Diploma Thesis

Grey Box Modeling of a Packed Bed Regenerator

carried out for the purpose of obtaining the degree of Dipl.-Ing., submitted at TU Wien,
Faculty of Mechanical and Industrial Engineering, by

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Vienna, July 2021
I confirm, that going to press of this thesis needs the confirmation of the examination committee.

**Affidavit**

I declare in lieu of oath, that I wrote this thesis and performed the associated research myself, using only literature cited in this volume. If text passages from sources are used literally, they are marked as such.

I confirm that this work is original and has not been submitted elsewhere for any examination, nor is it currently under consideration for a thesis elsewhere.

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Preface

The grey box models created for this Diploma Thesis showed great results. Therefore, parts of the Diploma Thesis have already been published in collaboration with Dipl.-Ing. Verena Halmschlager and Univ.Prof. Dipl.-Ing. Dr.techn. René Hofmann in the journal Energies under the title: 'Mechanistic Grey-Box Modeling of a Packed-Bed Regenerator for Industrial Applications', [1]. The paper is attached to the Diploma Thesis in Appendix B. Model structures created for this Diploma Thesis have been used for the creation of the paper.

I wish to express my gratitude to my thesis supervisors Dipl.-Ing. Verena Halmschlager and Univ.Prof. Dipl.-Ing. Dr.techn. René Hofmann for the possibility to write my master thesis under their supervision. I am especially thankful for the good collaboration, in cases of difficulty, they always found time to help.

I would further like to thank my family for their never-ending support. Particularly, I would like to thank my parents for encouraging my brother and me to follow our interests and for their support to further educate ourselves in any way, shape, or form we liked. Only because of the never-ending support of my parents, my brother, and his wife the emotional support, countless discussions, and proofreading it was possible to create this master thesis in its entirety.
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Abstract

In the transition from fossil fuels to renewable energy, energy storage solutions are needed to bridge time differences of energy production and consumption. To efficiently implement energy storage systems, accurate models thereof are needed. This thesis deals with the creation of a grey box model of a packed bed regenerator, a sensible thermal energy storage system. A mechanistic grey box modeling approach is used which combines prior knowledge (white box) and data (black box) of the packed bed regenerator. The model equations are derived from prior knowledge and parameters of these equations are optimized using data. To reduce the model error, different models with varying parameters and equations are created and compared with each other. The final model, being the most accurate one, is compared to an already existing white box model and an already existing mainly data-driven neural network model.

The final grey box model accurately predicts the behaviour of the packed bed regenerator for a wide variety of inputs and enables for insights into the temperature distribution of the packed bed regenerator. Further, it is computationally efficient and allows for fast adaption to operational and material changes when data is available.
Zusammenfassung


Das endgültige Grey-Box-Modell sagt das Verhalten des Festbettregenerators für einen großen Bereich an Eingangswerten akkurat voraus und ermöglicht Einblicke in die Temperaturverteilung des Festbettregenerators. Darüber hinaus ist es rechnerisch effizient und erlaubt eine schnelle Anpassung an betriebliche und materielle Änderungen, wenn Daten verfügbar sind.
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<td>Computational fluid dynamics</td>
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<td>HTF</td>
<td>Heat transfer fluid</td>
</tr>
<tr>
<td>I</td>
<td>Insulation</td>
</tr>
<tr>
<td>NARMAX</td>
<td>Non-linear autoregressive moving average model with exogenous inputs</td>
</tr>
<tr>
<td>NN</td>
<td>Neural network</td>
</tr>
<tr>
<td>PBR</td>
<td>Packed bed regenerator</td>
</tr>
<tr>
<td>SM</td>
<td>Storage medium</td>
</tr>
<tr>
<td>TES</td>
<td>Thermal energy storage</td>
</tr>
<tr>
<td>W</td>
<td>Wall</td>
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Symbols

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<tr>
<td>$\alpha$</td>
<td>Heat transfer coefficient $[W/(m^2K)]$</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Emissivity $[1]$</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>Reflection coefficient $[1]$</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Contraction coefficient $[1]$</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Expansion coefficient $[1]$</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Thermal diffusivity $[m^2/s]$</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Thermal conductivity $[W/(mK)]$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density [$kg/m^3$]</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stefan-Boltzmann constant [$W/(m^2K)$]</td>
</tr>
<tr>
<td>$\psi$</td>
<td>Porosity [1]</td>
</tr>
<tr>
<td>$\nabla$</td>
<td>Nabla operator</td>
</tr>
<tr>
<td>$A_{con}$</td>
<td>Contact surface [$m^2$]</td>
</tr>
<tr>
<td>$A_{cross}$</td>
<td>Cross section [$m^2$]</td>
</tr>
<tr>
<td>$A_{surf}$</td>
<td>Surface area [$m^2$]</td>
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<tr>
<td>$a_1$ and $a_2$</td>
<td>Constants of proportionality [$1/s$]</td>
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<tr>
<td>$B_i$</td>
<td>Biot number [1]</td>
</tr>
<tr>
<td>$c_{HTF}$</td>
<td>Specific heat capacity of the HTF [$J/(kgK)$]</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat capacity [$J/(kgK)$]</td>
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<tr>
<td>$c_{SM}$</td>
<td>Specific heat capacity of the SM [$J/(kgK)$]</td>
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<tr>
<td>$\epsilon$</td>
<td>Errors</td>
</tr>
<tr>
<td>$H$</td>
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<tr>
<td>$h$</td>
<td>Height of layer [m]</td>
</tr>
<tr>
<td>$i$</td>
<td>Layer number, counting from the bottom up</td>
</tr>
<tr>
<td>$k$</td>
<td>Time step</td>
</tr>
<tr>
<td>$k_f$</td>
<td>First time step used to calculate the cost function</td>
</tr>
<tr>
<td>$k_l$</td>
<td>Last time step used to calculate the cost function</td>
</tr>
<tr>
<td>$l$</td>
<td>Number of layers</td>
</tr>
<tr>
<td>$m$</td>
<td>Number of parameters to be optimized</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>Mass flow [$kg/s$]</td>
</tr>
<tr>
<td>$P$</td>
<td>Point defining a simplex</td>
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<tr>
<td>$P_{rad}$</td>
<td>Power radiated by a body [W]</td>
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<td>$p$</td>
<td>Model parameters</td>
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<tr>
<td>$\hat{p}$</td>
<td>Optimized parameters</td>
</tr>
<tr>
<td>$\Delta p$</td>
<td>Shift vector</td>
</tr>
<tr>
<td>$Q$</td>
<td>Transferred heat [$J$]</td>
</tr>
<tr>
<td>$\dot{Q}$</td>
<td>Rate of heat flow [W]</td>
</tr>
<tr>
<td>$\dot{q}$</td>
<td>Heat flux density [$W/m^2$]</td>
</tr>
<tr>
<td>$R$</td>
<td>Radius of a sphere [m]</td>
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ABBREVIATIONS AND SYMBOLS

r
Radius of the PBR under the assumption of a cylindrical PBR [m]

T
Temperature [°C]

∆T
Temperature difference [°C]

T_1 to T_4
Temperatures of the measurement layers 1 to 4 [°C]

T_m
Input temperature [°C]

T_{out}
Output temperature [°C]

t
Time [s]

∆t
Length of a time step [s]

U
Inputs in the form of a Matrix

u
Inputs

V_i
Volume of layer i [m^3]

v
Velocity [m/s]

x
State variables

y
Model outputs

y_t
True outputs

Model Parameters and Variables

α_1
Describes the heat transfer coefficient between HTF and SM [kg/s]

α_{11}, c_{HS1}, v_{SM1}
First parameter set of the model with an additional second parameter set used during charging

α_{12}, c_{HS2}, v_{SM2}
Second parameter set of the model with an additional second parameter set used during discharging

α_2
Describes the heat transfer coefficient between SM and wall [1]

α_{HS}
Share of potentially exchanged heat between HTF and SM [1]
ABBREVIATIONS AND SYMBOLS

\( \alpha_{SW} \) Share of potentially exchanged heat between SM and wall [1]

\( \alpha_{WI} \) Share of potentially exchanged heat between wall and insulation [1]

\( \gamma \) Ratio of the heat capacities of contacting materials [1]

\( b_{SM} \) Represents the temperature change of the SM by heat conduction between layers [1]

\( b_{W} \) Represents the temperature change of the Wall by heat conduction between layers [1]

\( c_{HS} \) Describes the heat capacity ratio between HTF and SM \([(m^3s)/kg]\)

\( c_{HSc} \) Describes the heat capacity ratio between HTF and SM independent of the temperature \([(m^3s)/kg]\)

\( c_{HSc1} \) Describes the heat capacity ratio between HTF and SM independent of the temperature, omitting the volume of the layer \([s/kg]\)

\( c_{HST} \) Describes the temperature dependent heat capacity ratio between HTF and SM \([(m^3s)/(kgK)]\)

\( c_{HST1} \) Describes the temperature dependent heat capacity ratio between HTF and SM, omitting the volume of the layer \([s/(kgK)]\)

\( c_{SW} \) Describes the heat capacity ratio between SM and wall [1]

\( c_{WI} \) Describes the heat capacity ratio between wall and insulation [1]

\( n \) Amount of historic time steps used to calculate the moving average used to adapt the heat loss [1]

\( T_{equiHS} \) Equilibrium temperature between HTF and SM [°C]

\( T_{equiSW} \) Equilibrium temperature between SM and wall [°C]

\( T_{equiWI} \) Equilibrium temperature between wall and insulation [°C]

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<td>$T_{HTF}$</td>
<td>Temperature of the heat transfer fluid [$^\circ$C]</td>
</tr>
<tr>
<td>$T_{HTF_0}$</td>
<td>Initial temperature of the heat transfer fluid [$^\circ$C]</td>
</tr>
<tr>
<td>$T_I$</td>
<td>Temperature of the insulation [$^\circ$C]</td>
</tr>
<tr>
<td>$T_{SM}$</td>
<td>Temperature of the storage medium [$^\circ$C]</td>
</tr>
<tr>
<td>$T_{sur}$</td>
<td>Temperature of the surroundings [$^\circ$C]</td>
</tr>
<tr>
<td>$T_W$</td>
<td>Temperature of the wall [$^\circ$C]</td>
</tr>
<tr>
<td>$v_I$</td>
<td>Describes the heat loss from the insulation to the surrounding via conduction [1]</td>
</tr>
<tr>
<td>$v_{MA}$</td>
<td>Describes the heat loss, dependent on the moving average temperature of the HTF, from the HTF to the surrounding [1]</td>
</tr>
<tr>
<td>$v_{SM}$</td>
<td>Describes the heat loss from the SM to the surrounding via conduction [1]</td>
</tr>
<tr>
<td>$v_{SM_r}$</td>
<td>Describes the heat loss from the SM to the surrounding via radiation $[K^{-3}]$</td>
</tr>
<tr>
<td>$v_W$</td>
<td>Describes the heat loss from the wall to the surrounding via conduction [1]</td>
</tr>
<tr>
<td>$z$</td>
<td>Describes the radiation between layers $[K^{-3}]$</td>
</tr>
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1. Introduction

1.1 Motivation

Facing climate change and finite fossil fuels, there is increasing political and societal commitment to increase the share of renewable energy sources. However, one of the main disadvantages of most renewable energy sources is their dependence on the weather. Thus energy can not always be produced exactly when needed. To match energy demand and availability, energy storage systems are used, [2]. It is one of the key technologies to support decarbonization with a need of 310GW of grid storage and significant thermal energy storage potential, [3].

