Development of an Optimization Framework and Grey-Box Modeling Concepts for Industrial Applications

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Vienna, July 2021

Verena Halmschlager

Abstract

This thesis covers two relevant aspects of industrial process optimization. Firstly, this thesis includes the development and application of an optimization framework for manufacturing processes. Although many studies dealt with the optimization of industrial energy systems, the optimization of manufacturing processes has been barely investigated. The framework uses a modular structure based on mixed-integer-linear-programming and is applied to a chipboard production plant using data-driven component models. The optimization of the use-case with and without design adaptations demonstrates the versatile and simple usability of the framework and the process's considerable potential for energy and costs savings. To show this potential, the main novelty of this framework, the combined optimization of energy and product, was pivotal. However, the process's full potential can only be realized if the framework is utilized for a real-time application.

Secondly, this work presents two grey-box modeling concepts for industrial component modeling – a Neural Network and a mechanistic grey-box modeling approach – to model a sensible thermal energy storage. A qualitative and quantitative analysis reveals that both models show increased accuracy and lower computational effort than a purely physical model. However, only the mechanistic grey-box model is also robust and reliable, and therefore applicable for real-time applications. In general, to facilitate the creation of industrial component models using data and physical information, systematic and universal grey-box modeling approaches are required.

Kurzfassung

Diese Arbeit befasst sich mit zwei Aspekten der industriellen Prozessoptimierung. Erstens beinhaltet diese Arbeit die Entwicklung und Anwendung eines Optimierungs-Frameworks für industrielle Fertigungsprozesse, die trotz vieler Studien über die Optimierung industrieller Energiesysteme nur am Rande untersucht wurden. Das modular aufgebaute Framework basiert auf gemischt-ganzzahliger-linearer Optimierung und wird auf eine Spanplattenproduktionsanlage angewandt, dessen Komponentenmodelle auf realen Prozessdaten basieren. Die Optimierung des Use-Cases mit und ohne Designänderung demonstriert die einfache und vielseitige Anwendbarkeit des Frameworks und die erheblichen Energie- und Kosteneinsparungspotenziale des Prozesses. Außerdem zeigen die Ergebnisse, dass die Berücksichtigung des Produkts als innovativer Kernbestandteil des Frameworks eine wesentliche Rolle im Energiemanagement des Gesamtsystems spielt. Dieses Potential kann allerdings nur mit der Echtzeitanwendung des Frameworks ausgeschöpft werden.

Zweitens werden in dieser Arbeit zwei Grey-Box Modellierungsansätze für industrielle Komponenten, ein Neuronales Netz und ein mechanistisches Grey-Box Modell, zur Modellierung eines sensiblen thermischen Energiespeichers untersucht. Eine qualitative und quantitative Analyse demonstriert, dass beide Modelle genauere Prädiktionen und einen geringeren Rechenaufwand als ein rein physikalisches Modell aufweisen, allerdings nur das mechanistische Grey-Box Modell auch robust und zuverlässig ist. Um die generelle Entwicklung von kombinierten physikalischen und daten-getriebenen Modellen zu erleichtern, sind universelle Grey-Box Modellierungsansätze erforderlich.

Acknowledgments

Throughout the course of this thesis, I have received a great deal of support and assistance from many people. Now it is time to express my deepest gratitude.

First of all, I want to thank my supervisor René Hofmann for his commitment, support, and faith – and especially for all the opportunities he opened to me. Also, I want to express my gratitude and appreciation to all members of the SIC! consortium who supported me throughout this thesis. Especially, I want to thank our industrial partner Fundermax, who played a decisive role in enabling this thesis and provided the data and information for the investigation of the chipboard production plant.

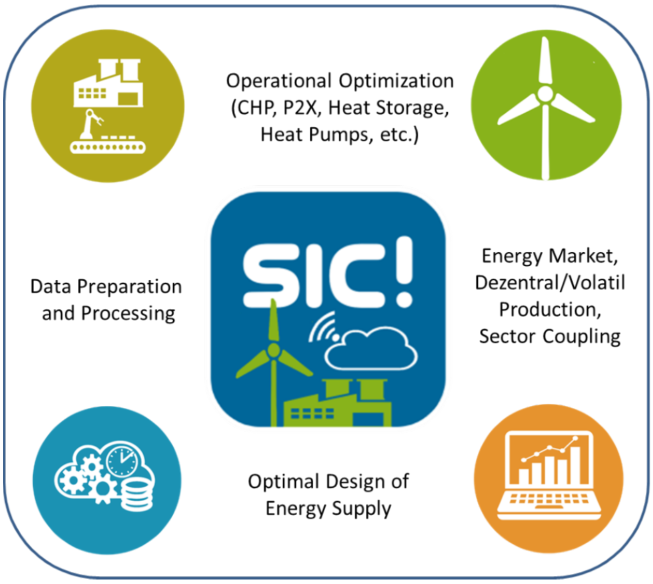
Next, I would like to acknowledge all my colleagues that I worked with during my employment at the TU Wien, for always having an ear and the wonderful discussions and coffee breaks. Here, I want to especially thank Felix, who guided and supported me throughout my thesis, always open for resourceful discussions to improve my ideas.

Apart from university, my time at the TU Wien would not have been the same without the countless cheerful, challenging, and (rarely) relaxing activities with my friends that always helped me stay focused and balanced. I especially want to thank my partner in crime, Manuel, for all the encouragement, mental support, and reminding me that *vo nix kummt nix*.

Finally and most importantly, I want to thank my family for their unconditional support - you made this possible!

Preface

This thesis was conducted during my employment at TU Wien in the research unit Industrial Energy Systems from 2018 to 2021 in the course of the cooperative doctoral school SIC! – Smart Industrial Concept[1]. SIC! is a doctoral school including three scientific partners, TU Wien, AIT Austrian Institute of Technology, and Montanuniversität Leoben and five industrial partners EVN, evon, FunderMax, ILF Consulting Engineers, and OSIsoft. SIC! primarily focuses on the research topics digitalization and decarbonization and aims to develop methods for the optimization of industrial plants, as well as relevant energy conversion, distribution and storage systems and their interaction with the energy industry. For this research aim, SIC! is composed of the following four pillars that can also be seen in the figure below: Data preparation and processing, operational optimization, energy markets, and optimal design of energy supply. The research within these four pillars is executed by 8 PhD students, whose cooperation is an essential part of this doctoral school.



Main pillars of SIC! ©TU Wien

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

My work in SIC! focused on the pillar operational optimization with the following main goals:

- Deployment and extension of modern optimization approaches – as mixed-integer-linear-programming (MILP) and thermal unit commitment problem (UC) – that enable the integration of external data in real-time (e.g. electricity market, district heating).
- Development of a simplified plant model (of the project partner's use-case) for operational optimization, including dynamic component models.
- Modeling and simulation of technologies that allow load shifting of thermal or electrical energy (e.g. thermal energy storage and heat pumps).

Another project that I was involved in during my employment at the TU Wien was the IEA IETS Annex XVIII with the topic "Digitalization, Artificial Intelligence and Related Technologies for Energy Efficiency and GHG Emissions Reduction in Industry". Within this Annex, I had the opportunity to join international meetings and I coordinated the drafting of the White Paper "Digitalization in Industry – An Austrian Perspective" [2].

Both the interdisciplinary work in the SIC! doctoral school and the participation in the Annex XVIII are closely tied to this thesis and shaped my research.

[2] `https://www.klimafonds.gv.at/publication/white-paper-digitalization-in-industry-an-austrian-perspective/`

Contents

List of Figures

Nomenclature

Acronyms

ARIMA Autoregressive Integrated Moving Average

CO_2 Carbon Dioxide

EH Energy Hub

GHG Greenhouse Gas Emissions

GRU Gated Recurrent Unit Neural Network

IEA International Energy Agency

IPCC Intergovernmental Panel on Climate Change

LMST Long-Memory-Short-Term Neural Network

MILP Mixed-Integer-Linear-Programming

ML Machine Learning

NN Artficial Neural Network

PSO Particle Swarm Optimization

RNN Recurrent Neural Network

SIC Smart Industrial Concept

UC Unit Commitment

Subscripts

f index for fuel costs

i index for the streams of a conversion constraint

n index for integer variables

o index for operation costs

q index for continuous variables

r index for rewards

t index for time

Symbols

A parameter matrix

a constant

B parameter matrix

b constant

bin binary variable

C coupling matrix parameters

c vector of parameters

D minimum required value for minimum output constraint

d vector of parameters

Dt time a unit needs to be off after it was shut down

F fuel costs

g vector of parameters

I energy hub inputs

L energy hub outputs

O operation costs

p stream of a unit

$p_{\max}$ maximal generation limit of a stream p

$p_{\min}$ minimal generation limit of a stream p

R rewards

Rd	maximal negative gradient of a stream p
Ru	maximal positive gradient of a stream p
S	slack variable
T	horizon of the optimization
u	on/off binary variable
Ut	time a unit needs to be on after it was started
v	start-up binary variable
w	shut-down binary variable
x	vector of n continuous variables
y	vector of q integer variables

Research summary

This chapter provides the backdrop for the publications that are the core element of this thesis. First, in Section 1, the work in this thesis is motivated by showing the big picture of today's energy system. After the Introduction, in Section 2, all relevant topics, methods, and applications for this thesis's publications are set into context and narrowed down to the specific content of this work. The description includes a rough theoretical background as well as an overview of essential research in literature. Following, in Section 3, the research objectives and questions of this thesis are stated. Next, Section 4 links all publications of this thesis. It includes the motivation of each paper and a short summary of content and results. Finally, in Section 5, relevant findings of this thesis are synthesized, and conclusions are drawn.

1 Introduction

Energy plays an essential role in human life. Around 1400 – 1800 kcal of energy are required by our body only to fulfill its vital tasks. On average, every human digests around 2900 kcal of energy every day (FAO 2018). However, the way we view at energy has drastically changed within the past centuries. Energy is not just used to fulfill our body's requirements but is necessary for nearly any process nowadays, e.g. in the industrial, agricultural, health or domestic sector. In Austria, about 35 times more than our body calorie intake – approximately 100,000 kcal per day – can be assigned to every person by human activities [3]. While too high energy uptake in humans typically leads to weight gain and higher risks of diseases, the increasing total energy consumption of our species and especially the high shares of conventional energy sources result in global consequences – the climate change.

The climate change stands for the nowadays increase of temperatures on our planet, including a change of weather patterns (Stocker 2014). These changes are caused by the human, more precisely by high emissions of greenhouse gases (GHG) that withhold the radiation of heat from earth towards space (Oreskes 2004). Although GHG emissions have entered our atmosphere since the beginning of life on our planet by natural animal or plant respiration processes, nowadays GHG emissions have taken dangerously high levels by human activities, threatening the delicate equilibrium that keeps our climate stable

[3] Assuming an average final energy consumption of 1400 PJ/year according to Umweltbundesamt (2017), and a population of 8.8 million in Austria

(Steffen et al. 2015). These activities include the use of fossil fuels, deforestation, synthetic fertilizers, and industrial processes (Lallanilla 2019). From all GHG emissions, carbon dioxide (CO_2) is the biggest driver of climate change. It is responsible for approximately 75 % of all GHG emissions worldwide (see Fig. 1) and rose 62 % between 1990 and 2019 (Peters et al. 2020)

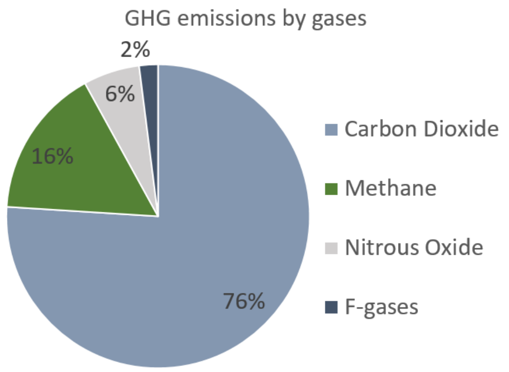


Figure 1: *Average worldwide GHG emissions by gases. Adapted from IPCC (2014)*

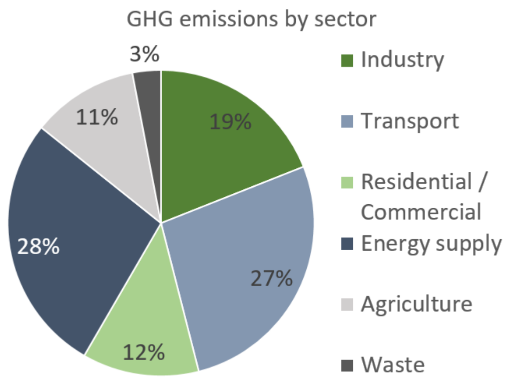


Figure 2: *GHG emissions by sector in the EU in 2017. Adapted from EEA (2017)*

To counteract today's high GHG emissions and the resulting climate change, the European Union has presented a long-term strategy to reach climate-neutrality by 2050 – meaning net-zero GHG emissions – which is a key element of the European Green Deal (European Comission 2019). Although this goal seems very resolute, experts question if the nowadays planned measures can actually prevent future hazardous scenarios. The Intergovernmental Panel on Climate Change IPCC (2018) predicts, that global warming needs to be kept below 1.5 °C to avoid dangerous tipping points. However, to reach this goal, climate neutrality might need to be reached already by 2040, according to the International Energy Agency (IEA 2016). These projections underline the urgency of this issue and the fact that we need to drastically change today's energy system. Especially the reduction of traditional, non renewable energy sources should be in focus of today's progression and every sector of our economy will need to contribute.

Focusing on the industry, this sector accounts for almost 20 % of the GHG emissions in Europe (see Fig. 2), and nearly 40 % of the worldwide CO_2 emissions (IEA 2018). The International Renewable Energy Agency (IREA) estimates that by 2050, four of the most energy-intensive industries and three key transport sectors could account for 38 % of energy and process emissions and 43 % of final energy consumption – unless major changes are realized now. Therefore, the combination of five emission reduction measures are suggested to achieve zero CO_2 emissions in these sectors by 2050 (IRENA 2020):

- Reduced demand and improved energy efficiency
- Direct use of clean, predominantly renewable electricity

- Direct use of renewable heat and biomass
- Indirect use of clean electricity via synthetic fuels and feedstock
- Use of carbon dioxide removal measures

From these five measures, the first – reduced demand and improved energy efficiency – is expected to achieve the highest reduction of GHG emissions of 28 % in the industrial sector. Methods like process optimization and energy storage integration can help achieve these measures by balancing energy peaks and troughs efficiently. Especially with the increased shares of fluctuating renewable energy sources like solar and wind energy, the balancing and compensation of energy becomes more and more relevant. According to IRENA (2019), this combination of renewable energy sources with energy efficiency measures can provide already 90 % of the CO_2 emission reductions required for the zero-emissions goal in 2050.

Nevertheless, to reach European and global climate goals and prevent hazardous future scenarios, government, industry, and society will all need to take responsibility and act. Long established habits and patterns of our society that contribute to the unsustainable exploitation of the worlds resources need to be reconsidered, even if this results in inconveniences in areas of every day live. From a technological point of view, on the one hand, it is essential to take advantage of the nowadays high level of knowledge and technical progress and to use already existing sustainable solutions to a significantly greater extent. On the other hand, many applications still require the development of new, innovative technologies and methods to which scientific research can contribute considerably.

2 Context

For the transition to a sustainable energy system, the efficient use of energy in the industrial sector plays an essential role. To reduce overall energy consumption and increase the efficiency of energy use and conversion in industrial applications, optimization methods have proven their universal applicability. Especially with today's complex energy market, new flexible technologies, and higher shares of volatile renewable energies from e.g. wind and solar, the scheduling of energy becomes essential to optimally use energy peaks and troughs in industrial processes. This scheduling of energy can be achieved by operational optimization, which is an optimization method that determines the optimal operation modes and capacities of every unit of a process. Particularly by combining operational optimization and the integration of e.g. energy storage technologies, fluctuations of renewable energy sources can be optimally utilized, leading to more sustainable and energy efficient processes.

Going one step further, generic energy management approaches, such as the Energy Hub concept, extend the operational optimization of a process. In these approaches, e.g. different energy sources such as gas, steam, oil, electricity, and the associated demand management options are considered, and dependencies between different energy systems can be displayed. In this way, interrelationships of different energy sources in single- to large-scale energy systems can be taken into account, leading to even better utilization of energy.

However, for these generic energy management approaches, same as for operational optimization, accurate and reliable component models of a process are required as a first step. For the modeling of existing industrial systems with a profound data basis, especially data-driven modeling methods like machine learning have attracted attention in the past years. Nevertheless, pure data-driven models – also called black-box models – often lack robustness and interpretability. In between these black-box models and the traditionally used physical modeling approach – also called white-box modeling – grey-box models are located. These models use data *and* physical relations and thus, can benefit from the advantages of both, black- and white-box models.

This thesis focuses on the aforementioned topics, operational optimization of industrial energy systems, and reliable yet accurate modeling methods based on data and physical knowledge, particularly for the modeling of thermal energy storage. Both approaches can contribute to today's challenges by increasing process' energy efficiency or reducing overall energy consumption. In this chapter, relevant principles, methods, and applications for each approach are outlined and set into context. At the beginning of each section, a general overview is given before the description is narrowed down to specific contents of this thesis.

2.1 Operational Optimization

In general, optimization can be defined as the search for the best possible solution, considering a defined goal and boundary conditions (Floudas et al. 2008). Although the term optimization is also widely used for any improvement, it is exclusively used for the former, the systematic search for the best solution, in this thesis.

Within optimization methods for industrial processes, typically, two types of optimization approaches are distinguished: Operational and design optimization. Operational optimization aims to determine the optimal operation of a process over a specified time horizon, including the choice of utilization, operation mode, and capacity of all components in a process. In contrast, design optimization deals with the optimization of the process's design. Thus this approach focuses on the adaption, replacement, and integration of new components in a process. Both operational and design optimization can be deployed independently, but combining the two approaches is currently investigated (Hofmann et al. 2019; Halmschlager et al. 2020a).

In this thesis, the main focus is on operational optimization of industrial processes, more specifically, applying the unit commitment problem to the Energy Hub concept.

Unit Commitment Problem

The unit commitment (UC) problem is an optimization problem in which the optimal commitment (on/off) and operation (loading level) of a set of units in a process is determined. A defined cost function acts as the objective function that is minimized, and operational constraints and demands are the boundary conditions of the optimization problem.

The UC problem originated in the power systems research in 1949 and, since then, has been frequently treated by many researchers (Abdou et al. 2018). Today, UC problems are widely used for operational optimization of energy systems and a variety of different solution techniques exist. They include dynamic programming, non-linear and linear programming approaches such as mixed-integer-linear-programming (MILP) and mixed-integer quadratic programming, heuristics, lagrangian relaxation, simulated annealing, and evolution inspired approaches (Carrion et al. 2006). As the UC problem includes the decision, whether a unit is on or off, it includes integer variables and results in a combination problem difficult to solve (Wood et al. 2014).

As a solution for the UC problem, the MILP formulation is widely used and also the method of choice in this thesis due to two major reasons: First, as only linear formulations are used, MILP problems can be solved with linear programming based solvers, leading to comparatively low computational times and a guaranteed minimum. Secondly, the MILP formulation offers high modeling flexibility. As for drawbacks, some systems cannot be represented precisely by linear formulations, and large optimization problems lead to considerable computational times. Nevertheless, MILP optimization problems have become a state-of-the-art method for the formulation of UC problems and have been applied successfully in a great variety of industrial applications. (Knueven et al. 2018)

Generally, mathematical programming formulations for optimization problems such as MILP aim to create an abstraction of a real system and consist of an objective function, constraints, and variables. To formulate the problem's constraints and define the objective function, a set of mathematical relationships, e.g. equalities, inequalities, and logical conditions, are used. In contrast to the general formulation of optimization problems, the MILP formulation only includes linear terms in the objective function and constraints, and includes at least one integer variable, according to Eq. (1). (Floudas 1995)

$$\min \ c^T x + d^T y \tag{1a}$$

$$s.t. \ \ Ax + By \leq g \tag{1b}$$

$$x \geq 0, \quad x \in X \subseteq \mathbb{R}^n \tag{1c}$$

$$y \in [0,1]^q \tag{1d}$$

Eq. (1a) describes the objective function of the optimization problem, were x is a vector of n continuous variables – see Eq. (1c) –, y is a vector of q integer variables – see Eq. (1d) – and c and d are n-column and q-column vectors of parameters. Eq. (1b) defines the constraints, where A and B are parameter matrices and g a parameter vector.

In the past decades, several efficient MILP formulations for the UC problem emerged, which primarily differ in their tightness, compactness, and use of integer, or rather binary variables. These binary variables are required to model the on/off behavior of a unit, formulate specific constraints, and differentiate between operation modes. A great number of binary variables, e.g. in large-scale optimization problems, can drastically increase the computational effort, and thus, several researchers aimed to minimize these integer variables. Initially, an approach with three binary variables was suggested (Arroyo et al. 2000), but today also approaches with two binary variables (Yang et al. 2017) and one binary variable exist (Carrion et al. 2006) to describe the behavior of one unit.

In the following paragraphs, an overview of commonly used constraints, an objective function, possible solvers, and the expected results of a UC-MILP problem are explained, based on a cost-based approach with three binary variables (Chang et al. 2004).

Start-up Constraint The start-up constraint defines the on/off behaviour of units, in this case with three binary variables u, v and w: Every time step t, a unit can either be *on* ($u = 1$) or *off* ($u = 0$) – according to Eq. (2) – and cannot be start-up ($v = 1$) and shut-down ($w = 1$) simultaneously – according to Eq. (3). In this and following equations, t is an index for the time that is limited by the horizon of the optimization T, being the simulation time.

$$u_t - u_{t-1} = v_t - w_t \qquad , \forall t \in [2, T] \tag{2}$$

$$v_t + w_t \leq 1 \qquad , \forall t \in [2, T] \tag{3}$$

Maximum/Minimum Generation Constraint With the maximum/minimum generation constraint, a stream p of a unit (e.g. thermal or electrical energy) can be limited by a minimum $p_{\min}$ and maximum $p_{\max}$ value, according to Eq. (4).

$$u_t \cdot p_{\min} \leq p_t \leq u_t \cdot p_{\max} \qquad , \forall t \in [1, T] \tag{4}$$

Ramp-Up/Ramp-Down Constraint Ramp-up/ramp-down constraints limit the gradient of a unit's stream with a maximal positive (Ru) gradient – according to Eq. (5) – or a maximal negative (Rd) gradient – according to Eq. (6).

$$(p_{t+1} - p_t) \leq \mathrm{Ru} \qquad , \forall t \in [1, T] \tag{5}$$

$$(p_t - p_{t+1}) \leq \mathrm{Rd} \qquad , \forall t \in [1, T] \tag{6}$$

Minimum-Up/Minimum-Down Time Constraint This constraint defines the time Ut that a unit needs to be on – see Eq. (7) – after it was started, and the time Dt that a unit needs to be off – see Eq. (8) – after it was shut down.

$$v_t + \sum_{k=t+1}^{t+Ut-1} w_k \leq 1 \qquad , \forall t \in [2, T] \tag{7}$$

$$w_t + \sum_{k=t+1}^{t+Dt-1} v_k \leq 1 \qquad , \forall t \in [2, T] \tag{8}$$

Conversion Constraint A constraint that is typically not described in MILP-UC models – probably because it is strongly dependent on the application – is a constraint that defines the linear relation between input and output streams of a unit, e.g. according to Eq. (9). This relation describes the conversion of e.g. energy streams that take place in a unit. For example, in a simplified model of a steam boiler, this constraint defines the relation between consumed fuel (input) and resulting steam (output).

$$a + \sum_i b_i \cdot |p_{i,t}| = 0 \quad , \forall t \in [1, T] \tag{9}$$

Here, a and b are constants, p represents any stream of a unit, and i is an index for the streams part of this constraint.

If a unit can not be described by a linear conversion constraint sufficiently, nonlinear behavior can be approximated by piece-wise linear segments. Binary variables bin are used to switch between associated linear functions according to Eq. (10), where n is an index for the linear segments. As only one linear function can be used at a time, Eq. (11) defines that only one of the binary variables can be unequal to zero every timestep.

$$\sum_n (a_n + \sum_i b_{i,n} \cdot |p_{i,t}|) \cdot bin_{n,t} = 0 \quad , \forall t \in [1, T] \tag{10}$$

$$\sum_n bin_{n,t} = 1 \quad , \forall t \in [1, T] \tag{11}$$

Minimum Output Constraint This constraint defines a minimum value D – e.g. an external demand – that needs to be fulfilled by a particular stream of a unit p, according to Eq. (12). If desired, a slack variable S – which can be penalized in the objective function – can be used to relax this constraint.

$$p_t + S_t = D_t \ , \quad S_t \geq 0 \qquad , \forall t \in [1, T] \tag{12}$$

Objective Function Typically, the objective function in the MILP-UC problem is a cost function and, therefore, is minimized when solving the optimization problem. The objective function includes different cost terms and can comprise real costs and auxiliary cost terms to drive the optimization towards a specific goal. For example, the objective function can include process costs such as fuel costs F, operation costs O, and rewards R, e.g. for selling electricity, heat or a product. This objective function can be described by Eq. (13), where f, o and r are the indices for the fuel costs, operation costs, and rewards.

$$\min \sum_{t=1}^{T} (\sum_f F_{f,t} + \sum_o O_{o,t} - \sum_r R_{r,t}) \tag{13}$$

Model Creation To create a MILP-UC model, fitting constraints and objectives for an application are chosen, and parameters are customized with available data and information. The above-described constraints and the objective function are examples of commonly used constraints and objectives, and several varying formulations exist in the literature (Abdi 2021). Before the formulated optimization problem can be solved, the prediction horizon of the optimization T needs to be defined, as well as a possible receeding horizon, also called rolling horizon. Using the rolling horizon approach, several optimization steps are conducted after each other, using the results of the previous optimization step as starting values. A detailed description of the rolling horizon approach can be found e.g. in Quoilin et al. (2017).

Model Solution After the formulation of the optimization problem is finalized, the MILP-UC problem can be handed to a solver. Nowadays, a number of very efficient solvers for MILP formulations exist that often use a mixture of different solution methods (e.g. Simplex-Methods, Branch & Bound, Branch & Cut). Finally, the optimization results in the values of all optimized variables of the optimization. These usually include the trajectories of all units' streams along the horizon, as well as the binary variables of all units that define whether a unit is on or off.

Summarized, by the formulation of a UC optimization problem, the optimal commitment and operation of a set of units in a process can be determined. Thus, this approach can be used to conduct operational optimization of industrial processes, resulting in economic and ecological savings. Also, in the bibliographical survey about the UC problems in Padhy (2004), the UC was considered one of the best available options to meet energy demand at minimum fuel costs. Nevertheless, the increasing complexity of today's energy systems, e.g. by distributed generation and the interconnection of different energy sources, further complicate the optimal use of energy in industrial processes. Thus, approaches that try to optimize one single energy carrier in one process are more and more displaced by holistic energy management concepts, such as the Energy Hub. (Cui et al. 2018)

Energy Hub Concept

The Energy Hub (EH) is a concept for optimal energy management of multi-energy-carriers, such as thermal and electrical energy, gas, and water. It was introduced in 2005 within a project called "a vision of future energy networks" (Favre-Perrod 2005) and since then has been covered in many publications.

Geidl et al. (2007) defined the Energy Hub (EH) as a unit where multiple energy carriers can be converted, conditioned, and stored. In other words, the EH concept aims to describe any multi-carrier-energy system that provides the features conversion, storage, input, and output. Therefore, this concept emphasizes the global view on energy systems, not only taking into account one energy carrier in one process, but considering the interactions between energy carriers, possibly in a network of several energy systems.

To better understand this seemingly abstract concept, the matrix model of an EH is shown in Fig. 3, and its corresponding matrix in Eq. (14), where $\boldsymbol{I}$ are the EH's inputs, $\boldsymbol{L}$ its outputs, and $\boldsymbol{C}$ is a parameter matrix. The EH in Fig. 3 consists of inputs and outputs, as well as a central area in which conversion and storage takes place. By correlating the different energy carriers at the input and output by the coupling matrix from Eq. (14), a model of an EH is created. For a more applied perspective, Fig. 4 shows a typical structure of an EH with four different energy carriers (electrical energy, thermal energy, energy from fuel A, and energy from fuel B), which could represent (a part of) an industrial energy system.

$$\begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_n \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1n} \\ C_{21} & C_{22} & \cdots & C_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \cdots & C_{mn} \end{bmatrix} = \begin{bmatrix} L_1 \\ L_2 \\ \vdots \\ L_m \end{bmatrix} \tag{14}$$

Figure 3: *Matrix model of the Energy Hub. Based on Mohammadi et al. (2017)*

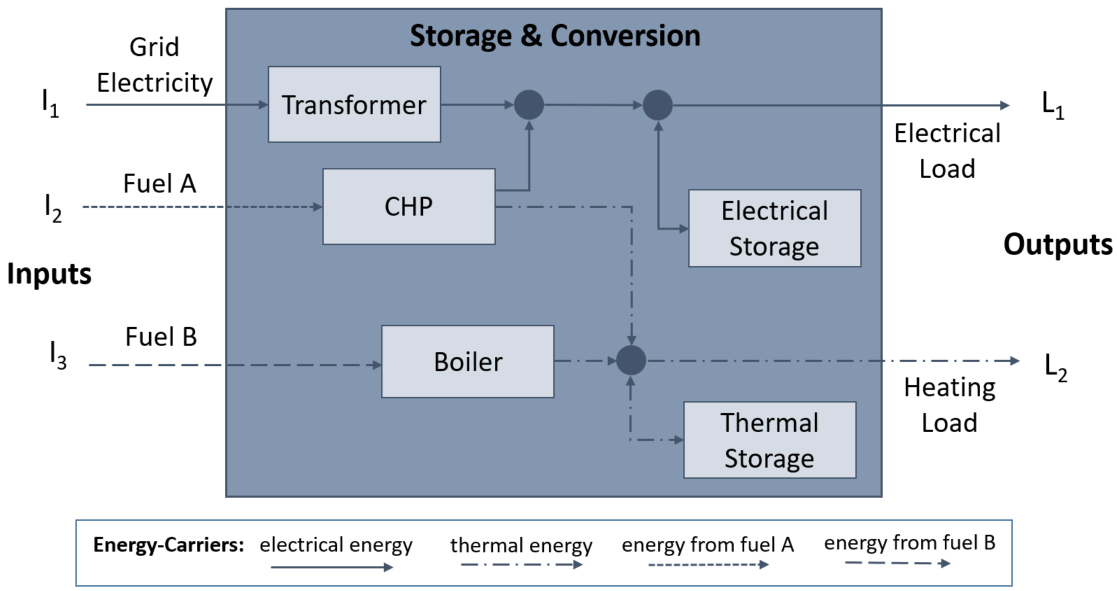


Figure 4: *Schematic structure of an Energy Hub. Based on Mohammadi et al. (2018)*

Over time, the Energy Hub concept has been applied to a variety of applications in different sectors. In Mohammadi et al. (2018), EHs are divided into macro and micro EHs, and into four sectors: residential, commercial, industrial, and agricultural. Micro EHs describe energy systems that aim to minimize their individual energy consumption, e.g. industrial power or manufacturing plants, and buildings. In contrast, macro EHs aim to optimize energy consumption from a controller perspective of an entire system, e.g. cities, and networks. According to the literature review in Mohammadi et al. (2018) and an overview of the state of the art of EHs in Sadeghi et al. (2019), most of the research conducted was in the fields of macro EHs and micro EHs in the residential sector, and only a few publications dealt with the optimization of industrial EHs.

However, in the last few years, several publications emerged – especially dealing with power plants – that cover different aspects of industrial EHs, e.g. new algorithms, applications, and technologies. Publications on this topic included the optimization of industrial EHs in smart grids (Paudyal et al. 2015), using a multi-objective model with heat and power (Nojavan et al. 2018), optimization of EHs with a demand response program (Majidi et al. 2017), or the optimization of an EH including water and energy (Vahid Pakdel et al. 2020). Also, publications dealt with flexibility measures in EHs (Niu et al. 2020), optimal planning and operation of multi-carrier networked microgrids (Ghanbari et al. 2020), or different aspects of uncertainties in EH systems (Pazouki et al. 2016; Najafi-Ghalelou et al. 2019; Roustai et al. 2018; Rakipour et al. 2019; Vahid-Pakdel et al. 2017). In most recent works, an optimization framework for multi-energy-carrier systems using Particle Swarm Optimization (PSO) algorithm was developed in Lingmin et al. (2020), and a multi-carrier energy network with thermal energy storage was optimized in Nazari-Heris et al. (2020).

The high number of recent publications underlines that this topic shows great interest in today's research. Nevertheless, previous works dealing with the EH approach in industry mainly focused on the optimization of power plants and only a few works dealt with the optimization of manufacturing processes. In fact, out of the significant number of articles presented in the extensive literature survey on Energy Hubs in Sadeghi et al. (2019), only the research in Calise et al. (2017) dealt with a manufacturing process, an engine manufacturing facility. However, with the manufacturing sector accounting for about one third of the final energy consumption in Austria according to IEA (2020), the application of the Energy Hub concept for manufacturing industrial processes seems to be a major research gap.

After this introduction of the Energy Hub concept and a literature review on industrial EHs, the focus is on the modeling and optimization approaches in EHs, particularly based on MILP and the unit commitment problem.

Optimization of Energy Hubs with MILP

First of all, being rather a concept than a method, the EH does not define a particular formulation or solution for the optimization problem to be solved. However, as EH optimization problems are usually large-scale, appropriate methods need to be chosen. In literature, for example, publications on EHs cover meta-heuristics and evolutionary optimization techniques like Particle Swarm Optimization, Quantum Particle Swarm Optimization, genetic algorithms (Shahrabi et al. 2021), or multi-agent genetic algorithms (Moeini-Aghtaie et al. 2014). However, as a (micro) EH optimization problem can be seen as an extended UC problem, comprising different energy carriers and interacting with external systems (e.g. district heating network, electricity grid), also MILP formulations have been widely applied (Shao et al. 2017).

Applying the MILP approach to the optimization of EHs, the constraints and objectives from the UC problem – see Eq. (2-13) – can be used as a basis, and the optimization problem can be solved with standard MILP solvers. However, for the formulation of EHs with MILP, additional constraints – for example for storage – are required in most applications, and the objective function might include multiple objectives (multi-objective function). Eventually, to optimize EHs with MILP and relevant for every optimization problem, the particular formulation, the used constraints, objectives, and solution technique always depends on the specific application.

Bottom line, the introduced UC problem can be used to optimize industrial processes and results in the optimal commitment and operation of a process' units. This approach can be extended, e.g. using different energy carriers and modeling interactions with external systems, to represent a more holistic perspective of today's energy systems, e.g. using the Energy Hub concept. Although many publications already dealt with Energy Hubs in industrial power systems, manufacturing EHs have only been marginally covered in the literature. Finally, regardless of the optimization approach used to optimize industrial processes, in the first step, accurate and reliable component models are required.

2.2 Modeling of Physical Systems

Basically, models of physical systems can be divided into two distinct approaches: Models that are derived from physical relations, called physical or white-box models, and models that are based on the analysis of data, called black-box, empirical, or data-driven models. The former traditionally used modeling approach uses a high level of mechanistic insights to create a model based on physical equations. The latter models use data and especially focus on finding a relationship between the system state variables (input and output) without explicit knowledge of the systems physical behavior (Solomatine et al. 2008). Compared to physical models, pure data-driven models can benefit from decreased modeling and computational effort. However, they are most often not transparent and lack robustness (Hamon et al. 2020).[4]

Models that use a mix of physical and data-driven approaches are referred to as grey-box models, and can therefore benefit from advantages of both approaches (Sohlberg et al. 2008). Depending on the amount of data or physical relations used, grey-box models can be either assumed to be more on the white-box side or on the black-side. An illustration of white-, grey- and black-box models can be seen in Fig. 5.

To create a grey-box model of a physical system, several approaches can be applied to combine data and physical knowledge. Thus, as a first step, the physical behavior of a system and possible data-driven modeling approaches need to be analyzed. For this reason, in the following sections, an overview of today's relevant data-driven modeling approaches is given before referring to grey-box modeling methods in particular. White-box models are not included in the description, as the choice of physical equations is always dependent on the specific application.

[4] The characteristics of black-box and white-box models are often generalized. Thus it is important to emphasize that not every data-driven model shows excellent accuracy and lacks robustness/reliability and not every purely physical model shows high computational effort and low accuracy, but only tendencies exist.

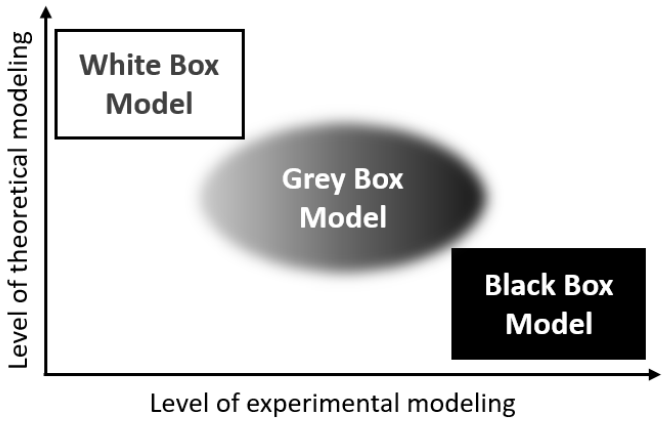


Figure 5: *Classification of black-box, grey-box and white-box models. Based on the presentation of Halmschlager et al. (2019) at NOLCOS conference.*

Data-Driven Modeling – Machine Learning

Especially with the developments in computational intelligence and machine learning, data-driven models have increased in significance in the past years. Common representatives for traditionally used data-driven modeling methods are linear regression or ARIMA (autoregressive integrated moving average). However, the increased capabilities of data-driven modeling techniques have brought many new and powerful modeling tools. These tools are often referred to as machine learning techniques and include e.g. Neural Networks. (Solomatine et al. 2008)

Machine learning (ML) is seen as a part of artificial intelligence and describes mathematical techniques/algorithms that independently improve through experience. These algorithms are fed with data – called training data – to build a prediction model that is automatically improved until a specific goal is reached. To create accurate and efficient models, the training data needs to be of a certain quality and magnitude. Thus, large amounts of data are required for machine learning, which can be a drawback for some applications. Nevertheless, due to the great potential of machine learning algorithms, they have been applied to various applications, including pattern and language recognition, transaction fraud detection, spam-identification, time-series-prediction, and many more. (Litzel 2016)

Usually, machine learning is separated into three major categories:

- **Supervised Learning:** In supervised learning, example inputs and desired outputs are predefined and the algorithms aim to find a general relation between input and output data. Supervised learning can be further divided into classification and regression. Typical applications of supervised learning are pattern and speech recognition and any type of prediction/forecasting, e.g. for price developments or prediction of machine behavior. (Ionos 2021a)

- **Unsupervised Learning:** In unsupervised learning, inputs and outputs are not predefined, but the algorithm aims to discover patterns in the data. Unsupervised learning is, e.g. used for anomaly detection, genetics (DNA patterns), or customer segmentation. (Heidmann 2021)
- **Reinforcement Learning:** In reinforcement learning, rewards are used for the algorithm to learn a desired strategy automatically. This form of learning is most often used by humans as well and can be applied to learn complex strategies. This type of machine learning is, e.g. used in parking assistance for cars or the management of smart grids. (Ionos 2021b)

For the modeling and prediction of time-series, e.g. for weather forecasts, price developments, or machine behavior, supervised regression learning and especially Artificial Neural Networks (NN) have attracted attention. Compared to classical time-series prediction methods like ARIMA models, NN can better deal with missing values, are able to recognize complex patterns in data, and can be applied to long term forecasts. In the past years, several approaches for time-series forecasting with NNs emerged, being inter alia Recurrent Neural Networks (RNN), Long-Memory-Short-Term (LMST), Gated Recurrent Unit (GRU), or Encoder-Decoder Model NN. Out of these approaches, RNNs are the most classical method for time-series predictions and many other approaches (e.g. LMST and GRU) are evolutions of the RNN. (Del Pra 2020)

Basically, the structure of RNNs is very similar to standard NNs, where neurons are divided into input layer, hidden layers, and output layer with corresponding weights and biases of each neuron's input. In contrast to standard NNs that only have forward connections, RNNs use feedback loops to address the temporal order and dependencies of sequences in a time-series (Schäfer et al. 2006). Same as standard NNs, RNNs are trained by optimizing the networks biases and weights and they require the specification of so-called hyperparameters. The hyperparameters include the variables that define the network's structure (number of hidden layers and amounts of neurons in each layer) and define how the network is trained. No exact rules or specifications exist to determine suitable values for these hyperparameters, but rules of thumb are usually applied.

