (T_{h2T} - T_{c2T}) \\
&CH_{2T,p+1} = CH_{2T,p} + \frac{\tau_p}{Q_{st\ 2T}} \\
&\Big[\sum_i \sum_k (\dot{Q}_{2T\ ikp} + \dot{Q}_{hpst\ ikp}) \\
&- \sum_j \sum_k (\dot{Q}_{2T\ jkp} + \dot{Q}_{hp\ st\ jkp})\Big] \\
&CH_{2T,p=1} = CH_{shift} = CH_{2T,p=NOP} \\
&S_{st\ 2T} = m_{2T}(max(CH_{2T}) - min(CH_{2T})) \\
&0 \le CH_{2T} \le 1
\end{aligned} \tag{A6}$$

energy balance heat pumps

$$\begin{aligned}
\dot{Q}_{hpst\ ikp} &= \dot{Q}_{hp\ ikp} + P_{el\ ikp} \\
\dot{Q}_{hpst\ jkp} &= \dot{Q}_{hp\ jkp} - P_{el\ jkp}
\end{aligned} \tag{A7}$$

constraints for binary variables for installations

$$
\begin{aligned}
&Z_{ijkp}\dot{Q}_{min} \leq \dot{Q}_{ijkp} \leq Z_{ijkp}\dot{Q}_{max\ ijkp} \\
&\dot{Q}_{max\ ijkp} = min(\dot{Q}_{ip}, \dot{Q}_{jp}) \\
\\
&Z_{2T\ ijkp}\dot{Q}_{min\ st} \leq \dot{Q}_{2T\ ijkp} \leq Z_{2T\ ijkp}\dot{Q}_{ijkp} \\
&Z_{1T\ ijkp}\dot{Q}_{min\ st} \leq \dot{Q}_{1T\ ijkp} \leq Z_{1T\ ijkp}\dot{Q}_{ijkp} \\
&Z_{cu\ ip} \leq \dot{Q}_{cu\ ip} \leq Z_{cu\ ip}\dot{Q}_{ip} \\
&Z_{hu\ jp} \leq \dot{Q}_{hu\ jp} \leq Z_{cu\ jp}\dot{Q}_{jp} \\
&Z_{st\ 2T} \geq Z_{2T\ ijkp}, \quad Z_{st\ 2T} \geq Z_{hp\ ijkp} \\
&Z_{st\ 1T} \geq Z_{1T\ ijkp}
\end{aligned}
\tag{A8}
$$

physical constraints

$$
\Delta T \geq \Delta T_{min}, \quad A^{\beta} \geq 0, \quad \dot{Q} \geq 0 \tag{A9}
$$

constraints for temperature differences

$$
\begin{aligned}
&LMTD_{ijkp} \leq CLMTD_{ijkp}(\Delta T_{ijkp}, \Delta T_{ij,k+1,p}) \\
&LMTD_{2T\ ijkp} \leq CLMTD_{2T\ ijkp}(\Delta T^{2T,1}_{ijkp}, \Delta T^{2T,2}_{ijkp}) \\
&LMTD_{1T\ ijkp} \leq CLMTD_{1T\ ijkp}(\Delta T^{1T,1}_{ijkp}, \Delta T^{1T,2}_{ijkp}) \\
&LMTD_{hp\ ijkp} \leq CLMTD_{hp\ ijkp}(\Delta T^{hp,1}_{ijkp}, \Delta T^{hp,2}_{ijkp}) \\
&\Delta T_{ijkp} \leq T_{ikp} - T_{jkp} + \Gamma_T(1 - Z_{ijkp}) \\
&\Delta T_{ij,k+1,p} \leq T_{i,k+1,p} - T_{j,k+1,p} + \Gamma_T(1 - Z_{ijkp}) \\
&\Delta T^{2T,1}_{ikp} \leq T_{ikp} - T_{h\ 2T} + \Gamma^{2T}_T(1 - Z_{2T\ ikp}) \\
&\Delta T^{2T,1}_{jkp} \leq T_{h\ 2T} - T_{j,k+1,p} + \Gamma^{2T}_T(1 - Z_{2T\ jkp}) \\
&\Delta T^{2T,2}_{ikp} \leq T_{i,k+1,p} - T_{c\ 2T} + \Gamma^{2T}_T(1 - Z_{2T\ ikp}) \\
&\Delta T^{2T,2}_{jkp} \leq T_{c\ 2T} - T_{j,k+2,p} + \Gamma^{2T}_T(1 - Z_{2T\ jkp}) \\
&\Delta T^{1T,1}_{ikp} \leq T_{ikp} - T_{1T\ p} + \Gamma^{1T}_T(1 - Z_{1T\ ikp}) \\
&\Delta T^{1T,1}_{jkp} \leq T_{1T\ p} - T_{j,k+1,p} + \Gamma^{1T}_T(1 - Z_{1T\ jkp}) \\
&\Delta T^{1T,2}_{ikp} \leq T_{i,k+1,p} - T_{1T\ p+1} + \Gamma^{1T}_T(1 - Z_{1T\ ikp}) \\
&\Delta T^{1T,2}_{jkp} \leq T_{1T\ p+1} - T_{j,k+2,p} + \Gamma^{1T}_T(1 - Z_{1T\ jkp}) \\
&\Delta T^{hp,1}_{ikp} \leq T_{ikp} - T_{i,k+1,p} + T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ ikp}) \\
&\Delta T^{hp,1}_{jkp} \leq T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ jkp}) \\
&\Delta T^{hp,2}_{ikp} \leq T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ ikp}) \\
&\Delta T^{hp,2}_{jkp} \leq T_{j,k+1,p} - T_{j,k+2,p} + T_{hp\ ap} + \Gamma_T(1 - Z_{hp\ jkp})
\end{aligned}
\tag{A10}
$$