Thermal energy storage can be utilized to store heat until it is used. This strategy is applied in energy-intensive industries with high temperature demands, such as the glass and the steel industry. Packed bed regenerators (PBRs) are thermal energy storage systems using solid materials as a storage medium. Their advantages are low cost, non-toxic materials, and an operating temperature range of around 50 °C - 300 °C, [4].

To optimize the integration of PBRs in industrial processes, it is crucial to predict their behavior accurately, [5]. To achieve this goal, a variety of different models can be used. One criterion to differentiate models is whether prior knowledge (white box) or data (black box) is used to create the model. White box models allow for high reliability and good understanding and do not need specific process data. However, the accuracy is restricted by the available knowledge and no data driven improvements are implemented. Black box models allow for fast development and a good fit when the available data are accurate.
However, they may not offer reliable extrapolation and offer no insights into the process. Especially neural networks and deep learning are rising in popularity due to increasingly available data and computing power. Examples range from creating a plausible high resolution image from a low resolution image [6] to lipreading [7]. Grey box models combine prior knowledge and data in an application-specific way to generate a model that achieves the desired model features. Dependent on the application, grey box model properties lie somewhere between the white box and black box model features. One commonly used approach is mechanistic grey box modeling. Hereby, equations based on physical knowledge are used and some parameters are optimized using data.

1.2 Aim

This thesis aims to create an accurate and reliable grey box model of a PBR situated at the TU Wien. Further beneficial model attributes are an accurate simulation of the internal temperature distribution and fast computational time. To achieve those model properties, a suitable grey box modeling approach is identified and implemented. Finally, to assess the attributes of the final grey box model, it is compared to an already existing white box model and an already existing data-driven neural network model.
2. Thermal Energy Storage

This chapter gives an overview of different energy storage systems. Focusing on thermal types, packed bed regenerators (PBRs), and the underlying heat transfer mechanisms of PBRs are described.

2.1 Energy Storage Types

In order to conserve energy between its production and consumption, energy storage systems perform three different processes: charging, storing, and discharging, [2]. Their applications range from stabilizing the power grid to ensuring continuous power supply to small devices via batteries such as phones, [8]. Therefore, energy storage systems are categorized by many different criteria. Table 2.1 shows different possible categorizations.

Especially energy storage to stabilize the grid is increasing in importance. The ambitious goals of the European Union presented in the energy road map 2050 include a target of approximately 50% renewable energy generation, [9]. Due to their volatile energy generation, more energy storage capacity is needed. An increase in renewable energy sources also increases the need for long-term energy storage, [10].

<table>
<thead>
<tr>
<th>Physical</th>
<th>Energetical</th>
<th>Temporal</th>
<th>Spatial</th>
<th>Economic</th>
</tr>
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<td>thermal</td>
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</table>
2.2 Thermal Energy Storage

Thermal energy storage (TES) either uses a sensible, latent, or thermo-chemical storage medium. Figure 2.1 shows a detailed breakdown of different types.

Sensible heat storage mediums/systems store energy in the form of heat by temperature increase. Water, thermal oil, metals, earth materials (sands, rocks), molten salt, and concrete are used as storage materials. Their thermal stability makes them an ideal candidate for high-temperature storage. One drawback is the low heat capacity compared to latent heat storage systems, especially given a small operating temperature range. Examples of sensible heat storage systems comprise domestic hot water storage, molten salt storage systems for solar thermal energy production, and PBRs for industrial applications. [4]

Latent heat storage mediums/systems store energy via latent heat. The heat is stored/released due to the phase change of the storage material. Mostly the phase change from solid to fluid and vice versa is used. Storage materials include organic (e.g. paraffin, esters) and inorganic (e.g. salts, salt hydrates) materials, [4]. Latent heat storage allows for a constant discharge temperature but typically has poor thermal conductivity. Use cases are e.g. building applications to reduce the temperature fluctuations during the day and incorporation into textiles to protect against high or low temperatures, [12].

Figure 2.1: Breakdown of different TES variants, in accordance with [11]
In thermo-chemical storage, heat can be stored or released by endotherm or exotherm chemical reactions. Used materials comprise e.g. magnesium or calcium hydroxides. Thermo-chemical storage has the highest energy storage density and long storage times with small heat loss. However, the storage material may undergo sintering during charging. The technology is currently in its laboratory state. [4]

2.3 Packed Bed Regenerators

PBRs are one kind of sensible TES. Their storage medium (SM) is arranged in a hollow structure as a packed bed. A heat transfer fluid (HTF) transfers heat into and out of the SM. Figure 2.2 shows the basic concept of a PBR. Rocks of different sizes can be used as SM and air, water, or oil can be used as HTF. One exemplary use case of PBRs is the application in concentrated solar power plants, whereby a pilot-scale demonstration plant is already built and an industrial design exists, [13].

![Figure 2.2: Packed bed regenerator](image-url)
2.3.1 Heat Transfer in a PBR

There are three different modes of heat transfer: Conduction, convection, and radiation. Conduction describes the energy transfer of adjacent molecules. In a PBR conduction takes place, for example, inside the SM, or in the walls. The heat flux density can be described by Fourier’s Law \( \dot{q} = -\lambda \nabla T \), with the thermal conductivity \( \lambda \), the nabla operator \( \nabla \) and the temperature \( T \). The energy balance and Fourier’s Law for the volume element of a stagnant, incompressible medium lead to \( \rho c_p \frac{\partial T}{\partial t} = -\nabla \dot{q} \), with the density \( \rho \) and specific heat capacity \( c_p \). Constant \( \lambda \), \( c_p \) and \( \rho \) lead to the heat equation \( \frac{\partial T}{\partial t} = \kappa \nabla^2 T \), with \( \kappa = \frac{\lambda}{\rho c_p} \) being the thermal diffusivity. \[14\]

Convection describes the heat transport in a fluid. It is a combination of the transported heat due to the movement of the fluid and conductive heat transport. Convection plays a fundamental part in the PBR since it describes heat transfer between the HTF and materials contacting the HTF (SM, wall, and pipes). It also describes the heat loss to the surrounding air. Convective heat transfer can either be free or forced. In the case of free convection, the flow of the fluid is a result of differences in density. In the case of forced convection, the flow is caused by external sources. The rate of heat transfer of a solid to a fluid can be described by \( \dot{q} = \alpha \Delta T \), with \( \alpha \) being the heat transfer coefficient and \( \Delta T \) the temperature difference. In the case of free convection, \( \alpha \) is a function of the temperature difference \( \Delta T \), because a different \( \Delta T \) causes a different density distribution and, therefore, a different flow caused by gravity. \[14\]

Further, heat is transferred by radiation. The amount of power radiated is described by the Stefan-Boltzmann law, which states \( P_{\text{rad}} = \sigma \epsilon A_{\text{surf}} T^4 \), in its simplest form. \( \sigma \) is the Stefan-Boltzmann constant, \( \epsilon \) is the emissivity, \( A_{\text{surf}} \) the surface of the object, and \( T \) the surface temperature of the object. \[14\]

2.3.2 HTF Flow in a PBR

The main cause of the flow of the HTF in PBRs is forced convection. It is caused by a pressure difference between the HTF that enters the PBR and the HTF that exits the PBR.
In the case of air as the HTF, this pressure difference can be generated by a fan. The air flow through a packed bed is mostly constant across its cross-section. However, in close range to the wall, the porosity of the packed bed is higher because the particles cannot fill up the space as efficiently. Therefore, the air has less flow resistance which results in a higher velocity in the proximity of the wall, [15]. The velocity close to the wall can be up to 4 times the average velocity, [15].
3. Grey Box Modeling Theory

This chapter gives a general introduction and overview of grey box modeling and related concepts. Modeling approaches can be characterized by many different metrics. One categorization is whether prior knowledge (white box) or data (black box) is used. A combination of prior knowledge and data-driven modeling is called grey box modeling. Since, white, grey, and black box models only refer to the use of prior knowledge/data during the modeling process, they may use similar model structures. Different models are discussed in the best fitting section of white, grey, and black box modeling. First, white and black box modeling is described. Optimization is discussed in the black box section, since optimization is an integral part of black box modeling. Thereafter, grey box modeling, different grey box modeling approaches, and exemplary use cases are described.

3.1 White Box Modeling

A white box modeling approach is used to develop a model that is only based on prior/physical knowledge. Therefore, white box models are also referred to as physical models. To create a white box model, the underlying system mechanics have to be known. These underlying mechanics can for example be physical laws (e.g. classical mechanics, Kirchoff’s Law). [16]

One area of white box modeling is computational fluid dynamics (CFD). During CFD simulations governing differential equations are solved. The governing equations for a fluid system are the Navier-Stokes system of equations that describe conservation of mass, impulse, and energy. Those differential equations can be solved numerically using finite difference
methods, finite element methods, or finite volume methods, [17].

3.2 Black Box Modeling

Black box models are only based on data of the underlying system and not on prior knowledge. System identification describes the development of a mathematical model of system behavior based on measured input and output values and can be used for the creation of black box models, [16]. Based on the underlying system, different modeling approaches are suitable. Some of the distinguishing system features are linearity or non-linearity, the number of inputs, the number of outputs, and continuous or discrete models. First, an overview of the steps of system identification is given. Second, different identification methods are discussed. This work only discusses dynamic systems in which system inputs cause a reaction in the system output.

3.2.1 General Approach for System Identification

The approach to system identification can be broken into 4 different steps [16]:

1. **Experiment planning:** The input signal is chosen to stimulate the system. The input signal is selected to have enough broadband to stimulate the system in its frequency domain.

2. **Data measurement:** During the system experiments, the data has to be captured. It is further examined for outliers and gaps.

3. **Choosing the identification method:** The identification method can for example be based on non-parametric models or on parametric models.

4. **Model validation:** The model validation depends on its planned application. It determines whether the model sufficiently achieves its desired goals. Finding a suitable model structure is usually an iterative process.
3.2.2 Model Structures

The success of a specific model structure is highly dependent on the underlying system. If the underlying system is linear and time-invariant, it can be for example modeled with transfer functions and state-space models. In the case of a linear system, the models are convertible into each other. If the underlying system is non-linear, it is important to choose the right model structure. There are a wide variety of different non-linear models. In general non-linear models can be described by input-output-models or state-space models. Examples of non-linear input-output-models are non-linear autoregressive moving average models with exogenous inputs (NARMAX) and neural network (NN) models.