To facilitate the development of NNs like RNNs, nowadays, a number of tools exist where only the type of NN, its hyperparameters, and the data need to be defined before a NN can be trained and tested. With these novel modeling tools, the creation and application of NNs and other ML tools became easier accessible, also for people with other backgrounds than in the field of ML.

Summarized, ML techniques such as NNs show very good performance for various tasks, including time-series predictions. However, for industrial applications, non-transparent and possibly unreliable predictions are a significant drawback of these models. To compensate for this disadvantage, they can be combined with physical modeling approaches. This combination is referred to as grey-box modeling and can be used to combine efficient and accurate ML modeling techniques with the robustness and reliability of physical modeling.

Grey-Box Modeling Methods and Applications

Grey-box models combine data-driven modeling approaches with physical considerations. According to Sohlberg et al. (2008), five different types of grey-box models can be differentiated, depending on how physical considerations and data are included in a model. Although most applications of grey-box modeling in literature do not explicitly identify with one of these five grey-box modeling types and often represent a mixture, the presented classification provides a good overview of the different approaches to grey-box modeling:

- **Constrained Black-Box Identification:** In constrained black-box identification, specific parameters of black-box models are constrained by physical relation. For example, in Aguirre et al. (2004), nonlinear polynomial models are constrained by steady-state information in a three-step approach.
- **Semi Physical Modeling:** In semi physical modeling, nonlinear transformations based on physical insights are applied to the existing data. The new input and output variables of the transformed data can be used as a regressor to create a black-box model.
- **Mechanistic Modeling:** In mechanistic modeling, physical equations of a system are formulated and one or more parameters are estimated/optimized by data. Typically, the primary chosen physical equations are refined continuously until a good fit is achieved. A systematic approach for this type of grey-box modeling is given in Sohlberg (1998).
- **Hybrid Modeling:** In hybrid modeling, a model is separated into a pure black-box modeling part and a white (or grey-box) modeling part. The black- and white-box modeling parts can either be used serially (e.g. the black-box part is used to model a small part of a system and included in a white-box model) or parallel (e.g. the black-box part is used to extend a too simple white-box model). As an example for this approach, in Thompson et al. (1994), a NN is employed as a black-box part in a model for a synthesizing chemical process.
- **Distributed Parameter Modeling:** For systems whose physical description includes partial differential equations, this grey-box modeling approach ensures that interferences between model reduction and model-data discrepancies are limited (Liu 2005).

Especially focusing on grey-box modeling of dynamic systems in industrial applications, e.g. thermal energy storage, only a few research in literature can be found. Particular on the topic of grey-box models that include ML approaches like NN, the research in literature is very rare.

In Tulleken (1993) a statistical estimation of the optimal linearly parametrized dynamic regression model was determined using physical knowledge and bayesian techniques. In

Oussar et al. (2001), a general methodology for grey-box modeling was proposed, building upon the mechanistic modeling approach. The grey-box modeling approach was applied to a dynamic industrial drying process. In Cen et al. (2011), an identification scheme for nonlinear dynamic systems using grey-box NNs was proposed and applied to a reaction wheel in a satellite attitude control system. Finally, Prada et al. (2018) identified a lack in literature dealing with the systematic development of dynamic grey-box models. Thus, a two-step approach for the development of grey-box models was presented, where physical relations are defined and a mixed-integer optimization algorithm is used to determine the remaining structure and parameters of the model. As a use-case, an acetone-butonal-ethanol fermentation process was analyzed. Pitarch et al. (2019) aimed to develop a grey-box model of limited complexity for process systems, e.g. for real-time optimization routines. A method based on data reconciliation and polynomial constrained regression was proposed and applied in an industrial evaporation plant.

This short literature survey in the field of dynamic grey-box modeling for industrial applications showed that research in this topic is still expandable. Especially the creation of grey-box models with ML techniques have been rarely dealt with, none of them focusing on the modeling of dynamic systems in industrial applications, e.g. for thermal energy storage. Although different types of grey-box models have already been developed for various applications and despite some attempts, there is still no universal approach for the development of grey-box models. In fact, the particular combination of physical considerations and amounts and method data is included in a model is strongly dependent on the application. Overcoming this challenge, grey-box models offer great potential to model dynamic systems in industrial applications. With their high flexibility of combining physical and data-driven models in various ways, they can be used for a multitude of applications, profiting from the benefits of both modeling approaches.

3 Problem Statement

Based on the aforementioned prospects towards more sustainable and efficient industrial processes, a state-of-the-art analysis, and the identification of research gaps, this thesis focuses on two essential aspects of industrial process optimization that can contribute to today's challenges:

Operational Optimization: Although there exist many publications on the optimization of power plants, there is a lack of research dealing with operational optimization approaches that focus on manufacturing processes, which significantly contribute to the total energy consumption in the industrial sector. In addition to the optimization of energy streams in, e.g. power plants, manufacturing processes include production units and product streams that further complicate the optimization problem. Thus, generic optimization approaches for manufacturing industries are required, where energy *and* product streams are optimized to exploit a process's full potential. This assessment leads to the following objective and sub-questions Q:

Objective: *Develop a modular tool for the operational optimization of manufacturing processes.*

Q1: *Does the tool improve the operation of a process?*

Q2: *Can the tool's models be adapted to changes of a process easily?*

Q3: *Is the tool applicable to other manufacturing processes?*

To achieve this objective and answer the formulated questions, a chipboard production process of the Fundermax GmbH served as a real industrial use-case. The chipboard production plant includes several energy conversion units (e.g. CHP plant, steam boilers), units for production (e.g. press, dryers), electricity can be sold to the grid, and a specified district heating demand needs to be fulfilled by the operators of the plant. The data and information basis of the use-case included time-series measurements, data-sheets, energy reports, and knowledge based on the experience of the plant operators.

Robust and Efficient Component Modeling: As an essential part of every optimization model, robust, accurate, and efficient component models are required. Traditionally, models of components in industrial processes have been based on physical equations – also referred to as white-box models –, leading to robust and reliable but often computationally expensive and not always highly accurate models. In contrast, advances in artificial intelligence enhanced the application of data-driven, also called black-box models, in the past years. These models are built on data and can benefit from decreased modeling effort, and high performance and accuracy while typically being less robust and reliable than white-box models. For industrial applications where efficient yet robust and reliable models are required, a mixture of the data-driven and physical modeling approach seems promising. Therefore, the following objective and questions can be formulated:

Objective: *Develop robust, accurate, and efficient modeling approaches for components in industrial processes, using data and physical information.*

> ***Q1:*** *How do the models perform compared to purely physical or data-driven models?*
>
> ***Q2:*** *How much effort is required to adapt these models to changes?*
>
> ***Q3:*** *Can these modeling approaches be applied to other, similar systems?*

For this research aim, one component of an industrial energy system, a sensible thermal energy storage located at the TU Wien laboratory – a packed-bed regenerator – was considered as a use-case. The packed-bed regenerator is a cost-efficient sensible thermal energy storage, especially suitable for industrial-scale, high temperature, short cycle storage applications. Several time series from experiments and a purely physical white-box model of the regenerator were available for the development and assessment of the modeling approaches.

4 Research Approach

This thesis deals with two important aspects of industrial process optimization: operational optimization, and component modeling. The central part of this thesis is a modeling and optimization framework for operational optimization, which I developed and applied to our project partners' use-case, a real-world chipboard production plant. The framework is based on mixed-integer-linear-programming (MILP) and thus, only uses linear models. The framework is addressed in three core publications of this thesis, Paper 1, Paper 2, and Paper 3. The second part of this thesis covers the modeling of an industrial sensible thermal energy storage – a packed-bed regenerator – using non-linear dynamic grey-box modeling concepts that combine data-driven and physical modeling approaches. The developed models are addressed in two core publications, Paper 4 and Paper 5, and are also dealt with in parts of the co-author publication Paper A. Figure 6 gives an overview of this thesis's core and co-author publications.

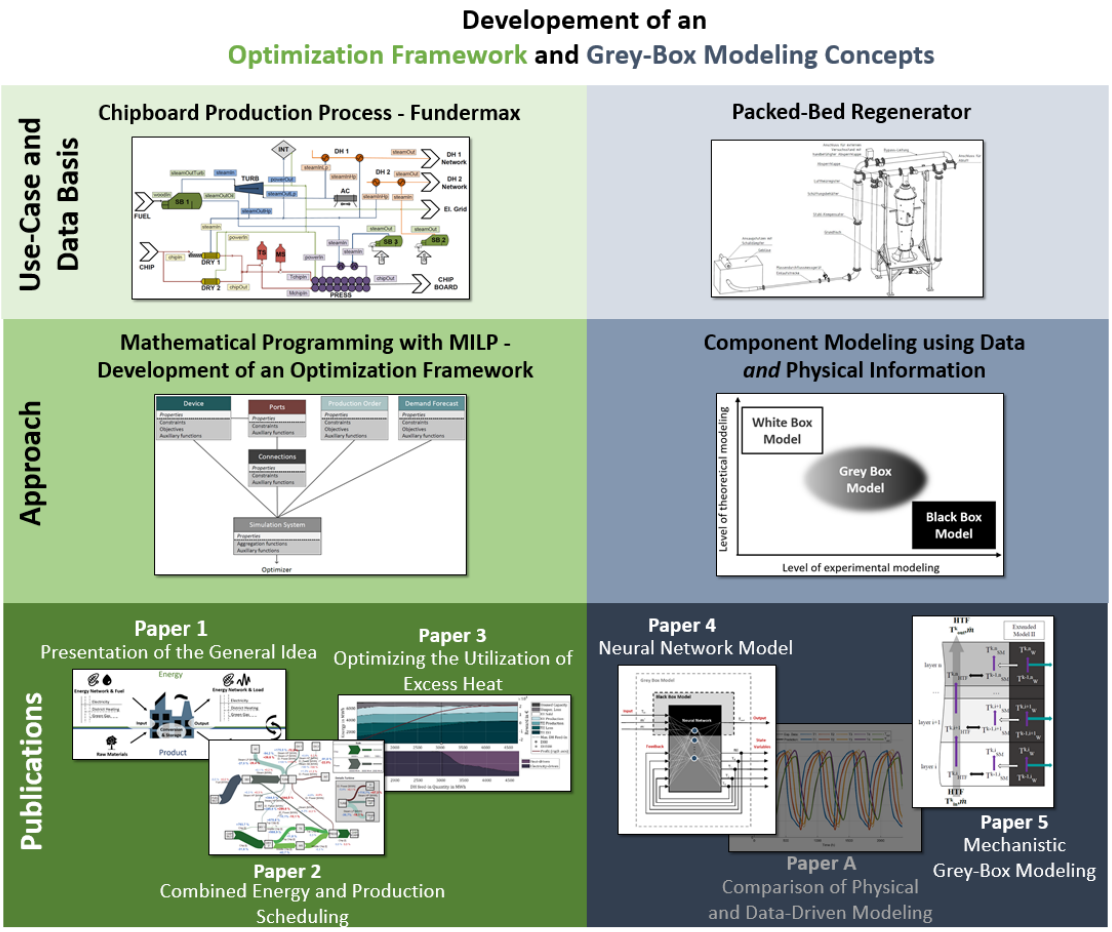


Figure 6: *Overview and links between the publications of this thesis*

4.1 Optimization Framework

The main part of this work covered the development of a modeling and optimization framework for industrial applications. The basic idea originated from my major goal within SIC! to develop a model for operational optimization of our project partner's use-case, a chipboard production plant. Out of the formulated goal and an analysis of state-of-the-art methods and identification of research gaps, we decided to not only create a model for the optimization of the use-case, but we wanted to develop an approach that allows to model and optimize (almost) any manufacturing process efficiently.

Inspired by the Energy Hub (EH) concept – a concept for optimal energy management in systems with multiple energy carriers – we aimed to develop a framework that can model and optimize industrial manufacturing EHs, also considering the product and production units. In **Paper 1**, we introduced this idea of the Industrial Energy Hub (IEH) and described the basic principles of the IEH modeling and optimization framework. The framework has a modular structure and is based on object-oriented programming to fit all the IEHs requirements and ensure maximal flexibility. For the formulation of the optimization problem, a MILP approach was used. In this first publication, we showed the applicability of our framework to a simplified and adapted version of the chipboard production process and analyzed the integration of storages. The results showed that, first, the framework allowed for straight-forward and efficient model creation and optimization of industrial manufacturing processes and second, that the included storages could improve the process's efficiency.

After the first application and proof of concept of our framework, we intended to apply the framework to the actual chipboard production process, using real process data and information from our project partner's plant. In **Paper 2**, we firstly published the optimization of the chipboard production process with the IEH modeling and optimization framework, based on process data. To assess the potential of the suggested IEH approach, we compared the sole optimization of energy streams (as typically done in the original EH approach) with the optimization of energy *and* product streams (done in the IEH approach). The results showed that the consideration of product streams is crucial for the optimization of the chipboard production plant and that energy losses could be reduced by approximately 30 % by optimization with the IEH approach. However, we also found out that this potential can only be exploited if process design is adapted accordingly and utilization of excess heat is improved.

As the logical next step, we investigated the optimal utilization of excess heat in the chipboard production process with design adaptations in **Paper 3**. Due to the flexible and modular structure of the framework, these design adaptations to the original chipboard production process could be modeled straight-forward and time-efficiently. The design adaptations included two thermal energy storage – a Ruth's steam storage and a stratified tank buffer storage – and the integration of an additional heat exchanger for district heating. A comparison between the original and the adapted process showed that the adaptations offer major advantages in terms of energy efficiency and costs. From all scenarios, the integration of the additional heat exchanger for district heating resulted in the highest profit. In contrast, the highest energy savings could be achieved with the integration of the Ruth's steam storage. Also, this application showed that the framework is well suited to model and optimize different scenarios within a process fast and efficiently.

4.2 Grey-Box Modeling Concepts

The starting point for this part of the thesis was the question, how to use existing data to efficiently model devices in industrial applications, e.g. for the integration in process optimization tools. For this approach, we decided to not only look into linear models that can be directly implemented in MILP optimization approaches, but also to analyze more complex non-linear models that we expected to show higher accuracy. In future research, on the one hand, these non-linear models could be linearized to be used in a MILP optimization approach. On the other hand, the non-linear modeling approaches could be used as a basis for other relevant topics within SIC!, e.g. general simulations, non-linear (design) optimization, and digital twin applications.

As a first step, I was looking into data-driven modeling approaches and black-box modeling. Within the variety of data-driven modeling approaches, machine learning techniques have seen a real hype in the past years because of their seemingly magical ability to make accurate predictions based on data. Especially Neural Networks have shown good performance for various (industrial) applications, and thus, they were my method of choice. After some research, though, we came to the conclusion that pure data-driven models might not be the best choice for industrial applications because they are difficult to interpret and can lead to unpredictable results. This conclusion led to the idea of incorporating physical knowledge into a data-driven model – in other words, to go for a grey-box modeling approach. We wanted to create a model that uses the best of both worlds: A model consisting of a data-driven part (e.g. Neural Networks) – aiming for accuracy and time-efficiency – and a physically-driven part – aiming for physical consistency and predictability.

In **Paper 4**, we realized this idea, creating a Neural Network (NN) model that was tailored to the specific use-case based on physical information. As a use-case, a sensible thermal energy storage, more precisely a packed-bed regenerator (PBR) situated at the TU Wien laboratory, could be employed. The model was built up by a recurrent NN as the data-driven part and considered the physical behavior of the use-case by choosing a network structure to account for the time-dependent, dynamic behavior of the thermal energy storage. The data basis for the model was generated by simulations of a validated white-box model of the PBR. Due to the importance of the predefined, physically-based structure of the NN, we decided to classify this model as grey-box. Regarding the NN model's results, the model could predict the PBRs outlet temperature over several loading and unloading cycles accurately with low computational effort. Essential for the successful model creation was the integration of state variables, the restructuring of state variables to account for changing physics, and last to keep the NN model simple and thus, limit the number of neurons and hidden layers in the NN architecture.

As a next step, we wanted to further evaluate the NN modeling concept and prove its applicability to measurement data. This was done as a part of the co-author **Paper A**, where we utilized measurement data of the PBR and compared the resulting NN model to the existing white-box model of the PBR. Again, the results of the NN model led to accurate predictions of the PBRs behavior, only showing minor deviations to the data. A quantitative and qualitative comparison with the white-box model demonstrated that the NN model yielded higher accuracy, showed decreased modeling and computational effort, and required less physical information of the use-case. However, drawbacks of this method were the relatively high amounts of required data and the decreased reliability compared to the white-box model. Although the NN model included some physical information of the PBR, the Neural Network was still the dominant part of the model, leading to a model that was rather data-driven than physical. This was also emphasized by the fact that partly incorrect data inevitably led to wrong, non-physical predictions, showing that the physical considerations were not able to prevent physically impossible results.

To recapitulate, the – rather data-driven than physically-driven – NN model showed very good performance but could still be improved in terms of robustness and reliability. To this end, we were curious to try other types of combining data-driven and physical modeling approaches for our use-case, which do not primarily focus on data. Considering the available data and physical information of the PBR, we chose a mechanistic grey-box modeling approach.

The mechanistic grey-box modeling approach was the content of **Paper 5** and also aimed to predict the outlet temperature of the PBR. However, in contrast to the previously developed NN models that were mainly built on data, the mechanistic grey-box model was mainly built on physical equations. The data-driven modeling part was included in the model by optimizing relevant parameters of these equations to fit the available measurement data of the PRB. A particular challenge within this approach was determining the most suitable physical equations to balance the contradiction between model simplicity and accuracy. In the end, the final model consisted of five equations and six parameters to be determined by optimization. The results of the mechanistic grey-box model were compared to the NN model and the white-box model. The mechanistic grey-box model not only showed higher accuracy than the NN model and the white-box model, but also improved robustness and reliability compared to the NN model, and reduced modeling and computational effort than the white-box model. In contrast to the NN model, partly incorrect data could be compensated by the model by its implemented physical equations that did not allow non-physical predictions.

5 Conclusion and Outlook

In this thesis, on the one hand, a modeling and optimization framework for industrial processes, particularly for the operational optimization of manufacturing plants, was developed and applied to a real-world use-case. On the other hand, two modeling approaches for a sensible thermal energy storage based on data and physical knowledge were investigated. The application of energy management systems like the optimization framework combined with efficient and reliable component models can contribute to today's energy and climate challenges by improving process efficiency and reducing overall energy consumption.

The modeling and optimization framework was inspired by the Energy Hub concept, a concept for optimal energy management in multi-energy-carrier systems. The framework aims for efficient and straight-forward optimization of industrial manufacturing processes and is built on a flexible and modular structure. As a basis for the formulation of the optimization problem, typical constraints and objectives of the unit commitment problem were implemented as MILP equations. Using this linear optimization approach, state-of-the-art solvers can solve the formulated optimization problem with low computational effort. As a novelty of this framework, the focus was laid on manufacturing processes and, thus, on the combined optimization of energy streams and optimal use of product streams and production units.

The framework was applied to a real-world use-case, a chipboard production plant. The model of the chipboard production plant included energy conversion and production units, electricity could be sold to the grid, a district heating demand needed to be met, and a specified amount of the product – chipboards – needed to be produced. Employing the optimization framework to the use-case with and without design adaptations yielded three relevant outcomes:

- The consideration of product streams in addition to energy streams is essential for the optimization of the chipboard production plant. Taking into account product *and* energy streams, energy losses can be reduced by approximately 30 %, compared to the sole optimization of energy streams.
- The integration of an additional heat exchanger and two types of sensible thermal energy storage revealed that these design adaptations yield significant benefits in energy efficiency and costs.
- The application of the framework to the chipboard production process within the three publications illustrated the potential of the framework to efficiently model and optimize industrial manufacturing processes. Also, design adaptations like the integration of thermal energy storage can be considered straight-forward due to the framework's modular structure.

Although the outcomes of the framework were satisfying, some ideas for improvements and future work could be identified: First, while the framework has been applied to a chipboard production plant using real process information and data, the optimization results have not yet been utilized for a real-time implementation in the plant. To do so, a great number of additional sensors in the production plant and an advanced control system would be necessary. Moreover, for a real-time implementation, the robustness of the framework against faulty predictions – due to unfeasible or unbounded optimization conditions – needs to be verified. Second, even though the use/application of the framework is straight-forward, the implementation of *additional* constraints or optimization options into the framework is quite complex and requires detailed knowledge of the framework's structure. Thus, to further extend the framework's application area, other processes' requirements need to be identified, and corresponding constraints or other features need to be implemented. Nevertheless, the framework's current built-in features should be adequate to model and optimize a wide variety of (manufacturing) processes efficiently, assuming that linear correlations can approximate their behavior. Last, as a *nice-to-have feature*, the development of a simple user-interface could further enhance the user-friendliness of the framework.

Regarding the formulated objective and research questions from Section 3, the developed optimization framework is well suited to model and optimize industrial manufacturing processes. Due to its flexible, modular structure, the framework can be easily adapted to process changes, also enabling the analysis of different scenarios. This flexible structure also allows the framework to be used for other manufacturing processes, however, only under the condition that linear correlations can describe these processes sufficiently accurately. Besides that, the application of the framework to the chipboard production plant showed that – in theory – the framework is capable of improving the use-case's energy consumption and energy losses by predicting the optimal trajectories of energy and product streams and suggesting suitable design adaptations. However, the expected improvements can only be realized if the process follows the predicted trajectories in a real-time implementation – only then, the actual potential of the optimization can be exploited. Thus, so far and without a real-time implementation, the framework has been primarily used to evaluate a process's potential. Nevertheless, the framework is a relevant step towards a more generic view of energy systems, considering most of the literature on industrial process optimization focuses on optimizing energy streams in, e.g. industrial power plants. It was shown that the product streams and production units play an essential role in the energy management of the entire chipboard production plant and, thus, should not be neglected. Therefore, the results underline the need for holistic optimization approaches for industrial (manufacturing) processes.

As the second part of this thesis, two modeling concepts for a sensible thermal energy storage - a packed-bed regenerator - were developed, aiming for models that are as accurate and efficient as data-driven models and at the same time as reliable as physical ones. As the models are based on data *and* physical knowledge, they were classified as grey-box models. The first model consists of a Neural Network (NN) as the data-driven part, which was tailored to the specific use-case based on physical information, e.g. by considering the time-dependent behavior of the thermal energy storage. The second model is based on a mechanistic grey-box modeling approach, in which parameters of physical equations were fitted to data. Compared to the NN model that was mainly built on data, the mechanistic grey-box model was principally based on physical equations. Both models were compared to an existing white-box model of the regenerator and showed improved performance in terms of accuracy, flexibility, and modeling and computational effort.

The application of the developed models to the packed-bed regenerator as an industrial use-case resulted in the following main conclusions:

- The NN model that was mainly built on data stands out by its accuracy and low modeling effort. Most important for the successful model creation was integrating state variables, the restructuring of variables to account for a change in physics, and keeping the NN architecture as simple as possible. However, with the NN model it is not possible to detect unplausible/unphysical effects in the data as the model will simply recreate the unphysical effects. This was recognized when the NN model predicted higher internal regenerator temperatures than physically possible due to inaccurate data.
- The mechanistic grey-box model convinces by very high accuracy, robustness, and low computational effort. Mainly based on physical equations, this approach can compensate for partly incorrect data. However, creating the mechanistic grey-box model was an iterative manual process, and a suitable set of equations could only be determined after several iteration steps.
- Although both models are accurate and efficient, three major advantages of the mechanistic grey-box model could be identified: First and most importantly, only the mechanistic grey-box model meets the goal of robustness/reliability, which is an essential feature, especially when it comes to real-time applications. In contrast, in the NN model, incorrect data will inevitably lead to wrong predictions. As a further advantage of the mechanistic grey-box model, it is easier adaptable to changes of the use-case. The reason is that – once the equations are set up – this model's parameter fitting can be conducted fast and only requires small amounts of new data. In contrast, the NN model requires large amounts of data, and model training can be challenging and might take several attempts with varying data sets. Last, the computational effort for the training, and for the testing of the mechanistic grey-box model is lower than for the NN model.

For future work, the modeling concepts should be applied to other industrial components, aiming to develop a universal systematic approach for combining data and physical knowledge. Even though the modeling effort of both models was still lower than for the existing white-box model, both models were developed iteratively and customized to the use-case to yield accurate predictions. Thus, a universal approach for creating grey-box models is essential to facilitate their creation. Besides that, the implementation of the models in process optimization tools, or e.g. in digital twin applications that are currently investigated intensively, could be evaluated. While the models can be integrated into any non-linear approach directly, the question remains open whether the models can be implemented into the developed linear optimization framework without losing too much information or being too complex.

Recapitulating and answering the formulated research questions in Section 3, both developed models stand out by their high accuracy and low computational effort compared to the white-box model, but only the mechanistic grey-box model also shows high robustness. Concerning flexibility, both models can be adapted to small changes (e.g. other materials, different operation ranges) of the use-case using the corresponding data to train/fit the models again. However, the training of the NN model can be challenging, and several attempts with varying data might be required. Due to the iterative and customized model creation, both models can only be used as a basis for modeling other similar systems, but they cannot be adopted directly. To do so, a universal modeling approach would be required. Last, it is essential to emphasize that there is no *correct* way of modelling, but that the assessment of a model always depends on the conditions and requirements of the specific use-case.

To sum it up, the developed optimization framework and modeling approaches showed promising results. For future research, the optimization framework could be extended to fit the needs of a real-time optimization tool and combined with advanced control systems. For the modeling concepts, a systematic approach for the combination of data and physical knowledge can further facilitate the use of these models. Finally, both of the presented approaches can make a small contribution to today's industrial challenges. However, in the end, a far-reaching change of our today's energy system can only be achieved if industry, society, and government all act together.

References

Abdi, H. (2021). "Profit-based unit commitment problem: A review of models, methods, challenges, and future directions". In: *Renewable and Sustainable Energy Reviews* 138, p. 110504. ISSN: 13640321.
DOI: 10.1016/j.rser.2020.110504.
URL: https://www.sciencedirect.com/science/article/pii/S1364032120307905

Abdou, I. and M. Tkiouat (2018). "Unit Commitment Problem in Electrical Power System: A Literature Review". In: *International Journal of Electrical and Computer Engineering (IJECE)* 8.3, p. 1357. ISSN: 2088-8708.
DOI: 10.11591/ijece.v8i3.pp1357-1372

Aguirre, L. A., M. Barroso, R. R. Saldanha, and E. Mendes (2004). "Imposing steady-state performance on identified nonlinear polynomial models by means of constrained parameter estimation". In: *IEE Proceedings - Control Theory and Applications* 151.2, pp. 174–179. ISSN: 1350-2379.
DOI: 10.1049/ip-cta:20040102

Arroyo, J. M. and A. J. Conejo (2000). "Optimal response of a thermal unit to an electricity spot market". In: *IEEE Transactions on Power Systems* 15.3, pp. 1098–1104. ISSN: 0885-8950.
DOI: 10.1109/59.871739

Calise, F., M. Dentice d'Accadia, L. Libertini, E. Quiriti, R. Vanoli, and M. Vicidomini (2017). "Optimal operating strategies of combined cooling, heating and power systems: A case study for an engine manufacturing facility". In: *Energy Conversion and Management* 149, pp. 1066–1084. ISSN: 01968904.
DOI: 10.1016/j.enconman.2017.06.028

Carrion, M. and J. M. Arroyo (2006). "A Computationally Efficient Mixed-Integer Linear Formulation for the Thermal Unit Commitment Problem". In: *IEEE Transactions on Power Systems* 21.3, pp. 1371–1378. ISSN: 0885-8950.
DOI: 10.1109/TPWRS.2006.876672

Cen, Z., J. Wei, and R. Jiang (2011). "A Grey-Box Neural Network based identification model for nonlinear dynamic systems". In: *2011 Fourth International Workshop on Advanced Computational Intelligence (IWACI 2011)*. Piscataway, NJ: IEEE, pp. 300–307. ISBN: 978-1-61284-375-9.
DOI: 10.1109/IWACI.2011.6160021

Chang, G. W., Y. D. Tsai, C. Y. Lai, and J. S. Chung (2004). "A practical mixed integer linear programming based approach for unit commitment". In: *2004 IEEE Power Engineering Society general meeting*. Piscataway, NJ: IEEE Service Center, pp. 221–225. ISBN: 0-7803-8465-2.
DOI: 10.1109/PES.2004.1372789

Cui, H. and K. Zhou (2018). "Industrial power load scheduling considering demand response". In: *Journal of Cleaner Production* 204, pp. 447–460. ISSN: 09596526.
DOI: 10.1016/j.jclepro.2018.08.270

Del Pra, M. (2020). “Time Series Forecasting with Deep Learning and Attention Mechanism”. In: *Towards Data Science*.
URL: https://towardsdatascience.com/time-series-forecasting-with-deep-learning-and-attention-mechanism-2d001fc871fc

EEA (2017). “Final energy consumption by sector and fuel in Europe”. In:
URL: https://www.eea.europa.eu/data-and-maps/indicators/final-energy-consumption-by-sector-10/assessment

European Comission (2019). *A European Green Deal*.
URL: https://ec.europa.eu/info/strategy/priorities-2019-2024/european-green-deal_en

FAO (2018). *Food and Agriculture Organization - New Food Balances*.
URL: http://www.fao.org/faostat/en/#data/FBS/visualize

Favre-Perrod, P. (2005). “A vision of future energy networks”. In: *Proceedings of the inaugural IEEE PES 2005 conference and exposition in Africa*. Piscataway, NJ: IEEE Service Center, pp. 13–17. ISBN: 0-7803-9326-0.
DOI: 10.1109/PESAFR.2005.1611778

Floudas, C. and P. Pardalos, eds. (2008). *Encyclopedia of Optimization*. Boston: Springer.

Floudas, C. A. (1995). *Nonlinear and mixed-integer optimization: Fundamentals and applications*. Topics in chemical engineering. New York: Oxford University Press. ISBN: 0195100565.
URL: http://site.ebrary.com/lib/alltitles/docDetail.action?docID=10358467

Geidl, M., G. Koeppel, P. Favre-Perrod, B. Klöckl, G. Andersson, and K. Fröhlich (2007). “The Energy Hub: A Powerful Concept for Future Energy Systems”. In: Electrical & Computer Engineering.

Ghanbari, A., H. Karimi, and S. Jadid (2020). “Optimal planning and operation of multi-carrier networked microgrids considering multi-energy hubs in distribution networks”. In: *Energy*, p. 117936. ISSN: 03605442.
DOI: 10.1016/j.energy.2020.117936

Halmschlager, D., A. Beck, M. Koller, S. Knöttner, and R. Hofmann (2020a). “Combined Optimization for Retrofitting of Heat Recovery and Thermal Energy Supply in Industrial Systems: Paper ID APEN-MIT-2020 211”. In: *Applied Energy Symposium: MIT A+B, August 12-14, 2020* Cambridge, USA.

Halmschlager, V., M. Koller, F. Birkelbach, and R. Hofmann (2019). “Grey Box Modeling of a Packed-Bed Regenerator Using Recurrent Neural Networks”. In: *IFAC-PapersOnLine* 52.16, pp. 765–770. ISSN: 24058963.
DOI: 10.1016/j.ifacol.2019.12.055

Halmschlager, V., F. Birkelbach, and R. Hofmann (2021a). “Optimizing the utilization of excess heat for district heating in a chipboard production plant”. In: *Case Studies in Thermal Engineering* 25, p. 100900. ISSN: 2214157X.
DOI: 10.1016/j.csite.2021.100900

Halmschlager, V. and R. Hofmann (2020b). “Holistic Approach for the Optimization of Industrial Hybrid Energy Hubs with MILP”. In: *30 European Symposium on Computer*

Aided Process Engineering. Ed. by S. Pierucci, F. Manenti, G. L. Bozzano, and D. Manca. Vol. 48. Computer-aided chemical engineering. Amsterdam, Netherlands and Cambridge, MA: Elsevier, pp. 1375–1380. ISBN: 9780128233771.
DOI: 10.1016/B978-0-12-823377-1.50230-5

– (2021b). "Assessing the potential of combined production and energy management in Industrial Energy Hubs – Analysis of a chipboard production plant". In: *Energy* 226, p. 120415. ISSN: 03605442.
DOI: 10.1016/j.energy.2021.120415

Halmschlager, V., S. Müllner, and R. Hofmann (2021c). "Mechanistic Grey-Box Modeling of a Packed-Bed Regenerator for Industrial Applications". In: *Energies* 14.11, p. 3174.
DOI: 10.3390/en14113174.
URL: https://www.mdpi.com/1996-1073/14/11/3174

Hamon, R., H. Junklewitz, and I. Sanchez (2020). *Robustness and explainability of Artificial Intelligence: from technical to policy solutions*. Publications Office.
DOI: 10.2760/57493

Heidmann, L. (2021). *Unsupervised Machine Learning: Use Cases & Examples*.
URL: https://blog.dataiku.com/unsupervised-machine-learning-use-cases-examples

Hofmann, R., S. Panuschka, and A. Beck (2019). "A simultaneous optimization approach for efficiency measures regarding design and operation of industrial energy systems". In: *Computers & Chemical Engineering* 128, pp. 246–260. ISSN: 00981354.
DOI: 10.1016/j.compchemeng.2019.06.007

IEA (2016). *World Energy Outlook 2016 – Analysis*. Paris.
URL: https://www.iea.org/reports/world-energy-outlook-2016

– (2018). *Global CO2 emissions by sector: IEA, Global CO2 emissions by sector, 2018, IEA, Paris https://www.iea.org/data-and-statistics/charts/global-co2-emissions-by-sector-2018*. Paris.
URL: https://www.iea.org/data-and-statistics/charts/global-co2-emissions-by-sector-2018

– (2020). "Energy Efficiency Indicators". In: Paris.
URL: https://www.iea.org/reports/energy-efficiency-indicators

Ionos (2021a). *Digitalguide: Supervised Learning - ein Lehrplan für Maschinen*.
URL: https://www.ionos.at/digitalguide/online-marketing/suchmaschinenmarketing/was-ist-supervised-learning/

– (2021b). *IONOS Digitalguide: Reinforcement Learning - wenn Maschinen Denken lernen*.
URL: https://www.ionos.at/digitalguide/online-marketing/suchmaschinenmarketing/was-ist-reinforcement-learning/

IPCC, ed. (2014). *Climate change 2014: Mitigation of climate change : Working Group III contribution to the Fifth assessment report of the Intergovernmental Panel on Climate Change*. Cambridge University Press. ISBN: 9781107415416.
DOI: 10.1017/CBO9781107415416

– (2018). *Global warming of 1.5°C. An IPCC Special Report on the impacts of global*

warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty.
URL: https://www.researchgate.net/publication/329841417_Global_warming_of_15C_An_IPCC_Special_Report_on_the_impacts_of_global_warming_of_15C_above_pre-industrial_levels_and_related_global_greenhouse_gas_emission_pathways_in_the_context_of_strengthening_the

IRENA, ed. (2019). *Global Energy Transformation: A Roadmap to 2050.* ISBN: 978-92-9260-121-8.
URL: https://www.irena.org/publications/2019/Apr/Global-energy-transformation-A-roadmap-to-2050-2019Edition

– ed. (2020). *Reaching Zero with Renewables: International Renewable Energy Agency Eliminating CO2 emissions from industry and transport in line with the 1.5^{0}C climate goal.*
URL: https://www.irena.org/publications/2020/Sep/Reaching-Zero-with-Renewables

Knueven, B., J. Ostrowski, and J.-P. Watson (2018). "Exploiting Identical Generators in Unit Commitment". In: *IEEE Transactions on Power Systems* 33.4, pp. 4496–4507. ISSN: 0885-8950.
DOI: 10.1109/TPWRS.2017.2783850

Lallanilla, M. (2019). "Greenhouse Gases: Causes, Sources and Environmental Effects". In: *Live Science.*
URL: https://www.livescience.com/37821-greenhouse-gases.html

Lingmin, C., W. Jiekang, W. Fan, T. Huiling, L. Changjie, and X. Yan (2020). "Energy flow optimization method for multi-energy system oriented to combined cooling, heating and power". In: *Energy* 211, p. 118536. ISSN: 03605442.
DOI: 10.1016/j.energy.2020.118536.
URL: http://www.sciencedirect.com/science/article/pii/S0360544220316443

Litzel, N. (2016). "So bereitet Machine Learning Big Data auf". In: *BigData-Insider.*
URL: https://www.bigdata-insider.de/so-bereitet-machine-learning-big-data-auf-a-544189/

Liu, Y. (2005). *Grey-box identification of distributed parameter systems.* Vol. 0503. Trita-S3-REG. Stockholm. ISBN: 9171780645.