constraints for heat exchange area

$$\begin{aligned}
&A^{\beta}_{ijkp} \geq CA^{\beta}_{ijkp} - \Gamma_A(1 - Z_{ijkp}) \\
&CA^{\beta}_{ijkp} = CA^{\beta}_{ijkp}(LMTD_{ijkp}, \dot{Q}_{ijkp}) \\
&A^{\beta}_{2T\ ijkp} \geq CA^{\beta}_{2T\ ijkp} - \Gamma_A(1 - Z_{2T\ ijkp}) \\
&A^{\beta}_{1T\ ijkp} \geq CA^{\beta}_{1T\ ijkp} - \Gamma_A(1 - Z_{1T\ ijkp}) \\
&A^{\beta}_{hp\ ijkp} \geq (CA^{\beta}_{hp\ ijkp} + CA^{\beta}_{hpst\ ijkp}) \\
&-\Gamma_A(1 - Z_{hp\ ijkp})
\end{aligned} \tag{A11}$$

summation constraints

$$A^{\beta}_{ijk} \geq A^{\beta}_{ijkp}, \quad Z_{ijk} \geq Z_{ijkp} \tag{A12}$$

heat pump constraints

$$\begin{aligned}
&\dot{Q}_{hp\ st\ ikp} / P_{el\ ikp} \geq COP_{min} \\
&\dot{Q}_{hp\ jkp} / P_{el\ ikp} \geq COP_{min} \\
&\Delta T_{hp\ ijkp} \leq \Delta T_{hp\ max} + \Gamma_T(1 - Z_{hp\ ijkp}) \\
&\Delta T_{hp\ ijkp} \geq \Delta T_{hp\ min} - \Gamma_T(1 - Z_{hp\ ijkp}) \\
&Z_{hp\ ijkp} Pel\ min \leq P_{el\ ijkp} \leq Z_{hp\ ijkp} P_{el\ max} \\
&Z_{hp\ ijkp} \dot{Q}_{min\ hp} \leq \dot{Q}_{hp\ ijkp} \leq Z_{hp\ ijkp} \dot{Q}_{ijkp} \\
&P_{el\ ijkp} \geq CP_{el\ ijkp} - \Gamma_{Pel}(1 - Z_{hp\ ijkp})
\end{aligned} \tag{A13}$$

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Further Publications

Parts of this work's content were not only published in the core publications of this thesis but were the subject of other dissemination activities. These contributions are listed below.

Presentations

The work on the SIC! cooperation doctoral school included a presentation in front of knowledgeable audience of the scope of SIC! with emphasis on the topics of this thesis:

R. Hofmann, L. Prendl, V. Halmschlager, S. Knöttner, A. Knöttner, J. Triebnig. Smart Industrial Concept - Holistic Approach with Digitalization of Industrial Processes and Applications for 2050 and beyond, *Presentation: Blickpunkt Forschung: Klimaschutz konkret @ TU Wien 23.10.2019 in Wien, Österreich.*

Scientific Reports

The SIC! community was invited to take part in the IEA IETS Annex XVIII on "Digitalization, Artificial Intelligence and Related Technologies for Energy Efficiency and GHG Emissions Reduction in Industry". In the course of this Annex, I participated in the creation of the White Paper "Digitalization in Industry – An Austrian Perspective":

R. Hofmann, V. Halmschlager, S. Knöttner, B. Leitner, D. Pernsteiner, L. Prendl, C. Sejkora,G. Steindl, and A. Traupmann. "Digitalization in Industry - An Austrian Perspective". *Tech.rep. accessed September 2021.* https://sic.tuwien.ac.at/fileadmin/t/sic/Dokumente/White-Paper-Digitalization-in-Industry.pdf

Supervised Theses

In the course of this thesis, I have supervised a master's thesis that added valuable contributions to my research.

M. Holzegger: "Framework for automated data acquisition and analysis of a fixed-bed regenerator using OSIsoft PI"; Betreuer/in(nen): R. Hofmann, L. Prendl; E302 - Institut für Energietechnik und Thermodynamik, 2021; Final exam: planned in spring 2022.

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