Applications of NN models range from mastering the game of GO [18] to developing self driving cars [19] and have already been used to model the behavior of packed bed regenerators [20]. Therefore a quick overview of NN is given.

Figure 3.1 shows a typical structure of a NN. Each circle represents a node. The structure is divided into vertical layers. The layer shown on the left side is called the input layer. The layer on the right is called the output layer. The layers in between are called hidden layers. Each layer can comprise an arbitrary number of nodes. The nodes are connected with other nodes, shown by arrows. In feed-forward neural networks, the outputs of one layer are used as input of the next layer. The arrows indicate which node output is used as input for the nodes in the next layer. Every node creates an output based on its weighted inputs, its activation function, and individual bias. [21]

During the training of NNs, different weights and biases are optimized to better fit the model outputs to the measured outputs. The effectiveness of a NN and its training is highly dependent on so-called hyperparameters. Hyperparameters are parameters that are chosen by the modeler, e.g. the number of input nodes or the number of hidden layers.

One of the main advantages of NNs is that they can be used for a wide variety of problems. Further, the models are computationally fast when trained. However, the training can be computationally intensive and may require a large data set. Also, due to the complexity of NNs, its behavior may not be predictable for inputs vastly different from its training
3.2.3 Optimization Techniques

Optimization describes the formulation and solution of an optimization problem, [22]. It is needed during the black box and grey box model creation since both use data-driven modeling techniques. Different optimization techniques have differing suitability dependent on the optimization problem. Optimization algorithms can be categorized by whether they use derivatives. Examples of algorithms using derivatives are least squares, recursive least squares, Newton’s method, Gauss-Newton’s method among others. Least square methods are the most fundamental methods and are discussed below. However, when derivatives are not available or otherwise not desirable, other algorithms have to be used. Therefore, the Nelder-Mead Simplex Algorithm is discussed below, due to its wide use.

Least Squares

One of the most basic concepts of parameter optimization consists of the ordinary least squares method. This method has been described, for example, in [16] or [23]. The least
Grey Box Modeling Theory

Black Box Modeling

square method minimizes the squares of the model errors $e$. For the linear least squares method a set of input variables $u$ for a data point with a true scalar output $y_t$ are given. A linear model $y = up$ is used, whereby $p$ are the model parameters and $y$ is the model output. The error of one data point equals $e = y_t - up$. For a plurality of data points this leads to:

$$e = y_t - Up$$

with $U$ being inputs in the form of a matrix. The parameters $p$ are optimized by minimization of the square of the errors:

$$e^T e = (y_t - Up)^T(y_t - Up).$$

Through derivation with respect to $p$ of the above formula and setting it equal to zero, the optimized parameterset $\hat{p}$ can be found to be:

$$\hat{p} = (U^T U)^{-1} U^T y_t$$

In case of a non-linear model, non-linear least square method can be used to minimize a cost function $cost(p) = \sum e^2(p)$. An initial set of parameters $p$ can be iteratively improved via $p^{k+1} = p^k + \Delta p$, with $\Delta p$ being the shift vector. This method is used for example in the Gauss-Newton algorithm in which $\Delta p$ is calculated via the use of Jacobi matrices.

Nelder-Mead Simplex Algorithm

The Nelder-Mead Simplex Algorithm, also called downhill simplex method, was published by Nelder and Mead [24]. It allows for optimization without the use of derivatives. It is an iterative approach beginning with a set of starting parameter values, which shall be optimized. The algorithm allows for a broad spectrum of applications and is widely used. However, the starting parameter values have to be chosen carefully, because they
may influence the optimized values of the parameters.

The method is used for an unconstrained minimization of a function \( f \) in \( m \) parameters \( p_1, p_2, \ldots, p_m \) with the output value \( y \). A simplex is defined by \( n+1 \) points \( P_1(p_{1,1}, p_{2,1}, \ldots, p_{m,1}) \), \( P_2(p_{1,2}, p_{2,2}, \ldots, p_{m,2}), \ldots, P_{m+1}(p_{1,m+1}, p_{2,m+1}, \ldots, p_{m,m+1}) \). In general, \( P_i(p_{1,i}, p_{2,i}, \ldots, p_{m,i}) \) for \( i = 1, 2, \ldots, m+1 \). \( h \) is the index of the point with the highest \( y \) value, so \( y_h = \max(y_i) \). \( \bar{P} \) describes the centroid of the points \( P_i \) without the point with the highest \( y \) value, \( P_h \). To find a minimum of the function, the point \( P_h \) is substituted by another point in the following way:

Beginning with reflection \( P^* \) of \( P_h \), whereby \( P^* = \bar{P} + \zeta(\bar{P} - P_h) \), \( \zeta \) is called the reflection coefficient and is a positive constant (e.g. 1). This means that the point \( P_h \) is moved to \( \bar{P} \) and beyond, the distance beyond being longer (or shorter) than the initial distance by a factor \( \zeta \). With \( y^* = f(P^*) \) four cases are differentiated:

First, \( y^* \) is a new minimum. In this case the point is moved further (expansion), by a factor \( \theta > 1: \) \( P^{**} = \bar{P} + \theta \zeta(\bar{P} - P_h) \) (e.g. \( \theta = 2 \)). If \( y^{**} = f(P^{**}) \) is lower than \( y^* \), \( P_h \) is substituted by \( P^{**} \), else by \( P^* \).

Second, \( y^* \) is not a new minimum, but is still smaller than at least one of the remaining \( y_i \), \( y^* < \max(y_i) \) for \( i \neq h \). In this case \( P_h \) is substituted with \( P^* \).

Third, \( y^* \) is larger than all of the remaining \( y_i \), but lower than \( y_h \), \( y^* > \max(y_i) \) for \( i \neq h \) and \( y^* < y_h \). Hereby, the point \( P^* \) is moved back towards \( \bar{P} \) (contraction). The new distance is by a factor \( \frac{1}{\eta} \) (0 < \( \eta < 1 \), e.g. 0.5) shorter than the initial distance \( \bar{P} - P^* \): \( P^{***} = \bar{P} + \eta \zeta(\bar{P} - P_h) \).

Fourth, if \( y^* \) is larger than \( y_h \), meaning a worse \( y^* \) is found, contraction is used on the initial point \( P_h \), it is moved towards \( \bar{P} \) but not beyond: \( P^{**} = \bar{P} - \eta(\bar{P} - P_h) \).

This is repeated until a termination condition is fulfilled. Many different termination conditions can be used. One of them compares the root mean square error to a predetermined value. When the error falls below the predetermined value, the optimization is stopped.
3.3 Grey Box Modeling

Grey box modeling is characterized by the usage of prior knowledge and data during the modeling process, [25]. The possibility of any combination of prior knowledge and data allows for a wide variety of outcomes. This also allows a grey box model to align more with the properties of a black box model or a white box model. Therefore, grey box models have different shades of grey [26], as indicated in Figure 3.2.

![Figure 3.2: Grey box models may have a black or white tint](image)

3.3.1 General Approach for Grey Box Modeling

The grey box approach is best suited when there is a benefit in combining prior knowledge and data. The procedure of creating a grey box model is in many cases iterative. Different model structures can be adapted or overthrown depending on their results. In general, the designer decides a starting model structure based on the available knowledge of the underlying system and its relevant properties. Further, the modeler decides what set of parameters are optimized using real-world data. Then the obtained model is trained on the real-world data, to find the values of the parameters that are optimized. Based on the results of the trained model, the model structure or parameters can be changed. The new model with a different structure or parameters can be evaluated against the previous model. The new model is used as a new reference if it shows improved results and is discarded otherwise. The parameter sets and model structures can be altered until a sufficiently good model is found. [27]
3.3.2 Grey Box Branches

Since grey box modeling allows for a wide variety of different models, efforts were made to categorize them into branches. However, different sources have different nomenclatures and different categories, compare [26] and [28]. Nevertheless, an overview of those branches described in [28] is given to show an overview of the possibilities.

**Constrained Black Box Identification**

Constrained black box identification uses a black box model which is modified to restrict its scope based on prior knowledge. For example, the model may have parameter limits or limits on the static gain of a model. In an extreme case, this modeling approach can consist of a black box model where, for example, only one output is given an upper limit. Further, steady-state information can be used to constrain the identification of non-linear models, [29].

**Semi Physical Modeling**

Semi physical modeling uses physical insights to transform a non-linear optimization problem into a linear optimization problem. This decreases the modeling difficulty for the black box model. In cases where the non-linear behavior is known, Hammerstein-, Wiener- or other block-oriented models can be used. For example, Forsell and Lindskog [30] used a semi physical model for a tank level modeling problem. Hereby, the optimization problem is reduced to be linear in the parameters, by setting the outflow in proportion to the square root of the tank level.

**Mechanistic Modeling**

The mechanistic modeling procedure includes a basic physical model which is derived from prior knowledge where some parameters or functions can be estimated by parameter fitting. The approach may be iterative. Hereby, a first simple model is created, which can further
be refined as long as an improved model can be found, [28]. In Section 3.3.5, a mechanistic approach for a storage vessel and a mechanistic approach of a biochemical process with a combined identification process is discussed.

**Hybrid Modeling**

Hybrid models use a white box model and a black box model. The results of one model are either used as input of the other model or the results of the models are combined to one final result. For example, it is possible to combine a semi physical model with a NN, [30]. This combination improves the previously mentioned tank level simulation model in comparison to only using a NN or only the semi physical model, [30].

**Distributed Parameter Modeling**

Distributed parameter modeling can be used when a system of PDEs should be modeled. It offers a systematic approach for grey box identification of distributed parameter models.

### 3.3.3 Grey Box Properties

Grey box properties are generally in between the properties of white box models and black box models, as the name suggests. Table 3.1 shows the properties of white and black box models. The information sources for grey box models include qualitative knowledge (rules), some insight and some data. All other grey box properties highly depend on the specific model. For example, a constrained black box model resembles mostly black box properties. However, a hybrid model may resemble white box or black box properties depending on the specific implementation. Generally, the grey box properties lie somewhere in between the white box and black box properties, [31]. Due to the wide range of possible grey box model properties, they are not shown in Table 3.1.
Table 3.1: Different attributes of white and black box models, according to [31]

<table>
<thead>
<tr>
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<th>Black box</th>
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<tr>
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<td></td>
<td>processes</td>
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3.3.4 State Space Models

State space models are mathematical models that use first order differential equations to relate inputs $u$, outputs $y$ and state variables $x$. The following State space models can be linear or non-linear and continuous or discrete. A linear model can be described in the continuous case by [16]:

$$\dot{x}(t) = Ax(t) + Bu(t) \quad (3.4)$$
$$y(t) = Cx(t) + Du(t). \quad (3.5)$$

Whereby $A$ is called state matrix, $B$ is called input matrix, $C$ is called output matrix and $D$ is called feed-through matrix. In the non-linear continuous case the model equations are [16]:

$$\dot{x} = f(x(t), u(t)) \quad (3.6)$$
$$y = h(x(t), u(t)). \quad (3.7)$$
Figure 3.3: Non-linear state space model, in accordance with [16]

Figure 3.3 shows a representation of the non-linear continuous case. The model equations for the non-linear discrete case with time steps k are [16]:

\[
\begin{align*}
    x(k+1) &= f(x(k), u(k)) \\
    y(k) &= h(x(k), u(k)).
\end{align*}
\] (3.8) (3.9)

State-space model equations can be fully derived using prior knowledge (white box). They can also be created using only data (black box). A black box model can be achieved in the case of linear time-invariant systems using the Ho-Kalman algorithm, which creates a minimal realization of a state-space model based on the external description, [32]. Further, state-space models allow for the creation of grey box models by using both prior knowledge and data. One grey box approach for state-space models consists of creating the model structure based on prior knowledge and fitting unknown model parameters using data (mechanistic modeling).