Majidi, M., S. Nojavan, and K. Zare (2017). "A cost-emission framework for hub energy system under demand response program". In: *Energy* 134, pp. 157–166. ISSN: 03605442.
DOI: 10.1016/j.energy.2017.06.003

Moeini-Aghtaie, M., A. Abbaspour, M. Fotuhi-Firuzabad, and E. Hajipour (2014). "A Decomposed Solution to Multiple-Energy Carriers Optimal Power Flow". In: *IEEE Transactions on Power Systems* 29.2, pp. 707–716. ISSN: 0885-8950.
DOI: 10.1109/TPWRS.2013.2283259

Mohammadi, M., Y. Noorollahi, B. Mohammadi-ivatloo, M. Hosseinzadeh, H. Yousefi, and S. T. Khorasani (2018). "Optimal management of energy hubs and smart energy

hubs – A review". In: *Renewable and Sustainable Energy Reviews* 89, pp. 33–50. ISSN: 13640321.
DOI: 10.1016/j.rser.2018.02.035

Mohammadi, M., Y. Noorollahi, B. Mohammadi-ivatloo, and H. Yousefi (2017). "Energy hub: From a model to a concept – A review". In: *Renewable and Sustainable Energy Reviews* 80, pp. 1512–1527. ISSN: 13640321.
DOI: 10.1016/j.rser.2017.07.030

Najafi-Ghalelou, A., S. Nojavan, K. Zare, and B. Mohammadi-ivatloo (2019). "Robust scheduling of thermal, cooling and electrical hub energy system under market price uncertainty". In: *Applied Thermal Engineering* 149, pp. 862–880. ISSN: 13594311.
DOI: 10.1016/j.applthermaleng.2018.12.108

Nazari-Heris, M., B. Mohammadi-ivatloo, and S. Asadi (2020). "Optimal operation of multi-carrier energy networks with gas, power, heating, and water energy sources considering different energy storage technologies". In: *Journal of Energy Storage* 31, p. 101574. ISSN: 2352152X.
DOI: 10.1016/j.est.2020.101574

Niu, J., Z. Tian, J. Zhu, and L. Yue (2020). "Implementation of a price-driven demand response in a distributed energy system with multi-energy flexibility measures". In: *Energy Conversion and Management* 208, p. 112575. ISSN: 01968904.
DOI: 10.1016/j.enconman.2020.112575

Nojavan, S., M. Majidi, and K. Zare (2018). "Optimal scheduling of heating and power hubs under economic and environment issues in the presence of peak load management". In: *Energy Conversion and Management* 156, pp. 34–44. ISSN: 01968904.
DOI: 10.1016/j.enconman.2017.11.007

Oreskes, N. (2004). "Beyond the ivory tower. The scientific consensus on climate change". In: *Science (New York, N.Y.)* 306.5702, p. 1686.
DOI: 10.1126/science.1103618

Oussar, Y. and G. Dreyfus (2001). "How to be a gray box: dynamic semi-physical modeling". In: *Neural Networks* 14.9, pp. 1161–1172. ISSN: 08936080.
DOI: 10.1016/S0893-6080(01)00096-X

Padhy, N. P. (2004). "Unit Commitment—A Bibliographical Survey". In: *IEEE Transactions on Power Systems* 19.2, pp. 1196–1205. ISSN: 0885-8950.
DOI: 10.1109/TPWRS.2003.821611

Paudyal, S., C. A. Cañizares, and K. Bhattacharya (2015). "Optimal Operation of Industrial Energy Hubs in Smart Grids". In: *IEEE Transactions on Smart Grid* 6.2, pp. 684–694. ISSN: 1949-3061.
DOI: 10.1109/TSG.2014.2373271

Pazouki, S. and M.-R. Haghifam (2016). "Optimal planning and scheduling of energy hub in presence of wind, storage and demand response under uncertainty". In: *International Journal of Electrical Power & Energy Systems* 80, pp. 219–239. ISSN: 01420615.
DOI: 10.1016/j.ijepes.2016.01.044

Peters, G. P., R. M. Andrew, J. G. Canadell, P. Friedlingstein, R. B. Jackson, J. I. Korsbakken, C. Le Quéré, and A. Peregon (2020). "Carbon dioxide emissions continue

to grow amidst slowly emerging climate policies". In: *Nature Climate Change* 10.1, pp. 3–6. ISSN: 1758-6798.
DOI: 10.1038/s41558-019-0659-6

Pitarch, J., A. Sala, and C. de Prada (2019). "A Systematic Grey-Box Modeling Methodology via Data Reconciliation and SOS Constrained Regression". In: *Processes* 7.3, p. 170.
DOI: 10.3390/pr7030170

Prada, C. de, D. Hose, G. Gutierrez, and J. L. Pitarch (2018). "DEVELOPING GREY-BOX DYNAMIC PROCESS MODELS". In: *IFAC-PapersOnLine* 51.2, pp. 523–528. ISSN: 24058963.
DOI: 10.1016/j.ifacol.2018.03.088

Quoilin, S., A. Zucker, and I. Hidalgo Gonzalez (2017). *Modelling future EU power systems under high shares of renewables: the Dispa SET 2.1 open source model*. Publications Office.
DOI: 10.2760/25400

Rakipour, D. and H. Barati (2019). "Probabilistic optimization in operation of energy hub with participation of renewable energy resources and demand response". In: *Energy* 173, pp. 384–399. ISSN: 03605442.
DOI: 10.1016/j.energy.2019.02.021

Roustai, M., M. Rayati, A. Sheikhi, and A. Ranjbar (2018). "A scenario-based optimization of Smart Energy Hub operation in a stochastic environment using conditional-value-at-risk". In: *Sustainable Cities and Society* 39, pp. 309–316. ISSN: 22106707.
DOI: 10.1016/j.scs.2018.01.045

Sadeghi, H., M. Rashidinejad, M. Moeini-Aghtaie, and A. Abdollahi (2019). "The energy hub: An extensive survey on the state-of-the-art". In: *Applied Thermal Engineering* 161, p. 114071. ISSN: 13594311.
DOI: 10.1016/j.applthermaleng.2019.114071

Schäfer, A. M. and H. G. Zimmermann (2006). "Recurrent Neural Networks Are Universal Approximators". In: *Artificial neural networks - ICANN 2006*. Ed. by S. Kollias, A. Stafylopatis, W. Duch, and E. Oja. Vol. 4131. Lecture Notes in Computer Science. Berlin: Springer, pp. 632–640. ISBN: 978-3-540-38625-4.
DOI: 10.1007/11840817{\textunderscore}66

Shahrabi, E., S. M. Hakimi, A. Hasankhani, G. Derakhshan, and B. Abdi (2021). "Developing optimal energy management of energy hub in the presence of stochastic renewable energy resources". In: *Sustainable Energy, Grids and Networks* 26, p. 100428. ISSN: 23524677.
DOI: 10.1016/j.segan.2020.100428

Shao, C., X. Wang, M. Shahidehpour, X. Wang, and B. Wang (2017). "An MILP-Based Optimal Power Flow in Multicarrier Energy Systems". In: *IEEE Transactions on Sustainable Energy* 8.1, pp. 239–248. ISSN: 1949-3037.
DOI: 10.1109/TSTE.2016.2595486

Sohlberg, B. and E. W. Jacobsen (2008). "GREY BOX MODELLING – BRANCHES

AND EXPERIENCES". In: *IFAC Proceedings Volumes* 41.2, pp. 11415–11420. ISSN: 14746670.
DOI: 10.3182/20080706-5-KR-1001.01934

Sohlberg, B. (1998). *Supervision and Control for Industrial Processes: Using Grey Box Models, Predictive Control and Fault Detection Methods*. Advances in Industrial Control. London: Springer. ISBN: 9781447115588.
DOI: 10.1007/978-1-4471-1558-8

Solomatine, D., L. M. See, and R. J. Abrahart (2008). "Data-Driven Modelling: Concepts, Approaches and Experiences". In: *Practical hydroinformatics*. Ed. by R. J. Abrahart. Water science and technology library. Berlin: Springer, pp. 17–30. ISBN: 978-3-540-79881-1.
DOI: 10.1007/978-3-540-79881-1{\textunderscore}2

Steffen, W., K. Richardson, J. Rockström, S. E. Cornell, I. Fetzer, E. M. Bennett, R. Biggs, S. R. Carpenter, W. de Vries, C. A. de Wit, C. Folke, D. Gerten, J. Heinke, G. M. Mace, L. M. Persson, V. Ramanathan, B. Reyers, and S. Sörlin (2015). "Sustainability. Planetary boundaries: guiding human development on a changing planet". In: *Science (New York, N.Y.)* 347.6223, p. 1259855.
DOI: 10.1126/science.1259855

Stocker, T., ed. (2014). *Climate change 2013: The physical science basis : Working Group I contribution to the Fifth assessment report of the Intergovernmental Panel on Climate Change*. Cambridge: Cambridge University Press. ISBN: 9781107415324.
DOI: 10.1017/CBO9781107415324

Thompson, M. L. and M. A. Kramer (1994). "Modeling chemical processes using prior knowledge and neural networks". In: *AIChE Journal* 40.8, pp. 1328–1340. ISSN: 0001-1541.
DOI: 10.1002/aic.690400806

Tulleken, H. J. (1993). "Grey-box modelling and identification using physical knowledge and bayesian techniques". In: *Automatica* 29.2, pp. 285–308. ISSN: 0005-1098.
DOI: 10.1016/0005-1098(93)90124-C.
URL: http://www.sciencedirect.com/science/article/pii/000510989390124C

Umweltbundesamt (2017). *Energieverbrauch und Energieeffizienz*.
URL: https://www.umweltbundesamt.at/umweltthemen/energie/energieverbrauch

Vahid Pakdel, M. J., F. Sohrabi, and B. Mohammadi-ivatloo (2020). "Multi-objective optimization of energy and water management in networked hubs considering transactive energy". In: *Journal of Cleaner Production* 266, p. 121936. ISSN: 09596526.
DOI: 10.1016/j.jclepro.2020.121936

Vahid-Pakdel, M. J., S. Nojavan, B. Mohammadi-ivatloo, and K. Zare (2017). "Stochastic optimization of energy hub operation with consideration of thermal energy market and demand response". In: *Energy Conversion and Management* 145, pp. 117–128. ISSN: 01968904.
DOI: 10.1016/j.enconman.2017.04.074

Wood, A. J., B. F. Wollenberg, and G. B. Sheblé (2014). *Power generation, operation, and control*. 3. ed. Hoboken, NJ: Wiley. ISBN: 9780471790556.

URL: http://site.ebrary.com/lib/alltitles/docDetail.action?docID=10768986

Yang, L., C. Zhang, J. Jian, K. Meng, Y. Xu, and Z. Dong (2017). "A novel projected two-binary-variable formulation for unit commitment in power systems". In: *Applied Energy* 187, pp. 732–745. ISSN: 03062619.
DOI: 10.1016/j.apenergy.2016.11.096

Publications

In this chapter, all relevant publications for this thesis are presented. This includes the core publications of this thesis – three journal and two conference papers – as well as further publications, comprising one co-author publication and other scientific contributions. For each core publication, the full paper, a short summary, my own contribution based on the CRediT author statement[5] and the reference are provided. The further publications are only briefly described.

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

Paper 1

Holistic Approach for the Optimization of Industrial Hybrid Energy Hubs with MILP

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

In this work, the idea of the Industrial Energy Hub (IEH) was first introduced. The IEH concept is based on the general EH concept but focuses on optimizing industrial manufacturing processes. Thus, the IEH approach not only considers energy streams but also takes into account product streams and production units. For proof of concept, the IEH approach is applied to a use-case that is inspired by the chipboard production plant. The modeling and optimization of the use-case with and without thermal energy storage shows that this holistic approach offers straight-forward and fast optimization of industrial manufacturing processes.

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

V. Halmschlager and R. Hofmann (2020b). "Holistic Approach for the Optimization of Industrial Hybrid Energy Hubs with MILP". in: 30 European Symposium on Computer Aided Process Engineering. *Ed. by S. Pierucci, F. Manenti, G. L. Bozzano, and D. Manca. Vol. 48. Computer-aided chemical engineering. Amsterdam, Netherlands and Cambridge, MA: Elsevier, pp. 1375–1380. ISBN: 9780128233771.*

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Holistic Approach for the Optimization of Industrial Hybrid Energy Hubs with MILP

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Abstract

This work presents a holistic approach for the optimization of Energy Hubs with mixed integer linear programming for industrial applications. As a use case, a chipboard production plant is used, which produces different products depending on current orders. The use case includes units for power and steam generation, energy conversion, energy and material storages as well as continuous and batch production machines. Additionally, power is sold to the grid and energy in form of heat covers the demand of two district heating suppliers. To model and optimize such extensive industrial systems efficiently, a generic and modular modelling approach is proposed. The entire process is modelled based on five generic modules, which can be configured for specific tasks. To evaluate the viability of the proposed approach, three different scenarios within the industrial use case (without storage, with thermal energy storage, with material storage) were optimized. The results show, that this approach is well suited for scheduling and the assessment of process design improvements of existing industrial plants, due to its easily adaptable modular structure and the ability to use simple data-driven models.

Keywords: Industrial Energy Hub (IEH), Optimization, Mixed Integer Linear Programming (MILP), Scheduling, Demand Side Response (DSR)

1. Introduction

The increased application of renewable energies, combined with the complex energy market and new flexible technologies, challenges today's industry. This increases the need for holistic energy efficiency solutions. In industry, optimal production scheduling - discussed in (Merkert et al., 2015) - and Demand Side Response (DSR) - discussed in (Lindberg et al., 2014) - are promising solutions. However, in many processes, other energy carriers like steam, oil or gases need to be considered as well as the product and electric power. (Hybrid) Energy Hubs (EH) are an option for integrated management of these Multi Energy Systems, where different energy carriers can be converted, coupled and stored. Only few publications deal with the optimization of EHs, most of them focusing on the residential or commercial buildings sector (Sadeghi et al., 2019).
The idea of the EH was first expressed in (Favre-Perrod, 2005) and further researched in several papers. (Mohammadi et al., 2017) and (Sadeghi et al., 2019) provide a good overview of recent publications within this topic. Terms such as "Multi-Energy System", "Multi-Carrier Energy Systems" and "Natural Gas Multi Energy Services" usually describe systems that are all based on the concept of the EH.

In this work, a concept for the modelling and optimization of an Industrial Energy Hub is proposed. The optimization of the Industrial Energy Hub is intended to be used for optimal production and energy scheduling as well as the analysis of different scenarios within an industrial process. The work is structured as follows: Section 2 describes the general concept of the Industrial Energy Hub. Section 3 deals with the holistic and modular modelling and optimization approach. In Section 4, the industrial use case - a chipboard production plant - is modelled and optimized and results are shown. The conclusion is presented in Section 5.

2. Industrial Energy Hub Concept

In contrast to the commonly used EH concept presented in (Geidl et al., 2007; Mohammadi et al., 2017; Sadeghi et al., 2019), we propose the Industrial Energy Hub (IEH) that also takes into account the production in an industrial plant. Thus, in addition to different energy carriers like electrical and thermal power, also the product acts as a carrier in the IEH. Figure 1 illustrates the concept of the IEH. This approach emphasizes the importance of energy in production processes and enables the integration of different energy carriers and networks into the modelling and optimization of an industrial production plant.

In analogy to a classification of general EH systems in (Mohammadi et al., 2017), the parts of the IEH can be divided into four units: *conversion, storage, input* and *output.* In contrast to the general EH system, the product is taken into account in each of these units in the IEH system. In *conversion* units, the characteristics and quality of a carrier can be changed (adapting converters) or a carrier can be transformed into other forms (changing converters). Both types of converters can be either operated continuously or in (semi-)batch mode. In the IEH, typical *conversion* units for energy are generators, thermal power plants or heat exchangers. *Conversion* units for the product are all machines or devices that are part of the production chain. *Storage* units in the IEH can be energy storages, but also material storages. *Input* and *output* units in the IEH are process requirements or limits that need to be considered. Typical *inputs* are energy from the grid, fuel for production machines and energy converters, as well as primary product materials. Typical *outputs* of the IEH are heat for district heating (DH) supply, power for the electricity grid, gas that is fed into the gas network as well as the product of the plant. Thus, the IEH concept and its classification to the four units *conversion, storage, input* and *output* enables a generic description of a variety of different industrial processes and can be used as a basis for the optimization of IEH systems.

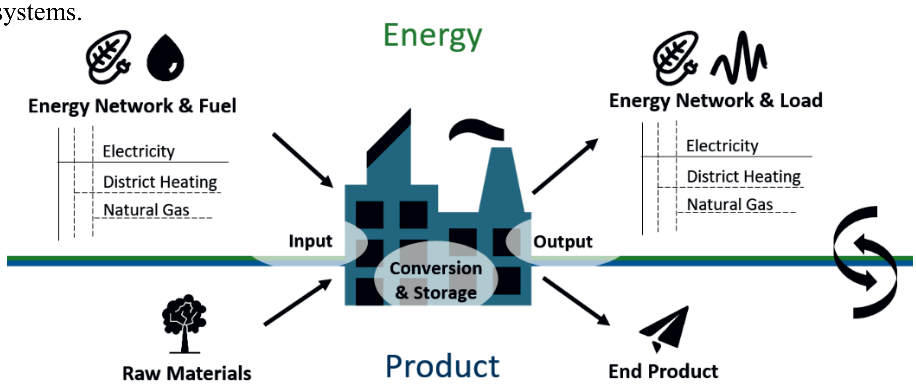

Figure 1: Illustration of the IEH concept

3. Modelling and Optimization Approach

The optimization of the IEH aims to determine the optimal energy and product flow in order to achieve minimal costs over a time horizon, whilst taking into account production specifications and external requirements.The approach is intended to be used for scheduling of existing industrial processes, but also for the assessment of different process design scenarios, e.g. to evaluate the implementation of additional machines/devices or storages. However, in existing industrial processes, the creation of detailed models is often not possible because only little data is available. Thus, simple and easily adaptable models are chosen for this applied approach. For this reason, the approach is based on an adaptable modular structure and uses a mixed integer linear programming (MILP) formulation with only linear, mostly data-based correlation. This way, modelling and optimization of an existing process and different design scenarios can be done in a time-saving manner with available process data.

3.1. MILP Formulation

The optimization problem is formulated as a MILP problem with linear constraints and a linear objective function. The optimization is set up in Matlab® with an object oriented approach. Process variables that can be varied and therefore optimized are called decision variables. These decision variables can be restricted by constraints. Binary decision variables (0 or 1) are used to indicate, if a device is switched on (1) or off (0). The objective function includes real costs, as well as penalties or rewards on decision variables to shift the optimization towards a desired goal. By using a MILP problem formulation, the optimization can be solved with state-of-the-art solvers (e.g. GUROBI) and results in a global optimum.

3.2. Holistic Modular Approach

To create an optimization model of the IEH with the MILP formulation, the industrial process is split into part models, called units. Based on the previous classification of the IEH system, all parts of the IEH can be divided in four units: *conversion, storage, input* and *output.* In addition to the former described first four units, also a *connection* unit is used in the optimization approach. For each of the five units, a generic module exists that acts as a basis model for all its parts/devices. Each generic module has an adaptable structure and offers the option to implement different preconfigured constraints and objectives. These are used to tailor a generic module to a specific device. The main advantage of this holistic approach is, that all part models can be easily adapted, omitted or added anywhere in the overall process model. In the following paragraphs, the structure, constraints and objectives of each module and its carriers (e.g. heat, product) are described in detail.

Conversion modules are used to model units that can adapt or transform a carrier in the IEH. Thus, converters are all machines/devices that consume or generate energy or a product. All converters are based on a generic input/output module and configured in detail by linear constraints. In the case that linear correlations are not capable to describe the behavior of the converter adequately, non-linear behavior can be approximated by piecewise linear relations and a differentiation in two or more operation modes. Constraints for converters can be divided into adaption/conversion constraints, carrier constraints and technical constraints. Constraints for adaption/conversion are used to describe the internal behavior of the converter, e.g. the amount of input that is required to generate a certain output. Carrier constraints are used to restrict the carriers when entering or exiting a converter. They include minimal and maximal constraints, as well as ramp up and ramp down constraints and represent limitations of the converter itself or the connection between different converters (e.g. pipes, conveyors). To model a converters technical limitations, start up and shut down times as well as minimal and maximal up and down times of a converter can be implemented. In addition to the constraints, the costs (start up or shut down costs, operation costs, material costs) of the converter can be added in the objective function.

Storage (energy or material) modules can have the same constraints as *conversion* modules. Additionally, constraints to model the integrative and dynamic charging and discharging behavior as well as thermal losses are added in the *storage* module.

The *input and output* module includes minimal and maximal constraints, as well as ramp up and ramp down constraints. If the input or output restriction varies over time, time sequence or integrative constraints can be used. Time sequence constraints can model demands or forecasts that need to be met by a certain carrier of a converter or storage. Integrative constraints are used to implement a production schedule over the time horizon. Both sequence and integrative constraints can be implemented directly as constraints, or added to objective function with a penalty or reward term.

The *connection* module connects the input and output streams of every module (converter, storage, in/outputs) with a mass or energy balance constraint.

The modelling of an IEH with the modular approach can be summarized as follows: Any carrier can be adapted and transformed in converters as well as stored in storages. Different converters and storages are connected with each other by connecting the according input and output streams of their carries with connections. External process inputs and outputs can be connected to converters or storages. They can represent time-dependent demands or a production sequence.

4. Use Case - Chipboard Production

To demonstrate the capability of the IEH approach, a simplified industrial chipboard production plant is considered as a use case, which is presented in Figure 2. The optimization model of the chipboard production is based on the IEH approach and uses industrial process data. A fictive district heating (DH) demand and a fixed price for electrical power are used. The optimization minimizes the overall process costs over a time horizon of 50 hours. For a design analysis of the process, three scenarios A, B and C are optimized.

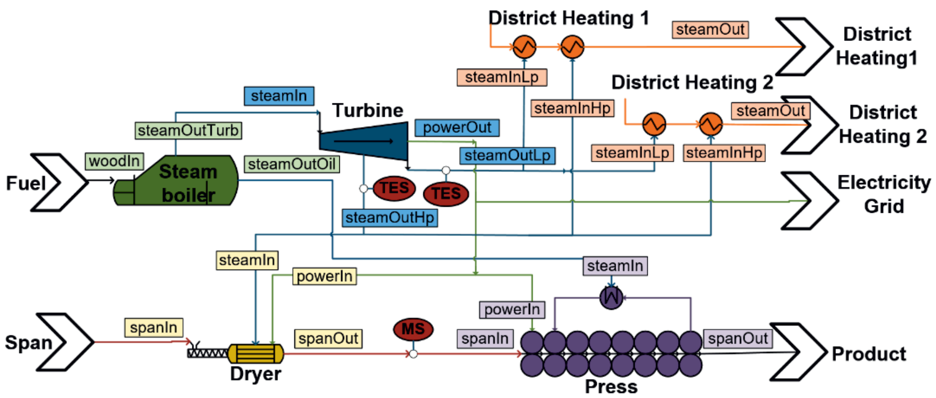

Figure 2: Use case - Flowchart of the simplified chipboard production

4.1. Analyzed Scenarios

In all scenarios, thermal and electrical energy that is required for the production is generated by a steam boiler and a steam turbine. As the amount of energy produced exceeds the demand of the production process, heat is fed into two DH networks with changing demands over time and electric power is sold to the grid. A production schedule defines the generation of two different products in two time intervals (product 1: 9-16 h, product 2: 23-38 h). Satisfying the production limits has highest priority in the process. The described external requirements are equal in all scenarios. The three scenarios only differ in the availability of storages. In the standard scenario A, no storages are available. In scenario B, two thermal energy storages (TES - steam accumulators for high and low pressure steam) with an efficiency of 99% are implemented. In scenario C, a material storage (MS) for dried span is added to scenario A. The location of the storages can be seen in the flowchart in Figure 2.

4.2. Optimization Results

Figures 3, 4 and 5 show the cumulative thermal energy (TE) that is used for the production process and fed into the DH network over a time horizon of 50 hours for the optimized scenarios A, B and C. Additionally, the charging and discharging behavior of the storages is depicted for scenarios B and C. In scenario A, the DH demand cannot be met over the entire time horizon (~93 % energy coverage), because not enough TE can be generated in times of high DH demand (after ~10 and 35 h) and production. In scenario B with the TES, more TE is produced in times of little production and used in times of high TE demand. In scenario C with the material storage, the generation of TE is shifted in time and used to process and store the chipboards in times of low DH demand. Hence, both storages can improve the processes efficiency by increasing its flexibility and enable the full coverage of DH demand.

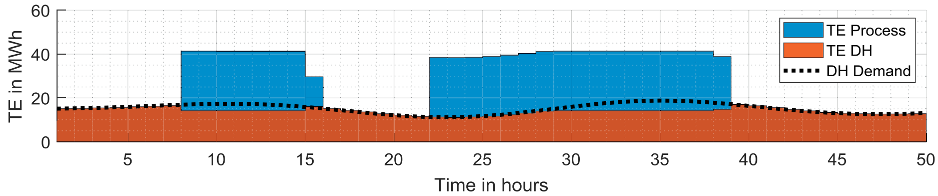

Figure 3: Optimization results of scenario A (no storage)

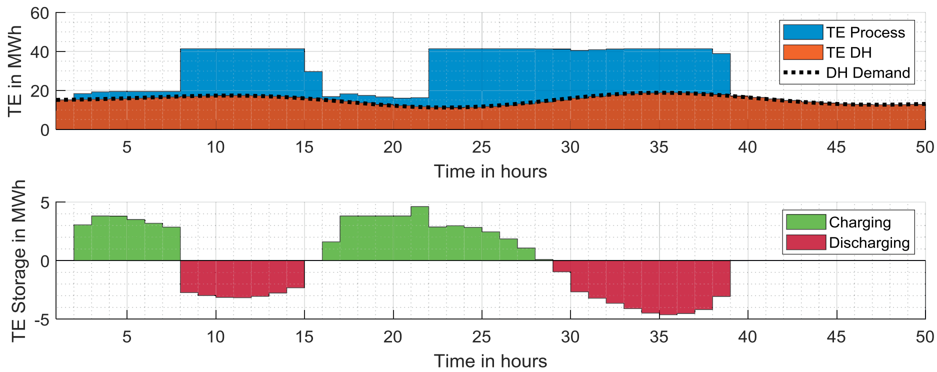

Figure 4: Optimization results of scenario B (thermal energy storage)

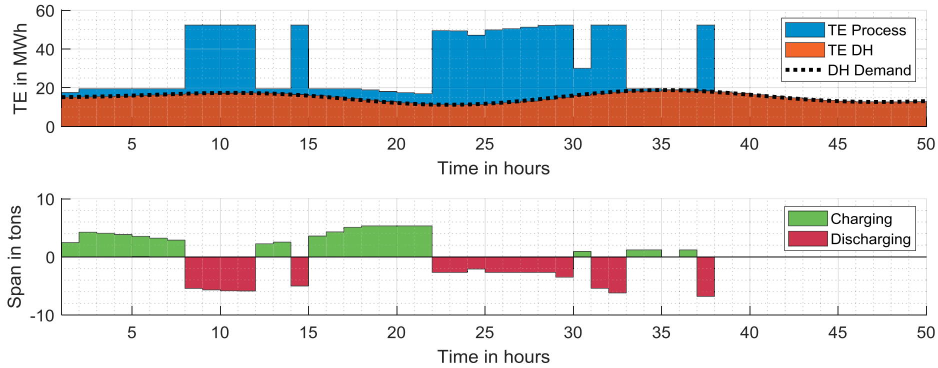

Figure 5: Optimization results of scenarios C (material storage)

5. Conclusion

The concept of the IEH and a holistic modelling and optimization approach were proposed. In the IEH, energy as well as the production of an industrial plant is considered. This enables the integration of different energy carriers and networks into the modelling and optimization of industrial plants. With the proposed approach, an industrial process can be modelled and optimized with five generic modules (converter, storage, input, output, connection). The generic and modular structure enables a fast implementation, combined with a high model adaptability. The results of the optimization can be used for scheduling, as well as for process design improvements. The viability of the approach was demonstrated with a use case. It confirms, that this holistic approach offers a straightforward and fast method to model and optimize industrial plants with process data. Future work will analyze the application of the proposed approach to extensive use cases and more comprehensive scenarios.

Acknowledgment

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References

Favre-Perrod P 2005. A vision of future energy networks. Proceedings of the inaugural IEEE PES conference and exposition in Africa. Piscataway, NJ: IEEE Service Center; 13–17.

Geidl M, Koeppel G, Favre-Perrod P, Klöckl B, Andersson G, Fröhlich K 2007. The energy hub-A powerful concept for future energy systems. Third Annual Carnegie Mellon Conference on the Electricity Industry: 13–4.

Lindberg C-F, Zahedian K, Solgi M, Lindkvist R 2014. Potential and Limitations for Industrial Demand Side Management. Energy Procedia; 61: 415–8.

Merkert L, Harjunkoski I, Isaksson A, Säynevirta S, Saarela A, Sand G 2015. Scheduling and energy – Industrial challenges and opportunities. Computers & Chemical Engineering; 72: 183–98.

Mohammadi M, Noorollahi Y, Mohammadi-ivatloo B, Yousefi H 2017. Energy hub. Renewable and Sustainable Energy Reviews; 80: 1512–27.

Sadeghi H, Rashidinejad M, Moeini-Aghtaie M, Abdollahi A 2019. The energy hub. Applied Thermal Engineering; 161: 114071.

Paper 2

Assessing the Potential of Combined Production and Energy Management in Industrial Energy Hubs – Analysis of a Chipboard Production Plant

Published in Energy in collaboration with René Hofmann

This paper covers the first optimization of the chipboard production plant with the developed framework and real process data. Relevant features of the optimization framework are described, including modeling paradigms and the used constraints and objectives. This paper also includes a detailed description of the devices and operation strategy of the chipboard production plant and shows a validation of the created component models of the plant. The main goal of this paper was to show the potential of optimizing a manufacturing process with the Energy Hub approach, considering the scheduling of product *and* energy streams. The results show that the optimization of product streams, in addition to energy streams, is essential for the energy management of the entire system, reducing the required energy for production units by 30 %. However, to exploit this potential, process design needs to be adapted accordingly.

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

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Assessing the potential of combined production and energy management in Industrial Energy Hubs – Analysis of a chipboard production plant

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ABSTRACT

To minimize energy consumption in today's industry, holistic energy efficiency solutions are required. The Energy Hub is a promising concept for optimal energy management of industrial systems with multiple energy carriers like electricity, heat, or gas. However, most of the research conducted in this field focuses on optimal energy management and does not consider the scheduling of product in manufacturing processes. Though, including production scheduling in the energy optimization of manufacturing processes can considerably increase energy efficiency, especially if batch processes are involved. This work identifies the potential of combined energy and production scheduling in Industrial Energy Hubs, using a chipboard production process as a use case. The chipboard production plant includes a combined heat and power unit, units for production, and has two district heating demands as external requirements. A generic modeling and optimization framework, based on mixed-integer linear programming, is used to model and optimize different scenarios. The results show that the scheduling of product has a significant impact on the energy management of the chipboard production plant: The required energy for the production units can be reduced by approximately 30 %. Nevertheless, this potential can only be exploited if process design is adapted and excess heat is utilized appropriately.

1. Introduction

The industrial sector accounts for approximately 25 % of the final energy consumption in Europe [1] and globally even more than one third [2]. Thus, energy savings in this sector are crucial to reach the global climate goals. New flexible technologies, increased application of renewables, decentralized systems and new digitalization measures can all contribute to the optimal use of energy in industry. However, the variety of measures and their interaction presents industrial companies with great challenges and increases the need for holistic energy efficiency solutions. In industry, optimal production scheduling (Merkert et al., 2015) and Demand Side Response (DSR) (Lindberg et al., 2014) are promising solutions. However, most of these approaches focus on individual aspects, e.g. the sole optimization of production or the optimization of electricity and heat. To exploit the full potential, not only heat and electricity, but also water, gas and other energy carriers should be implemented in an industrial energy management system [3]. The Energy Hub addresses this topic.

The Energy Hub (EH) is a recently established concept for optimal management of systems with multiple energy carriers, e.g. electricity, thermal power, or gas. It was first introduced within the framework of a project called “a vision of future energy networks (VOFEN)” [4]. In recent years, the EH was further discussed by many researchers and several definitions emerged. In Favre-Perrod [4], the EH was defined as an interface between consumers, producers, storage devices, and transmission devices. The interface can either be direct or via conversion equipment and one or more energy carriers can be handled. In Geidl et al. [5], the EH was defined as a unit, where multiple energy carriers can be converted, conditioned, and stored. More precisely, the EH can be seen as a unit that provides the basic features input and output, conversion, and storage of different energy carriers [6]. A very good overview of EHs was provided in Mohammadi et al. [7] and the state of the art and researches in the context of EHs were summarized in Sadeghi et al. [8].

In the latest review about EHs [9], EHs were divided into four sectors: residential, commercial, industrial, and agricultural micro

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Acronyms

AC	air condenser
CHP	combined heat and power
DH	district heating
DRY	dryer
EH	energy hub
El. Grid	electricity grid
Ext. Req	external requirement
HP	high pressure steam
IEH	industrial energy hub
INT	internal constant heat and electricity demand
LP	low pressure steam
MILP	mixed integer linear programming
MS	middle-chip storage
Prod. Sched	production schedule
SB	steam boiler
TS	top-chip storage
TURB	steam turbine

Parameters

$p_{\max}$	upper limit of a stream p
$p_{\min}$	lower limit of a stream p
a	constant offset
b	constant factor
C	process costs
D	demand of external requirement
Dt	amount of time, a device needs to be off after being shut down
E	demand penalty
O	demand of production schedule
R	rewards
Rd	maximal negative gradient of a stream p
Ru	maximal positive gradient of a stream p
T	horizon
Ut	amount of time, a device needs to be on after being started

Indices

c	process costs
e	penalties
i	streams in conversion constraint
k	connections
n	linear segments
r	rewards
t	time

Variables

$\overline{bin}$	binary variable - piecewise linear approx.
$\bar{f}$	storage fill level
$\bar{p}$	stream of a device
$\overline{si}$	storage total input stream
$\overline{so}$	storage total output stream
$\bar{S}$	slack variable
$\bar{s}$	stream that enters (+) or leaves (−) storage
$\bar{u}$	binary variable - on/off
$\bar{y}$	binary variable - start up
$\bar{z}$	binary variable - shut down

EHs. In this context, “micro” stands for self-contained energy systems that aim to minimize their individual energy consumption/costs. In contrast, macro EHs comprise an entire system and thus aim to optimize the energy consumption from a controller perspective. According to the literature review in Mohammadi et al. [9], most of the researches in the field of EHs focused on the residential sector and macro EHs and only few research has been done on the optimization of industrial EHs. However, most recently, several new papers were published that deal with industrial EHs. Furthermore, a number of publications described applications of this concept without explicitly declaring it as industrial EH.

Already before the term “Energy Hub” became popular, several researchers dealt with the optimal energy management in industrial cogeneration systems, respectively combined heat and power (CHP) systems. According to the definition of the EH and also exemplified in Mohammadi et al. [7], these systems are already a simple case of an EH. A good overview of publications on CHP-based energy systems was given in Majidi et al. [10]. Besides, a broad variety of publications emerged in the past few years that deal with industrial EHs in general, most of them focusing on industrial power plants. These publications cover different aspects of the EH, e.g. new methods, algorithms, applications, and technologies, described in the following. The research ranged from optimization of industrial EHs in Smart Grids [11], optimization of energy hubs with a multi-objective model including power and heat [12], a demand response program [13], or water and energy [14]. Other works focused on optimal planning and operation of multi-carrier networked microcrids [15] or flexibility measures in EHs [16]. Also, a great number of publications dealt with uncertainties in EH systems: In Pazouki et al. [17], a mathematical formulation for optimal planning of an EH with deterministic and stochastic circumstances of wind power, electricity price, and hub electricity demand was presented. Najafi-Ghalelou et al. [18] dealt with a robust optimization approach in the presence of market price uncertainty and multi-demand response programs. In Roustai et al. [19], a stochastic model for electricity, natural gas prices, and user’s demand was proposed, using conditional value at risk technique. The research in Rakipour and Barati [20] covered the optimal operation of an EH, based on uncertainty modeling of electrical, heating, and cooling demands, wind speed and solar irradiances, and prices of electricity and natural gas. Last, in Vahid-Pakdel et al. [21], stochastic programming was implemented to model the system uncertainties of demands, market prices, and wind speed in an EH.

To summarize, there exist a great number of publications dealing with scheduling of multi-energy-systems and optimization of industrial EHs. Interestingly, very little research deals with the optimization of industrial manufacturing processes with the EH approach, although this sector shows big potential for energy efficiency improvements. Also in the extensive literature survey on Energy Hubs [8], only one article dealt with the optimization of a manufacturing process, an engine manufacturing facility [22]. Obviously, there is a gap in EH research focusing on manufacturing processes.

If applying the EH approach for the optimization of a manufacturing process, also the production - more precisely the scheduling of product streams - should be considered. Actually, in many manufacturing processes, the production adds a considerable amount of flexibility to the process. This is the case in production processes that include either machines with (semi-) batch operation, storages, several equal or similar machines for a task, or a number of different production steps that do not require a specific order. For these applications, the production can be shifted in time and energy peaks and troughs can be optimally used, improving a process's efficiency.

In this work, we therefore aim to show the potential of optimizing a manufacturing process with scheduling of energy *and* product streams. To assess the effects of including the scheduling of product, we compare the classical EH approach - where only energy streams are considered - with the combined optimization of energy and product streams.

To model and optimize the energy and product flows in the manufacturing processes effectively, a modeling and optimization framework with a modular approach was developed. Using this generic optimization approach, different scenarios of the use case can be analyzed and compared in a time-efficient manner. The main contributions of this work are:

- Development of a generic optimization framework for process industry, able to model multi-energy carriers, production as well as external requirements
- Analysis of a real-world use case - a chipboard production plant - based on process data and data-driven, as well as physical models
- Comparison of different scenarios to demonstrate the potential of combined energy and production scheduling in manufacturing processes with the Energy Hub concept

The paper is organized as follows: Section 2 describes the general idea behind the Industrial Energy Hub concept. In Section 3, the modeling and optimization approach for the Industrial Energy Hub is presented. Section 4 deals with the use case - a chipboard production plant - and states the different scenarios. In Section 5, the results of the different scenarios are analyzed and compared to each other. Last, the most important outcomes and results are summarized in the Conclusion in Section 6.

2. Industrial Energy Hub concept

The Industrial Energy Hub (IEH) concept was first introduced in previous work [23] and is illustrated in Fig. 1. In contrast to the commonly used EH concept, e.g. described in Geidl et al. [5], the IEH also takes into account the processing of a product. This approach emphasizes the interaction between production and different energy carriers in an industrial manufacturing process.

Similar to the general EH concept in Mohammadi et al. [9], the IEH is built up by four main units: conversion, storage, input, and output. However, in addition to different energy carriers, also the product acts as a carrier in the IEH. In conversion units, carriers can be transformed to other carriers (changing converter), and/or the characteristics and quality of carriers can be changed (adapting converter). Conversion units in the IEH can be e.g. generators, combined heat and power (CHP) units, heat exchangers, or machines and devices that are part of the production. They can be operated continuously or in (semi-)batch mode. In the storage units, energy or product can be stored, e.g. in thermal energy storages or mass storages. Input and output units represent the flows of different carriers at the system boundary. Typical energy carriers in industrial systems are electricity, heat, and natural/green gas, which all can be bought from, or sold to the grid. Additionally, all production streams (e.g. raw materials, product) are considered as carriers as well in the IEH.

3. IEH modeling and optimization approach

For the IEH modeling and optimization approach, a framework is developed. In the following, underlying considerations and the implementation of the modeling and optimization framework are presented.

3.1. Modeling paradigms

3.1.1. Effectivity

The modeling and optimization framework for the IEH must be able to represent an entire industrial process accurately. Thus, the process model must include relevant characteristics of all internal units of a process (being all machines, devices, and storages) and their input and output streams (being carriers). Additionally, external requirements need to be considered, e.g. district heating (DH) demand, production schedule, selling electricity to the grid. To create accurate models of all internal units and external requirements, data and process information is required. The framework should be capable, of using data-driven as well as physical models, to be able to use the best modeling source available.

3.1.2. Flexibility

To be able to model and optimize different scenarios within an industrial process fast and efficiently, a flexible structure is required. Thus, all part models should be easily adaptable and additional machines/devices/requirements should be implemented fast and straight-forward. This aims for a modular approach.