### 3.3.5 Grey Box Application

Depending on the underlying system, different grey box models and optimization methods should be used. To achieve a deeper insight into the grey box modeling process, examples are described below for different simulation tasks.
Grey Box Model of a Biochemical Process

C. de Prada et al. [33] described different grey box models for a process called Acetone-Butanol-Ethanol fermentation process. The basic equations of the process were known. They comprised the mass balances for the cells, substrate, and products. The five equations had five unknown parameters. Further, the growth rate of the cells was unknown. However, there were several approximations of the growth rate. Further, it was known that the growth rate depends on the biomass, substrate, and solvent concentrations. However, the exact relations were unknown.

Two different approaches were used. First, a mechanistic grey box approach was chosen. An approximation function of the growth rate was selected and the unknown parameters were optimized. Difficulties in finding an accurate formula for the growth rate, lead to problems in realizing an accurate model. Using prior approximations of the growth rate and parameter optimization was not sufficient, because the approximation of the growth rate was not accurate.

The second approach considered the growth rate as an optimization parameter for every time step. To prevent large jumps in the growth rate, the cost function penalized changes in the growth rate between time steps. Through minimizing the cost function, the parameters and the growth rate of every time step were optimized. Having values for the growth rate for every time step allowed for the use of automatic learning of algebraic models to find a function for the growth rate.

Even though both approaches were grey box modeling methods, the second approach was superior. First, the results achieved with the second approach were more accurate than the ones achieved by the first approach. Second, after the basic equations were expressed no detailed knowledge about the growth rate had to be known. Third, the assumption of the growth rate as parameters saved computational time and prevented the trial and error of the implementation of different growth rates.
Grey Box Modeling Theory

Grey Box Model of a Thermal Storage Vessel

Ridder and Coomans [34] described a mechanistic modeling approach, which they called a parametric grey box model, with a non-linear optimization problem. Their main goal was to find a model that can be applied to a wide range of thermal storage vessels with no model structure change. Only parameter settings shall be changed based on the given operational data of the storage vessel.

A one dimensional model was used to calculate the temperature change of the water in the thermal storage vessel. The change in the temperature was dependent on four terms. The first term described the heat exchange between corresponding layers and the heat loss to the surrounding. The second term described the draining of hot water and, also, an inflow of cold water. The third term described heating via heating devices. The fourth term described the mixing of layers. The mixing of layers was only considered if a temperature inversion occurs, meaning when a lower layer had a higher temperature than the corresponding upper layer. This resulted in a lower density in the lower layer, leading to a current caused by gravity. Therefore, the fourth term equaled zero, when no temperature inversion was present.

The squared temperature difference of each measurement layer was used as cost function. For the parameter estimation, a Markov-Chain-Monte-Carlo method was chosen. The Markov-Chain-Monte-Carlo method allows for the optimization of non-differentiable systems.

This simple mechanistic approach delivered a structure with different parameter values for four different vessels. The grey box approach achieved accurate results for all considered vessels.
4. Experimental Setup

The development of the grey box model in this thesis is based on a packed bed regenerator (PBR) situated at the laboratory of the Institute for Energy Systems and Thermodynamics (IET) at the TU Wien. As the creation of a grey box model requires knowledge of the physical system, it is discussed in detail. The design, components, and operation modes of the PBR are described in the first section. In the second section, measurements of the charging and discharging cycles are discussed.

4.1 Design of the PBR

The basic design of the investigated PBR has been created in the course of a masters thesis by Drochter, [35]. The thesis comprises a detailed description of the parts used and the interested reader may look there for further details. A redesign took place in the course of another master thesis by Rasinger, [36]. Therein the data sets of the PBR were created, which were used for the development of the grey box models. A brief overview of the design and the most important parts is given below.

The PBR is a sensible energy storage system, that uses a packed bed of gravel to store heat. The gravel is stored in a storage vessel, which is approximately 2 meters high. To transfer the heat into and out of the gravel air is blown through the packed bed. As shown in Figure 4.1, air is getting aspirated by the fan and the air passes through a mass flow sensor of the PBR. Before and after the mass flow sensor there are straight pipes to reduce the turbulence, enabling a more precise measurement. Afterward, the air passes through an air heating register in which the air can get heated. Thereafter, the air flows into the
storage vessel and through the packed bed. Lastly, the air leaves the vessel and the air flows to the outside.

4.1.1 Main Components

A brief summary of the main components of the PBR is given below.

Fan

The fan Aerzen Roots can achieve a flow rate of up to 0.035 m³/s and is used to create the pressure difference needed to sustain the air flow through the packed bed.

Air Heating Register

The air heating register was produced by Carlo Loysch GmbH and the model number is HRR AK-16-10-107-15kW. This model comprises 12 heating coils with a heating power of up to 1250 kW. The heating coils can reach a temperature of up to 650 °C and transfer the
Experimental Setup

Design of the PBR

Figure 4.2: Detailed view of the storage vessel, adapted from [5]

heat to the air through convective heat transfer.

Storage Vessel

The storage vessel used is made of steel and has the form of a truncated cone with its smallest diameter at the bottom. When the storage vessel gets heated, it expands and the storage material fills up the additional space. When the storage vessel gets cooled, the storage vessel is forced to contract and tensions arise. The cone shape allows the storage material to move and to lessen the tensions. The exact dimensions of the storage vessel can be seen in Figure 4.2.

The storage vessel comprises four modules. First, the lowest module is intended to position and support the upper modules. Air enters the storage vessel via this first module. The two central modules are measuring modules. Each comprises two measuring layers and four temperature sensors per layer. A grid is placed between the first module and the lower measuring module to support the storage medium (SM). On top of the upper measuring module, a hopper connects the storage vessel to the outgoing pipes. SM is only placed
inside the measuring modules.

Storage Material

In the course of the operation of the PBR, different storage materials have been used. However, for the purpose of this thesis, only the data sets of one storage material are considered. The storage material comprises gravel with an average particle diameter of 6mm. A list of the most important material properties can be found in Table 4.1.

<table>
<thead>
<tr>
<th>Material properties</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>average particle diameter</td>
<td>6</td>
<td>mm</td>
</tr>
<tr>
<td>density</td>
<td>2590</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>porosity</td>
<td>0.375</td>
<td>1</td>
</tr>
<tr>
<td>bulk density with porosity of 0.375</td>
<td>1619</td>
<td>kg/m$^3$</td>
</tr>
<tr>
<td>storage mass in reactor</td>
<td>595</td>
<td>kg</td>
</tr>
<tr>
<td>specific heat capacity</td>
<td>840</td>
<td>J/(kgK)</td>
</tr>
<tr>
<td>thermal conductivity</td>
<td>1</td>
<td>W/(mK)</td>
</tr>
</tbody>
</table>

Insulation

The pipes and the vessels are covered in mineral wool for improved thermal insulation. The pipes are covered with a thickness of 100 mm and the thermal vessel is covered with a thickness of 200 mm. In addition to the mineral wool, an aluminum layer is added to reduce thermal radiation. The thermal conductivity of the mineral wool equals 0.085 W/(Km).

4.1.2 Measuring Devices

The data received by the measuring devices are an integral part of our modeling efforts and, therefore, the measuring devices are considered in detail.
Experimental Setup

Design of the PBR

The used temperature sensors were manufactured by Kobold Messring GmbH and are named TTE-164-102-K1-E. They are screw-in thermocouples with a tube of stainless steel in which the thermocouples are positioned. Figure 4.3 shows an illustration of the thermocouples used.

Mass Flow Sensor

The mass flow sensor uses the calorimetric principle. The model installed is named t-mass A 150 produced by Endress & Hauser GmbH. For this type of mass flow sensor, it is important, that the flow of the measured fluid is undisturbed. Therefore, a straight pipe with a constant diameter is leading into the sensor and out of it.

Differential Pressure Sensor

A differential pressure sensor is used to measure the difference in pressure between the air flowing into and out of the storage vessel. The model used is called Gems 5266-250-D-AC-Ti-C and is produced by Gems Sensors and Controls.
4.1.3 Arrangement of the Measuring Devices

Figure 4.4 shows the general arrangement of the measuring devices. The exact height of the four measurement layers inside the SM of the PBR can be seen in Figure 4.2.

The temperature sensors are screwed into the storage vessel. The sensors extend into the vessel for a length of approximately 9 cm. Figure 4.5 shows the placement of the sensors in the vessel. Since the distance of the sensor to the vessel wall is constant and the diameter of the vessel increases with its height, the sensors are placed further from the vessel center for higher measuring layers. The four temperature sensors of each layer are spaced evenly across the circumference.
4.1.4 Operating Modes

The PBR has two different operating modes called continuous current flow and counter current flow. During continuous current flow operation, the heat transfer fluid (HTF) flows through the bottom to the top during charging and discharging. Figure 4.6 shows the flow of the HTF during continuous current flow operation.

During counter current flow operation, the hot air enters the reactor from the top during charging. The discharging air flows from the bottom to the top, as displayed in Figure 4.7.

4.1.5 Heat Transfer in the PBR

To further understand the PBRs behavior the most important heat transfer processes are discussed.

Heat Transfer between Heat Transfer Fluid and Storage Medium

The heat transfer between the HTF and SM is the process with the most transferred heat. The rate of heat flow can be calculated using \( \dot{Q} = \alpha A_{\text{con}} (T_{\text{HTF}} - T_{\text{SM}}) \), whereby \( T_{\text{SM}} \) describes the temperature of the SM, \( T_{\text{HTF}} \) the temperature of the HTF, \( A_{\text{con}} \) the
Figure 4.6: HTF flow during continuous current flow operation. Charging on the left, discharging on the right, [37]

Figure 4.7: HTF flow during counter current flow operation. Charging on the left, discharging on the right, [37]
contact surface and $\alpha$ the heat transfer coefficient. $\alpha$ is dependent on various parameters, most importantly the velocity of the HTF, the temperature of the HTF, and the particle diameter. In the design phase $\alpha$ is calculated to be around $37 \, W/(m^2 \cdot K)$, for a particle diameter of 30 mm, [35]. The temperature distribution inside the pebble is dependent on the Biot number, which expresses the temperature deviation inside a body while its surface is heated or cooled. It can be calculated as the ratio between the internal and external heat transfer resistance: $B_i = \frac{R\alpha}{\lambda}$, with the Radius of the sphere $R$ and the thermal conductivity $\lambda$. A Biot number smaller than 0.1 implies that the difference between the surface temperature of the sphere and the core temperature of the sphere is at any given moment smaller than 9% of the initial temperature difference, [14]. Due to the small radius the Biot number is considered small.

**Heat Transfer between the SM, HTF and Wall**

Heat gets transferred between the casing and the HTF or the SM. The SM is in direct contact with the wall and heat can be conducted between them. However, the contact surface between the SM and the wall is small. Further, the HTF is also in contact with the wall and heat is transferred via convective heat transfer. Additional heat transfer occurs through radiation which means proportional to the fourth-order of the temperature.

**Heat Loss to the Surrounding**

Heat loss occurs mainly through heat conduction at the outer surface area of the PBR and is only dependent partly on heat radiation. The casing conducts the heat to the isolation. The isolation transfers the heat to the surrounding air. This results in heat loss to its surrounding. Across five conducted experiments, during which the input temperature of the HTF ranged from 50-250 °C and the HTF mass flow from 150 to 250 kg/h, the heat loss was in a range between 1-2 % per hour with regard to the stored heat, [37].
Heat Conduction between Pebbles

Each pebble is in contact with other pebbles and at all those contact areas heat can be conducted. The contact surface of one pebble to another is small and the temperature difference between each adjacent pebble is also small. Therefore, in comparison to the heat transfer between the HTF and the SM, this effect is considered negligible.

4.2 Charging and Discharging Cycle of the PBR

![Graph showing temperature over time during multiple charging cycles]

Figure 4.8: PBR behaviour during multiple charging cycles

Typical charging and discharging cycles of the PBR can be seen in Figure 4.8. The input temperature of the air, which is measured directly under the storage vessel, is changing rapidly at the beginning of the heating process and is reaching an equilibrium about 150 min after the beginning of the charging cycle. This is due to the fact, that the heating register and the pipes take time to warm up. When the heating register gets turned off,
the change in temperature of the incoming air occurs rapidly. However, the change slows down due to the remaining heat of the heating registers and pipes, which is transferred to the air. The temperature profile of the input temperature $T_{in}$ and the mass flow $\dot{m}$ of the air flowing into the storage vessel are needed for an accurate modeling approach. $T_1$ to $T_4$ are the temperatures measured in the measuring layers 1 to 4. The values shown are the average of the four temperature sensors of each layer. The temperature of $T_4$ should be in between the temperature $T_3$ and $T_{out}$ most of the time. However, $T_4$ does not behave as expected as seen in Figure 4.8. This suggests some errors in the measurement of the internal temperatures.

Furthermore, the individual sensors of a measurement layer measure different temperatures. The temperature profiles of each individual temperature sensor can be seen in Figures 4.9 to 4.12. Here e.g. $T_{12}$ denotes the second sensor of the first measuring layer.

Most sensors of one layer return similar temperatures. Even though the PBR is radially symmetric, the measured temperatures sometimes vary substantially within one layer, as Figure 4.9: Temperature of the first measurement layer
Experimental Setup

Charging and Discharging Cycle of the PBR

Figure 4.10: Temperature of the second measurement layer

Figure 4.11: Temperature of the third measurement layer
Experimental Setup

Charging and Discharging Cycle of the PBR

Figure 4.12: Temperature of the fourth measurement layer

seen in Figure 4.10 and Figure 4.12. One explanation is that the air flow is not symmetrical, [37]. This could lead to faster temperature changes in places with more air flow, due to a non-homogeneous packed bed. Figure 4.13 shows the potential formation of an air channel and its relation to the sensor arrangement. If the explanation of an acentric airflow was correct, we would expect all sensors on the same side of the reactor to behave similarly. However, the measurements on one side, i.e. $T_{12}, T_{22}, T_{32},$ and $T_{42},$ show different behaviors. In particular, $T_{12},$ and $T_{32}$ behave in accordance with the other sensors of their layers. Sensor $T_{22}$ provides lower temperatures while charging. Meanwhile, sensor $T_{42}$ shows higher temperatures while charging. Thus, if an air channel were present, it would need to be substantially curved. Therefore, an asymmetric air channel gives no simple explanation of the occurring phenomenon.

Another explanation could be that some of the measurements are inaccurate. One indication is that only sensor $T_{22}$ diverges significantly from the other three sensors of the second layer. Second, the average temperature of layer 4 lags the output temperature. These two factors strongly question the accuracy of the sensors.
Figure 4.13: Model of an acentric air flow in measurement layer 4, adapted from [37]
5. Grey Box Modeling of the PBR

The aim of the grey box modeling of the packed bed regenerator (PBR) is to accurately and robustly simulate the output temperature of the heat transfer fluid (HTF) based on the input temperature and the mass flow of the HTF. An iterative mechanistic model, which uses prior knowledge to create a model structure and uses data to optimize the parameters, is chosen. This decision is based on prior physical knowledge of the PBR, which allows the creation of a suitable model structure to accurately predict the output of the PBR with high robustness. Further, the small set of parameters in a mechanistic model, allows for accurate parameter fitting, even when the amount of data is limited. The first basic model structure only considers the heat transfer between the HTF and storage medium (SM). To achieve a better fit, an iterative approach is used to allow for changes in the model structure and parameters. Those changes comprise data driven changes, as using different parameter sets dependent on operating conditions or using the moving average of the SM temperature to adapt the heat loss. Physically driven adaptions comprise the implementation of heat transfer between layers, temperature dependent heat capacities and additional parts of the model (wall, insulation).

5.1 Basic Model Structure

In the first step, only the most basic characteristics of the PBR are modeled. Since the PBR is a dynamic system, sufficiently accurate state representation as well as an accurate change of the state variables and the corresponding output is necessary to accurately predict its behavior. The model of the PBR has two input parameters, namely the input temperature
and mass flow of the HTF, summarized by the input vector $u$. The desired output of the model $y$ is a scalar, namely the output temperature of the HTF. Figure 5.1 shows a representation of a discrete model, whereby $x$ describes the state variables of the PBR. The function $f(x, u, p)$ returns the output and $h(x, u, p)$ returns the change of the state variables and $k$ describes the time step. $f(x, u, p)$ and $h(x, u, p)$ depends on a parameter set $p$ that characterizes the behavior of the PBR. The functions $f(x, u, p)$ and $h(x, u, p)$ and the model parameters $p$ are derived from prior knowledge, whereby the values of $p$ are derived from data. The function can further comprise other known parameters such as the shape of the PBR.

5.1.1 State Representation of the Basic Model

In general, the relevant state variables of the PBR comprise the temperature distribution in the SM, HTF, wall, pipes, isolation, surroundings, and everything else in thermal contact. Parts with small heat capacities and little thermal interactions like the pipes do not influence the output temperature of the HTF as much as parts with large heat capacities and high thermal interactions like the SM. To achieve a simple model, the state variables of the model contain only the most important parts. Therefore, for the basic model, only the temperature distribution of the SM is used. To further simplify, the temperature is assumed to be homogeneous in horizontal layers. Those horizontal temperature layers are connected in series in the model. In a real-world interpretation, they are stacked vertically above each other to describe the PBR. Therefore, the state variables $x$ list the temperature of each layer. The temperature change in the layers and the output temperature of the HTF can be modeled based on the input temperature of the HTF and its state variables $x$. This
results in a model structure with layers as shown in Figure 5.2. \( u(k, i) \) describes the inputs of the layer \( i \) at the time step \( k \). Whereby \( l \) denotes the number of layers. The output of a layer is used as input for the next layer.

### 5.1.2 Model Equations

In the first basic model, the model equations are based only on the heat transfer between the HTF and the SM and the heat loss to the surrounding. All other effects are neglected for now.

#### Heat Transfer between HTF and SM

The most important model equations describe the heat transfer between the HTF and the SM. The heat transfer between the HTF and the SM is modeled via the convective heat transfer described in Section 4.1.5 - it is assumed that the Biot number is 0. Using Newton’s law of cooling the following equation can be used:

\[
\begin{align*}
\frac{d}{dt} \begin{pmatrix}
T_{HTF}(t) \\
T_{SM}(t)
\end{pmatrix} &= \begin{pmatrix}
a_1 & a_1 \\
a_2 & -a_2
\end{pmatrix} \begin{pmatrix}
T_{HTF}(t) \\
T_{SM}(t)
\end{pmatrix}.
\end{align*}
\] (5.1)

\( a_1 \) and \( a_2 \) describe how fast the temperature of the HTF \( T_{HTF}(t) \) and temperature of the SM \( T_{SM}(t) \) change and in reality may not be constant. For example, \( a_1 \) and \( a_2 \) may be dependent on the mass flow of the HTF. The temperature change for one time step can be calculated analytically by solving the differential equation. However, for reduced
computational effort, few discrete equations are desirable. Since the heat capacity of the SM is much larger than the heat capacity of the HTF, we assume that during one time step the temperature of the SM is constant. The rate of heat transfer to the HTF is given by 
\[ \frac{dQ(t)}{dt} = \alpha A_{\text{con}}(T_{SM} - T_{HTF}(t)), \]
with \( A_{\text{con}} \) being the contact surface and \( \alpha \) the heat transfer coefficient. For a layer in the PBR of Volume \( V \), the heat capacity of the HTF equals \( \rho_{HTF}c_{HTF}V \), whereby \( \rho_{HTF} \) is the density of the HTF and \( c_{HTF} \) its specific heat capacity. The transferred heat \( Q \) equals \( \rho_{HTF}c_{HTF}V \Delta T_{HTF} \). This results in 
\[ \frac{dT_{HTF}(t)}{dt} = \alpha A_{\text{con}} \rho_{HTF}c_{HTF}V \left( T_{SM} - T_{HTF}(t) \right), \]
for constant \( \rho_{HTF}c_{HTF}V \). With the solution:

\[ T_{HTF}(t) = T_{SM} + (T_{HTF0} - T_{SM}) \exp\left(-\frac{\alpha A_{\text{con}}}{\rho_{HTF}c_{HTF}V}t\right), \]  
(5.2)

whereby \( t \) is the time the HTF and SM are in contact and \( T_{HTF0} \) is the initial temperature of the HTF. When the HTF passes through a layer of the SM, the contact time depends on the layer height \( h \) and the velocity \( v \) of the HTF. The velocity can be calculated using the mass flow \( \dot{m} \) of the HTF, the density \( \rho \) of the HTF, the porosity \( \psi \) of the SM as well as the cross-section area \( A_{\text{cross}} \) of the PBR. This leads to:

\[ t = \frac{h}{v} = \frac{h \psi \rho_{HTF} A_{\text{cross}}}{\dot{m}}, \]  
(5.3)

and consequently:

\[ T_{HTF} = T_{SM} - (T_{SM} - T_{HTF0}) \exp\left(-\frac{\alpha A_{\text{con}}}{c_{HTF}V} \frac{h \psi A_{\text{cross}}}{\dot{m}}\right). \]  
(5.4)