3.1.3. Simplicity

Last but not least, modeling and optimization should be as

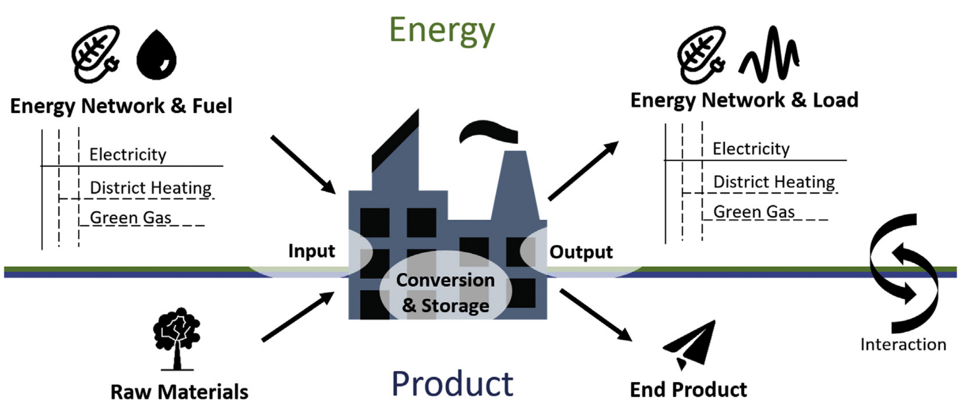

Fig. 1. Industrial Energy Hub concept. According to Ref. [23].

simple as possible, while still satisfying all requirements. Optimization performance is strongly dependent on the complexity of the models and the size of the total optimization problem. Additionally, the complexity of the models is often limited by the availability of data. Large amounts of data might not be available for all relevant measures and models need to be built on a limited data basis. To this end, simple, linear models are chosen for the framework.

3.2. Implementation

Following the described considerations, the IEH modeling and optimization framework is based on a modular and flexible structure, using object-oriented programming in Matlab and a mixed-integer linear programming (MILP) approach. The use of a linear formulation has the advantage, that every local optimum is a global optimum as well, and state-of-the-art (linear) optimization solvers (e.g. GUROBI) can be used to solve the linear optimization problem in satisfactory time. Besides, the part models, their constraints and objectives, are less complex than in non-linear formulations. For processes with highly nonlinear dependencies, accurate piecewise linear approximations are required. In our experience, (piecewise) linear models are able to approximate the most relevant features of industrial processes well.

To model and optimize an industrial process with the IEH approach, the process is split into one (or a combination of) units that are represented by *part models*. Each part model can have several different streams that enter or leave this unit. The streams can either be energy carriers or a product stream. The streams of all part models can be connected to form the process system.

For this approach, a class structure is developed that predefines different part models, their streams, and connections. With this class structure, the part models, their streams and their connections are automatically translated into a MILP formulation that can be optimized by state-of-the-art solvers. This approach has the advantage, that minimal effort is required for the MILP formulation when creating the process model. The constraints, objectives, and required formulations for the optimization are already predefined in the classes and just need to be instantiated. With this modular approach, it is possible to develop optimization models of industrial processes very fast and efficiently and compare different scenarios. New streams of energy carriers (e.g. gas, water) as well as new part models can be implemented straightforward and thus, making this approach an optimal tool for the optimization of multi-carrier industrial processes, respectively IEHs.

In the following paragraphs, relevant part models in the IEH framework, their constraints and objectives are described. The implemented constraints and objectives are based on a cost-based unit commitment problem, according to G. W. Chang et al. [24]. The implemented constraints and objectives consist of parameters, which are fixed values in the optimization, and variables, which are determined during optimization. In the following description, variables are always marked with an overline, e.g. $\overline{p}$.

3.2.1. Devices

Device part models can describe any machine, device, or storage in an industrial process. Every device part model can have an arbitrary number of input and output streams, which can be either energy carriers or product streams. The characteristics of a device are predefined by constraints and objectives of the underlying class and can be customized/adapted for every single device part model. The linear correlation between input and output streams in the device part model is defined by conversion constraints, the on/off behavior is described by the start-up constraint and the minimum-up/minimum-down time constraints. Additionally, every input and output stream can have maximum/minimum generation limits as well as ramp-up/ramp-down limits. With these constraints, the most important characteristics of an industrial process can be modeled. Fig. 2 illustrates a device part model with its constraints, two input streams $\overline{p}_1$ and $\overline{p}_2$, and three output streams $\overline{p}_3$, $\overline{p}_4$ and $\overline{p}_5$.

Conversion Constraint. Conversion constraints describe the relation between input and output streams of a device according to Eq. (1). This relation is defined by the conversion of energy or product streams that take place in a device. E.g., in a simplified model of a steam boiler, the conversion constraint can define the relation between consumed fuel (input stream) and resulting steam (output stream). However, not only the relation between input and output streams, but also between two (or more) input streams, or two (or more) output streams can be defined.

$$a+\sum_i b_i\cdot\left|\left(\overline{p}_{i,t}\right)\right|=0 \quad ,\forall t\in[1,T] \tag{1}$$

Here, a is constant offset, b is a factor and $\overline{p}$ represents any stream (input or output) of a device, depending on the relation to be described. t is the index for the time that is limited by the horizon of the optimization T and i is the index for the streams that are part of one conversion constraint. For the streams $\overline{p}$, the absolute value is used, because output streams are defined to be positive and input streams are always negative. The constant offset a and the factor b can be set to positive or negative values, according to the required relation. This way, any kind of linear relation between streams can be modeled, regardless if the streams are input or output. One device can have one or more conversion constraints to describe its behavior.

In cases that a linear function can not describe the behavior of a device accurately, non-linear behavior can be approximated by piecewise linear segments. The total conversion function is thus based on several linear functions that are associated to linear segments. The switching between the associated linear functions is done by binary variables $\overline{bin}$ for every linear segment, according to Eq. (2), where n is the index for the linear segments. Additionally, Eq. (3) defines that only one of the binary variables is unequal to zero and thus, only one of the linear functions can be used at a time.

$$\sum_n\left(a_n+\sum_i b_{i,n}\cdot\left|\left(\overline{p}_{i,t}\right)\right|\right)\cdot\overline{\mathrm{bin}}_{n,t}=0 \quad ,\forall t\in[1,T] \tag{2}$$

$$\sum_n\overline{\mathrm{bin}}_{n,t}=1 \quad ,\forall t\in[1,T] \tag{3}$$

3.2.2. Start-up constraint

Using an approach with three binary variables, the start-up constraints defines that every time step t, a unit can either be *on* (binary variable $\overline{u}=1$) or *off* ($\overline{u}=0$) - see Eq. (4) - and cannot be start-up (binary variable $\overline{y}=1$) and shut-down (binary variable $\overline{z}=1$) at the same time - see Eq. (5).

$$\overline{u}_t-\overline{u}_{t-1}=\overline{y}_t-\overline{z}_t \quad ,\forall t\in[2,T] \tag{4}$$

$$\overline{y}_t+\overline{z}_t\leq 1 \quad ,\forall t\in[2,T] \tag{5}$$

3.2.3. Maximum/minimum generation limits

The minimum and maximum generation constraint limits a selected stream $\overline{p}$ of a device by its maximum p_{max} and minimum p_{min}, using the binary on/off variable $\overline{u}$, according to Eq. (6).

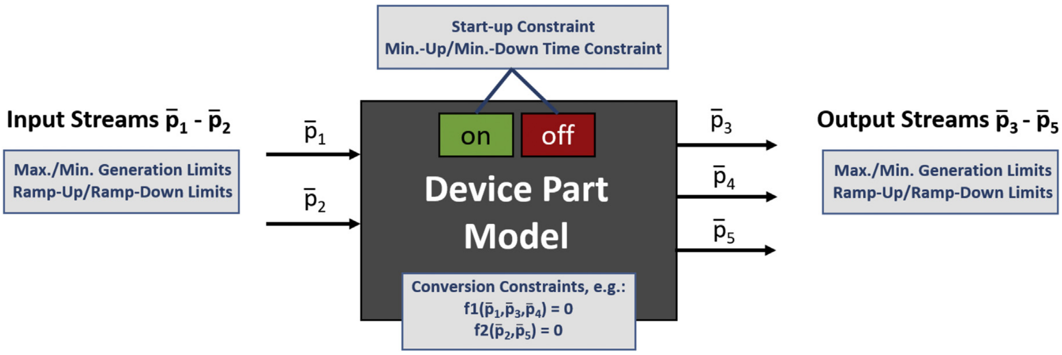

Fig. 2. Illustration of a generic Device Part Model.

$$\bar{u}_t \cdot p_{\min} \leq \bar{p}_t \leq \bar{u}_t \cdot p_{\max} \quad , \forall t \in [1, T] \tag{6}$$

3.2.4. Ramp-up/ramp-down limits

Ramp-up/ramp-down constraints limit the maximal positive (Ru) - see Eq. (7) - and negative (Rd) gradient of a selected stream $\bar{p}$ - see Eq. (8).

$$\left(\bar{p}_{t+1} - \bar{p}_t\right) \leq \mathrm{Ru} \quad , \forall t \in [1, T] \tag{7}$$

$$\left(\bar{p}_t - \bar{p}_{t+1}\right) \leq \mathrm{Rd} \quad , \forall t \in [1, T] \tag{8}$$

3.2.5. Minimum-up/minimum-down time constraint

The minimum-up/minimum-down time constraint defines the amount of time, a device needs to be on (Ut) - Eq. (9) - and off (Dt) - Eq. (10) - after being started ($\bar{y} = 1$) and shut down ($\bar{z} = 1$).

$$\bar{y}_t + \sum_{k=t+1}^{t+Ut-1} \bar{z}_k \leq 1 \quad , \forall t \in [2, T] \tag{9}$$

$$\bar{z}_t + \sum_{k=t+1}^{t+Dt-1} \bar{y}_k \leq 1 \quad , \forall t \in [2, T] \tag{10}$$

3.2.6. Storage constraint

For the use of storages, additional storage constraints - Eq. (11) and Eq. (12) - need to be implemented. They use the storage total output $\overline{so}$, input $\overline{si}$, the fill level $\bar{f}$, and the amount $\bar{s}$ that enters or leaves the storage every time step t. $\bar{s}$ can be positive or negative, depending if the storage is charged or discharged. The fill level can be limited by a maximum value, using the maximum generation limit constraint from Eq. (6).

$$\overline{so}_t = \overline{si}_t + \bar{s}_t \quad , \forall t \in [1, T] \tag{11}$$

$$\bar{f}_t = \bar{f}_{t-1} - \bar{s}_{t-1} \quad , \forall t \in [1, T] \tag{12}$$

3.2.7. External requirements

External requirements are another type of part model in the IEH framework. These part models can represent every external demand that is not directly defined by the chipboard production itself, e.g. district heating demand or required electrical energy sold over time. The predefined constraint - see Eq. (13) - for external requirements connects a selected output stream of a device part model $\bar{p}$ with its demand D, using a slack variable $\bar{S}$ that can be penalized in the objective function.

$$\bar{p}_t + \bar{S}_t = D_t \ , \ \bar{S}_t \geq 0 \quad , \forall t \in [1, T] \tag{13}$$

3.2.8. Production schedule

The production schedule is another part model in the framework. It includes an arbitrary number of different orders of a certain product that need to be produced along a specified time interval. The predefined constraint of this part model connects a selected product stream $\bar{p}$ of a device part model with its product demand O, according to Eq. (14). Additionally, a deadline and a penalty for not fulfilling the deadline can be set in the objective function.

$$O_t = O_{t-1} - \bar{p}_{t-1} \ , \ O_t \geq 0 \quad , \forall t \in [1, T] \tag{14}$$

3.2.9. Objectives

Typically, the objective of the optimization of industrial processes is the reduction of costs, energy, or emissions. In this work, we use a cost-based optimization approach. The objective function includes energy and production costs, rewards, and penalties for not fulfilling external requirements and the production schedule. All considered costs of the process can be implemented by adding a linear cost term to the objective function. The IEH framework uses a multi-objective function that inhabits internal process costs C, demand penalty E, and rewards R, e.g. for selling electricity to the grid. The multi-objective optimization problem is solved by a weighted-sum approach, in which penalties and reward terms need to be set according to a companies production strategy. Similar to the constraints, also all objectives are predefined in the classes of each part model and can be added to every stream in the process. The multi-objective optimization function can be described by Eq. (15), where c, e and r are the indices for the costs, penalties, and rewards.

$$\min \sum_{t=1}^{T} \left(\sum_{c} C_{c,t} + \sum_{e} E_{e,t} - \sum_{r} R_{r,t} \right) \tag{15}$$

3.3. Aggregated process model

To create a model of an entire industrial process, the previously described part models need to be connected. Fig. 3 illustrates the combination of three different device part models A-C with two external requirements and one production schedule. To connect the different device part models, their input and output streams are connected. This is done by setting the sum of the input streams - which are negative - equal to the sum of the output streams - which are positive - for every connection with the index k, according to Eq. (16). The connection of an output stream to an external requirement or a production schedule is already defined in the corresponding part model constraints in Eq. (13) and Eq. (14).

$$\sum_{k} \overline{p}_{k,t} = 0 \quad , \forall t \in [1, T] \tag{16}$$

After the definition of all part models and their connections, the development of the model is completed and the process can be optimized.

3.4. Optimization and outcomes

To solve the formulated MILP optimization problem, the Yalmip Optimization Toolbox in Matlab in combination with the solver GUROBI is used. A receding horizon approach is used, where the optimization is conducted over a specified time interval - the horizon - and the optimized variables are shifted in time to conduct the optimization in the next time interval.

The results of the optimization show the optimal operation of all devices and streams in the process (= all variables), with regard to minimum costs, depending on the used parameters. Thus, for every time step along the horizon, the optimization predicts the optimal quantity of all energy and product streams $\overline{p}$, the optimal operation modes defined by $\overline{bin}$ (in case different operation modes are implemented), and if a device is on or off by the binary variables $\overline{u}$, $\overline{y}$ and $\overline{z}$. For storages, also the variables $\overline{f}$, $\overline{si}$, $\overline{so}$ and $\overline{s}$ are predicted by the optimization. Additionally, the results show the total costs (including penalties, rewards and process costs) and, if the external requirements and production schedule could be fulfilled, using the slack variable $\overline{S}$. By adapting the objective function, also energy consumption or emissions can be minimized with the IEH modeling and optimization approach. However, in this work only the cost-based optimization is analyzed. Therefore, the optimization results do not provide information about minimal energy input or emissions.

4. Use case - Chipboard production plant

As a use case, a real-world chipboard production plant is analyzed. The process includes two dryers and a press for production, two chip storages, as well as a steam boiler and a steam turbine that act as a combined heat and power (CHP) unit. The output steam and electrical power of the CHP unit is used for the production process and can also be sold to the district heating (DH) network and the electrical grid. The plant has contracts with two DH companies and is the main supplier for one of them.

A flowchart of the simplified process is displayed in Fig. 4. In the flowchart, *SB* stands for steam boiler, *TURB* for the turbine, *DRY* for the dryers, *MS* for middle-chip storage, *TS* for top-chip storage, *AC* for air condenser, *DH* for district heating and *INT* for an additional internal constant demand of heat and electricity.

To model and optimize the chipboard production process, in the first step the process is split into units. The following energy conversion units are modeled:

- **Turbine:** The turbine has a capacity of 10 MW and converts the major part of the steam from the steam boiler SB 1 to electrical power, high pressure steam (HP), and low pressure steam (LP). The relations between electrical power, LP, and HP are defined by conversion constraints that are based on turbine specifications and process data. Most of the turbine's electrical power is used for the process itself, the remaining electricity is sold to the grid. The turbine can be operated in four different modes, resulting in different relations between steam and electrical power with pressures of the low pressure steam (LP) of 0.3, 0.7, 0.9, or 1.2 bar.

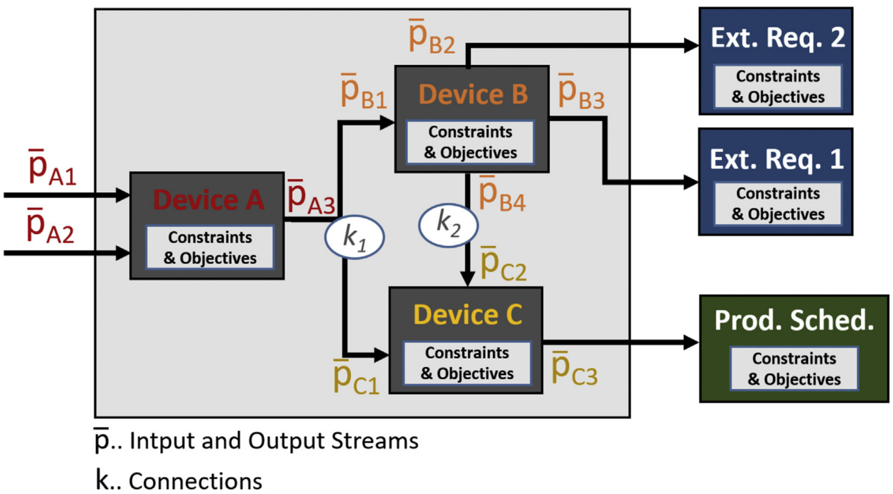

Fig. 3. Example of the combination of five part models A-E with two external requirements 1–2 and one production schedule.

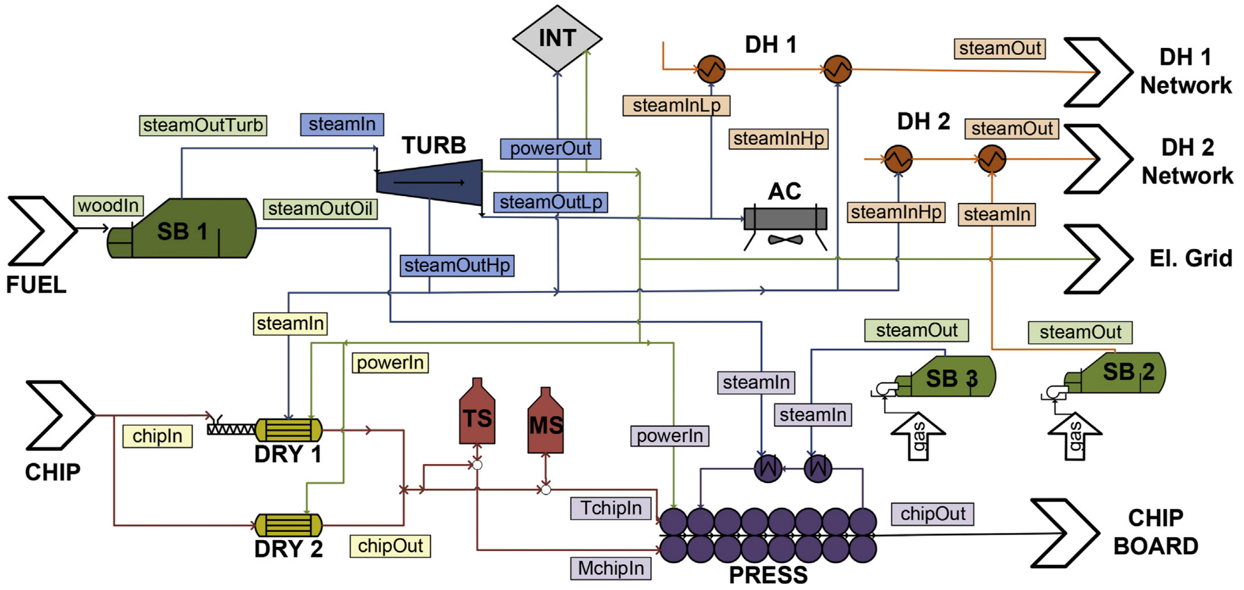

Fig. 4. Flowchart of the chipboard production process.

- **Steam Boiler (SB) 1**: The SB 1 converts fuel (wood) to steam that is fed to the turbine and used to heat up the thermal oil in the press. The steam boiler has a capacity of approximately 50 MW and requires approximately 36,000 MWh fuel (wood) every month. Currently, a little more than 1/3 of the produced steam from the steam boiler SB 1 and the turbine is used internally for the process, a little less than 1/3 for the district heating demand, and about 1/3 of the steam is a loss.
- **Steam Boiler (SB) 2**: The SB 2 has a capacity of 9 MW and can be used to generate additional steam out of gas to meet the DH 1 demand at all times. The operation of SB 2 is costly and therefore, it is only used if required.
- **Steam Boiler (SB) 3**: SB 3 has a capacity of 6 MW and produces additional steam to heat the thermal oil for the press. Same as SB 2, the operation of SB 3 is expensive and thus, only used when necessary.
- **Air Condenser (AC)**: The AC condenses excess LP steam from the turbine. Thus, the steam that leads to the AC is a loss. The AC is limited by a maximal capacity.

The following units for production are included:

- **Dryer 1**: Dryer 1 uses HP steam and electrical power to dry chips, according to the defined conversion constraints.
- **Dryer 2**: Dryer 2 includes a combined gas and dust burner to generate flue gas, which is used to dry the chips directly. As dust is a waste product of the process, it is used preferably and assumed to be available all time at no cost. In the model, gas is only used to start up the dryer. Additionally, dryer 2 uses electrical power. After drying, the chip is separated to top-chip and middle-chip, which differ in their size/fineness. The top-chip and middle-chip are used in different shares in the press, depending on the type of product.
- **Top-chip/Middle-chip Storage (TS/MS)**: In the TS/MS, top-chip/middle-chip can be stored. The storages are identical in construction and are limited by a maximal amount of chip that can enter and exit the storage, as well as a maximal fill level.
- **Press**: The press uses electrical power and thermal oil to produce chipboards out of different shares of top-chip and middle-chip. The volume of production is approximately 30,000 tons of chipboard per month. The press is implemented with four different operation modes. Each operation mode is tailored to one type of product with a specific thickness, shares of middle-/top-chip, and operation time.

As external requirements, the operators of the chipboard production plant need to fulfill two district heating demands, which are defined by the district heating companies. Not fulfilling the demands is penalized by a fixed price. For both demands, realistic time-series are used, based on real data. Additional, electrical energy can be sold to the grid to a fixed price to either of the district heating companies, whereas company 2 has a higher price. As a production schedule, four different products (according to the operation modes of the press) can be specified. For each product, an arbitrary number of orders with a penalty and deadline can be set.

4.1. Operation mode and strategy

In general, the chipboard production process is operated 24/7. However, not all of the devices are active all of the time, as this depends on the current production schedule, the district heating demand, and also on maintenance works. All modeled devices except the press are operated continuously. The press only operates continuously when producing chipboards with constant thickness. When switching to another type of chipboard, the press has a short downtime and is thus operated semi-continuously.

Currently, the goal of the operators is to fulfill the production schedule, the district heating demand, and to sell as much electricity as possible. Due to a fixed subsidized feed-in tariff, electricity can be sold at a good price. The high price for electricity leads to the fact that the steam boiler SB 1 and turbine operate in full load whenever possible - even if this is not required by the production. To this end, the energy input of the steam boiler SB 1 and the turbine will not be reduced by the operational optimization of the process. However, optimal operation and scheduling of the process can lead to reduced internal energy consumption (energy consumption of all devices), reduced energy consumption of the steam boilers SB 2 and SB 3, as well as increased feed-in of electricity. Additionally, optimization can be used to evaluate the maximal district heating demand that can be met and thus, showing the process's full potential.

4.2. Chipboard production optimization model

To optimize the described chipboard production process, the developed IEH modeling and optimization approach from Section 3 is applied. All described energy conversion and production units of the chipboard production plant are modeled as device part models. Their input and output streams are defined according to the flowchart of the chipboard production process in Fig. 4. The two district heating networks are modeled as external requirements and the amounts of chipboards that need to be produced are defined by a production schedule. The behavior and characteristic of each unit in the process is described by the predefined constraints and objectives (see Section 3), whereas the variables are to be determined by the optimization and the parameters are defined based on the data basis.

Resulting from the described process units of the chipboard production plant, the objective function includes the following terms: Fuel costs of the steam boilers, rewards for selling electricity to the grid, and penalties for not fulfilling the district heating demand or the production schedule.

The final MILP optimization model of the chipboard production can be solved with state-of-the-art solvers, e.g. GUROBI. Most importantly, the outcomes of the optimization show the optimal trajectories of all input and output streams of all devices, and whether the district heating demands and the production schedule can be fulfilled.

4.3. Data basis

For the modeling and optimization of the chipboard production plant, real process data of the industrial site is used. On the one hand, process information is used to determine which constraints and objectives (and thus parameters) are implemented in each part model. On the other hand, process data is used to define the values of the constraints' parameters. The data basis comprises time-series data of one year, energy reports, data-sheets, as well as additional process information based on experience. Whereas time-series data is logged every few seconds, most of the other data/information is available on a daily or monthly base. Time-series data is always used to create models in the first step, because this data basis is expected to be the most accurate. As time-series data is not available for all required measures, energy reports and data-sheets are utilized for some of the models to create either data-driven or physical models. Additionally, some of the required information for the modeling and optimization are based on process knowledge and experience of employees of the company.

These heterogeneous data sources are not rare in industrial plants and complicate the effective modeling and optimization. All data needs to be gathered, sorted, and brought to the same units and time frame, which is a complex and time-consuming task. Also, this reinforces the need for a thorough model validation, in order to check the models and assumptions and enable reliable predictions with the optimization.

4.4. Model validation - static simulation

Fig. 5 shows a Sankey diagram of the chipboard production plant, based on process data for a representative data set of one month. For validation of the models, static modeling results are compared with process data. For this purpose, required input, output, and production data is used to calculate the energy demand of each unit. The red numbers beside the streams in Fig. 5 stand for the deviations from the calculated static modeling results to the real process data. A deviation of e.g. ±5 % means, that the static modeling results are 5 % higher/lower than the real process data. It can be seen, that the model is able to predict the output variables of the steam boiler and the turbine, as well as the energy inputs of the dryers and press fairly accurately, with a mean error of 2.4 %. Due to the use of linear models, measurement inaccuracies in the time-series data, and the heterogeneous data basis in general, a small error is inevitable.

4.5. Simulation scenarios

To show the differences between the classical EH approach - where only energy streams are considered - with the combined optimization of energy and product streams, three scenarios are simulated and compared with the real-world case **S0**.

- **Scenario S1:** Constant production - The production schedule is not included in the optimization. Instead, a constant production rate is assumed that is based on monthly averages. Thus, also the steam and power demand for the production units (dryers, press, internal demand) are constant. This scenario represents the sole optimization of energy streams and neglects the flexibility of production units. To this end, the optimization in this scenario determines the optimal operation of the steam boiler and turbine in order to fulfill the variable district heating demands, maximize the sale of electricity and cover the constant heat and power demand for production.
- **Scenario S2:** Flexible production - The production schedule is included in the optimization. The steam and power demand for the production units depend on the operation of the process. Thus, the production units can be operated flexibly and the utilization and scheduling of the dryers, the storages, and the press can be optimized. This scenario includes all previously described devices, the variable district heating demands, and the production schedule of the process. It represents the combined energy and production management in the chipboard production process.

In the course of the evaluation of the results, we identified that the specified district heating demands are limiting factors in the optimized scenario with flexible production S2. To this end, another scenario is analyzed:

- **Scenario S3:** Flexible production without district heating limitation - This scenario is equal to S2, except that the steam for the district heating demand 2 is not limited, but rewarded by a fixed price. This scenario shows the potential of a combined optimization of production and energy, where excess heat can be exploited.

To be able to compare the results of all scenarios, the external requirements are kept the same. The scenarios include the same district heating demand (except district heating demand 2 in S3) and the same amount of chipboards are produced. A time span of 30 days is simulated in all scenarios. The optimization is conducted with a horizon of 5 days (120 h) for 6 times (total 720 h) with the receding horizon approach. One time step in the simulation is representative for 1 h in the real process. With the linear optimization approach, computational times could be held comparatively low (approximately 2 h per scenario), despite the complex process

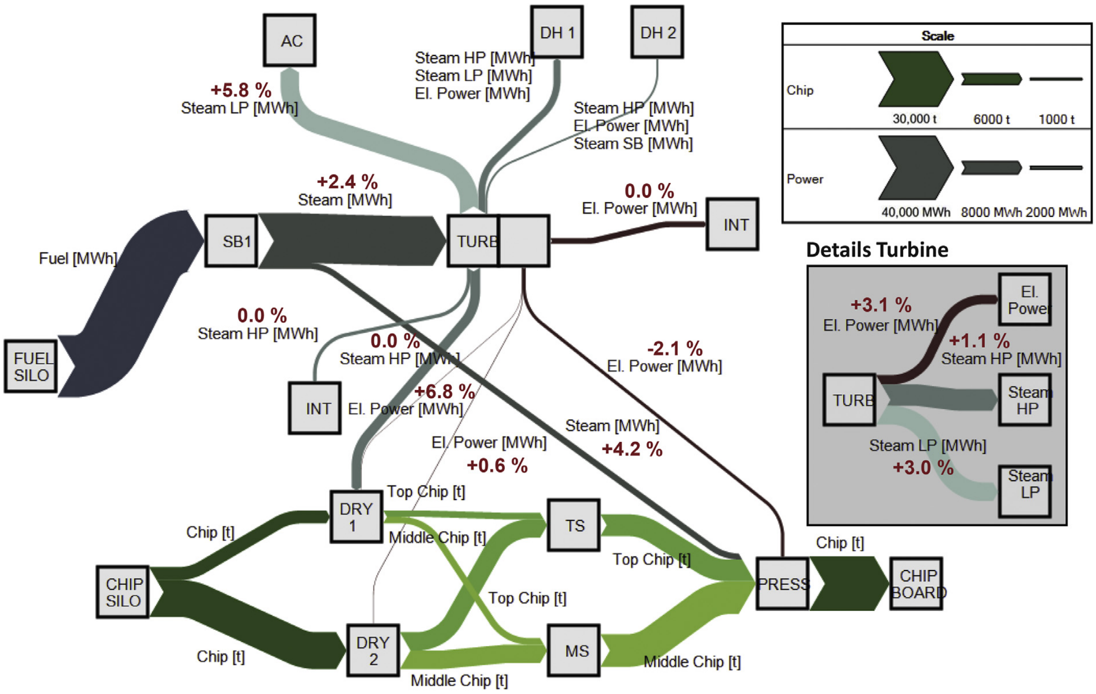

Fig. 5. Sankey diagram of the real-world case with deviations to the static simulation results (red).

and long simulation time span.

5. Results

Figs. 6–8 show a comparison of the following relevant energy-measures for the three optimized scenarios and the real-world case S0:

- Electrical Power (El. Power): Total electrical power, produced by the turbine. Additionally, the amount of electrical power sold to the grid is given in Fig. 8.
- Production Steam (Prod. Steam): Steam used for the dryer, the press, and the internal constant steam demand.
- DH Steam HP/LP (DH HP/DH LP): High pressure steam (HP)/low pressure steam (LP), used for the district heating (DH) demand.

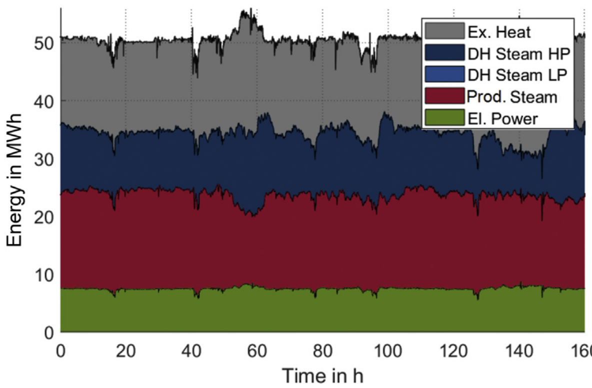

Fig. 6. Relevant energy-measures in the real-world case S0.

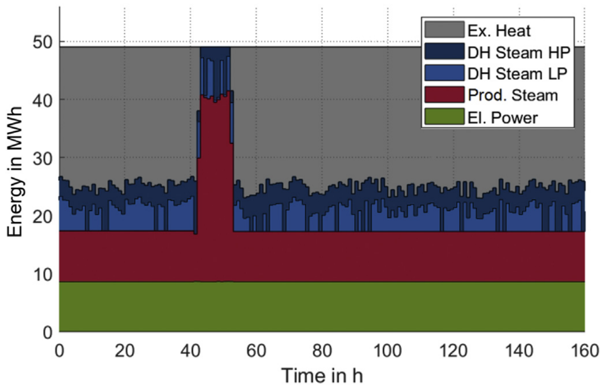

Fig. 7. Relevant energy-measures in scenario S2.

- Excess Heat (Ex. Heat): LP steam that leads to the air condenser (AC) and thus, is a loss.

In Figs. 6 and 7, the energy-measures over a time horizon of 160 h for the real-world case S0 and scenario S2 are shown. A comparison of the cumulative results of the energy-measures of all scenarios over a time horizon of one month can be found in Fig. 8. The deviations of the results of scenarios S1–S3 to the real-world case S0 are depicted by a percentage in Fig. 8. A deviation of e.g. ±5 % means that the value in this scenario is 5 % higher/lower than in S0. In the following paragraphs, the energy-measures of the scenarios are compared to each other.

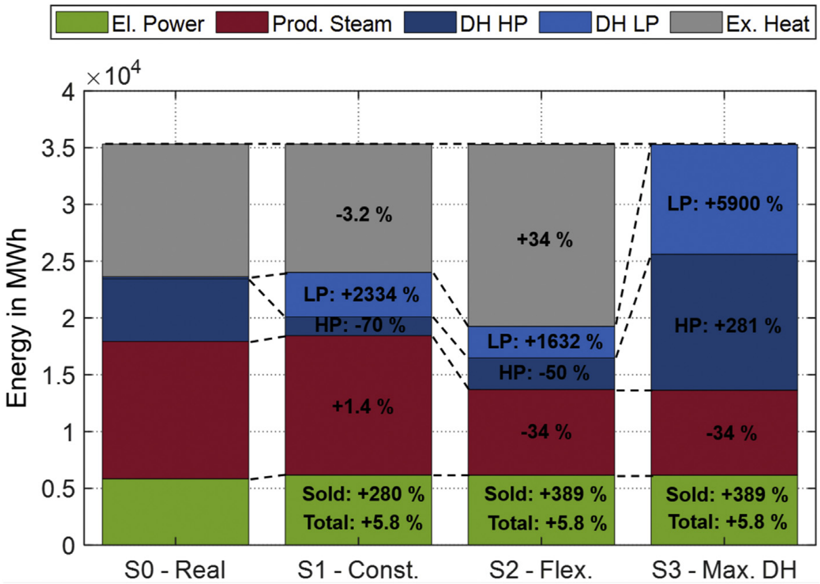

Fig. 8. Comparison of relevant energy-measures of all scenarios.

5.1. Electrical power

In all scenarios, the cumulative electrical power is higher (total +5.8 %, see Fig. 8) than in the real case S0, as selling power to the grid is rewarded with a good price. Approximately 280 % more electricity in S1, and approximately 390 % more electricity in S2 and S3 can be sold, compared to the real-world case S0. The steam boiler and the turbine always operate at full load to produce maximum electricity in S1–S3. In contrast in S0, the turbine is partly operated with a higher end pressure, which results in increased energy in forms of steam and reduced electrical power. Although the total electrical power is equal in S1–S3, a little more electricity can be sold to the grid in S2 and S3 than in S1. The reason is, that fewer electrical energy is required for the production in S2 and S3, because the dryers - that require a different amount of electrical energy according to their loading - are operated optimally.

5.2. Production steam

In S1, the steam required for the production is almost equal to the one in the real-world case S0, because the constant power and steam demand in this scenario are based on real data. In the scenarios S2 and S3 that include the scheduling of production, the cumulated production steam is reduced drastically by approximately one third. This significant deviation is caused by the shifting of the production, especially by the optimal operation of the two dryers. Whereas dryer 1 requires HP steam and only few electrical power if little loaded, dryer 2 does not require any HP steam and operates most efficiently fully loaded. Depending on the utilization of the steam and electricity from the steam boiler and turbine, either dryer 1 or dryer 2 is preferably used. Besides that, the storages in S2 and S3 after the dryers allow for a more flexible capacity utilization of the dryers: In times of excess heat, the utilization of dryer 1 is increased and the resulting additionally dried chips can be stored and used when required. This behavior can be seen in Fig. 7, that shows a peak between hour 40 and 60, compared to Fig. 6. During this peak, excess heat is available and used to dry chips in dryer 1. The described behavior of the dryers, combined with the varying DH demand, can be optimally utilized in S2 and S3 and leads to the drastic reduction of production steam. Although the model of dryer 1 shows an error of 6.8 % for the electrical power (see Fig. 5), the optimization results only vary marginally if the dryer 1 model is adapted in different ways to realize an error below 1%. Thus, this error is not responsible for the deviations of the production steam between the different scenarios.

5.3. DH steam LP & HP

In the scenarios S1–S3, the total DH demand can be met without the additional steam boiler SB 2. Only the relations between LP and HP vary between the different scenarios.

5.4. Excess heat

In the real-world case S0, a considerable amount of LP steam leads to the AC and thus, is a loss. Due to the fixed DH demand and the full-load operation of SB 1 and the turbine, the amount of excess heat can not be reduced significantly in scenarios S1 and S2, see Fig. 8. To the contrary, the excess heat in S2 is even higher, because less HP steam is required for the production and the total energy stays the same. The depiction of S3 in Fig. 8 therefore shows the potential of the optimization, in case that unlimited HP steam can be sold to the district heating network. Considering an average fixed reward of 20 €/MWh, steam with a value of more than 31,000 € could be sold additionally in one month, if all excess HP steam is utilized for district heating.

For a more detailed analysis, the differences between all energy streams of the scenarios S0–S2 can be seen in Fig. 9. It shows a Sankey diagram of S2 and compares energy and product streams with S0 and S1. The width of the arrows/lines show the magnitudes of the resulting energy and product streams in the optimized Scenario 2. Deviations to S0 are depicted by a blue percentage, deviations to S1 by a red percentage. Thus, a blue/red percentage of 1 % means that the results in S0/S1 for this stream are 1 % lower than in S2. The biggest deviations can be identified at the dryers 1 and 2

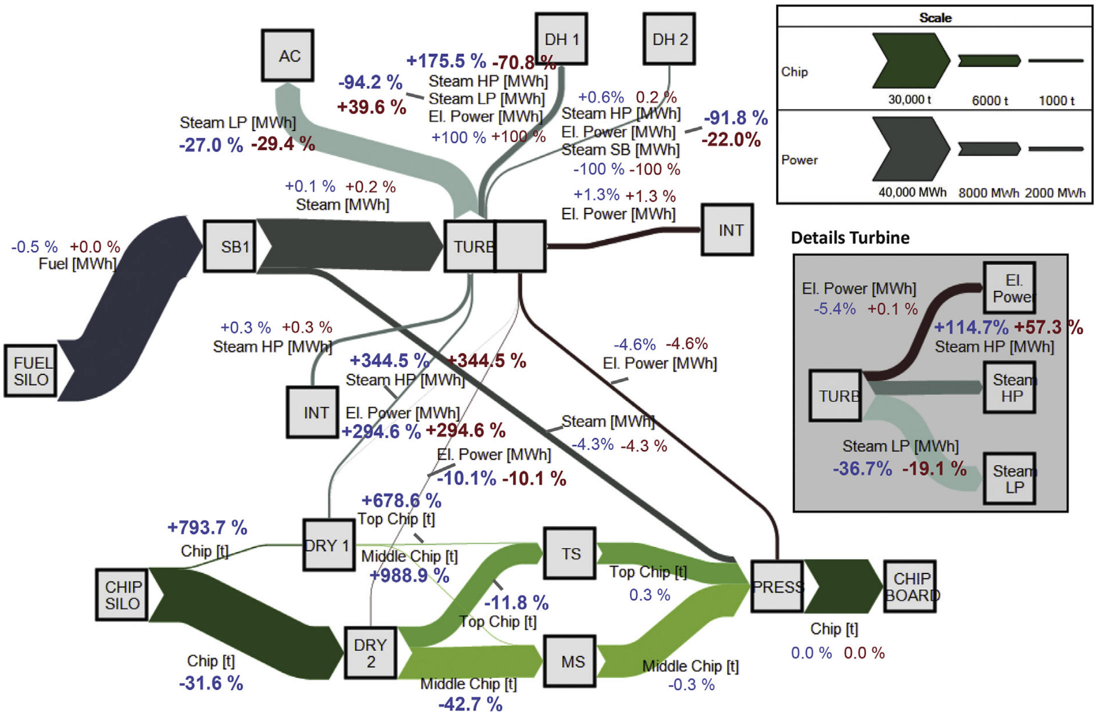

Fig. 9. Sankey diagram of S2, with deviations to the real-world case S0 (blue) and constant production S1 (red). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

and the DH demand. Although the total DH demand is equal in the scenarios S0–S2, the shares of LP, HP, and sold electrical power differ. Regarding the dryers, it can be seen that significantly less chip is processed in dryer 1 and more in dryer 2 in S1 and S2 than in the real-world case S0. The optimal operation of the dryers leads to a reduced electrical power and HP steam demand for the production.