The assumption of the layers being cylindrical leads to \( h = V/A_{\text{cross}} \). As \( \psi \) and \( c_{HTF} \) are constant we obtain the following equation, using the constant \( \alpha_1 = \alpha A_{\text{con}} \psi / c_{HTF} \):

\[ T_{HTF} = T_{SM} - (T_{SM} - T_{HTF0}) \exp\left(-\frac{\alpha_1}{\dot{m}}\right). \]  
(5.5)

The introduction of layers \( i \) stacked above each other leads to:

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Grey Box Modeling of the PBR

Basic Model Structure

\[ T_{HTF,i} = T_{SM,i} - (T_{SM,i} - T_{HTF,i-1}) \exp(-\frac{\alpha_1}{\dot{m}}). \]  
(5.6)

The equation is implemented for discrete time steps \( k \):

\[ T^k_{HTF,i} = T^k_{SM,i} - (T^k_{SM,i} - T^k_{HTF,i-1}) \exp(-\frac{\alpha_1}{\dot{m}^k}). \]  
(5.7)

The temperature change of the SM is calculated via the exchanged heat, which leads to the following equation:

\[ (T^{k+1}_{SM,i} - T^k_{SM,i})(c_{SM}\rho_{SM}(1 - \psi)V_i) = (T^k_{HTF,i-1} - T^k_{HTF,i})(\Delta t\dot{m}^k c_{HTF}) \]  
(5.8)

Hereby is \( c_{SM} \) the specific heat capacity of the SM. The time \( \Delta t \) describes the length of a time step. This is different from the time \( t \), which describes the time the HTF is in contact with the layer of the PBR. Finally, this leads to:

\[ T^{k+1}_{SM,i} = T^k_{SM,i} + (T^k_{HTF,i-1} - T^k_{HTF,i}) \frac{\Delta t\dot{m}^k c_{HTF}}{c_{SM}\rho_{SM}(1 - \psi)V_i}. \]  
(5.9)

Since \( c_{HTF}, c_{SM}, \rho_{SM}, \psi \) and \( \Delta t \) (for constant time steps) are constant, a new constant \( c_{HS} = \frac{\Delta t c_{HTF}}{c_{SM}\rho_{SM}(1 - \psi)} \) can be introduced. This constant can be seen as a ratio between the heat capacity of the HTF and the SM. This leads to:

\[ T^{k+1}_{SM,i} = T^k_{SM,i} + (T^k_{HTF,i-1} - T^k_{HTF,i}) \frac{\dot{m}^k c_{HS}}{V_i}. \]  
(5.10)

This model assumes the input into each layer of the PBR as constant for one time step. The input temperature of the lowest layer equals the input temperature of the HTF. The input temperature of every other layer equals the output temperature of the layer below. A more accurate modeling approach can set the modeling time step equal to the time it takes the HTF to pass through one layer and to have the input temperature in a layer to be the output temperature of the past layer. However, this approach is not used due to its
increased computational cost.

The time step length is set to be equal to the sampling rate of 1 min. This time step length is appropriate due to the inertia of the system. The time during which the HTF passes through the whole PBR is calculated by

\[ t = \frac{r^2 \pi H \rho}{m} = \frac{0.25^2 \pi \times 2.03 \times 0.375 \times 150}{150} \approx 0.001 \text{h} = 0.06 \text{ min} = 3.6 \text{ s}, \]

with the assumption of a cylindrical PBR with the radius \( r \) assumed to be 0.25 m and height \( H \). The length of a time step is more than 15 times longer than the time it takes the HTF to pass the PBR. Therefore, it is assumed that the input temperature of a layer is only dependent on the output temperature of the current time step of the layer below.

**Heat Loss to the Surroundings**

The heat loss is mostly dependent on the temperature of the wall of the PBR. The wall temperature is assumed to be equal to the temperature of the SM. The heat loss is only expressed in a temperature decrease in the SM. The heat flow is assumed to be constant during the time step, with \( T_{SM} \) and \( T_{sur} \), the temperature of the surrounding air, being constant. Furthermore, it is assumed that the heat loss is proportional to the difference between \( T_{SM} \) and \( T_{sur} \). Thus, \( T_{SM,i}^{k+1} \) needs to be corrected by a heat loss term which is proportional to the temperature difference between the SM and the surroundings. This is implemented by reducing \( T_{SM,i}^{k+1} \) by:

\[ v_{SM}(T_{SM,i}^k - T_{sur}), \]

whereby \( v_{SM} \) is a fitted parameter that represents the heat loss from the SM. The smaller the constant \( v_{SM} \) the smaller the heat loss. Therefore, \( v_{SM} \) resembles the quality of the isolation.
5.1.3 Training Data Set

In a first approach, only one data series is used to optimize the parameters and to rank the model. This enables fast optimization and shows whether the model complexity is sufficient to accurately simulate the output temperature. However, overfitting may not be detected. Once the model achieves sufficiently good results on a single data set, the size of the training data set is increased by adding different measurement series and the model is tested on a test data set. Figure 5.3 shows the input values of the training data. During the measurement, the length of the charging and discharging cycles is continuously shortened.

5.1.4 Parameter Optimization

The parameters that are optimized using data are $\alpha_1$, $v_{SM}$ and $c_{HS}$ for the basic model. The root mean square error (RMSE) of the output temperature is used to calculate the cost function:

$$cost = \sqrt{\frac{\sum_{k=k_l}^{k_f} (T_{HTF,l}^k - T_{out}^k)^2}{k_l - k_f + 1}},$$  \hspace{1cm} (5.12)
whereby $T_{HTF,l}^k$ is the simulated output temperature for a model with l layers at the time $k$, $T_{out}^k$ is the measured output temperature of the PBR at the time $k$, $k_f$ is the first and $k_l$ is the last time step used to calculate the cost function. Internal temperatures are not considered due to the uncertainty of their accuracy.

The cost function only includes the time steps in which changes in the output temperature are present, due to its regular operation. Therefore, the cost function comprises the time steps 800 to 4200 of the training data set.

As parameter optimization tool the Nelder-Mead simplex algorithm - see Subsection 3.2.3 - is chosen. Since future grey box model iterations may not be differentiable, the main advantage of this algorithm is that it does not require any derivatives. Further, the Nelder-Mead simplex algorithm allows for fast implementation in Matlab by using the function \texttt{fminsearch}. However, it takes hundreds of iterations to find accurate parameters. This is acceptable because of the low computational cost of the model. The algorithm requires initial starting values of the parameters that shall get optimized. It is possible that different starting parameters lead to different optimization results and therefore, multiple sets of starting points are used.

5.1.5 Basic Model Summary and Results

The model uses 29 layers each 7 cm high, representing the height of 2.03 m of the PBR. The model equations used are Equations (5.7, 5.10 and 5.11). The Nelder-Mead simplex algorithm is used with a wide spectrum of starting parameters. Every parameter is tested within a range from $10^{-10}$ to $10^{10}$ with a constant step width of $10^4$ and every possible combination of starting parameters is tried. The best fit is achieved with the following parameter values shown in Table 5.1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HS}$</td>
<td>0.0483</td>
<td>$(m^3/s)/kg$</td>
</tr>
<tr>
<td>$a_1$</td>
<td>0.109</td>
<td>$kg/s$</td>
</tr>
<tr>
<td>$v_{SM}$</td>
<td>0.000328</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure 5.4: Output of the basic model

Figure 5.4 shows the model results of the optimized model. The corresponding RMSE is 5.17 °C for the used data set. The main goal is to reduce the RMSE, while not overfitting the model. The main flaw of the model seems to be at the end of each loading cycle where the temperature increases too fast. Further, the decrease of the output temperature occurs too early, and the rate of temperature decrease is not high enough. Nevertheless, the fit is already quite accurate, for such a simple model.

The output of the model is dependent on the number of layers used to calculate the models. One might assume that, if the number of layers is increased (equal to decreasing the layer height), the accuracy should be improved. However, in this case, the accuracy of the model decreases with an increase in layers. With the height reduced to 1 cm per layer, the achieved RMSE increases to 5.36 °C with the same optimization procedure as described above. This indicates that this model is not accurately describing the underlying system and most likely misses some relevant properties. The next models aim to decrease the RMSE and to have a decreasing RMSE when the number of layers increases.
5.2 Data Driven Adaption

To further reduce the RMSE of the model, data-driven adaptions are implemented. In this section, the RMSE calculation, training data, and optimization remain the same as in Section 5.1.

5.2.1 Addition of a Second Set of Parameters

In this approach, two different sets of parameters are used during charging and discharging. The first parameter set is used during charging. Specifically, when the simulated output temperature of the previous time step is smaller than the input temperature of the current time step. When the output temperature is larger (discharging), the second parameter set is used. Within each set, the same parameters as in the basic model are used and an index is used to differentiate between the first and second set of parameters. The optimized parameter values of the basic model are used as a starting point for the optimization for both parameter sets. The optimized parameter values can be found in Table 5.2.

Table 5.2: Parameter values of the basic model adapted with an implementation of a second parameter set

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HS1}$</td>
<td>0.0493</td>
<td>(m³s)/kg</td>
</tr>
<tr>
<td>$c_{HS2}$</td>
<td>0.0491</td>
<td>(m³s)/kg</td>
</tr>
<tr>
<td>$\alpha_{11}$</td>
<td>0.101</td>
<td>kg/s</td>
</tr>
<tr>
<td>$\alpha_{12}$</td>
<td>4.75</td>
<td>kg/s</td>
</tr>
<tr>
<td>$v_{SM1}$</td>
<td>0.000515</td>
<td>1</td>
</tr>
<tr>
<td>$v_{SM2}$</td>
<td>-1.03e-05</td>
<td>1</td>
</tr>
</tbody>
</table>

The loss parameter $v_{SM2}$ is smaller than 0. This means that during the use of parameter set 2, the temperature of the SM increases with respect to the temperature difference between $T_{SM}$ and $T_{sur}$. At first glance, this has no physically valid explanation. However, it can be interpreted that heat stored in parts of the PBR, which is not modeled in this simulation, is transferred into the HTF.

This model achieves an RMSE of 4.44 °C. This is a clear reduction in comparison to the
Figure 5.5: Output of the basic model with two parameter sets

Figure 5.6: Step function response of the basic model with two parameter sets
RMSE of 5.2 °C when only one parameter set is used. Figure 5.5 shows the modeled output temperature for the training data set. One can see the sudden temperature increase in the simulated output temperature when the input temperature decreases below the output temperature and the parameter set is changed. For comparison, Figure 5.6 shows the model output for a step function as input. The input temperature is set to be 300 °C for the first 2000 minutes. Thereafter the input temperature is set to be 22 °C. The mass flow is constant at 150 kg/h. At minute 2001 the new parameter set is used and the output temperature is increased with no underlying physical explanation. Due to this behavior, this model is not further used to improve the grey box model, because it limits its accuracy given unfavorable of inputs (robustness).

5.2.2 Adaptation of the Heat Loss Function

Another way to adapt the grey box model is to change the heat loss function. Therefore, the heat loss is adapted using the sum of the last \( n \) temperatures of each layer, weighted with the parameter \( v_{MA} \). This allows the model to optimize two more parameters. The temperature \( T_{SM,i}^{k+1} \) is adapted with:

\[
-T_{SM,i}^{k+1}(T_{SM,i}^{k} - T_{sur}) + \frac{v_{MA}^n}{n} \sum_{j=k-n}^{k} T_{SM,i}^{k-j},
\]

The optimization comprises 5 parameters. The 3 parameters of the basic model plus \( v_{MA} \) and \( n \). The initial values for optimization are the optimized values of the basic model with \( v_{MA} \) set to 0 and \( n = 100 \). Table 5.3 shows the optimized parameters.

Table 5.3: Parameter values of the basic model adapted with a heat loss dependent on previous HTF layer temperatures

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{HS} )</td>
<td>0.0493</td>
<td>((m^3s)/kg)</td>
</tr>
<tr>
<td>( \alpha_1 )</td>
<td>1.15</td>
<td>( kg/s )</td>
</tr>
<tr>
<td>( v_{SM} )</td>
<td>0.000844</td>
<td>1</td>
</tr>
<tr>
<td>( v_{MA} )</td>
<td>0.000457</td>
<td>1</td>
</tr>
<tr>
<td>( n )</td>
<td>215</td>
<td>1</td>
</tr>
</tbody>
</table>

The RMSE of this model is 3.94 °C. This is a significant improvement from the basic model.
Figure 5.7 shows the results for the training data set. In comparison to the basic model the increase of the output temperature is slower and fits the measured output temperature better.

5.3 Physically Driven Adaption

The basic model comprised only the most important mechanics of the PBR. To further increase the accuracy different physically inspired model changes are tested. The RMSE calculation, training data, and optimization remain the same in this section as in Section 5.1.

5.3.1 Heat Conduction between Layers

To implement the heat transfer between layers, a parameter $b_{SM}$ is introduced. $b_{SM}$ represents the amount of temperature changed by heat conduction between layers. $b_{SM}$ should be positive since the heat flows from hotter layers to colder layers. The calculation is performed after the heat transfer between the HTF and SM. Therefore, the temperature of the SM is adjusted by:
\[ T_{SM,i}^{k+1} = T_{SM,i}^{k} + b_{SM}(T_{SM,i-1}^{k} - 2T_{SM,i}^{k} + T_{SM,i+1}^{k}). \] (5.14)

As a starting point for the optimization, the optimized parameters of the basic model are used. Three different starting points 0.1, 0.01, and 0.001 for \( b_{SM} \) are tested. This leads to the following optimized parameter set shown in Table 5.4.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{HS} )</td>
<td>0.0478</td>
<td>( (m^3/s)/kg )</td>
</tr>
<tr>
<td>( a_1 )</td>
<td>2.02</td>
<td>( kg/s )</td>
</tr>
<tr>
<td>( v_{SM} )</td>
<td>0.000313</td>
<td>1</td>
</tr>
<tr>
<td>( b_{SM} )</td>
<td>0.0185</td>
<td>1</td>
</tr>
</tbody>
</table>

The RMSE reaches a value of 4.95 °C. This is only slightly better than the basic model. Also, there is no change in the characteristics of the output temperature. This slight improvement in the RMSE does not justify the higher model complexity. Therefore, this effect is not included in future models.

### 5.3.2 Temperature Dependent \( c_{HS}(T) \)

Another model adaption which can be introduced is a temperature dependency of \( c_{HS} \). A linear temperature dependency is implemented using:

\[ c_{HS}(T) = c_{HSc} + T_{SM}c_{HST}. \] (5.15)

Hereby, \( c_{HSc} \) is the constant part of \( c_{HS}(T) \) and \( c_{HST} \) is a constant which represents the temperature dependency of \( c_{HS}(T) \). As the starting point for the optimization, the optimized values of the basic model are used together with \( c_{HST} = 0 \). The optimized results can be found in Table 5.5.

The RMSE decreases to 5.09 °C compared to approximately 5.2 °C of the basic model. No significantly better fitting abilities are found. The temperature dependency of \( c_{HS} \) is not considered further, until significant changes of the model structures are made.
Table 5.5: Parameter values of the basic model adapted with a temperature dependent \( c_{HS}(T) \)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{HS_c} )</td>
<td>0.0512</td>
<td>( (m^3\text{s})/\text{kg} )</td>
</tr>
<tr>
<td>( c_{HS_T} )</td>
<td>-2.82e-05</td>
<td>( (m^3\text{s})/(\text{kgK}) )</td>
</tr>
<tr>
<td>( \alpha_1 )</td>
<td>0.112</td>
<td>( \text{kg/s} )</td>
</tr>
<tr>
<td>( v_{SM} )</td>
<td>0.000325</td>
<td>1</td>
</tr>
</tbody>
</table>

5.3.3 Radiation Loss

The influence of the implementation of heat loss via radiation is supposed to be low - because the surface of the mineral wool has only a small temperature difference to its surroundings, [37]. Nevertheless, in cases of holes in the isolation or not well covered pipes, radiation losses could occur. To test the effects of radiation, the model is expanded with a term of radiation loss which assumes that the wall has the same temperature as the SM and has a direct radiation loss to the surrounding, with an additional parameter \( v_{SM_r} \):

\[
T_{SM,i}^{k+1} = T_{SM,i}^{k+1} - v_{SM_r}(T_{SM,i}^k)^4. \tag{5.16}
\]

For correct calculation, \( T_{SM} \) has to be denoted in Kelvin. The optimization is initialized with the optimized values of the basic model and \( v_{SM_r} \) is set to 0 \( K^{-3} \). This leads to no improvement of the RMSE while \( v_{SM_r} \) was optimized to be 0 \( K^{-3} \). When the starting value of \( v_{SM_r} \) is set to 10\(^{-10} \) \( K^{-3} \), the optimized value is in the range of 10\(^{-13} \) \( K^{-3} \), having almost no influence and indicating that almost no radiation loss occurs. Therefore, radiation loss is not considered any further.

5.3.4 Radiation Between Layers

Radiation between layers could be a relevant process for the heat transfer between layers. It is implemented using the following formula:

\[
T_{SM,i}^{k+1} = T_{SM,i}^{k+1} + z(T_{SM,i}^k)^4 - 2T_{SM,i}^k + T_{SM,i}^{k+1} + T_{SM,i+1}^k)^4). \tag{5.17}
\]
Hereby, \( z \) is an additional optimization parameter describing the radiation between layers. For correct calculation, the temperatures have to be denoted in Kelvin. Again the starting values of the optimization are the results of the basic model. The starting value of \( z \) is set to \( 10^{-10} \). This leads to the optimized values seen in Table 5.6.

Table 5.6: Parameter values of the basic model adapted with radiation between layers

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{HS} )</td>
<td>0.0480</td>
<td>(m(^3)s)/kg</td>
</tr>
<tr>
<td>( \alpha_1 )</td>
<td>2.29</td>
<td>kg/s</td>
</tr>
<tr>
<td>( v_{SM} )</td>
<td>0.000323</td>
<td>( 1 )</td>
</tr>
<tr>
<td>( z )</td>
<td>6.49e-11</td>
<td>( K^{-3} )</td>
</tr>
</tbody>
</table>

The RMSE shrinks to 5.09 °C - again only a slight improvement with one additional parameter. No significantly different behavior of the output function occurred. Therefore, the radiation between layers is not further considered.

### 5.3.5 Implementation of the Wall

For every layer, we introduce one temperature value of the wall \( T_W \) for every layer. Therefore, the implementation of the wall of the PBR doubles the state variables. The wall is set to be in thermal conduct with the SM and it is assumed that the temperature change of the SM is small compared to the temperature change of the wall. The calculation is done after the heat transfer between the HTF and SM is calculated. The temperate change of the wall is calculated by:

\[
T_{W,i}^{k+1} = T_{SM,i}^{k+1} - (T_{SM,i}^{k+1} - T_{W,i}^k)\alpha_2.
\]  

(5.18)

\( \alpha_2 \) describes the heat transfer coefficient between SM and wall. The corresponding temperature change of the SM is calculated by:

\[
- (T_{W,i}^{k+1} - T_{W,i}^k)c_{SW}.
\]  

(5.19)

Hereby \( c_{SW} \) describes the heat capacity ratio between the SM and the Wall. It is assumed
that the heat capacity ratios in every layer are constant. This assumption neglects that the
thickness of the wall is not constant and that the heat capacity ratio between the SM and
wall changes for layers of different heights due to the truncated cone shape of the PBR.
The temperature change due to the heat loss to the surrounding is now implemented by
adapting the temperature of the wall with:

\[-v_W(T_{W,i}^k - T_{sur}).\] (5.20)

$v_W$ describes the heat loss from the wall to the surrounding. This results in a model with two
additional optimization parameters $\alpha_2$ and $c_{SW}$. The parameters $\alpha_2$ and $c_{SW}$ not necessarily
represent the wall in a physical way. The model will use those parameters to minimize the
RMSE. Essentially the model can now include a rough temperature distribution within
one layer. Whereby the heat capacity of the different parts and the degree of thermal
conductivity is determined using data.

The starting values for the optimization are based on the results of the basic model. How-
ever, a wide variety of starting values is tested, because the optimization sometimes failed
to produce low errors. Table 5.7 shows the optimized parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HS}$</td>
<td>0.0495</td>
<td>$(m^3s)/kg$</td>
</tr>
<tr>
<td>$c_{SW}$</td>
<td>0.150</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>34.0</td>
<td>$kg/s$</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>0.993</td>
<td>1</td>
</tr>
<tr>
<td>$v_W$</td>
<td>0.00259</td>
<td>1</td>
</tr>
</tbody>
</table>

This approach leads to a decreased RMSE of 3.94 °C which is a strong decrease from
the original value of 5.2 °C. Also, the simulated temperature output fits the temperature
profile of the PBR better, as Figure 5.8 shows. This model improves the RMSE and is still
physically sound. Therefore, the performance of future models is measured against this
model and it is used as a starting point for further model iterations.
5.4 Changes in Calculation and Data

Due to the limited robustness during the optimization process, a change in the calculation of the heat transfer between the HTF and SM is made. Since a model with high accuracy for the single training data set is found, a training and test data set with multiple data sets is introduced and used to evaluate the models. This further demands that the cost function is adapted.