Summarized, the analysis of relevant measures shows that the steam demand for the production is reduced significantly (34 %) in the scenarios that include production scheduling. Additionally, more energy can be sold to the grid in these scenarios. In a detailed observation of all process streams, it can be seen that production is shifted towards dryer 2, which uses less electricity if fully loaded and no HP steam. In combination with the varying DH demand, the dryers can be operated optimally in S2 and S3, leading to a reduced electrical and steam demand for the production and different shares of LP and HP for district heating. However, although considerably less steam for the production is required in S2 and S3, the total amount of energy stays the same in all scenarios and the excess heat in the AC can not be reduced. Thus, the cost-based optimization of the chipboard production plant is only beneficial, if excess heat is utilized. Excess heat could be used to either cover a higher DH demand - as exemplified in S3 - or e.g. recycled/fed back to the process and used for preheating.

6. Conclusion

The optimization of energy and product streams in an industrial chipboard production process was conducted with a holistic modeling and optimization framework. The chipboard production plant includes a combined heat and power unit, units for production, and has two district heating demands as external requirements. The units for production include storages, a press, and two dryers, which allow a shifting of operation. Three different scenarios were analyzed, to show the potential of the combined energy and production management in a manufacturing process, based on the Energy Hub concept. The results show that the optimization of product streams, in addition to energy streams, plays a crucial role in the management of the entire system: The required energy for the production units could be reduced by 34 %, using a cost-based optimization approach. However, this potential can only be exploited, if also external requirements and process design are adapted. Excess heat needs to be utilized appropriately, e.g. for district heating or internal preheating/recycling, to benefit from the optimization. Future work will investigate the use of excess heat in extended scenarios with process design modifications.

Credit author statement

Verena Halmschlager: Conceptualization, Methodology, Validation, Investigation, Formal analysis, Writing – original draft, Visualization, René Hofmann: Conceptualization, Writing – review & editing, Supervision, Project administration, Funding acquisition.

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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References

[1] EEA. Final energy consumption by sector and fuel in europe. European Environment Agency ENER 016; 2020. URL, https://www.eea.europa.eu/data-and-maps/indicators/final-energy-consumption-by-sector-10/assessment.

[2] IEA. Digitalization and energy – technology report. URL, https://www.iea.org/reports/digitalisation-and-energy; 2017.

[3] Cui H, Zhou K. Industrial power load scheduling considering demand response. J Clean Prod 2018;204:447–60.

[4] Favre-Perrod P. A vision of future energy networks. In: Proceedings of the inaugural IEEE PES 2005 conference and exposition in Africa. Piscataway, NJ: IEEE Service Center; 2005. p. 13–7.

[5] Geidl M, Koeppel G, Favre-Perrod P, Klöckl B, Andersson G, Fröhlich K. The energy hub: a powerful concept for future energy systems. Electrical & Computer Engineering; 2007.

[6] Geidl M, Andersson G. A modeling and optimization approach for multiple energy carrier power flow. In: IEEE Russia power tech. Piscataway, NJ: IEEE; 2008. p. 1–7. 2005.

[7] Mohammadi M, Noorollahi Y, Mohammadi-ivatloo B, Yousefi H. Energy hub: from a model to a concept – a review. Renew Sustain Energy Rev 2017;80:1512–27.

[8] Sadeghi H, Rashidinejad M, Moeini-Aghtaie M, Abdollahi A. The energy hub: an extensive survey on the state-of-the-art. Appl Therm Eng 2019;161:114071.

[9] Mohammadi M, Noorollahi Y, Mohammadi-ivatloo B, Hosseinzadeh M, Yousefi H, Khorasani ST. Optimal management of energy hubs and smart energy hubs – a review. Renew Sustain Energy Rev 2018;89:33–50.

[10] Majidi M, Mohammadi-ivatloo B, Anvari-Moghaddam A. Optimal robust operation of combined heat and power systems with demand response programs. Appl Therm Eng 2019;149:1359–69.

[11] Paudyal S, Cañizares CA, Bhattacharya K. Optimal operation of industrial energy hubs in smart grids. IEEE Transactions on Smart Grid 2015;6(2):684–94.

[12] Nojavan S, Majidi M, Zare K. Optimal scheduling of heating and power hubs under economic and environment issues in the presence of peak load management. Energy Convers Manag 2018;156:34–44.

[13] Majidi M, Nojavan S, Zare K. A cost-emission framework for hub energy system under demand response program. Energy 2017;134:157–66.

[14] Vahid Pakdel MJ, Sohrabi F, Mohammadi-ivatloo B. Multi-objective optimization of energy and water management in networked hubs considering transactive energy. J Clean Prod 2020;266:121936.

[15] Ghanbari A, Karimi H, Jadid S. Optimal planning and operation of multi-carrier networked microgrids considering multi-energy hubs in distribution networks. Energy; 2020. p. 117936.

[16] Niu J, Tian Z, Zhu J, Yue L. Implementation of a price-driven demand response in a distributed energy system with multi-energy flexibility measures. Energy Convers Manag 2020;208:112575.

[17] Pazouki S, Haghifam M-R. Optimal planning and scheduling of energy hub in presence of wind, storage and demand response under uncertainty. Int J Electr Power Energy Syst 2016;80:219–39.

[18] Najafi-Ghalelou A, Nojavan S, Zare K, Mohammadi-ivatloo B. Robust scheduling of thermal, cooling and electrical hub energy system under market price uncertainty. Appl Therm Eng 2019;149:862–80.

[19] Roustai M, Rayati M, Sheikhi A, Ranjbar A. A scenario-based optimization of smart energy hub operation in a stochastic environment using conditional-value-at-risk. Sustainable Cities and Society 2018;39:309–16.

[20] Rakipour D, Barati H. Probabilistic optimization in operation of energy hub with participation of renewable energy resources and demand response. Energy 2019;173:384–99.

[21] Vahid-Pakdel MJ, Nojavan S, Mohammadi-ivatloo B, Zare K. Stochastic optimization of energy hub operation with consideration of thermal energy market and demand response. Energy Convers Manag 2017;145:117–28.

[22] Calise F, Dentice d'Accadia M, Libertini L, Quiriti E, Vanoli R, Vicidomini M. Optimal operating strategies of combined cooling, heating and power systems: a case study for an engine manufacturing facility. Energy Convers Manag 2017;149:1066–84. URL, http://www.sciencedirect.com/science/article/pii/S0196890417305733.

[23] Halmschlager V, Hofmann R. Holistic approach for the optimization of industrial hybrid energy hubs with milp. first ed. Vol. 130 of Part C. Elsevier, 30th european symposium on computer aided chemical engineering; 2020.

[24] Chang GW, Tsai YD, Lai CY, Chung JS, editors. A practical mixed integer linear programming based approach for unit commitment. IEEE Power Engineering Society General Meeting; 2004. 2004.

Paper 3

Optimizing the Utilization of Excess Heat for District Heating in a Chipboard Production Plant

Published in Case Studies in Thermal Engineering in collaboration with Felix Birkelbach and René Hofmann

This paper was developed based on the results of Paper 2 and analyzes design modifications in the chipboard production plant to optimally use excess heat for district heating. In this paper, the focus is on the modular structure of the framework that allows for the fast creation of optimization models of different scenarios. The three scenarios/design adaptations in this paper include the integration of two thermal energy storage, a Ruth's steam storage and a stratified tank buffer storage, and the activation of an additional heat exchanger for district heating. The results of the analysis demonstrate that all of the design modifications yield significant benefits over the original process.

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

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Optimizing the utilization of excess heat for district heating in a chipboard production plant

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ABSTRACT

The industry is responsible for about one third of the global energy consumption, and thus, reducing energy and emissions in this sector is crucial to reach global climate goals. Methods like operational optimization can improve industrial processes' efficiency, leading to a decrease of excess heat or total energy. By combining operational optimization with flexibility measures like thermal energy storage, intermittent heat can be optimally utilized.

This work analyzes the optimal utilization of excess heat for district heating in a real-world industrial use case, a chipboard production plant. The process includes a combined heat and power unit and units for production. Electricity can be sold to the grid, and two district heating demands need to be met while satisfying the production schedule of the plant. To exploit the utilization of excess heat, four adaptations to the process are considered: Increased district heating feed-in capacities, the integration of two different thermal energy storages, and the activation of an additional heat exchanger for district heating.

To optimize the process's operation with and without the adaptations, an optimization framework is developed. Its modular structure allows for straight-forward design adaptations. The outcomes show that the process's efficiency can be significantly improved by applying operational optimization and considering the process adaptations. In all scenarios, the currently contracted district heating feed-in capacity can be significantly increased, leading to profits up to 108,000 € per month and reduction of energy losses up to 87 %. Although the heat exchanger's activation yields the highest profits of all scenarios, thermal energy storages can increase the process's flexibility. In the end, the decision, which modification is most viable depends on the operator's objectives.

1. Introduction

With a share of more than 30 % of the global energy consumption, the industrial sector plays a crucial role to reach global climate goals [1]. In order to decrease the energy consumption and fully utilize available energy in existing industrial plants, different approaches can be pursued. On the one hand, the operation of an existing process can be optimized without changing the process design. This is generally known as operational optimization and often referred to with terms like optimal energy scheduling, production scheduling, optimal energy management, or Demand Side Response (DSR) in the industrial context [2]. On the other hand, the process design can be modified by adapting existing devices or integrating new devices [3]. In this paper, we aim to minimize excess heat by

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combining these two approaches. A multi-carrier-energy system with a combined heat and power (CHP) unit is optimized to exploit the use of excess heat for district heating. As design modifications, an additional heat exchanger and two sensible thermal energy storages are considered due to their widespread use in industry and their low investment costs [4].

In literature, a great number of publications deal with the optimization of industrial CHP systems and multi-energy-carrier systems, also known as Energy Hubs [5]. A good overview of recent publications for the optimization of CHP systems can be found in Refs. [2,6] and for Energy Hubs in Refs. [7,8] and [9].

Though, narrowing down the literature to the optimal operation/use of excess heat (for district heating) in industrial multi-carrier energy systems with thermal energy storage, the number of publications reduces sharply. In Ref. [10] the optimal operation of multi-carrier energy networks with energy storage technologies is analyzed. The energy-carriers gas, power, heating, and water are considered. The main focus is laid on the effects of interconnections between energy-carriers and their impacts on the operation of these energy networks. In Ref. [11] the excess heat recovery in industrial-city networks is addressed. The paper proposes measures to enable heat flexibility (including thermal energy storage) and evaluates their technical, environmental and economic feasibility by a reference scenario. Also, researches deal with the use of excess heat from the industrial sector for the district heating network in e.g. Denmark [12] or Great Britain [13]. In Ref. [14] the economic and environmental benefits of a CHP plant with seasonal thermal energy storage are analyzed. In Ref. [15] a framework for the optimization of multi-energy systems, using wind and solar energy is established with Particle Swarm Optimization (PSO) algorithm. Combined cooling, heating and power, as well as storage are considered, and an office building is used for a case study.

The literature review shows that although many publications provide methods and tools for the optimization of multi-energy-systems with thermal energy storage, there are gaps in applying these methods in real-world industrial applications, especially in manufacturing industries. This work, therefore, presents a real-world industrial manufacturing case study, a chipboard production process. The plant includes a CHP system, production units, heat can be sold to the district heating network, and electrical power sold to the grid. In previous work [16], we conducted the operational optimization/scheduling of energy and production in the chipboard production plant. The optimization resulted in a significant reduction (approx. 1/3) of the production units' energy consumption. However, a non-negligible amount of heat in the process is still unused and dissipated to the surrounding. This unused heat could be used for district heating if the process was adapted appropriately. Therefore, this work focuses on the optimal use of excess heat for district heating in the chipboard production process. The previously conducted operational optimization is now combined with the analysis of different process adaptations. First of all, the company can renegotiate its district heating contracts and increase the contracted feed-in capacities. This modification is a precondition to use the surplus energy, which is currently dissipated, for district heating. In addition to the elevated district heating feed-in capacities, three design adaptations are considered: Two different thermal energy storage are implemented to increase the process's flexibility. This way, the available energy can be shifted in time, leading to higher efficiency and reduced losses. Last, an already existing heat exchanger for district heating, which is currently unused, is reactivated to further increase the district heating feed-in capacities.

The main contributions of this work are:

- Development of an optimization framework for (manufacturing) process industry, whose structure allows for straight-forward design adaptations
- Optimization of the use of excess heat for district heating in a real-world chipboard production plant by implementing two thermal energy storages and an additional heat exchanger
- Demonstration of improved utilization of energy and increased profits by combined operational optimization and process adaptations

The remainder of this paper is organized in the following sections. In Section 2, the underlying concept - the Industrial Energy Hub concept - is presented, and the used modular optimization framework is described. In Section 3, the use case and its operation mode/strategy are introduced. Possible design modifications are discussed, and the analyzed scenarios are stated. In Section 4, the results are

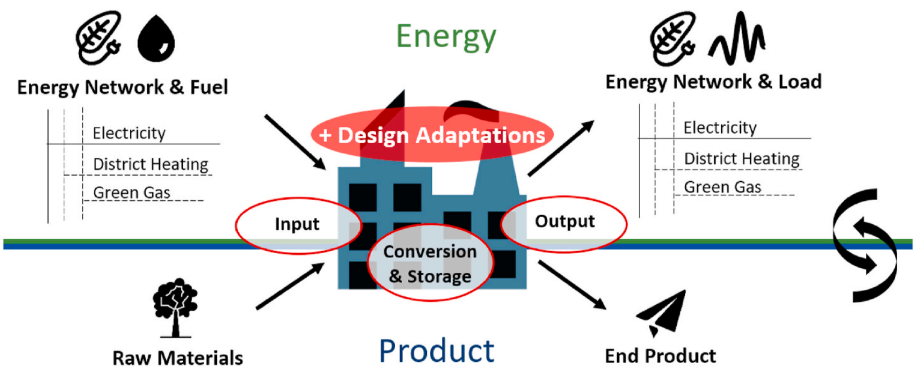

Fig. 1. Industrial Energy Hub concept. According to Ref. [17].

presented, including a detailed analysis of the total energy consumption, remaining excess heat, and amortization time in all scenarios. In Section 5, the major contributions of this paper are summarized.

2. Methods

For the optimization of the chipboard production plant, a modeling and optimization framework [17], with a Mixed-Integer-Linear-Programming (MILP) formulation was developed. The modular structure of the framework allows for straight-forward design adaptations of a process. The framework was developed to optimize any multi-energy-carrier industrial process and is based on the Industrial Energy Hub concept.

2.1. Industrial Energy Hub concept

The Industrial Energy Hub (IEH) concept was introduced in previous works [16,17], and is illustrated in Fig. 1. The IEH approach is based on the commonly used EH concept [8,18], where a system is built up by four units: conversion, storage, input, and output. To take into account the production of an industrial plant, in addition to the different energy carriers of the EH, also the product acts as a carrier in the IEH. In conversion units, energy and product carriers can be converted to other carriers, or their characteristics can be changed. Storages are presented by storage units, where energy (e.g. thermal energy storage) or product (e.g. mass storage) can be stored. Last, with the input and output units, the flows at the system boundaries are described. Typical input and output flows in industrial systems are electricity, heat, and natural/green gas that can all be sold to or bought from the grid. Additionally, resources/raw material for the process, as well as the end product, are represented by input and output units. For a more detailed description of the IEH, we refer to Refs. [16,17].

In contrast to the authors' previous publications, this paper does not consider a fixed system but aims to optimize the plant in operation *and* design. Design adaptations can be made in all four units of the IEH (see Fig. 1), e.g. by implementing additional devices (conversion or storage), changing flows of energy or product carriers, or changing input and output units.

2.2. Modeling and optimization framework

The modeling and optimization framework is based on the IEH concept and thus, aims to model and optimize any combination of input, output, and conversion/storage units. For this purpose, a modular approach based on Mixed-Integer-Linear-Programming (MILP) formulation is used. It is realized by object-oriented programming in Matlab and the use of an elaborate class structure shown in Fig. 2. The framework consists of the six classes: device-class, ports-class, connections-class, production order-class, demand forecast-class, simulation system-class. In the following sections, instances of a class are always named after their class (e.g. instance of

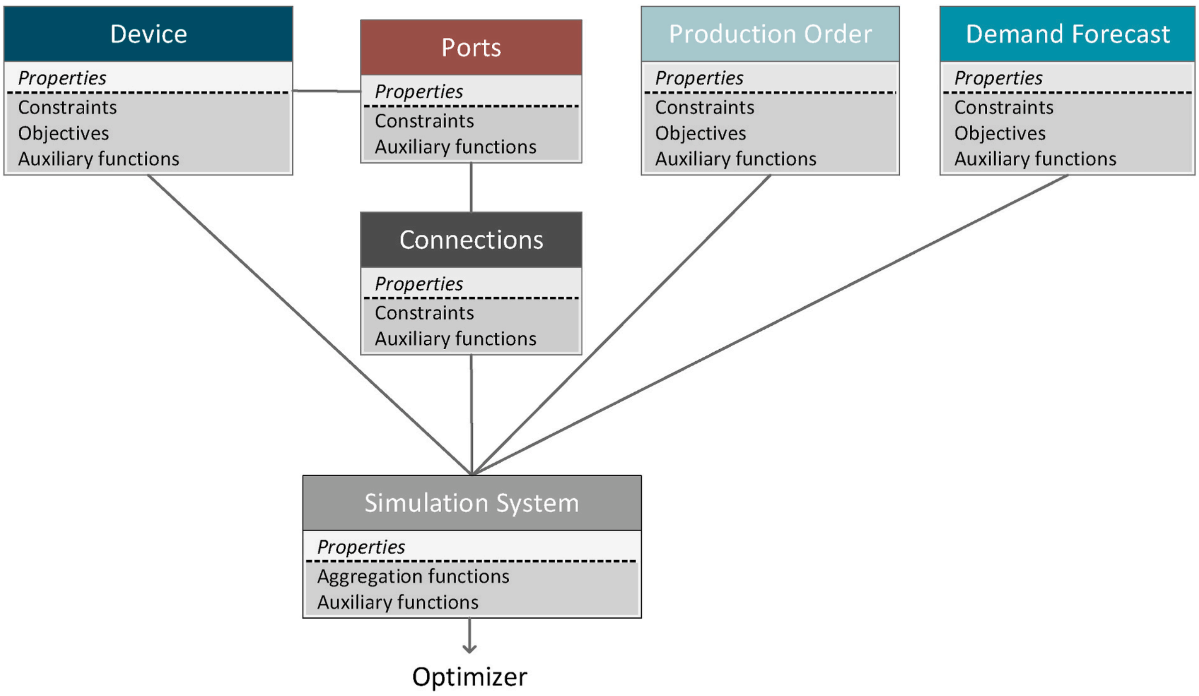

Fig. 2. Class structure of the modeling and optimization framework.

the device-class = Device).

- **Device:** Instances of the device-class describe any conversion or storage unit in a process, and thus, they are the core components of the process model.
- **Ports:** Ports are always assigned to a Device and describe a stream that enters or leaves a Device. One Device can have an arbitrary number of different Ports that can reflect either an energy or a product stream.
- **Connections:** Connections connect different Devices, more specifically their Ports, to form the process model.
- **Production Order:** A Production Order describes external requirements of the process that need to be met over a specified time horizon. Production Orders are therefore suitable to implement a production schedule, where a certain amount of product needs to be produced until a specified point in time.
- **Demand Forecast:** A Demand Forecast describes external requirements of the process that need to be met at every time step. Demand Forecasts are therefore suitable to implement a required district heating demand, where a certain amount of heat needs to be fed to the network at every time step.
- **Simulation System:** In the Simulation System, the previously described Devices (and Ports), Production Orders, and Demand Forecasts are connected (by Connections) to form the total process model.

Each of the six classes has several properties and functions, which are summarized in the class diagram in Fig. 2. First, the classes set the basic structure (properties) and predefine constraints and objectives of an object. Second, the classes automatically translate all objectives, constraints, and properties of their instances into a MILP formulation, with Auxiliary Functions. The Simulation System uses Aggregation Functions to summarize all other classes' functions, and Auxiliary Functions to translate these functions into a suitable form for the optimizer. The implemented constraints and objectives of the framework are based on a cost-based unit commitment problem [19]. The following constraints are defined: Three-Bin Constraint, Down/Up Time Constraint, Hot/Cold Start Up Constraint, Min/Max Constraint, RampUp/RampDown Constraint, Conversion Constraint and Storage Constraint. Objectives can be either real costs, which can be assigned to every stream (represented by Ports), or imaginary costs, usually implemented as rewards or penalties. In the case of a multi-objective function, a weighted-sum approach is used. The resulting linear optimization problem can be solved by state-of-the-art solvers (e.g. GUROBI). The output are trajectories of every optimized variable and the state (on or off) of every device. For a more detailed description of the frameworks implemented constraints and objectives, we refer to Ref. [16].

The described modular approach has the advantage that minimal effort for the formulation of the optimization problem is required. To optimize a process, the underlying models, constraints and objectives need to be known. However, the formulation of the optimization problem is done by the predefined auxiliary functions of the framework. With this modular and flexible structure, all parts of the process model (Devices, Ports, Production Orders, Demand Forecasts, Connections) can be easily adapted, added, or omitted, without the need to change the entire process model. This makes the framework suitable not only for operational optimization but also for the analysis and comparison of different scenarios with design adaptations.

2.3. Exemplary process compilation

To close the gap between theory and implementation, an example for the compilation of a Simulation System with the framework is demonstrated. Fig. 3 shows a Simulation System that consists of four Devices, two Demand Forecasts, and one Production Order. Each Device has several associated Ports that define input and output streams (energy or product carriers). Each Device, Demand Forecast, Production Order, and Port has constraints and/or objectives, and properties, defined by the user while instantiating. To form the process model, the different Devices - more precisely their Ports -, Demand Forecasts, and the Production Order are connected by Connections. Now, the Simulation System can be compiled and directly solved by the solver. A second, (or third, ect.) Simulation

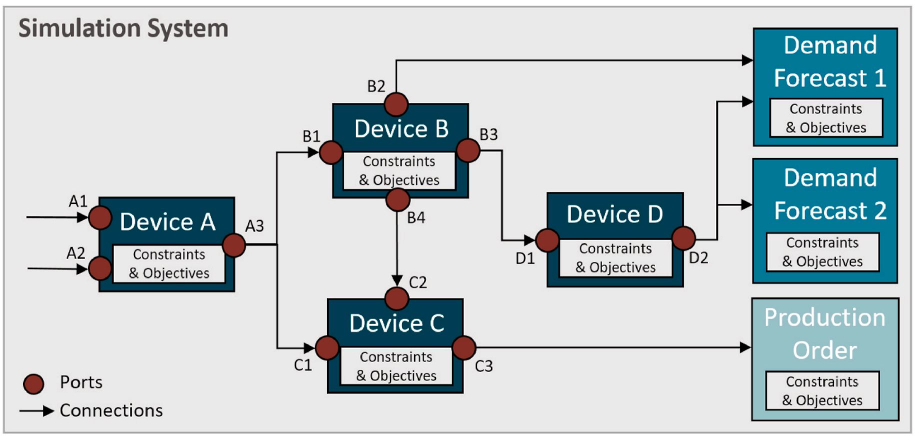

Fig. 3. Exemplary process compilation of a Simulation System.

System can be easily built by changing constraints/objectives, switching Connections, or adding/omitting Devices, Ports, Production Orders, and Demand Forecasts.

3. Use case - chipboard production plant

A real-world industrial plant - a chipboard production - is considered as a use case. The simplified process flowchart can be seen in Fig. 4. The chipboard production mainly consists of a CHP unit (steam boiler and steam turbine), and units for production, including two mass storages. Also, heat is used to meet the district heating demand of two suppliers, and electricity can be sold to the grid. The design modifications analyzed in this paper and described in Section 3.3 are shown in dashed yellow.

The optimization model of the chipboard production is compiled according to the description in Section 2.3. All process units are modeled as Devices with Ports. The two district heating networks are modeled as Demand Forecasts, and the Production Order represents the chipboards that need to be produced over time. The models of the process units are based on both data-driven and physical models, depending on the data basis. The created optimization model was validated in Ref. [16] and showed high accuracy with a mean error of approx. 2.4 %. In that publication, also more information about the underlying data can be found.

3.1. Original chipboard production process

The following heat and power generation/conversion units are part of the chipboard production plant:

- **Steam Turbine:** The turbine converts a share of the steam from the steam boiler SB 1 to heat (high pressure (HP) steam and low pressure (LP) steam) and electrical power. Its electricity and heat are used for the production process and can be sold to the electrical grid and district heating network. The turbine has a capacity of 10 MW and can be operated in four different modes. The operation modes differ in the pressure and temperature of the LP steam according to Table 1, resulting in different shares of HP steam, LP steam, and electricity. Due to the coupled generation of steam and electricity in the steam turbine, the ratio between HP steam, LP steam, and electricity can not be varied arbitrarily but depends on the operation mode and the temperature and pressure of the LP steam. A maximal output of electricity is achieved with the lowest pressure/temperature LP steam, which is currently the most used operation mode, referred to as *electricity-driven* in Table 1. However, due to the coupled generation of heat and electricity, also the amount of heat is rather high in this operation mode. In the heat-driven operation modes - see Table 1 - the electricity output is lower than in the electricity-driven operation, leading to increased shares of heat.
- **Steam Boiler (SB)**: The steam boilers in the process convert fuel to steam. They differ in their capacity and type of fuel. SB 1 has a capacity of 50 MW and requires approx. 36,000 MWh of wood every month. The produced steam by SB 1 and the turbine is currently used in the following shares: a bit more than 30 % are used for production, approx. 30 % are used for district heating and slightly less than 30 % are a loss. Steam boiler SB 2 (9 MW) uses gas to generate additional steam to meet the district heating demand at all times. Steam boiler SB 3 (6 MW) uses gas to heat the press's thermal oil. The operation of both SB 2 and SB 3 is costly, and therefore, they are only used if required.
- **Air Condenser (AC):** The AC condenses excess LP from the turbine and thus, the steam that leads to the AC is a loss.

The following units for production are part of the chipboard production plant:

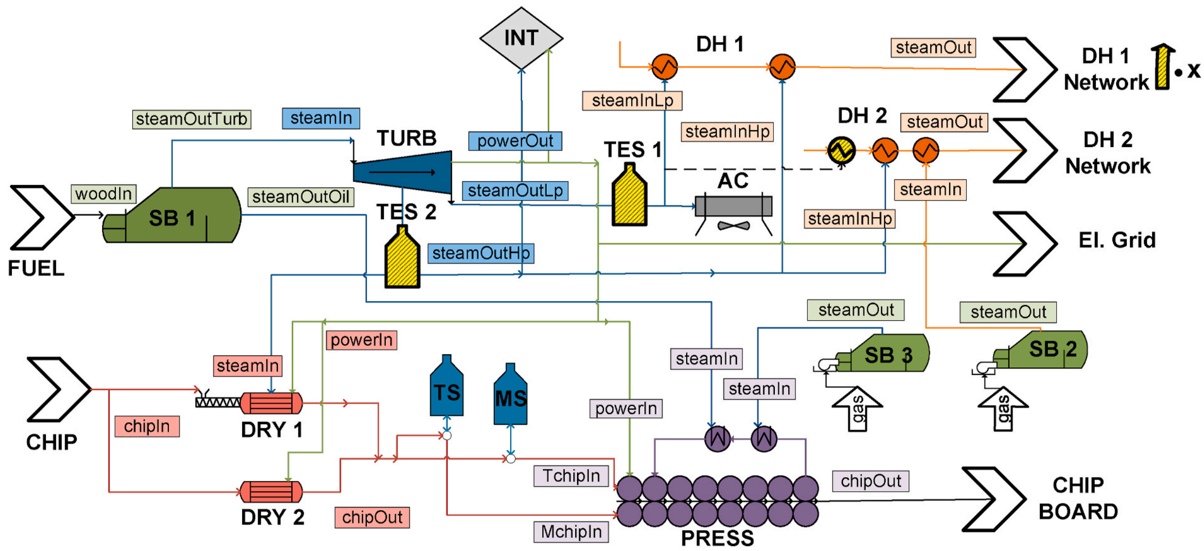

Fig. 4. Simplified process flowchart of the chipboard production.

Table 1
Operation modes of the turbine.

Operation Mode	Pressure LP Steam	Temperature LP Steam	Type of Operation
1	0.3 bar	65 °C	electricity-driven
2	0.7 bar	90 °C	heat-driven
3	0.9 bar	97 °C	heat-driven
4	1.2 bar	105 °C	heat-driven

- **Dryer**: Dryers are used to dry the chips before they enter the press or the mass storages. Dryer 1 uses HP steam and electrical power to dry chips, whereas dryer 2 uses flue gas - generated by a combined gas and dust burner - to dry the chips directly. After drying, the chips are separated into top-chip and middle-chip, which differ in their size/fineness. Top-chip and middle-chip are used in different ratios in the press, depending on the type of product.
- **Top-chip/Middle-chip Storage (TS/MS)**: In the top-chip and middle-chip mass storages, top-chips and middle-chips can be stored. Both storages are identical in construction and are limited by a maximal fill level and a maximal amount of chips entering/exiting the storages.
- **Press**: The press produces chipboards out of different shares of top-chip and middle-chip. The press requires electrical power and thermal oil and has a production volume of approx. 30,000 tons of chipboards every month.

As external requirements, two district heating demands and a production schedule need to be fulfilled, and electricity can be sold to the grid:

- **District Heating (DH)**: The plant operator has contracts with two district heating companies, each specifying a district heating demand. The chipboard production is a secondary supplier for DH company 1 and the main supplier for DH company 2. This makes it obligatory to fulfill the DH 2 demand at all times, also during failures and maintenance works. For these occasions, SB 2 can fulfill the entire DH 2 demand on its own, however, with higher costs. In contrast, DH 1 only needs to be fulfilled during normal operation and allowing small deviations.

To fulfill the district heating demand of DH 1 (required temperature ≈ 130 °C), either HP steam or LP steam can be used. However, only LP steam above the temperature level of the ingoing DH stream (≈ 65 °C) can be used. Thus in the electricity-driven operation mode (see Table 1), the temperature of LP steam is 65 °C, and thus, none (or marginal) LP steam can be used for district heating. For the heat-driven operation modes, an increasing share of the required energy for the DH 1 demand can be supplied by LP steam. In contrast, the DH 2 demand (required temperature ≈ 95 °C) can only be fulfilled by HP steam. Although there already exists a heat exchanger to use LP steam for DH 1, it is currently not used/required.

- **Production Schedule**: The production schedule defines the number of chipboards that need to be produced until a certain time. For this use case, four products with different shares of top- and middle-chip span are considered.
- **Electricity Grid**: Although most of the electrical energy of the turbine is used for the production units, excess electricity can be sold to the grid at a fixed, subsidized price. However, the subsidy for electricity is expected to end in the near future and electricity generation is not economic with the current fixed (unsubsidized) market price. Nevertheless, by participating in the day-ahead market, electricity can still be sold at a favorable price during peak hours of electricity demand. For this reason, day-ahead electricity prices - based on real-market prices in Austria - are used for this use case.

3.2. Operation mode and strategy

In general, the chipboard production process is operated 24/7. The operation mainly depends on the production schedule and the DH demand. The operators' strategy is to fulfill the district heating demand as the first priority, the production schedule as the second priority, and to sell as much electricity as possible and profitable. Usually, maximal production and full DH coverage do not affect each other significantly. Thus, it is possible to fully fulfill the DH demand and run production at highest capacity utilization anyway.

All modeled devices of the process - except the press - operate continuously. The press is considered to be operated semi-continuously. It is operated continuously when chipboards of the same thickness are produced. However, when switching between different type of chipboards, the press has a short down time.

With the current operation strategy and without operational optimization, the utilization of energy is not fully exploited because the operators cannot predict the operation of the process in detail and will always consider a buffer to minimize risks and fulfill the process demands at all times. In contrast, using operational optimization, the operation of the process *can* be predicted, changing the currently used heuristic operation strategy towards optimal control. Using operational optimization, all boundary conditions and contingencies are already considered, and buffer can be mostly eliminated. However, to fully exploit the utilization of excess heat, operational optimization *and* process modifications are required.

3.3. Utilization of excess heat - process modifications

The previously conducted study of the chipboard production process showed that a considerable amount of excess heat - up to 40 % of the total thermal energy - is led to the air condenser and is not utilized [16]. For this reason, this work seeks to optimize the utilization of excess heat in the chipboard production process. In addition to the optimization of the original process in Ref. [16], we aim to optimize the chipboard production plant with process adaptations in this work. These adaptations are intended to achieve the following objectives:

1. Minimizing excess heat and/or total energy consumption
2. Maximizing profit
3. Increasing the process's flexibility

In addition to these objectives, three relevant boundary conditions need to be considered: First, the power and heat generation units and the production units should not be changed/replaced. Second, limited data of the process hinders the analysis of recycling excess heat, e.g. to preheat water or the span before it enters the press. Third, the amount of produced heat exceeds the demand at maximum capacity, whereas the plant's electricity demand can be just about covered. Thus, any electrical storage or heat pump (which converts electrical energy to thermal one) is not expected to be of any advantage. In fact, to decrease excess heat, the surplus of thermal energy needs to be utilized appropriately.

Considering the objectives and conditions mentioned, we identified the following promising process adaptations: First, the company could renegotiate its district heating contracts and increase the contracted feed-in capacities. This way, excess heat can be used to cover higher district heating feed-in quantities, leading to reduced excess heat and increased profit. Second, thermal energy storage could be used to increase the process's flexibility. These storages can improve energy utilization in the process, leading to reduced total energy consumption, reduced excess heat, and even higher district heating feed-in quantities. Third, the activation of the currently unused heat exchanger for DH 2 is considered. This heat exchanger enables the use of LP steam for DH 2, which is otherwise dissipated by the air condenser. In the following paragraphs, these four process adaptations are described more detailed:

- **District Heating (DH) Demand - Renegotiation of Contracts**: To use excess heat for DH, the operators of the plant could renegotiate the DH contracts and assure the DH companies a higher feed-in quantity. The magnitude of this quantity is to be determined by the analysis of the optimization. However, as the steam boiler 2 must cover the entire demand for DH 2 at any time, this demand can not be elevated without exchanging the steam boiler. For this reason, a higher feed-in quantity is only considered for DH 1.
- **HP Energy Storage - Ruth's Steam Storage**: As thermal energy storage (TES) for the high pressure steam of the steam turbine ($\approx$ 200 °C and up to 13 bar), a Ruth's steam storage is considered (see TES 1 in Fig. 4). The Ruth's steam storage is a sensible thermal energy storage that stores steam in a cylindrical pressure vessel filled with liquid water and steam as a two-phase fluid. Ruth's steam storages have already been applied in various industrial processes and power plants to increase their flexibility and efficiency [20–22].

To determine the investment costs of a Ruth's steam storage in the chipboard production, the volume is calculated based on [23]. For the calculation, a fill level of 0.9 is assumed, the steam in the storage can vary between 13 bar (state 1) and 4 bar (state 2), and maximal 25 t/h HP steam can be extracted from the storage, based on simulations without storage size limitations. This results in a volume of approx. 310 m^3.

- **LP Energy Storage - Stratified Tank Buffer Storage**: As thermal energy storage for the low pressure steam, a stratified tank buffer storage is considered (see TES 2 in Fig. 4). The stratified tank buffer storage consists of an insulated tank, which is filled with water of different temperature levels from hot to cold. Hot water can be directly fed into and extracted from the tank, while the same amount of cold water is removed from or fed to the tank. Stratified tanks usually operate with water temperatures between 0 and 95 °C, making the storage suitable for water storage for DH 2 with a temperature of up to 95 °C.

The size of the buffer storage is based on the maximal fluctuations of the DH 2 demand and results in a required tank size of 100 m^3 for hot and cold water (or two separated tanks for hot and cold water with a size of 50 m^3 each). As investment costs for a stratified tank buffer storage of 100 m^3, prices starting from 50,000 € were found [24]. Including proper insulation and installation, we expect investment costs of $\approx$ 100,000 € for the buffer storage.

Both the Ruth's steam storage and the stratified tank buffer storage are implemented in the optimization model with the Storage Constraints from Ref. [16], assuming a loss of 2 % of the stored energy per hour.

- **Activation LP Heat Exchanger**: In addition to the use of HP steam for the district heating demand 2, also the use of LP steam is considered (yellow symbol in Fig. 4). The heat exchanger for the use of LP steam is already installed in the chipboard production but is currently not used. Similar to DH 1, LP steam can only be used if the temperature level is higher than the ingoing DH temperature (up to 65 °C for DH 2). Thus, only in the heat-driven operation mode of the turbine, LP steam can be used for DH 2, see Table 1.

3.4. Simulation scenarios

In line with the described adaptations, the following scenarios are analyzed in this work:

- **S0:** Reference Process - Includes all original parts of the process described in Sec. 3.1 and considers increased DH feed-in quantities.
- **S1:** Stratified Tank Buffer Storage - Same as S0 but including the LP storage described.
- **S2:** Ruth's Steam Storage - Same as S0 but including the HP storage described.
- **S3:** Activation LP Heat Exchanger: Same as S0 but including the heat exchanger to use LP steam for DH 2.

The optimization models of all scenarios are created with the optimization framework and solved with GUROBI. For all scenarios, the hourly varying day-ahead market price and the production schedule are the same. The defined production schedule leads to maximal production at all times in all scenarios. To analyze the feed-in quantity that can be guaranteed to the DH suppliers, the district heating demand is increased by multiplying the original DH demand, which varies every time step. The optimization is conducted with a horizon of 1 day (24 h) for 6 times (total 144 h) with a receding horizon approach. 1 h in the real process is represented by one time step in the simulation.

4. Results and discussion

The analysis of the results is done in three steps. First, energy and profit are evaluated for increased feed-in quantities of heat for DH in S0. For the evaluation of the profits, fuel costs and earnings by selling heat to the DH network and electricity to the grid are considered. Rewards by selling chipboards are not taken into account, as production in all scenarios is equal. Thus, profits in this analysis can also be negative. Second, the maximal feed-in quantity that can be guaranteed to the DH companies is determined for each scenario. The maximum feed-in quantity is the basis for a possible renegotiation of the companies' district heating contracts. It is defined by a point (further referred to as DH100), at which the increased DH demand can still be fulfilled 100 % in every step of the optimization. Beyond this point, not all of the demand can be fulfilled anymore. At this point DH100, energy and costs are evaluated and compared with the currently contracted DH demand at point DH0. Third, investment costs and profit at DH100 are used to determine the amortization time of the scenarios with process adaptations.

In Fig. 5, the used energy and costs of S0 are displayed for increasing DH feed-in quantities. Here, the used energy for the process is divided into thermal energy (TE) for district heating (DH), TE loss (TE that is fed to the air condenser), TE used for the production, electrical energy (EE) for the production, EE that is sold to the grid, as well as unspecified losses (e.g. heat losses). Additionally, the unused capacity of the process is displayed, and the points DH0 (1170 MWh) and DH100 (3025 MWh) are marked. Besides the energy, the profit of the plant - excluding profit from production that is equal in all scenarios - is given on the right hand. In the bottom subfigure of Fig. 5, the turbine's operation mode can be seen, which can be either electricity-driven or heat-driven, according to Table 1. In the former operation mode, maximal electricity can be produced, but the LP steam has a too low temperature to be used for DH. In the latter, the temperature of LP steam is higher, and thus, LP steam can be used for DH.

Relevant conclusion that can be drawn from Fig. 5 are:

- TE DH and the profit increase constantly until DH100 is reached, while TE loss decreases. After DH100 is reached, the curves of TE DH and profit flatten and approach a maximum.

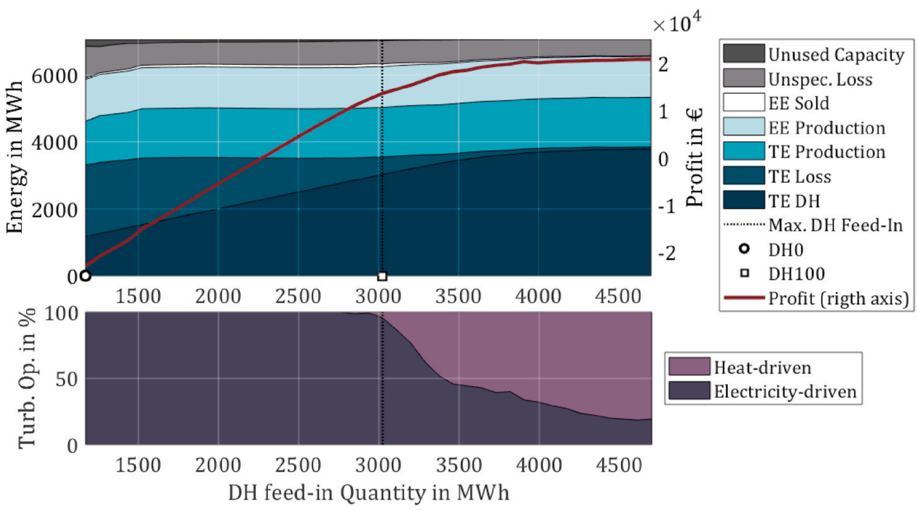

Fig. 5. Shares of used energy and costs for S0 along an increasing DH feed-in quantity, as well as operation mode of the turbine for one week.

- At high DH feed-in quantities, the turbine increasingly switches from the electricity-driven operation mode to the heat-driven operation mode to fulfill the higher DH demand. This results in LP steam with a higher temperature, but also in decreased amounts of electricity that can be sold.
- At DH100, almost 2.6 times more heat can be fed into the DH network compared to DH0, and the thermal energy losses are reduced by 76 %. This leads to more than 91,000 € higher profits per month than in DH0, where fuel costs exceed earnings from selling heat and electricity (−23,000 € per month).

The evaluation of the scenarios S1–S3 showed that the first two of the described findings above are almost identical in all scenarios. However, the scenarios differ in their maximal DH feed-in quantity (at DH100) and their profits. Thus, energy and costs of all scenarios at DH100 are compared in Fig. 6. In the top diagram of Fig. 6, the shares of used energy - in accordance with Fig. 5 - are displayed at DH100 for all scenarios. The respective feed-in quantities in MWh can be found below each bar. In the bottom diagram, the fuel costs - which are negative - and the earnings from selling heat and electricity - which are positive - are displayed. The addition of costs and earnings results in the profit, shown for S0 in Fig. 5.

It can be seen that the scenarios S1–S3 show at least minor improvements to S0. S1 (including the LP storage) has a slightly higher profit than S0, as more electricity can be sold to the grid while less energy is used in total. Same as in S2 (including the HP storage), this leads to a reduction of fuel costs. In both S2 and S3, the maximal feed-in rate of heat for DH is higher than in S0, and thus, internal losses decrease while profits increase. In S3, the feed-in rate at DH100 as well as the profit are the highest since a larger share of LP steam can be used for district heating. In this scenario, the turbine operates in the heat-driven operation mode more often. On the one hand, this leads to lower amounts of electricity and thus, fewer electricity can be sold to the grid. On the other hand, it leads to a higher temperature LP steam, which does not need to be dissipated by the air condenser but can be used for DH.

As the last step, the amortization times of the scenarios S1–S3 are evaluated. In Fig. 7, the investment costs - separated into uncovered costs and covered costs - and the profit of all scenarios at DH100 is compared to S0 at DH100. Additionally, the net profit after 5 years is marked. It can be seen that, although the HP storage in S2 shows good results in Fig. 6, the high investment costs of this storage lead to the longest amortization time of 5 years. For S1 with the LP storage, the profit is less than in S2, but this storage's lower investment costs lead to only 1 year amortization time. With zero investment costs and high profits, S3 shows the best results of all scenarios regarding total profit.

Finally, the most important outcomes from the analysis of Figs. 5–7 are summarized in Table 2 and described:

- **Max. Feed-In Quantity:** In all scenarios, the maximal feed-in quantity (at DH100) is far higher than the contracted feed-in quantity (at DH0). Thus, in all scenarios, a significantly higher feed-in quantity could be guaranteed to the DH companies, leading to higher profits. From all scenarios, S3 shows the highest maximal feed-in quantities, leading to additional profits of 108,711 € per month compared to the original DH demand.

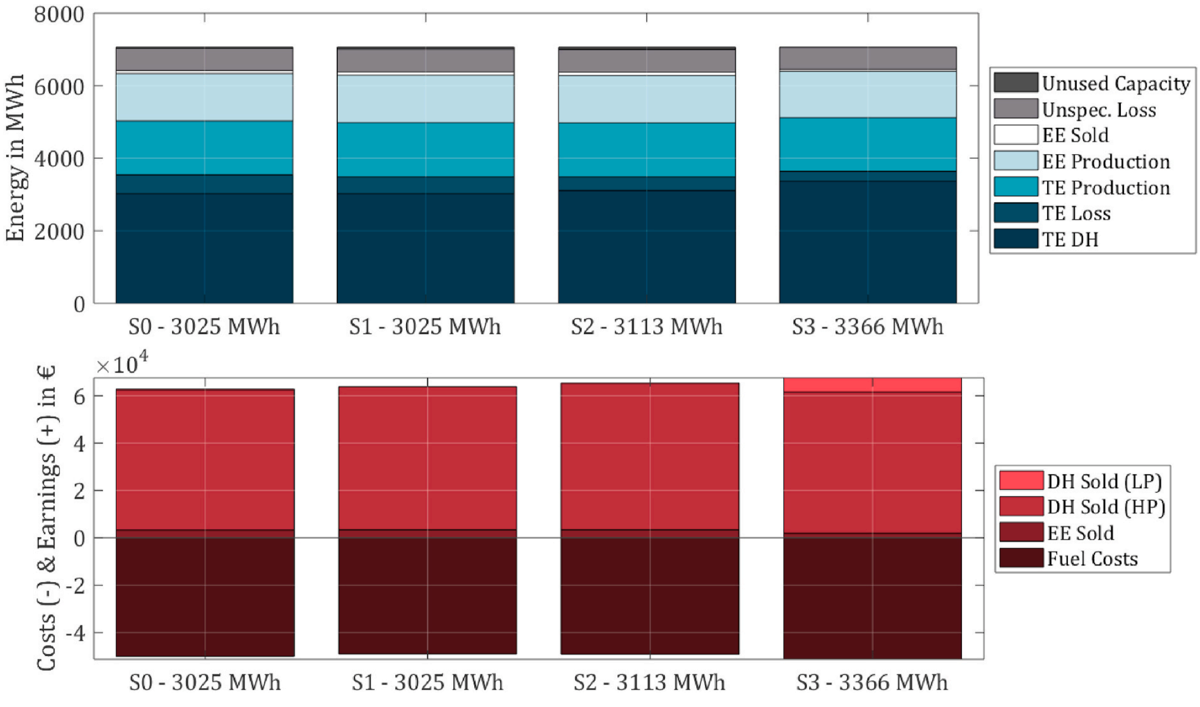

Fig. 6. Shares of used energy and costs/earnings at DH100 for all scenarios for one week.

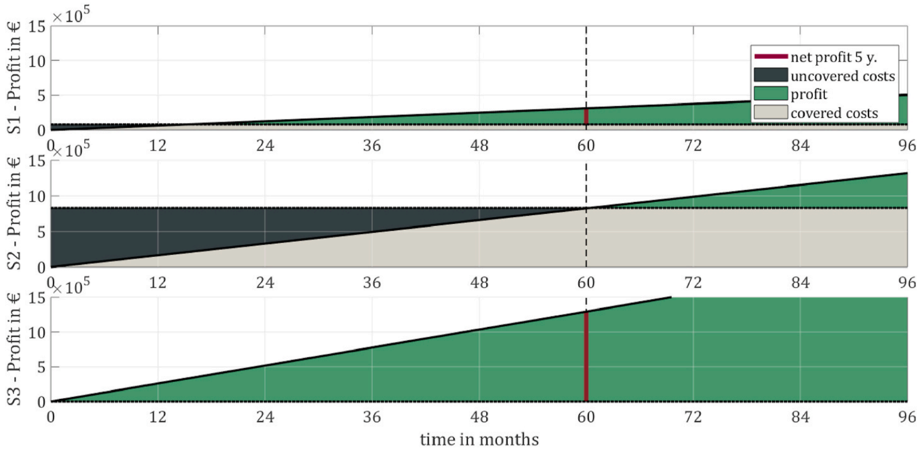

Fig. 7. Investment costs vs. profit along 8 years.

Table 2
Summary of the most important outcomes.

	S0	S1	S2	S3
Investment Costs	0	100,000	830,000	0
Amortization Time in years	0.0	1.3	5.0	0.0
Multiple of original DH demand at DH100	2.6	2.6	2.7	2.9
Reduction of TE loss at DH100 in %	76	79	79	87
Total Energy Consumption at DH100 per month in MWh	7023	7013	7001	7057
Profit at DH0 per month in €	−23,013	−22,288	−22,036	−18,036
Profit at DH100 per month in €	68,395	73,585	81,635	90,675
Diff. Profit at DH100 and at DH0 per month in €	91,408	95,873	103,671	108,711

- **Thermal Losses:** In all scenarios, thermal energy losses are significantly reduced (by up to 87 %) by increasing the DH feed-in quantities. In S3, thermal losses at DH100 are the lowest from all scenarios. However, the scenarios with the thermal energy storages S1 and S2 are the only ones with reduced total energy consumption.
- **Profit:** The scenarios S1–S3 yield (at least slightly) higher profits at DH100 than the reference scenario S0. However, S2 has the longest amortization time of 5 years, followed by S1 with 1 year. With zero amortization time and high profits, S3 performs best in terms of profit.
- **Scenario Assessment:** Although S3 shows the best results in terms of profit and utilization of excess heat, the scenarios with the thermal energy storage S1 and S2 yield more flexibility and security. The energy storage can shift the conversion and consumption of energy in time and provide improved security by retaining heat as a buffer. Deciding which of the factors - profit, utilization of excess heat, or flexibility - are most relevant depends on the operator's objectives.

5. Conclusion

The optimal utilization of excess heat for district heating in a chipboard production process was analyzed. An increase of the district heating feed-in capacity is considered, which reduces excess heat and simultaneously increases the companies' profit. Also, different design adaptations are considered, including two thermal energy storages and the activation of an existing heat exchanger. The optimization of the process with and without modifications was conducted with a modular optimization framework, which modular structure allows for straight-forward design adaptations. The outcomes show that the process's efficiency can be significantly improved by applying operational optimization and considering the process adaptations. The results of the optimization yield three important outcomes:

1. The maximal feed-in quantity for district heating is far higher (between 2.6 and 2.9 times) than the currently contracted feed-in quantity. If district heating contracts are renegotiated accordingly, this would lead to additional earnings between 91,408–108,711 € per month.
2. Thermal energy losses can be reduced by 76 %–87 % in the different scenarios by increasing the district heating feed-in quantities. In the scenarios with thermal energy storages, also the primary energy consumption can be slightly reduced.
3. All scenarios with design adaptations result in higher profits than the reference process. However, the Ruth's steam storage has the highest amortization time of 5 years, followed by the buffer storage (1 year) and the activation of the heat exchanger with zero investment costs.

Although the activation of the heat exchanger yields the best results in terms of profit, further considerations are required to decide which modification is best suited. First, the economic analysis only includes fuel costs, investment costs, and earnings for selling heat for district heating and electricity to the grid. However, also other cost factors like maintenance costs or personnel costs are important aspects. Second, the assessment of the scenarios should not only depend on profit and energy consumption but also on flexibility. In fact, the considered thermal energy storages can yield additional benefits in the real application. They can increase the process's flexibility and can provide improved security by retaining heat as a buffer. Thus, the decision, whether and which modifications are implemented also depends on the operators' objectives.

CRediT author statement

Verena Halmschlager: Conceptualization, Methodology, Validation, Investigation, Formal analysis, Writing - Original Draft, Visualization, Fel**ix Birkelbach:** Conceptualization, Formal analysis, Writing - Review & Editing, R**ené Hofmann:** Conceptualization, Writing - Review & Editing, Supervision, Project administration, Funding acquisition.

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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References

[1] IEA, Digitalization and energy – technology report, URL, https://www.iea.org/reports/digitalisation-and-energy, 2017.
[2] Y. Xu, C. Yan, H. Liu, J. Wang, Z. Yang, Y. Jiang, Smart energy systems: a critical review on design and operation optimization, Sustainable Cities and Society 62 (2020) 102369. URL, http://www.sciencedirect.com/science/article/pii/S2210670720305916.
[3] H. Jouhara, N. Khordehgah, S. Almahmoud, B. Delpech, A. Chauhan, S.A. Tassou, Waste heat recovery technologies and applications, Thermal Science and Engineering Progress 6 (2018) 268–289.
[4] G. Alva, Y. Lin, G. Fang, An overview of thermal energy storage systems, Energy 144 (2018) 341–378. URL, http://www.sciencedirect.com/science/article/pii/S036054421732056X.
[5] P. Favre-Perrod, A vision of future energy networks, in: Proceedings of the Inaugural IEEE PES 2005 Conference and Exposition in Africa, IEEE Service Center, Piscataway, NJ, 2005, pp. 13–17.
[6] M. Majidi, B. Mohammadi-ivatloo, A. Anvari-Moghaddam, Optimal robust operation of combined heat and power systems with demand response programs, Appl. Therm. Eng. 149 (2019) 1359–1369.
[7] M. Vahid-Ghavidel, M.S. Javadi, M. Gough, S.F. Santos, M. Shafie-khah, J.P. Catalão, Demand response programs in multi-energy systems: a review, Energies 13 (17) (2020) 4332.
[8] M. Mohammadi, Y. Noorollahi, B. Mohammadi-ivatloo, M. Hosseinzadeh, H. Yousefi, S.T. Khorasani, Optimal management of energy hubs and smart energy hubs – a review, Renew. Sustain. Energy Rev. 89 (2018) 33–50.
[9] H. Sadeghi, M. Rashidinejad, M. Moeini-Aghtaie, A. Abdollahi, The energy hub: an extensive survey on the state-of-the-art, Appl. Therm. Eng. 161 (2019) 114071.
[10] M. Nazari-Heris, B. Mohammadi-ivatloo, S. Asadi, Optimal operation of multi-carrier energy networks with gas, power, heating, and water energy sources considering different energy storage technologies, Journal of Energy Storage 31 (2020) 101574.
[11] K. Karner, R. McKenna, M. Klobasa, T. Kienberger, Industrial excess heat recovery in industry-city networks: a technical, environmental and economic assessment of heat flexibility, J. Clean. Prod. 193 (2018) 771–783.
[12] F. Bühler, S. Petrović, K. Karlsson, B. Elmegaard, Industrial excess heat for district heating in Denmark, Appl. Energy 205 (2017) 991–1001.
[13] S.J. Cooper, G.P. Hammond, J.B. Norman, Potential for use of heat rejected from industry in district heating networks, gb perspective, J. Energy Inst. 89 (1) (2016) 57–69. URL, http://www.sciencedirect.com/science/article/pii/S1743967114203588.
[14] B. McDaniel, D. Kosanovic, Modeling of combined heat and power plant performance with seasonal thermal energy storage, Journal of Energy Storage 7 (2016) 13–23. URL, http://www.sciencedirect.com/science/article/pii/S2352152X1630055X.
[15] C. Lingmin, W. Jiekang, W. Fan, T. Huiling, L. Changjie, X. Yan, Energy flow optimization method for multi-energy system oriented to combined cooling, heating and power, Energy 211 (2020) 118536. URL, http://www.sciencedirect.com/science/article/pii/S0360544220316443.
[16] V. Halmschlager, R. Hofmann, Assessing the Potential of Combined Production and Energy Management in Industrial Energy Hubs – Analysis of a Chipboard Production Plant, Manuscript submitted for publication, 2020.
[17] V. Halmschlager, R. Hofmann, Holistic approach for the optimization of industrial hybrid energy hubs with milp, in: first ed.Of Part C. Elsevier, 30th European Symposium on Computer Aided Chemical Engineering, vol. 130, 2020.
[18] M. Geidl, G. Koeppel, P. Favre-Perrod, B. Klöckl, G. Andersson, K. Fröhlich, The Energy Hub: A Powerful Concept for Future Energy Systems, Electrical & Computer Engineering, 2007.
[19] G.W. Chang, Y.D. Tsai, C.Y. Lai, J.S. Chung (Eds.), A Practical Mixed Integer Linear Programming Based Approach for Unit Commitment, IEEE Power Engineering Society General Meeting, 2004.
[20] W.-D. Steinmann, M. Eck, Buffer storage for direct steam generation, Sol. Energy 80 (10) (2006) 1277–1282.
[21] E. González-Roubaud, D. Pérez-Osorio, C. Prieto, Review of commercial thermal energy storage in concentrated solar power plants: steam vs. molten salts, Renew. Sustain. Energy Rev. 80 (2017) 133–148.
[22] R. Hofmann, S. Dusek, S. Gruber, G. Drexler-Schmid, Design optimization of a hybrid steam-pcm thermal energy storage for industrial applications, Energies 12 (5) (2019) 898.
[23] B. Glück, Dampfgefaellespeicher: berechnungsverfahren "dampfgefaellespeicher (ruthsspeicher), URL, http://berndglueck.de/waermespeicher.php, 2012.
[24] Hansegger, Pufferspeicher, URL, www.hansegger.at, 2020, http://www.hansegger.at/120122768.

Paper 4

Grey Box Modeling of a Packed-Bed Regenerator Using Recurrent Neural Networks

Oral presentation at NOLCOS Conference 2019 and published by IFAC PapersOnLine in collaboration with Martin Koller, Felix Birkelbach and René Hofmann

In this paper, the NN grey-box modeling approach of the packed-bed regenerator was firstly published. The NN model in this publications is based on results of an existing validated white-box model of the use-case. The basic principles of the developed NN model, its structure, the NN network architecture and training are described, and the results are analyzed. Using a suitable NN model and accounting for the physics of the packed-bed regenerator by restructuring variables and including state variables, the NN model yields accurate predictions. This paper can therefore be seen as a proof of concept for the developed NN grey-box modeling approach.

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

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Grey Box Modeling of a Packed-Bed Regenerator Using Recurrent Neural Networks

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Abstract: A data-driven modeling approach for a pilot scale Packed-Bed Regenerator is examined and insights are generalized. Training data is generated with a one dimensional physical simulation model, which covers a wide variety of operation conditions including full load and partial load behavior. The NARX Recurrent Neural Network architecture is used to create a model that is able to describe the complex behavior of the regenerator. A grey box modeling approach is proposed that utilizes feedback state variables and incorporates knowledge about the internal behavior of the device. Using this approach, the behavior of the Packed-Bed Regenerator can be described accurately with multi-step ahead predictions. This work presents a first step towards data-driven modeling of dynamic processes in industrial applications. In addition to the presentation of important modeling key points for the proposed grey box model, important steps regarding data preprocessing are identified and insights in the applicability of different Neural Network architectures are discussed.

Keywords: Data-driven Modeling, Grey Box Modeling, Neural Networks, Thermal Energy Storage, Non-Linear Dynamic Systems

1. INTRODUCTION

Over the last decades, the collection and processing of large quantities of data, known as *data mining*, has gained in significance and found application in a variety of sectors, including industry. In today's advanced industrial processes, large amounts of data are analysed in order to obtain insights that can be used to improve the performance of a process. The increased availability of data also expanded the possibilities for data-based modeling techniques, e.g. Machine Learning or Neural Networks (Nisbet et al., 2009, pp.15-32). Models created with these techniques are most often referred to as black-box models that are based solely on data and do not consider any physical characteristics of a system. Black box models hide their internal logic, which makes the interpretation of these models difficult or even impossible (Benitez et al., 1997, p.1156). The opposite approach are white box models that are solely built on deterministic equations and physical knowledge. They are transparent and often based on relations for heat transfer and flow dynamics in case of thermal systems. Their creation requires detailed knowledge of the process and is often a challenging task (p.523 Prada et al., 2018; Solomatine et al., 2008, pp.17-27).

In between these two contrary approaches, the grey box models are placed. Grey box models are constructed based on both physical knowledge and data, using the advantages of both white and black box models. They have been gaining in importance in industrial processes, due to their low modeling effort and their improved transparency compared to pure data-driven models (Herceg et al., 2017, p.1361). A discussion of grey box models in dynamic systems can be found in (Prada et al., 2018; Cen et al., 2011; Oussar and Dreyfus, 2001). Different definitions and classifications for grey box models exist, depending on the amount and type of additional information and the way the physical knowledge is taken into account. In this work, no explicit physical equations are implemented in the model but physical knowledge is used to choose suitable variables and the structure of the model. In this way, relations that would need to be described by complex equations can be approximated. This type of model can be classified as a semi-physical model, according to (Sohlberg and Jacobsen, 2008, p.11416). Semi-physical models are grey box models that use physical insights to transform input and output to new variables, in cases where physical modeling is challenging and the results of pure black box models are poor.

As a use case, a pilot scale Packed-Bed Regenerator (PBR) is modeled. The PBR is a cost-efficient sensible thermal energy storage system that presents a promising option to efficiently store excess heat. They are used for industrial scale, high temperature, short cycle storage applications (Michalka, 2018, pp.20-37). To create a data-driven model of the PBR, training data was generated by a 1D physical simulation model. This way, the required data can be generated conveniently for a great number of cycles, different operating conditions and full and partial load behavior.

The aim of the data-driven model is the prediction of the outlet temperature of the PBR for a defined number

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of timesteps. This task is commonly known as "time series prediction" or "time series forecasting". For these kind of modeling tasks, Neural Networks (NN), or more specifically, Recurrent Neural Networks (RNN) have been successfully applied in numerous works and were chosen for this investigation. An overview of advances in time series forecasting with Neural Networks can be found in (Tealab, 2018). In general, NNs are a technique used in Machine Learning. They can be trained in order to solve complex problems. Recurrent Neural Networks represent a special case of NNs that can "memorize" parts of the inputs and/or outputs by using feedback connections that loop back layers of the network (Nelles, 2001, pp.645-650). This way, RNNs can account for the time dependent behavior of the PBR. As the focus of this work lies on the presented grey box modeling approach rather than on the creation of a NN, predefined RNNs from MATLAB R2018b are utilized for the creation of the model.

Following the introduction in Section 1, Section 2 describes the Packed-Bed Regenerator. In Section 3, the generation of training data with the physical 1D simulation model is discussed. Section 4 deals with the proposed grey box modeling approach for the PBR and its distinction to commonly used black box and white box models. Here, also the parameters of the model, namely input, output and state variables, are presented and their adaptation is discussed. In Section 5, the network architecture and its training procedure is stated. For the evaluation in Section 6, the performance of different models as well as important modeling key points are described. Additionally, advantages and limitations of the NN grey box model are presented. Finally in the conclusion in Section 7, the most important outcomes are highlighted and possible future research topics are discussed.

2. USE CASE: PACKED-BED REGENERATOR

A pilot scale PBR test rig (see Fig. 1) is chosen as a use case to analyse the applicability of the proposed data-driven modeling approach. It is located in the laboratory of the Institute for Energy Systems and Thermodynamics (IET) at TU Wien. The PBR has a conic steel casing surrounded by an insulation, is filled with gravel as storage medium (SM) and uses ambient air as heat transfer fluid (HTF). The HTF can heat the ambient air up to 330 °C. During the charging process, the HTF flows from top to bottom and the heat is absorbed by the SM. During discharging, the flow direction is switched and the HTF enters at bottom with ambient temperature, flows to top and absorbs heat from the SM. In the test rig, temperature is measured at the inlet, outlet and at four locations along the vertical axis within the storage (T_1 – T_4). In Figure 2, the PBR is illustrated and the internal temperature sensors are indicated. A detailed description of the PBR can be found in (Michalka, 2018).

3. TRAINING DATA GENERATION

To build a data-driven model of the PBR, data that represents the complex dynamic full and partial load operating behavior of the PBR is required. For this task, a validated 1D simulation model was employed (Koller and Hofmann, 2018, p.926). The 1D model uses physical

Fig. 1. Picture of the insulated test rig

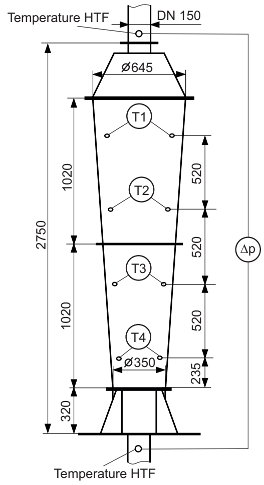

Fig. 2. Sketch of the regenerator (Michalka, 2018)

properties as model parameters and consists of three components: the SM (gravel), the HTF (air) and the steel casing. All components are modeled as 1D elements. Figure 3 shows a comparison of the real storage and the physical 1D modeling approach. The heat transport is modeled along the vertical axis for each component and between the components within each 1D element. The correlations for the heat exchange between SM and HTF, thermal conductivity along the 1D-axis for SM and HTF, and heat transfer between SM and casing are taken from (VDI, 2013).

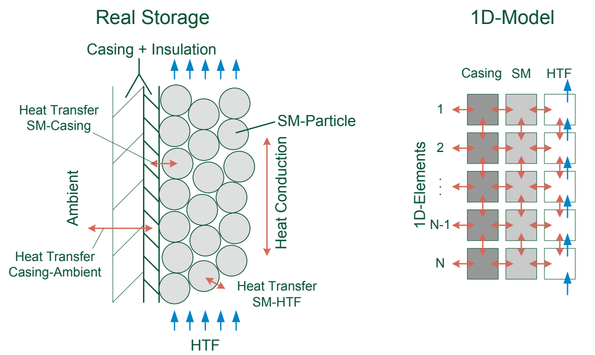

Fig. 3. Scheme of the real storage and the 1D model from (Koller and Hofmann, 2018, Fig.2)

The simulated training data consists of the HTF temperatures at the bottom and the top of the reactor T_b and T_t, the mass flow of the HTF $\dot{m}$, the temperatures at the four measuring points within the storage (T_1–T_4) and the fill level, which is defined as the total thermal energy of the storage. The data covers a total simulation time of 1000 h (120.000 time steps). Charging and discharging processes are alternated and the cycle duration and mass flow for each cycle were varied randomly within the operating range. The inlet temperature of the HTF is always 325 °C during charging and 22 °C during discharging. For training, the data was prepared to be zero-mean and split into training (70%), validation (15%) and test data (15%).

4. GREY BOX MODELING APPROACH

In many industrial applications, only little information about the physical behavior of already existing devices is available. This can impede the creation of detailed white box models. In these cases, data-driven modeling approaches provide a promising alternative (Herceg et al., 2017, p.1361). To minimize computational as well as modeling effort, the data-driven models should be as complex as necessary and as simple as possible. Thus, the number of variables and parameters should be kept as low as possible. In a pure black box model, solely ingoing and outgoing data is used to build a model of the system. No additional information is taken into account. Hence, a simple black box model of the PBR would use mass flow and inlet temperature as inputs and the outlet temperature as an output. However using only this information, the resulting model is not able to predict the complex non-linear behavior of the PBR, since the output of the PBR model does not only depend on the input but also on its current state. Thus, it is essential to chose an appropriate model structure and incorporate additional information. In the proposed grey box model, the additional information is based on known physical relations and incorporated by

(1) including feedback state variables and

(2) restructuring in/output variables.

In contrast to the white box physical 1D model of the PBR, the grey box model does not require relations for internal processes such as heat transfer or flow dynamics. The neural network is trained to "learn" these relations from the training data with the right choice of model structure, variables and characteristic values. Thus, this approach is well suited for industrial processes, where plenty of data as well as basic physical information about the process are available but where the development of a white box model would be a challenging task. The structure of the grey box model for the PBR and its distinction to the black box model are depicted in Figure 4.

In general, a state variable is a quantity that describes the current state of a dynamic system. To make use of state variables in data-driven modeling approaches, it is necessary that they can be either measured or calculated. The state variables are implemented as feedback variables and can be utilized to train the network with additional information in the training. Once the network training is completed, only one starting value for each state variable and the input data is needed to conduct multi-step ahead predictions. The state variables are calculated iteratively. In contrast to the input variables, the state variables do not need to be known during operation, but only during the training. With this approach, additional information about the physics of the device can be included in the model conveniently. Another feature of the state variables is, that they are physical properties of the system that can help to interpret the output of the model.

Regardless, the number of state variables should always be minimized, as the incorporation of state variables increases the complexity of a model. Only state variables that significantly improve the performance of the model should be included.

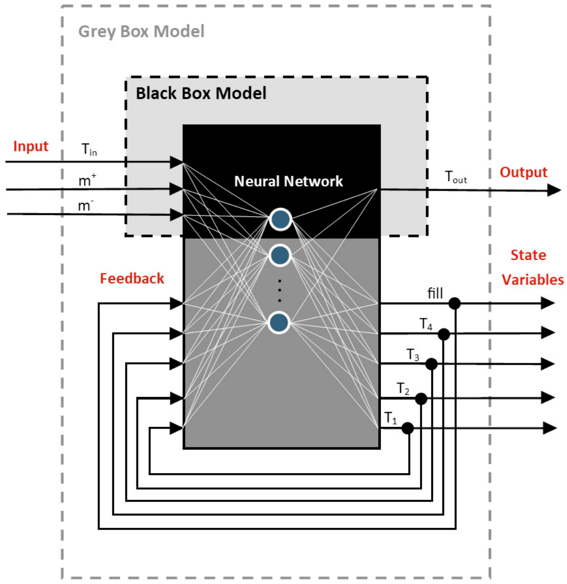

Fig. 4. Grey box vs. black box modeling approach for the model of the PBR

As state variables in the PBR model, the temperatures (T_1–T_4) inside the reactor (see Fig. 3) and the fill level of the regenerator are considered. The state variables (T_1–T_4) capture the effect of the temperature front that develops during charging and discharging inside the reactor. The fill level represents another important characteristic of the PBR: It describes the energy that is stored in the PBR.

Another feature of the approach is the adaptation of input variables to account for a change in physics. Separate input variables should be used for each operation mode, so that the model can recognize the variation more clearly. In the grey box model, the mass flow is separated in a positive and negative component to account for the change of the flow direction when switching between charging and discharging, according to

$$\dot{\mathrm{m}}^+ = \begin{cases} \dot{\mathrm{m}} & \text{charge} \\ 0 & \text{discharge} \end{cases} \tag{1}$$

$$\dot{\mathrm{m}}^- = \begin{cases} 0 & \text{charge} \\ \dot{\mathrm{m}} & \text{discharge.} \end{cases} \tag{2}$$

Similarly to the mass flow, the input and output temperatures of the model are modified to account for the switched flow direction during charging and discharging. The input and output temperatures T_{in} and T_{out} are set either to the bottom (T_b) or top temperature (T_t) of the PBR, depending on the flow direction, given by

$$\mathrm{T_{in}} = \begin{cases} \mathrm{T_t} & \text{charge} \\ \mathrm{T_b} & \text{discharge} \end{cases} \tag{3}$$

$$\mathrm{T_{out}} = \begin{cases} \mathrm{T_b} & \text{charge} \\ \mathrm{T_t} & \text{discharge.} \end{cases} \tag{4}$$

5. NETWORK ARCHITECTURE AND TRAINING

For the grey box model of the PBR, the nonlinear autoregressive NN architecture with exogenous inputs (NARX) is chosen. NARX is a recurrent dynamic network architecture that can enclose every layer of the network by a feedback connection. In this way, it is possible to feed back the input as well as the output variables. The feeback connection can be an interval of several timesteps or only one, as in the proposed model. The number of feedback timesteps is characterized by a hyperparameter called delay. A delay of 0 stands for no feedback, delay 1 means that only one timestep is fed back. In the default NARX architecture, either all variables of an output layer are fed back or non of them. Thus, to implement our network architecture in MATLAB, an additional output layer was added to the default NARX network. The resulting network architecture can be seen in Figure 5.

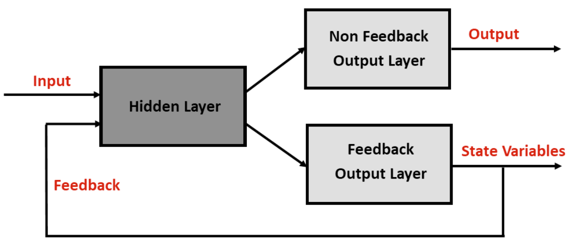

Fig. 5. Network architecture of the NARX NN for the PBR

For the creation of the NARX network, two training methods can be used: open loop and closed loop training. To build an accurate model for multi-step ahead predictions, a closed loop training of the network is required. However in contrast to open loop, the closed loop training only converges if the starting values are already sufficiently close to optimum. To solve this issue, a two-stage training of the network was conducted. First, the network is trained open loop to obtain good starting values. Then, the network is trained again in closed loop with identical hyperparameters.

To find the best settings for the training, the following hyperparameters of the NN were adjusted: Number of neurons, number of hidden layers, training function, number of input and feedback delays and transfer function. As data-driven models are not completely transparent, there is no universally applicable rule to choose the right hyperparameters - however rules of thumb exist. Commonly, rather simple models with few variables, hidden layers and neurons are recommended. Also in our model, we achieved good results with few neurons (approx. 10), one hidden layer and a delay of one timestep for the feedback variables. A large number of neurons (more than 20-30) and/or more than one hidden layer led to overfitting and an overestimation of small deviations. Consequently, a NARX network with 1 hidden layer, 10 neurons and 1 output delay for the state variables is chosen for the evaluations in the next section.

6. EVALUATION

With the grey box modeling approach, it is possible to create Neural Network models that can describe the behavior of the PBR. The following evaluation discusses the performance of models with different input, output and state variables as well as varying network characteristics. A summary of the considered models can be found in Table 1. In this way, features of the grey box model can be illustrated and the most important key points for modeling are highlighted. As a measure for the performance of the different models, the mean squared error (MSE) between the simulated data and the closed loop prediction of the test data set is calculated. In all figures, *Data* stands for the simulated data and *Prediction* for the closed loop prediction. The results are displayed for a representative time interval of several hours.

First, the performance of three simplified models is evaluated. *Model X* is a simple black box model with $\dot{\mathrm{m}}$ and $\mathrm{T_{in}}$ as inputs and $\mathrm{T_{out}}$ as an output. *Model Y* features split mass flows $\dot{\mathrm{m}}^{+}$ and $\dot{\mathrm{m}}^{-}$, while *Model Z* includes all state variables but only one variable for the mass flow. A summary of the three simplified models can be found in Table 1. All models exhibit very poor performances with a MSE around 0.4 and fail to follow the trend of the data. This is exemplified by *Model Z* in Figure 6.

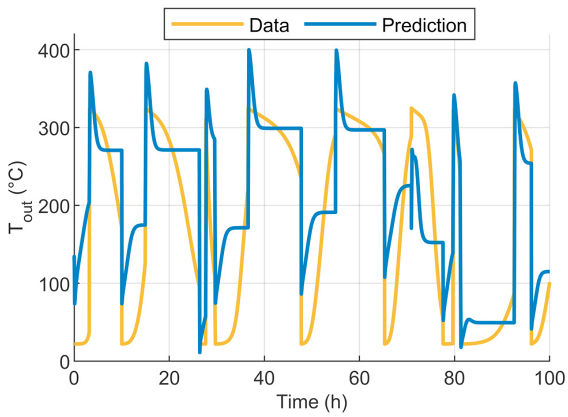

Fig. 6. Prediction of $\mathrm{T_{out}}$ by *Model Z*

The three simplified models demonstrated that additional information about the device is required in order to achieve good results. This information is incorporated in the grey box model by including state variables and by adapting input and output variables.

However, as the model should be as simple as possible, it is important to determine, which state variables are actually essential to improve the performance of the model and which can be omitted. For this reason, two models that incorporate different state variables are compared with each other. In *Model A*, all suggested state variables (T_1–T_4, fill level) are included. *Model B* only utilizes the fill level.

Although both models *A* and *B* result in a good closed loop performance (MSE of 0.011 for *Model A*, MSE of 0.0039 for *Model B*), differences can be identified visually. Figure 7 and 8 show the predicted outlet temperature by *Model*

Table 1. Overview of the different models

Model	Input	Output	State Variables	MSE	Suitable	Description
X	T_{in}, $\dot{m}$	T_{out}	none	0.43	✗	Simpl. model: Pure black box
Y	T_{in}, $\dot{m}^+$, $\dot{m}^-$	T_{out}	none	0.43	✗	Simpl. model: Black box, split mass flow
Z	T_{in}, $\dot{m}$	T_{out}	fill level, (T_1–T_4)	0.55	✗	Simpl. model: Including state variables
A	T_{in}, $\dot{m}^+$, $\dot{m}^-$	T_{out}	fill level, (T_1–T_4)	0.011	✓	Prediction is oscillating slightly
B	T_{in}, $\dot{m}^+$, $\dot{m}^-$	T_{out}	fill level	0.0039	✓	Best model reg. MSE and simplicity

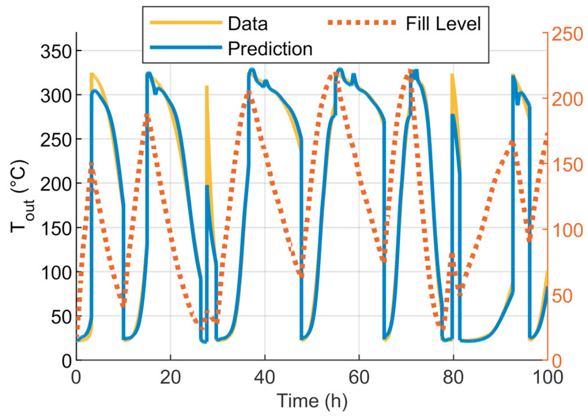

Fig. 7. Prediction of T_{out} by *Model A*

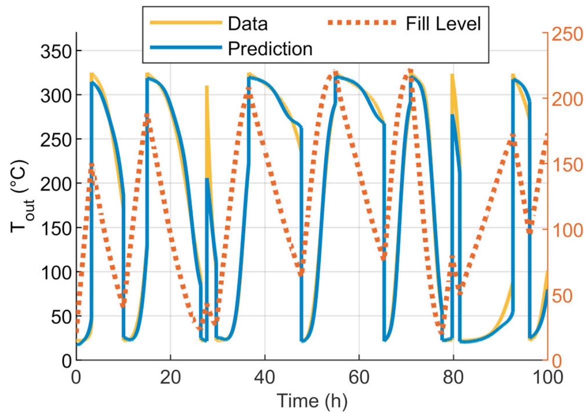

Fig. 8. Prediction of T_{out} by *Model B*

A and *Model B* and the fill level of the PBR. In *Model A*, oscillations in regions of high outlet temperatures, just after switching from charging to discharging, can be seen. A detailed observation of the state variables (T_1–T_4) (see Fig. 9) reveals, that also the temperature state variables oscillate in these regions. Additionally, it can be seen that the temperature state variables exhibit high gradients when switching between charging and discharging. Apparently, some time is necessary before a steady temperature front develops after changing the flow direction of the PBR. The oscillations seem to be a result of these high temperature gradients, which impede an accurate prediction when switching between charging and discharging.

In contrast, *Model B* is able to predict the outlet temperature more accurately in these regions and results in an improved overall performance. However, also *Model B* reveals inaccuracies in some areas, especially when predicting the temperature drop while discharging. Figure 10 shows a comparison of the prediction from *Model* A and *B* for a small interval to illustrate their inaccuracies. Although both models show inaccuracies in some parts of the prediction, it is remarkable that the multi-cycle performance is not affected by this issue. In a prediction over more than 12000 timesteps, no drift can be noticed. *Model A* as well as *Model B* can account for the change of flow direction correctly and manage to stabilize after few iterations.

Even though the comparison of *Model A* and *B* showed, that the additional use of temperature state variables in *Model A* does not lead to better performances, this approach could still yield benefits in even more complex modeling tasks. In case of the PBR, this may become relevant if the model was extended by operation modes with varying input temperatures or different storage materials.

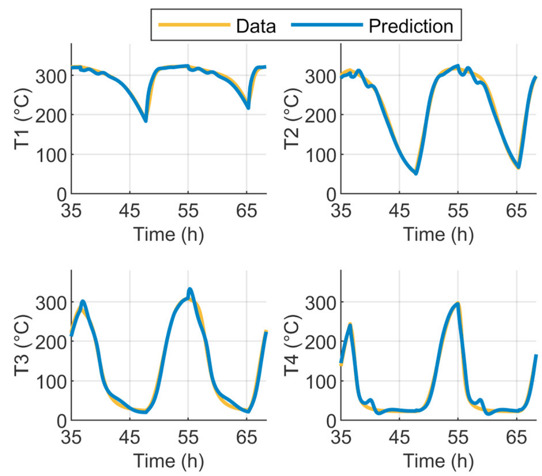

Fig. 9. Prediction of T_1–T_4 by *Model A*

Finally, it is important to keep in mind that this data-driven modeling approach is only valid for the operating conditions and the data limits of the data that it was trained with. Changing the input temperature or mass flow to values that outreach the range of the training data would not lead to meaningful results at all. Although the grey box model yields higher transparency and improved interpretability of the results compared to pure black box models, it still shows some peculiarities of these input-output models. For example, small changes of hyperparameters or input variables sometimes led to variations that could not be explained in a meaningful way.

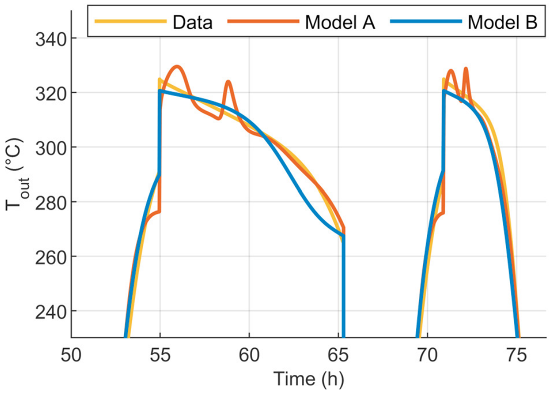

Fig. 10. Prediction of T_{out} by *Model A* and *Model B*

Nevertheless, in the case of strictly prescribed operation conditions that often characterize industrial processes, the grey box model is a promising modeling approach due to its low modeling effort, once all the data is gathered. Not only the modeling but also the computational effort of the grey box model is significantly lower compared to e.g. the white box 1D model. Whereas the calculation of the simulation data lasted for several hours with the 1D model, the Neural Network can predict the outlet temperature within seconds with sufficient accuracy.

7. CONCLUSION

The investigation showed that the proposed grey box modeling approach is well suited to predict the behavior of the Packed-Bed Regenerator. The performance of the grey box model was evaluated and the advantages and limitation were discussed. For the Packed-Bed Regenerator, three important modeling key points can be summarized:

(1) Include state variables: Use fill level (and optionally internal temperatures) as feedback variables
(2) Restructure variables to account for a change in physics: Use separate input variables for each operation mode "charging" and "discharging" and split input and output variables according to the flow direction
(3) Keep it simple: Reduce number of neurons and feedback variables as far as possible

These key points were essential in order to achieve accurate predictions with the model of the Packed-Bed Regenerator and should also yield major benefits in similar modeling tasks. For devices with prescribed operation conditions e.g. in industrial applications, a Neural Network grey box model is a convenient alternative to complex and elaborate physical models, offering the advantage of increased transparency and improved interpretability compared to pure black box models.

To examine the applicability of the proposed approach in real processes, future work will analyze the application of this method based on experimental data from the Packed-Bed Regenerator test rig at TU Wien.

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REFERENCES

Benitez, J.M., Castro, J.L., and Requena, I. (1997). Are artificial neural networks black boxes? *IEEE transactions on neural networks*, 8(5), 1156–1164. doi:10.1109/72.623216.

Cen, Z., Wei, J., and Jiang, R. (2011). A grey-box neural network based identification model for nonlinear dynamic systems. In *Fourth International Workshop on Advanced Computational Intelligence, 2011*, 300–307. IEEE. doi:10.1109/IWACI.2011.6160021.

Herceg, D., Georgoulas, G., Sopasakis, P., Castano, M., Patrinos, P., Bemporad, A., Niemi, J., and Nikolakopoulos, G. (2017). Data-driven modelling, learning and stochastic predictive control for the steel industry. In *2017 25th Mediterranean Conference on Control and Automation (MED)*, 1361–1366. IEEE. doi:10.1109/MED.2017.7984308.

Koller, M. and Hofmann, R. (2018). Mixed integer linear programming formulation for sensible thermal energy storages. In *28th European Symposium on Computer Aided Process Engineering*, volume 43, 925–930. Elsevier. doi:10.1016/B978-0-444-64235-6.50163-7.

Michalka, A. (2018). *Experimentelle Untersuchungen eines Festbettregenerators mit feinem Kies als Speichermaterial*. Ph.D. thesis, Technicacl University of Vienna.

Nelles, O. (2001). *Nonlinear system identification: From classical approaches to neural networks and fuzzy models*. Engineering online library. Springer, Berlin.

Nisbet, R., Elder, J.F., and Miner, G. (eds.) (2009). *Handbook of statistical analysis and data mining applications*. Academic Press/Elsevier, Amsterdam and Boston.

Oussar, Y. and Dreyfus, G. (2001). How to be a gray box: Dynamic semi-physical modeling. *Neural networks*, 14(9), 1161–1172.

Prada, C., Hose, D., Gutierrez, G., and Pitarch, J.L. (2018). Developing grey-box dynamic process models. *IFAC-PapersOnLine*, 51(2), 523–528. doi:10.1016/j.ifacol.2018.03.088.

Sohlberg, B. and Jacobsen, E.W. (2008). Grey box modelling – branches and experiences. *IFAC Proceedings Volumes*, 41(2), 11415–11420. doi:10.3182/20080706-5-KR-1001.01934.

Solomatine, D., See, L.M., and Abrahart, R.J. (2008). Data-driven modelling: Concepts, approaches and experiences. In *Practical Hydroinformatics*, volume 68 of *Water Science and Technology Library, 68*, 17–30. Springer-Verlag, s.l. doi:10.1007/978-3-540-79881-1_2.

Tealab, A. (2018). Time series forecasting using artificial neural networks methodologies: A systematic review. *Future Computing and Informatics Journal*, 3(2), 334–340. doi:10.1016/j.fcij.2018.10.003.

VDI (2013). *VDI-Wärmeatlas*. Springer Vieweg, Berlin, Heidelberg. doi:10.1007/978-3-642-19981-3.

Paper 5

Mechanistic Grey-Box Modeling of a Packed-Bed Regenerator for Industrial Applications

Published in Energies in collaboration with Stefan Müllner and René Hofmann

In this paper, the mechanistic grey-box model of the packed-bed regenerator is presented. The use-case and all relevant physical equations of the model are described, as well as the parameters that were fitted by data with optimization methods. Three models with different numbers of equations and parameters are presented and compared with the created NN model and with the existing white-box model. Especially the mechanistic grey-box model with the highest number of equations (5) and parameters (6) shows excellent accuracy and stands out by its robustness and reliability compared to the NN model.

My contribution: Conceptualization, Validation, Visualization, Investigation, Formal Analysis, Writing – Original Draft, Writing – Review & Editing, Supervision

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Article

Mechanistic Grey-Box Modeling of a Packed-Bed Regenerator for Industrial Applications

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Abstract: Thermal energy storage is essential to compensate for energy peaks and troughs of renewable energy sources. However, to implement this storage in new or existing industries, robust and accurate component models are required. This work examines the development of a mechanistic grey-box model for a sensible thermal energy storage, a packed-bed regenerator. The mechanistic grey-box model consists of physical relations/equations and uses experimental data to optimize specific parameters of these equations. Using this approach, a basic model and two models with extensions I and II, which vary in their number from Equations (3) to (5) and parameters (3 to 6) to be fitted, are proposed. The three models' results are analyzed and compared to existing models of the regenerator, a data-driven and a purely physical model. The results show that all developed grey-box models can extrapolate and approximate the physical behavior of the regenerator well. In particular, the extended model II shows excellent performance. While the existing data-driven model lacks robustness and the purely physical model lacks accuracy, the hybrid grey-box models do not show significant disadvantages. Compared to the data-driven and physical model, the grey-box models especially stands out due to their high accuracy, low computational effort, and high robustness.

Keywords: grey-box modeling; physical modeling; data-driven modeling; packed-bed regenerator; sensible thermal energy storage

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1. Introduction

Reaching future climate goals is a major issue in today's society. Key elements of the transition towards more sustainable energy systems are the pervasive application of renewable energies and reduction of total energy consumption. For example, the worldwide electricity demand has increased by almost 75% from 2000 to 2018, whereas the share of renewable energies was still around 28% in 2018 [1]. However, renewable energy sources such as wind or solar energy can show high fluctuations due to their dependence on the weather. To compensate for these energy peaks and troughs efficiently, thermal energy storage is required [2]. Thermal energy storage can match intermittent heat supply with demand, leading to better use of excess heat, which is still one of today's key challenges in the industrial sector [3]. Especially the combination of innovative storage technologies with energy optimization/management tools can significantly increase process' efficiency. Nevertheless, for integrating thermal energy storage in new or existing processes and their use in optimization tools, reliable and accurate component models for behavior prediction are required.

Typically, modeling of physical systems is separated into two distinct approaches: white-box and black-box modeling. In white-box modeling—also called physical or first principle modeling—a model of a system is based on deterministic equations using in-depth physical knowledge. These models are usually robust, but their modeling and computational effort can be high [4]. In contrast, black-box models—also called data-driven or empirical models—are based on data. Traditional data-driven modeling approaches include ARIMA (autoregressive integrated moving average) models and regression models [5].

However, with the advances in data-driven modeling techniques, Machine Learning (ML) methods have seen increased hype in recent years. These models can independently improve through experience and are able to capture complex patterns. In contrast to physical models, data-driven models—especially using ML techniques—can lack robustness due to their non-transparent structure. Though, modeling and computational effort can be decreased compared to physical models. [6]

In between these two distinct approaches of white- and black-box modeling, grey-box models are located. Grey-box models can be seen as a mixture of physical and data-driven modeling, using physical considerations/equations *and* data. Thus, grey-box models can benefit from both modeling approaches, being robustness and low modeling and computational effort. [7]

According to Sohlberg and Jacobsen [8], grey-box models can be divided into five categories. Although most studies in the literature do not explicitly identify with one of these five categories, they still give a good overview of grey-box modeling methods:

- **Constrained black-box modeling:** In constrained black-box modeling, constraints based on prior knowledge–e.g., limits on a model's output or static gain–are added to a black-box model. E.g., non-linear polynomial models were constrained by steady-state information in a three-step approach in Aguirre et al. [9].
- **Mechanistic modeling:** Mechanistic modeling, also called parameterized physical modeling [10], uses physical equations based on prior knowledge and optimizes parameters based on data. A systematic approach for mechanistic grey-box models was proposed in Sohlberg [11].
- **Semi-physical modeling:** Semi-physical modeling uses prior knowledge to transform a non-linear optimization task into a linear optimization task.
- **Hybrid modeling:** Hybrid modeling combines white- and/or grey- and/or black-box models. The combination can either be in series or parallel arrangement. E.g., in Thompson and Kramer [12], a model for a synthesizing chemical process is developed with a Neural Network as a black-box modeling part.
- **Distributed parameter modeling:** Distributed parameter modeling allows for model reduction based on moving finite elements and grey-box identification [13].

Focusing on grey-box modeling of dynamic systems in industrial applications, e.g., for thermal energy storage, the research in the literature is limited: First, Tulleken [14] determined a statistical estimation of the optimal linearly parametrized dynamic regression model, using physical knowledge and bayesian techniques. Oussar and Dreyfus [15] proposed a general methodology for mechanistic grey-box modeling and applied the approach to a dynamic industrial drying process. Cen et al. [7] investigated an identification scheme for non-linear dynamic systems using grey-box Neural Networks and applied them to a reaction wheel in a satellite attitude control system. de Prada et al. [4] identified a lack in the literature for the systematic development of dynamic grey-box models and proposed a two-step approach for developing grey-box models. Therein, physical relations were defined, and a mixed-integer-linear-programming optimization approach was used to identify suitable parameters and the remaining structure. This approach was applied to an acetone-butonal-ethanol fermentation process. Pitarch et al. [16] developed grey-box models of limited complexity for process systems, based on data reconciliation and polynomial constrained regression. As a use-case, the approach was applied to an industrial evaporation plant. Finally, in the authors' previous works [17,18], a sensible thermal energy storage, a packed-bed-regenerator (PBR), was modeled using Neural Networks and physical considerations. Although the Neural Network models showed good performance and high accuracy, their robustness/reliability was limited due to their mainly data-driven nature.

Regarding the modeling of packed-bed thermal energy storage such as the PBR in general, a good overview of different types and modeling approaches can be found in [19–21] analyzes the transient response of packed-bed thermal storage. Focusing on the modeling of packed-bed thermal energy storage with gaseous flow, continuous solid phase/Schumann models [22] have been widely used in the literature. These models use a uniform temperature between fluid and solid [23]. The continuous solid phase/Schumann models were used, for example, in Zanganeh et al. [24], where the sensible part of a combined sensible-latent high temperature energy storage is modeled numerically, considering separate fluid and solid phases with variable thermo-physical properties, thermal losses, and axial dispersion by conduction and radiation. Additionally, Hänchen et al. [25] used this approach and formulated the combined convection and conduction heat transfer of a high-temperature packed-bed energy storage for air-based concentrated solar power plants as a numerical model with 1D two-phase energy conservation equations. White et al. [26] investigated the thermal wave propagation in packed-bed thermal reservoirs with numerical and theoretical analysis, focusing on thermal losses due to irreversible heat transfer. Additionally, recently, König-Haagen et al. [27] modeled a packed-bed thermal energy storage in combination with an Organic Rankine Cycle using numerical modeling based on the Schumann model. Last, this modeling approach was also applied in Hoffmann et al. [28] and compared to a single-phase model. Moreover, the continuous solid phase/Schumann models, also dispersion concentric models have been applied to packed-bed thermal energy storage with gaseous flow, e.g., in Barton [29] for the storage of solar thermal energy. Furthermore, numerical modeling is used in Odenthal et al. [23] to model a horizontal packed-bed energy storage considering regularly shaped channels with gaseous flow with a one-dimensional dispersion concentric model. Finally, [30] developed a one spatial dimension transfer model of a packed-bed thermal energy storage for simulating the performance of a combined cycle concentrated solar power plant with storage.

In contrast to existing publications, this work investigates a mechanistic grey-box modeling approach to model the PBR, with the main research goal to develop an accurate and reliable model. Within this approach, physical information about the PBR is used to determine essential physical relation/equations, and measurement data are used to optimize physical, or physically inspired parameters of these equations. This way, a physically based model is built, while using far fewer equations than a traditional white-box model. Compared to the authors' previously published mainly data-driven and solely physical models of the PBR [17,18], the proposed mechanistic grey-box modeling approach is preliminary based on physical knowledge and uses data for refinement.

To the authors' best knowledge, a mechanistic grey-box modeling approach has not been applied yet to model sensible thermal energy storage systems such as the PBR. Thus, as the main research goal, this work presents a novel, robust and efficient modeling method for dynamic industrial systems and in-depth investigates the mechanistic grey-box modeling approach. Additionally, the presented grey-box model is a major addition to the authors' previous publication [18], where the PBR was modeled with a primarily data-driven modeling approach using Neural Networks and also with a purely physical modeling approach. The new mechanistic grey-box model can be seen as an in-between approach of the previously used methods, using advantages of both physical and data-driven modeling.

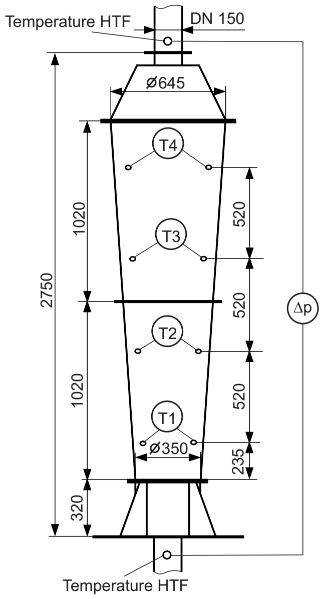
This work is organized as follows: In Section 2, the PBR and its experimental setup and operation characteristics are presented. In Section 3, the grey-box modeling approach is described, and governing equations and parameters are given. In Section 4, the results of the developed grey-box models are discussed. In Section 5, the grey-box models are compared qualitatively and quantitatively to the existing physical and data-driven model of the PBR. Finally, a conclusion and outlook is given in Section 6, followed by the Nomenclature and references.

2. Experimental Setup

As a use-case, a sensible thermal energy storage—a packed-bed regenerator (PBR)—is used. The semi-industrial scale PBR test rig is situated at the TU Wien laboratory and is depicted in Figure 1a and illustrated in Figure 1b. The main part of the PBR is the insulated conical vessel which is filled with the storage medium (SM) gravel. In this vessel, air as the heat transfer fluid (HTF) enters from the bottom and flows through the SM to the top. While charging, the HTF is heated up by an electric heater before it enters the vessel, and heat is transferred from the HTF to the SM. While discharging, cold HTF flows from the bottom to the top through the hot SM, and heat is transferred from the SM to the HTF.

For temperature measurements, the PBR is equipped with 18 temperature sensors: one at the HTF inlet and outlet (calibrated resistance temperature sensors) and four pieces of calibrated NiCr-Ni thermocouples located uniformly in each of the four horizontal layers of the vessel, according to Figure 1b. In addition, the mass flow of the HTF is measured at the inlet of the vessel with a mass flow sensor. Thus, relevant measurement data from the PBR include the HTF inlet temperature T_{in}, the HTF outlet temperature T_{out}, an average temperature for every horizontal layer of the vessel T1–T4, and the mass flow of the HTF $\dot{m}$. A more detailed description of the PBR test rig can be found in Michalka [31] and Hofmann et al. [18].

(**a**) Picture of the insulated PBR



(**b**) Illustration of the PBR

Figure 1. Visualization of the PBR test rig [18].

Measurement Series

In this work, experimental data from eight different measurement series of the PBR test rig are employed, which are displayed in Table 1. Each of the eight measurement series covers 3 or 4 charging/discharging cycles and includes varying HTF mass flows $\dot{m}$. The cycles are specified by a target inlet temperature T_{in} of the HTF for the operation modes charging and discharging. This target temperature is the desired HTF inlet temperature of the PBR to be reached by the electric heater. If the maximum (during charging) or minimal (during discharging) temperature T_{out} at the top of the PBR vessel is reached, the PBR switches from one operation mode to the other one.

Table 1. Measurement series of the PBR.

Series	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Number of Cycles	3	3	3	3	3	3	3	4
Mass Flow $\dot{m}$ in kg/h	150	150	126	150	175	200	250	146
Target Temp. Charging: T_{in} in °C	310	310	230	230	230	230	230	310
Target Temp. Discharging: T_{in} in °C	20	20	50	50	50	50	50	20
Max. Temp. Charging: T_{out} in °C	290	200	185	185	185	185	185	265
Min. Temp. Discharging: T_{out} in °C	200	150	80	80	80	80	80	50

3. Grey-Box Modeling Approach

The main aim of the developed grey-box model is the accurate and robust prediction of the HTF outlet temperature T_{out} of the PBR. Based on the detailed available physical knowledge and existing measurement data of the PBR test rig, a mechanistic modeling approach was chosen. In this mechanistic modeling approach, the PBR is described by physical (inspired) equations. Relevant parameters of these equations are fitted to the existing data by optimization techniques. These parameters can either be (a combination of) real physical properties, physically inspired, or empirically chosen to achieve a good fit of the model. This combination of physical and empirical modeling approaches leads to an iterative process in which essential governing equations are formulated, altered, and extended to yield an accurate and robust model.

Thus, in the first step, governing model equations are formulated, and optimization parameters are determined to create a basic model. To improve the fit of this basic model, the model is extended by additional equations and optimization parameters in the next step. In total, three different grey-box models, the basic model and two extended models, are presented and compared in this work.

3.1. General Model Features

The three developed mechanistic grey-box models of the PBR are all based on the same basic structure and use time series data of the mass flow $\dot{m}$ and inlet temperature of the HTF T_{in} to predict the outlet HTF temperature T_{out}. As a modeling basis, the vessel is vertically separated into n horizontal layers, and assumed cylindrical. Each layer of the vessel is modeled by a state-space model and the layers are connected in series to form the complete model of the PBR. This way, the calculation of the HTF temperature T_{out} is conducted for every time-step of a measurement series.

For each of the three developed grey-box models, the models of these layers are based on different assumptions and equations. Whereas the basic model only assumes heat transfer between the HTF and SM, and heat loss to the surrounding, the extended models include additional or more detailed correlations. The following list gives an overview of the three models' assumptions:

- **Basic Model:** Considering convective heat transfer between HTF and SM, and heat loss to the surrounding that is only dependent on the temperature of the SM of the current layer.
- **Extended Model I–Heat Loss Dependency:** Same as the basic model, including the dependency of the heat loss on the SM temperature of the previous time-steps.
- **Extended Model II–Inclusion of a Wall and Non-Constant Heat Capacity:** As the basic model, including an additional medium–the wall–that is set in thermal contact with the SM. Additionally, the heat capacity of the HTF and SM is not considered constant, but dependent on the temperature of the SM.

Although other modifications to the basic model were tested, they did not show relevant outcomes or significantly improved efficiency compared to the presented models. Thus, their modifications are only briefly listed for the sake of completeness. They included: Heat radiation losses, heat radiation between layers, the conical vessel shape, different part models for charging and discharging, and heat conduction between the SM of the layers. A general overview of the influences of several packed-bed thermal energy storage properties (radiation, temperature-dependent material properties, etc.) can e.g., be found in Allen [32].

3.2. Basic Grey-Box Model

In the basic grey-box model, only heat transfer between HTF and SM, and heat loss to the surrounding are considered in each layer i of the PBR vessel for every time-step k. The following procedure is used for all layers: HTF is entering layer i and flows through the SM in this layer. While charging, this leads to a warming of SM by the hot HTF and a reduction of the HTF temperature, and vice versa for discharging. Also taking into account a heat loss of the SM, this results in new temperatures of SM T_{SM} and HTF T_{HTF} in layer i and time-step k. These new SM and HTF temperatures can be used as a basis to calculate the temperatures of the subsequent layers $i+1$ and time-steps $k+1$. As the HTF flows through the solid SM, the HTF temperature depends on the HTF temperature of the previous layer $i-1$, while the SM temperature depends on the SM temperature of the previous time-step $k-1$. This approach is also illustrated in Figure 2. Note here that the presented approach is strongly dependent on the used time-step size. However, similar to the parameters fitted by optimization, the evaluation of a fitting time-step size is part of this partly empirical modeling approach.

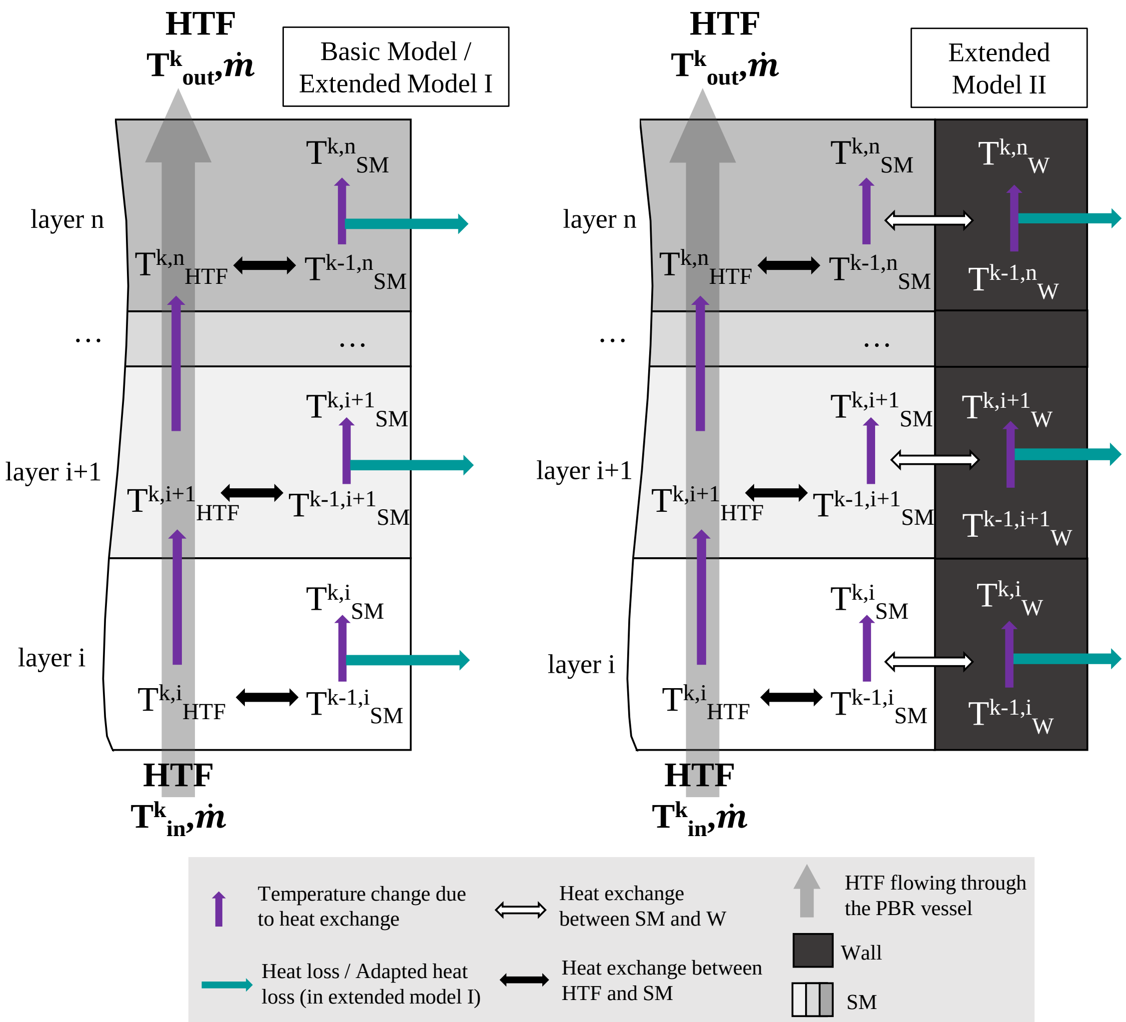


Figure 2. Modeling procedure of the basic model (**left**), extended model I (left, using adapted heat loss), and extended model II (**right**).

For the presented procedure, it is assumed that the HTF and SM in each layer i approach (but do not entirely reach) an equilibrium temperature T_{eq}. This equilibrium temperature can be calculated by equating the heat transferred between the HTF–see Equation (1)–and SM–see Equation (2)–, according to Equation (3).

$$Q_{\mathrm{SM}}^{k,i} = (T_{\mathrm{eq}}^{k,i} - T_{\mathrm{SM}}^{k-1,i})(c_{\mathrm{SM}}\,\rho_{\mathrm{SM}}\,(1-\varphi)\,V) \tag{1}$$

$$Q_{\mathrm{HTF}}^{k,i} = (T_{\mathrm{eq}}^{k,i} - T_{\mathrm{HTF}}^{k,i-1})(\Delta k\,\dot{m}\,c_{\mathrm{p,HTF}}) \tag{2}$$

$$(T_{\mathrm{eq}}^{k,i} - T_{\mathrm{SM}}^{k-1,i})(c_{\mathrm{SM}}\,\rho_{\mathrm{SM}}\,(1-\varphi)\,V) = -(T_{\mathrm{eq}}^{k,i} - T_{\mathrm{HTF}}^{k,i-1})(\Delta k\,\dot{m}\,c_{\mathrm{p,HTF}}) \tag{3}$$

Considering constant values for the (isobaric) heat capacity of the HTF $c_{\mathrm{p,HTF}}$ and SM c_{SM}, the density of the SM ρ_{SM}, the porosity of the SM φ, the volume of each layer V, and time-steps Δk, a new parameter β_{SH} can be introduced, according to Equation (4). Then, the equilibrium temperature can be formulated by Equation (5), where $\dot{m}$ is the time-dependent HTF mass flow.

$$\beta_{\mathrm{SH}} = \frac{\Delta k\,c_{\mathrm{p,HTF}}}{c_{\mathrm{SM}}\,\rho_{\mathrm{SM}}\,(1-\varphi)\,V} \tag{4}$$

$$T_{\mathrm{eq}}^{k,i} = \frac{\beta_{\mathrm{SH}}\,\dot{m}\,T_{\mathrm{HTF}}^{k,i-1} + T_{\mathrm{SM}}^{k-1,i}}{\beta_{\mathrm{SH}}\,\dot{m} + 1} \tag{5}$$

This equilibrium temperature can be theoretically reached at full heat exchange between HTF and SM. However, in practice, heat exchange between HTF and SM is not completely performed, and the equilibrium temperature is not reached. To determine the actual temperatures of HTF and SM after heat exchange, the following approach is used: A new empiric parameter α_{SH} is introduced that describes the share of heat exchange between HTF and SM. α_{SH}=0 stands for a complete heat exchange and α_{SH}=1 stands for no heat exchange between HTF and SM. This leads to the physically inspired equation Equation (6) to determine the temperature of the HTF. Using the parameter β_{SH} from Equation (4) that includes the heat transfer ratio between HTF and SM, Equation (7) can be formulated to calculate the SM temperature in layer i and time-step k.

$$T_{\mathrm{HTF}}^{k,i} = T_{\mathrm{eq}}^{k,i} - (T_{\mathrm{eq}}^{k,i} - T_{\mathrm{HTF}}^{k,i-1})\,\alpha_{\mathrm{SH}} \tag{6}$$

$$T_{\mathrm{SM}}^{k,i} = T_{\mathrm{eq}}^{k,i} - (T_{\mathrm{eq}}^{k,i} - T_{\mathrm{SM}}^{k-1,i})\,\alpha_{\mathrm{SH}} \tag{7}$$

To consider the heat loss to the surrounding that is assumed only linearly dependent on the temperature of the SM of the previous time-step, Equation (7) can be extended by the empirical parameter ν_{SM} and the temperature difference between the surrounding T_{sur} and T_{SM} of the previous time-step. Including the heat loss, the temperature of the SM can be determined by Equation (8).

$$T_{\mathrm{SM}}^{k,i} = T_{\mathrm{eq}}^{k,i} - (T_{\mathrm{eq}}^{k,i} - T_{\mathrm{SM}}^{k-1,i})\,\alpha_{\mathrm{SH}} - \nu_{\mathrm{SM}}(T_{\mathrm{SM}}^{k-1,i} - T_{\mathrm{sur}}) \tag{8}$$

Resulting, the basic model of the PBR consists of three equations, namely Equation (5) to calculate the equilibrium temperature in layer i, and Equations (6) and (8) to determine the temperatures of the HTF and SM for every time-step k in layer i after heat exchange. These equations include three parameters—α_{SH}, β_{SH}, and ν_{SM}—that aggregate or estimate relevant characteristics of the heat transfer between HTF and SM, and heat loss. β_{SH} describes the relation of heat capacity between HTF and SM according to Equation (4) and the two empirical parameters α_{SH} and ν_{SM} describe the heat transfer rate between HTF and SM, and the heat loss. Using the mechanistic grey-box modeling approach, these three parameters can be fitted by optimization methods to achieve good modeling results. Finally, to further improve this basic model, model extensions can be formulated.

3.3. Extended Grey-Box Model I—Heat Loss Dependency

The first extended model additionally considers the dependency of the heat loss on the SM temperature of previous time-steps. For this purpose, Equations (5) and (6) from the basic model are kept the same, and only Equation (8) is altered by including the moving average of the SM temperature of the previous time-steps. For the integration of the moving average, two new empirical parameters ν_{MA} and γ are introduced. ν_{MA} describes the weighting of the moving average and γ is the number of temperatures from previous time-steps used for the calculation of the moving average. The equivalent equation to Equation (8) of this extended model can be found in Equation (9).

$$T_{\text{SM}}^{k,i} = T_{\text{eq}}^{k,i} - (T_{\text{eq}}^{k,i} - T_{\text{SM}}^{k-1,i})\,\alpha_{\text{SH}} - \nu_{\text{SM}}(T_{\text{SM}}^{k-1,i} - T_{\text{sur}}) - \frac{\nu_{\text{MA}}}{\gamma}\sum_{j=1}^{\gamma} T_{\text{SM}}^{k-j,i} \tag{9}$$

Thus, this extended grey-box model also uses three equations, Equations (5), (6) and (9). However, compared to the basic model, it includes five instead of three parameters to be fitted during optimization, being the parameters of the basic model α_{SH}, β_{SH}, and ν_{SM}, and the new parameters ν_{MA} and γ.

3.4. Extended Grey-Box Model II—Inclusion of a Wall and Non-Constant Heat Capacity

In the second extended grey-box model, in addition to the SM and HTF, another medium—the wall W—is introduced, according to Figure 2. This wall represents the steal wall (and insulation) of the PBR. In the model, the wall is set into thermal contact with the SM, allowing a horizontal temperature gradient within one layer of the PBR. Similar to the heat transfer between HTF and SM—see Equation (3)—heat transfer between SM and the wall W is described by an equilibrium temperature, according to Equation (11). Here—in accordance with Equation (4)—a parameter β_{SW} is introduced in Equation (10) that describes the heat capacity ratio between SM and W, using the wall's heat capacity c_{W} and the auxiliary parameter m_{A}, being the mass of the wall in one layer.

$$\beta_{\text{SW}} = \frac{c_{\text{W}}\, m_{\text{A}}}{c_{\text{SM}}\,\rho_{\text{SM}}\,(1-\varphi)\,V} \tag{10}$$

$$T_{\text{eqSW}}^{k,i} = \frac{\beta_{\text{SW}}\,T_{\text{SM}}^{k,i} + T_{\text{W}}^{k-1,i}}{\beta_{\text{SW}}+1} \tag{11}$$

With the equilibrium temperature between SM and W, the temperatures of the SM and W—see Equations (12) and (13)—can be determined, using a new empirical parameter α_{SW} that describes the share of heat exchange between SM and W. In accordance with α_{SH} described in the basic model, α_{SW} = 0 stands for a complete heat exchange and α_{SW} = 1 for no heat exchange.

$$T_{\text{SM}}^{k,i} = T_{\text{eqSW}}^{k,i} - (T_{\text{eqSW}}^{k,i} - T_{\text{SM}}^{k,i})\,\alpha_{\text{SW}} \tag{12}$$

$$T_{\text{W}}^{k,i} = T_{\text{eqSW}}^{k,i} - (T_{\text{eqSW}}^{k,i} - T_{\text{W}}^{k-1,i})\,\alpha_{\text{SW}} \tag{13}$$

In the model of the wall, the heat loss of the PBR is dependent on the temperature of the wall, the surrounding temperature T_{sur}, and the empirical parameter ν_{W} that describes the heat loss of the wall, leading to Equation (14) for the calculation of the wall temperature in one layer.

$$T_{\text{W}}^{k,i} = T_{\text{eqSW}}^{k,i} - (T_{\text{eqSW}}^{k,i} - T_{\text{W}}^{k-1,i})\,\alpha_{\text{SW}} - \nu_{\text{W}}(T_{\text{SM}}^{k-1,i} - T_{\text{sur}}) \tag{14}$$

In addition in this extended model, the parameter β_{SH}—describing the heat capacity ratio between HTF and SM that was assumed constant in the basic model in one layer—is now considered dependent on the temperature of the SM. This new dependent parameter is defined as β_{SHT} and includes the parameters for the constant β_{SH} and temperature dependent β_{SHt} heat capacity ratio, according to Equation (15).

$$\beta_{\mathrm{SHT}} = \beta_{\mathrm{SH}} + T_{\mathrm{SM}}^{k,i}\,\beta_{\mathrm{SHt}} \tag{15}$$

Thus, this extended grey-box model uses five equations, Equation (5) with the new β_{SHT} instead of β_{SH}, Equations (6), (11), (12) and (14). It includes six parameters to be fitted during optimization, being α_{SH}, α_{SW}, ν_{W}, β_{SW}, and β_{SH} and β_{SHt} that can be combined to β_{SHT}.

3.5. Parameter Fitting–Optimization

To fit the parameters of the three developed grey-box models to the existing data, the root mean squared error (RMSE) of the model outlet T_{out} is optimized with the function *fminsearch* (using the Nelder-Mead Simplex Algorithm) in Matlab. Thus, the cost function of the optimization problem can be formulated by Equation (16), where T_{out} is the predicted outlet temperature of the HTF of the top layer with the grey-box models, $\overline{T_{\mathrm{out}}}$ the measured outlet temperature, and k the index for the time.

$$\sqrt{\sum_{k}(\overline{T_{\mathrm{out}}} - T_{\mathrm{out}})^2} \tag{16}$$

For the three developed grey-box models, different parameters are optimized with this approach, which are all dimensionless. The basic model optimizes α_{SH}, β_{SH}, and ν_{SM}. The extended model with heat loss dependency adds two parameters ν_{MA} and γ. In the extended model with the wall and non-constant heat capacity, the parameters α_{SH}, α_{SW}, ν_{W}, β_{SW}, β_{SH} and β_{SHt} are optimized.

3.6. Simulation Procedure

Using the corresponding equations and parameters for each of the three models, the simulation of the PBR is conducted by solving the equations for every layer i and time-step k (representing one minute) of the measurement series in Matlab. For all models, the PBR is separated into 203 layers (which were empirically chosen) with a height of 1 cm, and the used measurement series include approximately 1000 to 4500 time-steps, being 16 to 75 h.

As input in every time-step, the measured inlet HTF temperature $\overline{T_{\mathrm{in}}}$ and HTF mass flow $\dot{m}$ are required. In addition, before starting the simulation, the starting values for the SM temperature in the first layer were set equal to the surrounding temperature of 22 °C. As a result, the models predict the outlet HTF temperature T_{out} for all time-steps of the measurement data. In addition, the temperatures $T1$–$T4$ along the PBR vessel can be determined by the HTF temperatures of the corresponding layers.

4. Results and Discussion

For the analysis of the results, the three developed grey-box models are applied to the existing measurement data of the PBR from Table 1. Out of the eight measurement series, Series 3 is used to train the models, meaning to fit the models' parameters to the data. The other series are used to test the models' performance on so far *unknown* data. However, all series show a similar general behavior and the choice of training and test series does not affect the results considerably.

First of all, in Table 2, the dimensionless parameters and the accuracy of the results–measured by the root-mean-squared-error (RMSE) of the training and test outlet temperature T_{out} in °C–of the three grey-box models are summarized. It can be seen that the test RMSE of the extended grey-box model II yields the best results with a RMSE of 3.03 °C, followed by the extended grey-box model I with a RMSE of 4.58 °C, and the basic model with a RMSE of 6.08 °C. Also, the results reveal that all models extrapolate well, meaning the models can predict *unknown* data almost as accurate as the data they were trained with. Due to the similar behavior of the time series, this outcome was expected and can be seen by the relatively low difference between training and test RMSE, especially in the extended models I and II.

Table 2. Comparison of parameters and prediction accuracy of the three grey-box models.

Type of Model	Basic Model	Ext. I Heat Loss	Ext. II Wall + β_{SHT}
α_{SH}	0.722	0.155	0
α_{SW}	-	-	0.99
β_{SH}	22.0	23.6	27.2
β_{SHt}	-	-	−0.0197
β_{SW}	-	-	4.75
ν_{MA}	-	−0.00117	-
ν_{SM}	0.000459	0.00174	-
ν_{W}	-	-	0.00135
γ	-	166	-
Training RMSE in °C	6.08	4.58	2.89
Test RMSE in °C	7.68	5.51	3.03

In the next step, the performance of the three grey-box models is evaluated by their prediction accuracy of the HTF temperature T_{out}. In addition, observing the internal HTF temperatures $T1$–$T4$ allows for a more detailed analysis of the models behavior and was essential to improve and extend the grey-box models. For example, only if the temperature inside the PBR decreases steadily from $T1$ to $T4$ while charging, physically correct behavior is displayed. Although it therefore seems evident to use the temperatures $T1$–$T4$ as additional model outputs, these measurements show inaccuracies ($T3$ and $T4$ are higher than T_{out} in some series) and their integration in the model did not yield better outcomes. The inaccuracies are probably caused by the unequal location of the sensors in the vessel and the building of flow strains resulting in non-uniform heat exchange. Thus, these measurement were only used for the analysis of the model behavior and not integrated into the model. However, the integration of accurate measurements of $T1$–$T4$ could further improve the models' accuracy.

For the basic grey-box model, the measured and predicted outlet temperature and two of the internal temperatures, $T1$ and $T3$, are displayed in the upper sub-figure of Figure 3 (only two internal temperatures are displayed to limit the complexity of the figure). The lower sub-figure shows the deviation of the measured to the predicted outlet temperature. (The high deviations at the beginning of a series result from manual adjustments of the regenerator that do not reflect its actual operation behavior. Thus, the deviations at the beginning of a time series are not included in the final RMSE value.) It can be seen that during charging (rising curve), the outlet temperature and also the internal temperatures are predicted quite accurately. During discharging (falling curve) and switching between the operation modes, relatively high deviations can be seen. Moreover, the results show that the model predicts the internal temperatures physically correct (decreasing temperatures from $T1$ to $T3$ to T_{out}) in contrast to the evidently inaccurate experimental data that shows higher values for $T3$ than $T1$. Summarized, although the basic grey-box model can approximate the general physical behavior of the PBR well, the prediction of the outlet temperature still shows significant deviations to the data.

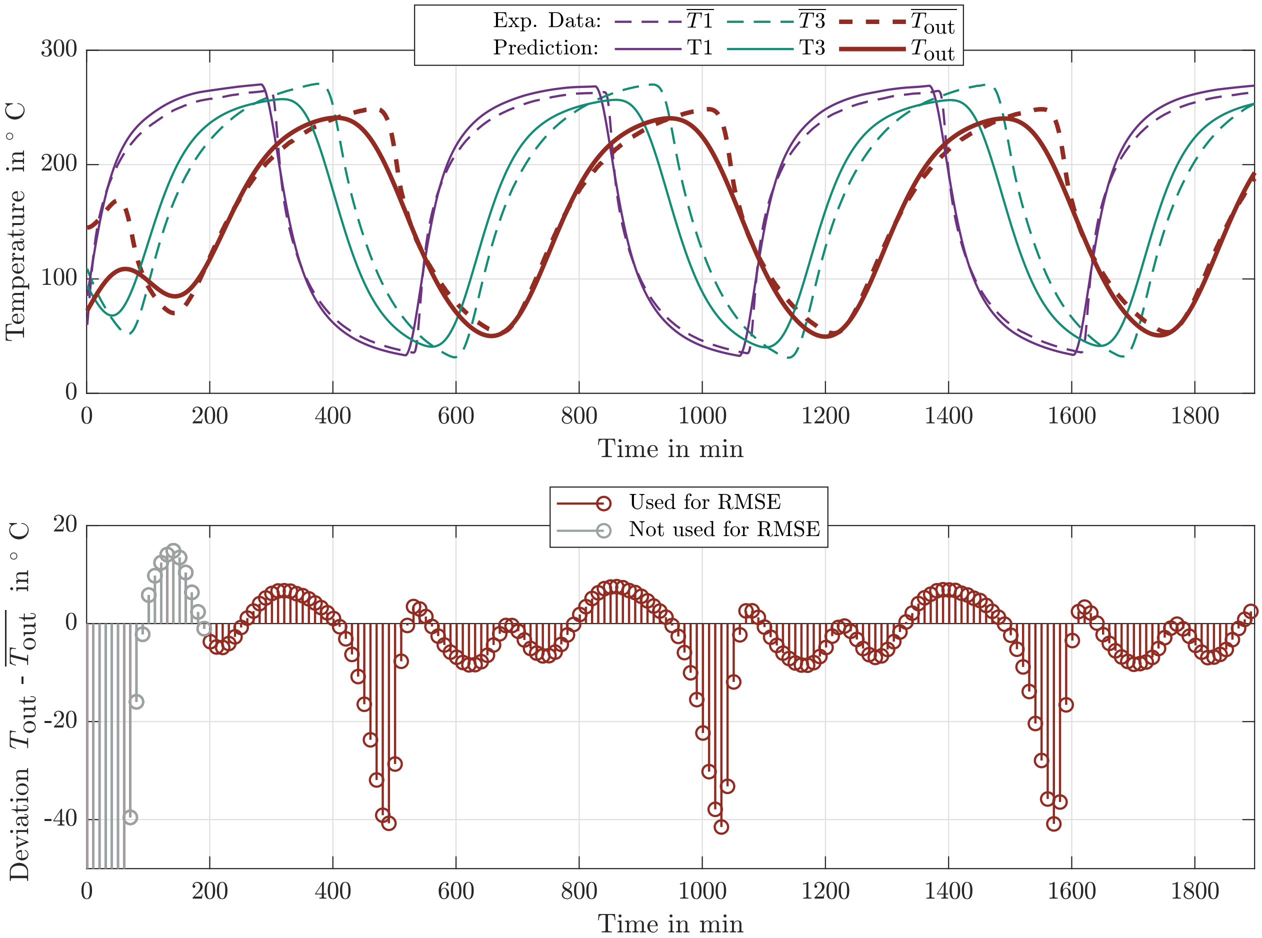


Figure 3. Results of the basic grey-box model for measurement series 1.

Next, the results of the extended grey-box model I that includes the heat loss dependency are shown in Figure 4. It can be seen that this model can predict the outlet temperature (and internal temperatures) when switching between the operation modes charging and discharging more accurately than the basic model, but still shows deviations to the experimental data. Also, same as the basic grey-box model, the internal temperatures are predicted physically correct in this model. Thus, although the inclusion of the heat loss dependency increases the accuracy of the results, also this extended grey-box model can still be improved.

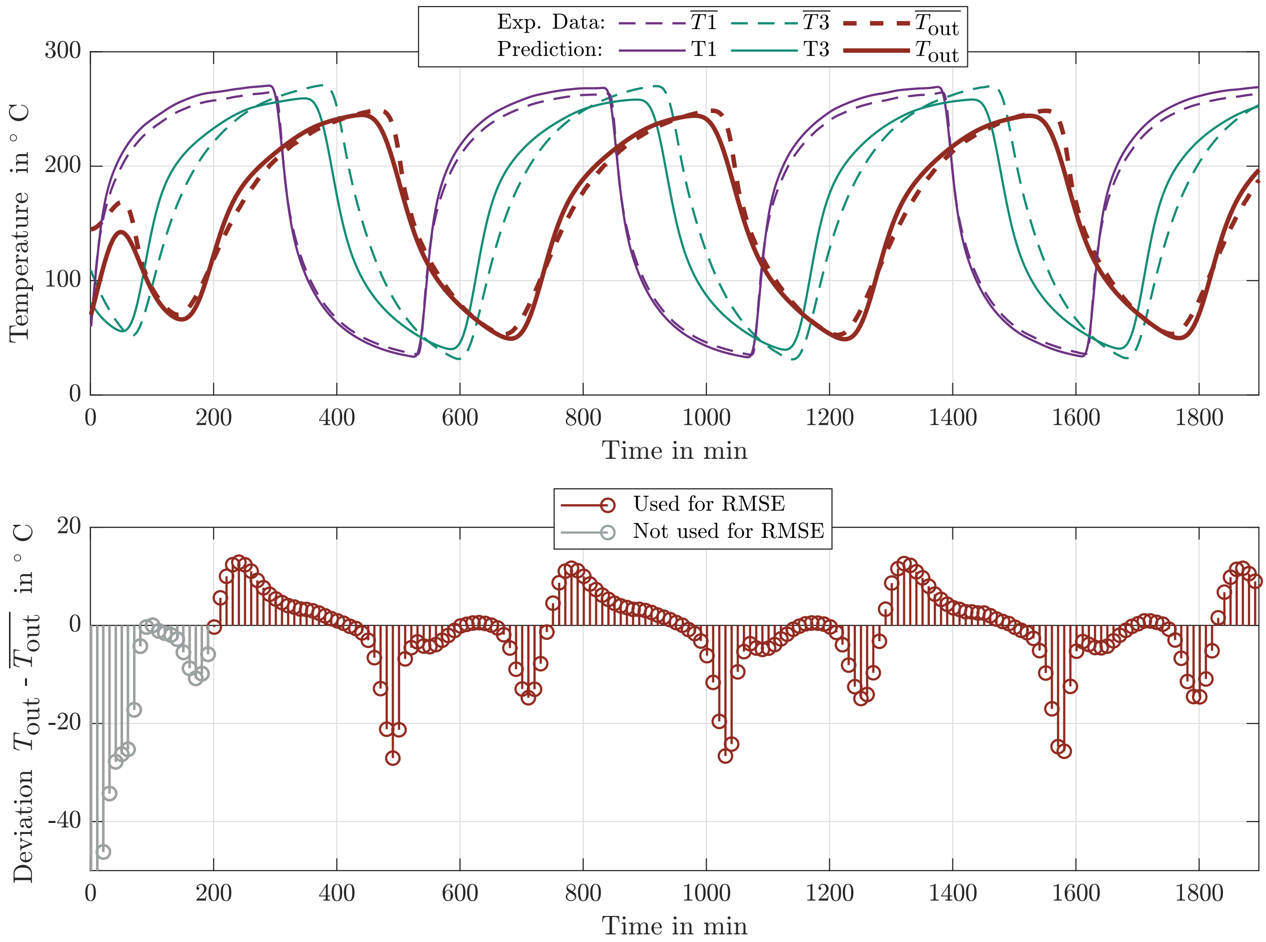


Figure 4. Results of the extended grey-box model I for measurement series 1.

Finally, the results of the extended grey-box model II that includes a wall and non-constant heat capacity are shown in Figure 5. It can be seen that this model predicts the outlet temperature very accurately with only minor deviations and approximates the internal temperatures physically correct. For a more detailed analysis of this model, the predicted wall temperatures $T1_{wall}$ and $T3_{wall}$ are also displayed in Figure 5. It can be seen that the wall temperature lags the temperature of the HTF in a consistent manner. This is achieved by the additional state variable of the wall that results in a horizontal temperature gradient in each layer of the model. Although the included optimization parameters of the wall do not necessarily represent actual physical constants of the wall, they allow for a suitable approximation of the horizontal temperature distribution within the PBR.

Regarding the non-constant heat capacity ratio of the HTF and SM that is also included in this model, this adaption also slightly contributes to the excellent results of this model. This was analyzed by comparing the test RMSE of this model (RMSE = 3.03 °C) and the basic model (RMSE = 7.68 °C), with the test RMSE of the model only with the implementation of the wall (RMSE = 4.34 °C) and only with the non-constant heat capacity ratio (RMSE = 7.24 °C). Thus, it can be seen that the introduction of the wall drastically decreases the RMSE of the basic model, and that the non-constant heat capacity ratio further slightly decreases the RMSE. Also, this conclusion is amplified by the relatively close to zero value of β_{SHt} in Table 2, which indicates a relatively low temperature dependence of β_{SHT}.

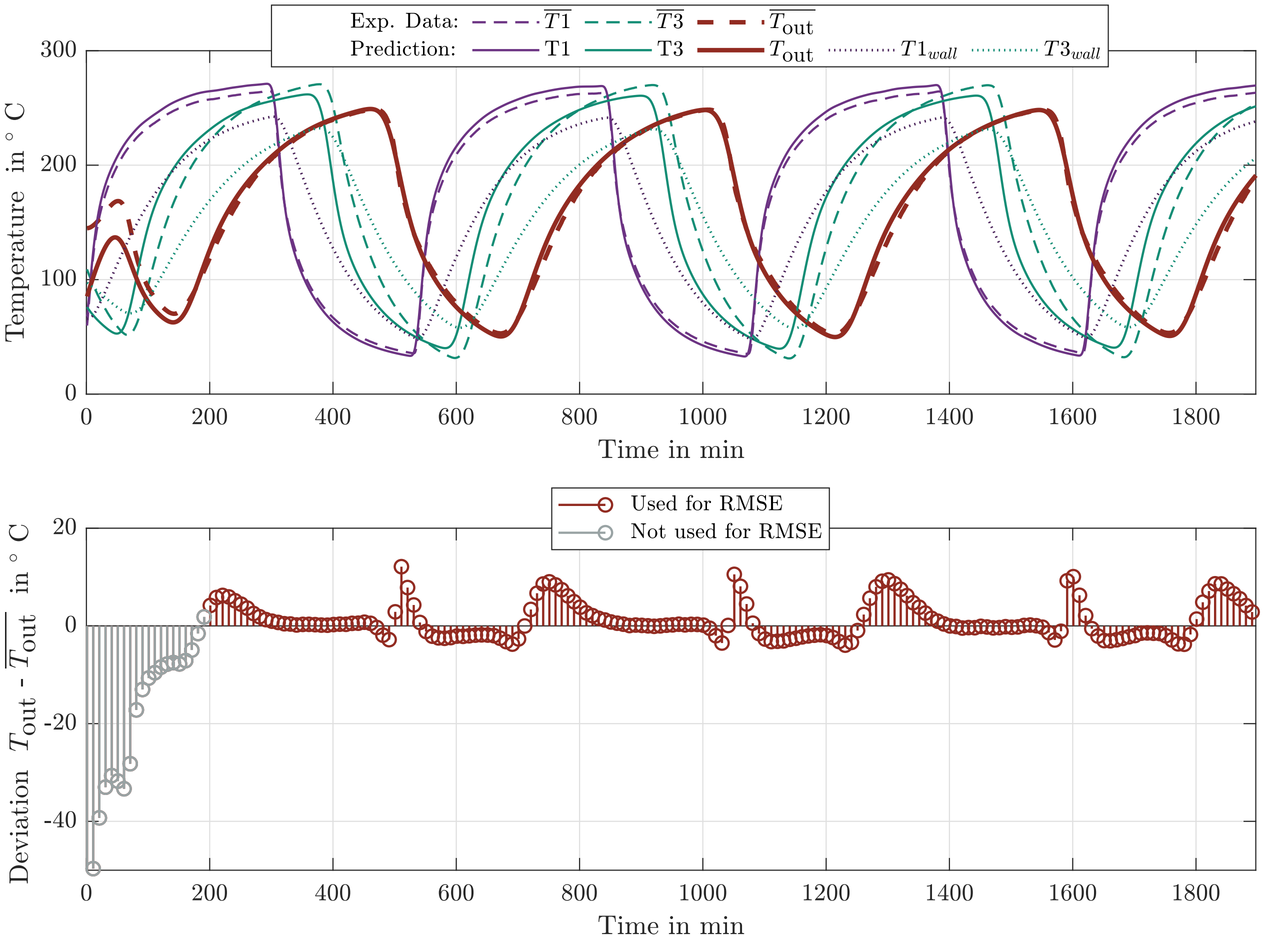


Figure 5. Results of the extended grey-box model II for measurement series 1.

Summarized, the results of the predictions with the three models lead to the following outcomes:

- All models can approximate the general physical behavior of the PBR well and display the internal temperatures physically correct. However, the extended grey-box model I, and especially the extended grey-box model II, result in significantly higher prediction accuracy than the basic model. With an RMSE of $\approx$3, the extended grey-box model II shows the best results.
- Especially the implementation of the wall and its additional state variable adds an essential extension to the basic grey-box model, approximating a horizontal temperature gradient in each layer.
- Although the extended grey-box model II includes two more equations and three more parameters than the basic model, the computational effort is still very low (0.12 s for predicting all measurement series on a conventional desktop computer). Thus, the slightly higher complexity does not diminish the excellent performance of this model.

Finally, to further evaluate the performance of the developed grey-box models, the models are compared to two existing models of the PBR: A purely physical model and a mainly data-driven Neural Network model.

5. Comparison of Physical, Data-Driven and Grey-Box Model

In a previous work [18], a primarily data-driven model using Neural Networks (NN) and a purely physical model of the PBR were developed. Like the grey-box models, both models aimed to accurately predict the outlet temperature T_{out} of the PBR. The data-driven model was based on a Recurrent Neural Network, using a specific structure to account for the time-dependent behavior of the PBR. For the creation and testing of the NN model, the same measurement series as for the grey-box models were employed. In contrast, the physical model was only based on physical relations, considering a finite difference 1D model with convective and conductive heat transfer in the mediums SM, HTF and the wall of the PBR.

For a quantitative comparison of the different models, the prediction of the outlet temperature T_{out} with the physical, the data-driven NN model, and the extended grey-box model II for one charging/discharging cycle of measurement series 1 is displayed in Figure 6. It can be seen that both the physical and data-driven NN model can predict the outlet temperature of the PBR fairly accurately. Nevertheless, similar to the basic grey-box model, the physical model shows inaccuracies when switching between charging and discharging. In contrast, the NN model can predict the outlet temperature more accurately, but shows small oscillations (e.g., around time-step 840) and most importantly, it is not as robust as the physical model. This was seen by the false/nonphysical predictions of this model, if the model was trained with inaccurate experimental data. In contrast to the NN and the physical model, the developed grey-box models stand out by accurate *and* robust predictions. A detailed analysis of the grey-box models' qualitative features and a short comparison with the NN and the physical model is presented below. For a more detailed description of the NN and physical model and their detailed quantitative and qualitative analysis, we refer to Hofmann et al. [18].

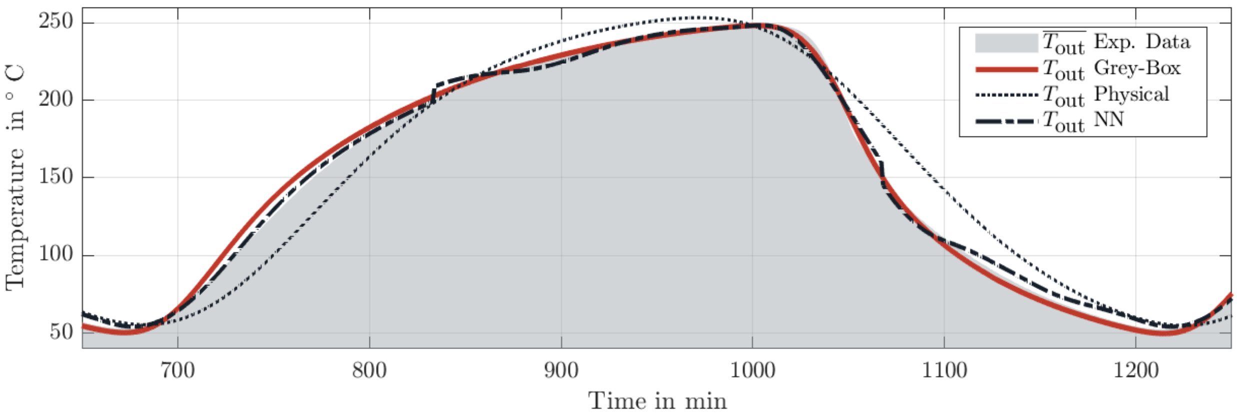


Figure 6. Results of the extended grey-box model II, physical, and NN model for one cycle of measurement series 1.

5.1. Qualitative Comparison

5.1.1. Modeling Effort

In the developed grey-box models, the determination of a suitable model structure was the most time-consuming step. Whereas the structure of the basic grey-box model was chosen almost right-away, the extensions of the basic model were an elaborate and iterative process. A significant number of attempts with varying physical or empirical parameters were conducted, before the extensions yielded significantly better results than the basic model, without being too complex. However, once a suitable structure was defined, its implementation, the optimization of the parameters and the actual prediction could be conducted very quickly. Compared to the existing models, the overall modeling effort for the grey-box model is a bit higher than for the data-driven NN model and lower than for the physical model. However, in the end, the modeling effort of grey-box modeling strongly depends on the application and requirements of a model.

5.1.2. Computational Effort

The developed grey-box models only use 3–5 five equations and 3–6 parameters to be optimized. Thus, the computational effort is small, leading to a maximal simulation time of 0.12 s for all eight measurement series on a conventional computer (4-core i5 processor with 8GB RAM). In contrast, the same predictions with the NN model required about 3 s and more than 100 s with the purely physical model.

5.1.3. Ability for Adaptation

For many applications, high flexibility and adaptability to changes are major modeling goals. These changes can include material or structural changes of a system, but also e.g., variations of the operation modes. Generally, physical models are able to adapt to small operational changes easily and can also conduct predictions outside their originally desired prediction-range. However, changes in material or a process's structure might require major model adaptations. This is also true for the existing purely physical model. In contrast, data-driven models are only valid in the operation modes and ranges they were trained for. E.g., for varying operation modes, material or structural changes, the model needs to be trained with the associated new data. However, if a data-driven model's structure can be maintained for these changes, the model can be adapted quickly and straight-forwardly with the new data. This is also valid for the existing data-driven NN model.

As a mixture of data-driven and physical models, the grey-box model allows for quick adaption to any changes. On the one hand, the grey-box model can conduct predictions outside its training range such as the physical model. On the other hand, varying operation modes, material or structural changes can be adapted straight-forwardly and quickly with the associated new data. As a further benefit of the grey-box model, in contrast to the NN model, less data for these adaptations is required. Finally, although the developed grey-box models are not directly applicable to other systems, the underlying mechanistic grey-box modeling approach offers high potential for various applications.

5.1.4. Robustness

The robustness is used as a measure for a model's probability to generate inaccurate results. In this sense, the grey-box models—same as the purely physical model—can be considered robust. As the grey-box models are built on physical equations, their results are comprehensible and plausible, leading to only physically correct predictions. This was also emphasized by the consistently physically correct predictions of the outlet and internal temperatures of the grey-box models. In contrast, data-driven models such as the NN model are not transparent and can lead to incomprehensible/nonphysical results. As a result in the NN model, inaccurate/nonphysical data automatically led to nonphysical predictions, being higher temperatures of $T3$ than $T1$.

5.1.5. Required Knowledge and Resources

For the mechanistic grey-box modeling approach, advanced physical knowledge of the PBR was required as well as experimental data. However, in contrast to the purely physical model, fewer physical insights in the PBR were required for the creation. In comparison to the NN model, the grey-box models required smaller amounts of data. In fact, only one measurement series was enough for fitting the parameters of the grey-box models, whereas the NN model used six measurement series on average for training—and more data would have still been beneficial. Regarding resources, the development of the mechanistic grey-box models required a numerical software with optimization tools.

5.2. Summary and Discussion

Table 3 summarizes the most important features of the grey-box models, compared to the purely physical and the data-driven NN model, where ↑ stands for *high* and ↓ for *low*, and ↑↓ for *moderate*.

The qualitative and quantitative analysis of the results showed that the developed grey-box models—especially the extended grey-box model II—yield excellent performance, also in comparison to the existing models. The extended grey-box model II cannot only predict the outlet temperature of the PBR very accurately, but is also robust and has low computational effort. As the only drawback of this grey-box model, its modeling effort is moderate to high due to the various possibilities to combine physical considerations and data.

Table 3. Summary of the comparison–grey-box model vs. physical model vs. data-driven NN model.

Modeling Approach	**Grey-Box Model**	**Physical Model**	**NN Model**
Accuracy	↑	↓	↑
Modeling Effort	↑↓	↑	↓
Computational Effort	↓	↑	↓
Effort for Small Adaptations	↓	↓	↓
Effort for Major Adaptations	↓	↑	↓
Robustness	**Robust**	Robust	Limited Robustness
Required Knowledge	**Advanced Process Knowledge**	Detailed Process Knowledge	Basic Process Knowledge
Required Resources	**Numerical Software + Optimization Tools, Test & Training Data**	Numerical Software, Validation Data	Numerical Software + ML Toolbox, Large Data Sets

Finally, it can be concluded that the results of the developed mechanistic grey-box models are promising and that this approach could be a sound alternative to traditionally used numerical modeling approaches for packed-bed thermal energy storage, as described in Section 1. Especially for thermal energy storage systems with limited physical information, existing experimental data, and models that require reduced complexity (e.g., for process optimization tools), this approach stands out by accurate predictions while being significantly less complex than physical, numerical models. However, compared to purely physical models, the presented approach is not applicable for the design of systems but only for analyzing a system after its erection. Thus, as an application area, the mechanistic grey-box modeling approach could be well suited to model parts of industrial energy systems, such as the PBR, for realizing operational or design optimization of a process.

6. Conclusions and Outlook

This work analyzed the development and performance of mechanistic grey-box models for a sensible thermal energy storage, a packed-bed regenerator. The models aimed to predict the outlet temperature of the regenerator accurately and robust, using physical consideration/equations *and* existing data. With this mechanistic modeling approach, the regenerator was described by physical equations, and specified parameters—being either physical or physically inspired/empirical—were fitted to the data by optimization methods.

Using this approach, three mechanistic grey-box models were developed: The basic model based on 3 equations and 3 parameters, the extended model I using 3 equations and 5 parameters, and the extended model II with 5 equations and 6 parameters. The results of the models revealed that the extended grey-box model II yields the best results and can predict the PBR outlet temperature very accurately. However, all developed grey-box models can extrapolate and approximate the physical behavior of the PBR well.

Finally, compared to an existing data-driven Neural Network model and a purely physical model of the regenerator, the grey-box models show very good performance. They can benefit from high accuracy, low computational effort, low effort for adaptations, high robustness, and only small amounts of data are required. The only minor drawback of the developed grey-box models is their moderate to high modeling effort. Although the basic grey-box model could be developed very quickly, especially finding suitable model extensions and parameters was rather time-consuming. Nevertheless, it was shown that this hybrid approach—a mixture of physical and data-driven model—shows excellent qualitative and quantitative results and can be a sound alternative to traditionally used numerical modeling approaches for e.g., optimization applications.

For future work, we plan to test the grey-box models for part-load operation of the regenerator. Although further extensions for this works' modeling purpose did not yield any significant improvements, the consideration of part-load operation or other modeling goals might require model adaptations, e.g., the implementation of accurate measurements of the internal temperatures $T1$–$T4$ or additional empirical factors. Furthermore, the approach could be applied to other industrial systems to generally evaluate the applicability of this approach to industrial process modeling.

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References

1. IEA. *Data Overview*; IEA: Paris, France. Available online: https://www.iea.org/fuels-and-technologies/electricity (accessed on 27 May 2021).
2. Arce, P.; Medrano, M.; Gil, A.; Oró, E.; Cabeza, L.F. Overview of thermal energy storage (TES) potential energy savings and climate change mitigation in Spain and Europe. *Appl. Energy* **2011**, *88*, 2764–2774. doi:10.1016/j.apenergy.2011.01.067.
3. O'Rielly, K.; Jeswiet, J. Strategies to Improve Industrial Energy Efficiency. *Procedia CIRP* **2014**, *15*, 325–330.
4. De Prada, C.; Hose, D.; Gutierrez, G.; Pitarch, J.L. Developing Grey-Box Dynamic Process Models. *IFAC-PapersOnLine* **2018**, *51*, 523–528, doi:10.1016/j.ifacol.2018.03.088.
5. Solomatine, D.; See, L.M.; Abrahart, R.J. Data-Driven Modelling: Concepts, Approaches and Experiences. In *Practical Hydroinformatics: Computational Intelligence and Technological Developments in Water Applications*; Water Science and Technology Library, 68; Abrahart, R.J., See, L.M., Solomatine, D.P., Eds.; Springer: Berlin/Heidelberg, Germany, 2008; Volume 68, pp. 17–30. doi:10.1007/978-3-540-79881-1_2.
6. Hamon, R.; Junklewitz, H.; Sanchez, I. *Robustness and Explainability of Artificial Intelligence: From Technical to Policy Solutions*; Publications Office of the European Union: Luxembourg, 2020; doi:10.2760/57493.
7. Cen, Z.; Wei, J.; Jiang, R. A Grey-Box Neural Network based identification model for nonlinear dynamic systems. In Proceedings of the Fourth International Workshop on Advanced Computational Intelligence (IWACI), Wuhan, Hubei, China, 19–21 October 2011; IEEE: Piscataway, NJ, USA, 2011; pp. 300–307. doi:10.1109/IWACI.2011.6160021.
8. Sohlberg, B.; Jacobsen, E.W. Grey Box Modelling–Branches and Experiences. *IFAC Proc. Vol.* **2008**, *41*, 11415–11420. doi:10.3182/20080706-5-KR-1001.01934.
9. Aguirre, L.A.; Barroso, M.; Saldanha, R.R.; Mendes, E. Imposing steady-state performance on identified nonlinear polynomial models by means of constrained parameter estimation. *IEE Proc. Control Theory Appl.* **2004**, *151*, 174–179, doi:10.1049/ip-cta:20040102.
10. Ljung, L. Approaches to identification of nonlinear systems. In Proceedings of the 29th Chinese Control Conference 29–31 July 2010, Beijing, China, 2010; pp. 1–5.
11. Sohlberg, B. *Supervision and Control for Industrial Processes: Using Grey Box Models, Predictive Control and Fault Detection Methods*; Advances in Industrial Control; Springer: London, UK, 1998; doi:10.1007/978-1-4471-1558-8.
12. Thompson, M.L.; Kramer, M.A. Modeling chemical processes using prior knowledge and neural networks. *AIChE J.* **1994**, *40*, 1328–1340, doi:10.1002/aic.690400806.

13. Liu, Y.; Jacobsen, E.W. Error Detection and Control in Grey-Box Identification of Distributed Parameter Processes. *IFAC Proc. Vol.* **2004**, *37*, 841–846.
14. Tulleken, H.J. Grey-box modelling and identification using physical knowledge and bayesian techniques. *Automatica* **1993**, *29*, 285–308, doi:10.1016/0005-1098(93)90124-C.
15. Oussar, Y.; Dreyfus, G. How to be a gray box: dynamic semi-physical modeling. *Neural Netw.* **2001**, *14*, 1161–1172, doi:10.1016/S0893-6080(01)00096-X.
16. Pitarch, J.; Sala, A.; de Prada, C. A Systematic Grey-Box Modeling Methodology via Data Reconciliation and SOS Constrained Regression. *Processes* **2019**, *7*, 170, doi:10.3390/pr7030170.
17. Halmschlager, V.; Koller, M.; Birkelbach, F.; Hofmann, R. Grey Box Modeling of a Packed-Bed Regenerator Using Recurrent Neural Networks. *IFAC-PapersOnLine* **2019**, *52*, 765–770, doi:10.1016/j.ifacol.2019.12.055.
18. Hofmann, R.; Halmschlager, V.; Koller, M.; Scharinger-Urschitz, G.; Birkelbach, F.; Walter, H. Comparison of a physical and a data-driven model of a Packed Bed Regenerator for industrial applications. *J. Energy Storage* **2019**, *23*, 558–578, doi:10.1016/j.est.2019.04.015.
19. Ismail, K.; Stuginsky, R., Jr. A parametric study on possible fixed bed models for pcm and sensible heat storage. *Appl. Therm. Eng.* **1999**, *19*, 757–788, doi:10.1016/S1359-4311(98)00081-7.
20. Schmidt, F.W., Willmott A.J. *Thermal Energy Storage and Regeneration*, 1st ed.; Hemisphere Publishing Corporation: Washington, D.C., USA, 1981; doi:10.1615/ICHMT.1981.AdvCourseHeatExch.370.
21. Beasley, D.E.; Clark, J.A. Transient response of a packed bed for thermal energy storage. *Int. J. Heat Mass Transf.* **1984**, *27*, 1659–1669, doi:10.1016/0017-9310(84)90278-3.
22. Schumann, T. Heat transfer: A liquid flowing through a porous prism. *J. Frankl. Inst.* **1929**, *208*, 405–416, doi:10.1016/S0016-0032(29)91186-8.
23. Odenthal, C.; Steinmann, W.D.; Zunft, S. Analysis of a horizontal flow closed loop thermal energy storage system in pilot scale for high temperature applications–Part II: Numerical investigation. *Appl. Energy* **2020**, *263*, 114576, doi:10.1016/j.apenergy.2020.114576.
24. Zanganeh, G.; Khanna, R.; Walser, C.; Pedretti, A.; Haselbacher, A.; Steinfeld, A. Experimental and numerical investigation of combined sensible–latent heat for thermal energy storage at 575 °C and above. *Sol. Energy* **2015**, *114*, 77–90, doi:10.1016/j.solener.2015.01.022.
25. Hänchen, M.; Brückner, S.; Steinfeld, A. High-temperature thermal storage using a packed bed of rocks–Heat transfer analysis and experimental validation. *Appl. Therm. Eng.* **2011**, *31*, 1798–1806, doi:10.1016/j.applthermaleng.2010.10.034.
26. White, A.; McTigue, J.; Markides, C. Wave propagation and thermodynamic losses in packed-bed thermal reservoirs for energy storage. *Appl. Energy* **2014**, *130*, 648–657, doi:10.1016/j.apenergy.2014.02.071.
27. König-Haagen, A.; Höhlein, S.; Brüggemann, D. Detailed exergetic analysis of a packed bed thermal energy storage unit in combination with an Organic Rankine Cycle. *Appl. Therm. Eng.* **2020**, *165*, 114583, doi:10.1016/j.applthermaleng.2019.114583.
28. Hoffmann, J.F.; Fasquelle, T.; Goetz, V.; Py, X. A thermocline thermal energy storage system with filler materials for concentrated solar power plants: Experimental data and numerical model sensitivity to different experimental tank scales. *Appl. Therm. Eng.* **2016**, *100*, 753–761, doi:10.1016/j.applthermaleng.2016.01.110.
29. Barton, N.G. Simulations of air-blown thermal storage in a rock bed. *Appl. Therm. Eng.* **2013**, *55*, 43–50.
30. Heller, L.; Gauché, P. Modeling of the rock bed thermal energy storage system of a combined cycle solar thermal power plant in South Africa. *Sol. Energy* **2013**, *93*, 345–356, doi:10.1016/j.solener.2013.04.018.
31. Michalka, A. Experimentelle Untersuchungen Eines Festbettregenerators Mit Feinem Kies Als Speichermaterial. Ph.D. Thesis, Technical University of Vienna, Vienna, 2018.
32. Allen, K.G. Rock Bed Thermal Storage for Concentrating Solar Power Plants. Ph.D. Thesis, Stellenbosch University, Stellenbosch, South Africa, 2014.

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.

Paper A – Co-Author Publication

Comparison of a physical and a data-driven model of a Packed Bed Regenerator for industrial applications

R. Hofmann, V. Halmschlager, M. Koller, G. Scharinger-Urschitz, F. Birkelbach, and H. Walter (2019). "Comparison of a physical and a data-driven model of a Packed Bed Regenerator for industrial applications". *Journal of Energy Storage 23, pp. 558–578. doi:10. 1016/ j. est. 2019. 04. 01*

This paper covers the application of the NN grey-box model and the white-box model to the packed-bed regenerator using real time-series data. The experimental setup, the white-box and the NN modeling approach are presented, and the results of the two models are compared. A quantitative and qualitative analysis reveals that the NN model shows higher accuracy, decreased modeling and computational effort, can be easier adapted to major changes of the model, and requires less physical knowledge of the use-case. However, the NN is less robust than the physical model and requires large data sets.

My contribution: Methodology, Validation, Investigation, Formal Analysis, Writing – Original Draft, Visualization (all regarding the NN model and the model comparison)

Presentations

Referring to contents of this thesis, three presentations in front of scientific and industrial audiences were given:

V. Halmschlager , E. Pleschutznig, R. Hofmann. „Betriebsoptimierung – Realität und Zukunft". *Webinar Dekarbonisierung der Industrie: Erneuerbare Prozesse und Energieeffizienz, Betriebsoptimierung neu Gedacht – Nutzung sämtlicher Abwärmepotenziale und Flexibilitäten, KLIEN, (19.11.2020)*, `https://www.klimafonds.gv.at/wp-content/uploads/sites/16/Betriebsoptimierung_AnnexXIX_new.pdf`

R. Hofmann, V. Halmschlager, S. Knötter: "Digitalisierung, Künstliche Intelligenz und verwandte Technologien - Annex XVIII"; Vortrag:Digitalisierung in der Industrie - Workshop, Wien; 14.11.2019.

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

As part of the IEA IETS Annex XVIII on "Digitalization, Artificial Intelligence and Related Technologies for Energy Efficiency and GHG Emissions Reduction in Industry", I had the opportunity to coordinate the drafting 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 three master's theses that made valuable contributions to my research.

M. Fischer: "Programmierung der Steuerung eines Festbettregenerators und Erstellung eines datengetriebenen Modells zur Beschreibung des Speicherverhaltens"; Betreuer/in(nen): R. Hofmann, V. Halmschlager; E302 - Institut für Energietechnik und Thermodynamik, 2019; Final exam: 06/2019.

E. Gütl: "Data-Driven Modelling of a Fixed Bed Regenerator using Machine Learning in Tensorflow"; Betreuer/in(nen): R. Hofmann, V. Halmschlager; E302 - Institut für Energietechnik und Thermodynamik, 2019; Final exam: 10/2019.

S. Müllner: "Grey-Box Model of a Packed-Bed Regenerator"; Betreuer/in(nen): R. Hofmann, V. Halmschlager; E302 - Institut für Energietechnik und Thermodynamik, 2021; Final exam: planned in summer 2021.

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