5.4.1 Change of the Heat Transfer Calculation

The previous calculation assumed that the change in $T_{SM}$ is small compared to the change in $T_{HTF}$. However, this assumption was not supported by the models, especially if $\dot{m}$ is large and the layers are small. If the model parameter $c_{HS}$ and $\alpha_1$ are chosen poorly and $\dot{m}$ is high the system is unstable because the temperature change of the SM overshoots the initial temperature of the HTF. Therefore, a different calculation structure is implemented. A more robust calculation is possible if both temperatures approach a temperature equilibrium which is based on the ratio $\gamma$ of the heat capacities of the contacting materials. The equilibrium temperature $T_{equiHS}$ between HTF and SM is calculated by:

![Figure 5.8: Output of the model with a wall](image)

Figure 5.8: Output of the model with a wall
\[ T_{\text{equi}HS,i}^k = \frac{\gamma T_{HTF,i-1}^k + T_{SM,i}^k}{\gamma + 1} \]  

(5.21)

with \( \gamma = c_{HS} \dot{m}^k / V_i \), this results in:

\[ T_{\text{equi}HS,i}^k = T_{HTF,i-1}^k - \frac{T_{HTF,i-1}^k - T_{SM,i}^k}{1 + c_{HS} \dot{m}^k / V_i}. \]  

(5.22)

Both temperatures approach this equilibrium during one time step. However, the term \( e^{-\alpha_1 \dot{m}} \) is replaced by \( \alpha_{HS} \) indicating that \( \alpha_1 \) is proportional to \( \dot{m} \). This results in the following equations:

\[ T_{HTF,i}^k - T_{\text{equi}HS,i}^k = (T_{HTF,i-1}^k - T_{\text{equi}HS,i}^k) \alpha_{HS} \]  

(5.23)

\[ T_{SM,i}^{k+1} - T_{\text{equi}HS,i}^k = (T_{SM,i}^k - T_{\text{equi}HS,i}^k) \alpha_{HS} \]  

(5.24)

and explicitly:

\[ T_{HTF,i}^k = T_{\text{equi}HS,i}^k + (T_{HTF,i-1}^k - T_{\text{equi}HS,i}^k) \alpha_{HS} \]  

(5.25)

\[ T_{SM,i}^{k+1} = T_{\text{equi}HS,i}^k + (T_{SM,i}^k - T_{\text{equi}HS,i}^k) \alpha_{HS}. \]  

(5.26)

\( \alpha_{HS} \) equal 0 indicates that all possible heat is exchanged and \( \alpha_{HS} \) equal 1 indicates that no heat is exchanged. The absolute value of \( \alpha_{HS} \) is used, to restrict negative values. A change in \( \alpha_{SM} \) changes the rate of approach and a change in \( c_{HS} \) changes \( T_{\text{equi}HS} \). This calculation method is used for the heat transfer between HTF and SM and between SM and wall. The heat loss calculation is unchanged.
5.4.2 Introduction of Training and Test Data

The training data is now extended to five data sets shown in Section A.1. The training data includes the cycles with the lowest and highest temperatures as well as some data sets in between. The maximal input temperature ranges from 150 °C to 280 °C and the mass flow ranges from 150 kg/h to 250 kg/h. The test data consists of six data sets, shown in Section A.2. The input temperature ranges from 160 °C to 250 °C and the mass flow ranges from 150 kg/h to 250 kg/h.

5.4.3 Adaption of the Cost Function

The cost function used for the optimization is now the average of the RMSE of each data set. The RMSE of one data set is obtained by setting a time window in which the PBR is in operation for which the RMSE is calculated.

5.4.4 Increase in Layers

The increase of the RMSE, due to an increase in the number of layers, is not present with the model with a wall. In fact, the RMSE decreases with an increase in layers. Therefore, the number of layers is increased to 203 from 29. The resulting layer thickness is decreased from 7 cm to 1 cm.

5.5 Results and Improvements of the Model with a Wall

The model with a wall and with the robust heat transfer calculation is used as a new standard. First, an initial evaluation of the most important metrics of the model with a wall is conducted. Afterward, improvements to the model are implemented and evaluated.
5.5.1 Performance of the Model with a Wall

Usage of the training data described in Section 5.4.2 for optimization of the model with a wall and with more robust heat transfer calculations, leads to the optimized parameters found in Table 5.8. As one can observe, the heat transfer between HTF and SM is large, as indicated by $\alpha_{HS}$ being in the range of zero ($10^{-7}$).

Table 5.8: Parameter values of the model with a wall

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HS}$</td>
<td>0.0502</td>
<td>$(m^3/s)/kg$</td>
</tr>
<tr>
<td>$c_{SW}$</td>
<td>1.46</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{HS}$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{SW}$</td>
<td>0.986</td>
<td>1</td>
</tr>
<tr>
<td>$v_W$</td>
<td>0.00168</td>
<td>1</td>
</tr>
</tbody>
</table>

The results of the model with a wall, using the more robust heat transfer calculations, lead to an RMSE of $6.03 \degree C$ for the training data and $5.17 \degree C$ for the test data. For comparison, the basic model, with the more robust heat transfer calculation and new test and training data, has an RMSE of $9.56 \degree C$ for the training data and $7.28 \degree C$ for the test data. The smaller RMSE in the test data is likely because the training data includes a higher temperature range than the test data. Since the error is calculated in absolute terms and not in relation to the actual temperature, higher temperatures tend to result in higher absolute errors.

5.5.2 Implementation of the Insulation

With the positive results of the implementation of the wall, the number of state variables are increased again. Another part, called insulation, is implemented in a similar manner as the wall. The additional part is called insulation due to its implementation. It is the new outermost part that is set in thermal contact to the wall and the surroundings. However, its model parameters do not necessarily represent the real-world insulation, since the model parameters are only optimized to achieve an accurate model. With the insulation implemented the model has more parameters to adjust to the output. The used equations are:
with $T_{\text{equiWI}}$ being the equilibrium temperature between the wall and the insulation, $T_I$ being the temperature of the insulation, $\alpha_{WI}$ representing the share of potentially exchanged heat between wall and insulation and $c_{WI}$ representing the heat capacity ratio between wall and insulation. The reduction of $T_{I,i}^{k+1}$ due to the heat loss being:

$$v_I(T_{I,i}^k - T_{\text{sur}}).$$

Whereby $v_I$ describes the heat loss from the isolation to the surrounding via conduction. The optimization uses the results of the model with a wall as a starting point. Initially $\alpha_{WI}$ is set equal to $\alpha_{SW}$ and $c_{WI}$ is set equal to $c_{SW}$. Table 5.9 shows the optimized parameters.

Table 5.9: Parameter values of the basic model adapted with a wall and insulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HS}$</td>
<td>0.0503</td>
<td>$(m^2/s)/kg$</td>
</tr>
<tr>
<td>$c_{SW}$</td>
<td>4.72</td>
<td>1</td>
</tr>
<tr>
<td>$c_{WI}$</td>
<td>1.59</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{HS}$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{SW}$</td>
<td>0.984</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{WI}$</td>
<td>0.992</td>
<td>1</td>
</tr>
<tr>
<td>$v_I$</td>
<td>0.00664</td>
<td>1</td>
</tr>
</tbody>
</table>

The RMSE of the training data declines to 6.02 °C which is only a minimal improvement from the grey box model with only the wall implemented. The RMSE of the test data declines to 5.16 °C - another minimal improvement. With two additional parameters and only a slight improvement, this model structure is not taken into further consideration.
5.5.3 Heat Conduction within the Wall

The wall is artificially split into layers for the computations. Thus, it seems natural to add heat conduction between these layers to our model. The equation is similar to the heat conduction between layers and is calculated after the heat conduction between the SM and the wall. The temperature change of the wall caused by heat conduction equals:

\[ T_{W,i}^{k+1} = T_{W,i}^k + b_W(T_{W,i-1}^k - 2T_{W,i}^k + T_{W,i+1}^k). \]  (5.31)

With \( b_W \) being the optimization parameter which represents the heat conduction between layers of the wall. Table 5.10 shows the parameter values of the optimized parameters. Those new results do not resemble physical behavior, because \( b_W \) is negative, indicating that heat is being transferred from a colder medium to a hotter medium.

Table 5.10: Parameter values of the model with a wall and thermal conductivity between wall layers

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>( c_{HS} )</td>
<td>0.0502</td>
<td>((m^3 s)/kg)</td>
</tr>
<tr>
<td>( c_{SW} )</td>
<td>4.32</td>
<td>1</td>
</tr>
<tr>
<td>( \alpha_{HS} )</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>( \alpha_{SW} )</td>
<td>0.986</td>
<td>1</td>
</tr>
<tr>
<td>( v_W )</td>
<td>0.00167</td>
<td>1</td>
</tr>
<tr>
<td>( b_W )</td>
<td>-0.00424</td>
<td>1</td>
</tr>
</tbody>
</table>

Due to the additional parameter, the training RMSE is unchanged at 6.03 °C. However, the test RMSE increased to 5.30 °C. We conclude that the model is not improved by the additional parameter of heat transfer between the wall layers.

5.5.4 Model with a Wall and Temperature Dependent \( c_{HS}(T) \)

The model with a wall gets adapted by an temperature dependent \( c_{HS} \), similarly to Subsection 5.3.2:

\[ c_{HS}(T) = c_{HS} + T_{SM}c_{HST}. \]  (5.32)
Table 5.11 shows the optimized parameters. The RMSE of the training data decreases significantly to 4.08 °C. The RMSE of the test data also decreases significantly to 3.66 °C. This results in the most accurate model so far with only one additional parameter.

Table 5.11: Parameter values of the model with a wall and temperature dependent $c_{HS}(T)$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HSc}$</td>
<td>0.0558</td>
<td>$(m^3 s)/kg$</td>
</tr>
<tr>
<td>$c_{HST}$</td>
<td>-3.69e-05</td>
<td>$(m^3 s)/(kg K)$</td>
</tr>
<tr>
<td>$c_{SW}$</td>
<td>4.65</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{HS}$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{SW}$</td>
<td>0.983</td>
<td>1</td>
</tr>
<tr>
<td>$v_W$</td>
<td>0.00160</td>
<td>1</td>
</tr>
</tbody>
</table>

5.5.5 Model with a Wall and Temperature Dependent $c_{HS}(T)$ and Cylindrical Form

In all previous models, the PBR is calculated by using its geometric form of a truncated cone for the calculation of temperature change caused by heat exchange between HTF and SM. However, the model does not need to have a truncated cone, because the output temperature is mainly dependent on the overall ratio between HTF and SM capacity. Therefore, a model with cylindrical shape, with no input for geometrical ratios is created, omitting the layer volumes $V_i$. Hence, the parameters $c_{HSc}$ and $c_{HST}$ are replaced by $c_{HSc1}$ and $c_{HST1}$. The only input used is the number of layers and the mechanistic equations. The number of layers used is 203. However, since the volume of a layer is not used in the calculation, there is no explicit layer height. The optimization leads to the parameter values found in Table 5.12.

Table 5.12: Parameter values of the model with a wall, temperature dependent $c_{HS}(T)$ and cylindrical form

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HSc1}$</td>
<td>27.9</td>
<td>s/kg</td>
</tr>
<tr>
<td>$c_{HST1}$</td>
<td>-0.0184</td>
<td>s/(kg K)</td>
</tr>
<tr>
<td>$c_{SW}$</td>
<td>4.62</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{HS}$</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{SW}$</td>
<td>0.983</td>
<td>1</td>
</tr>
<tr>
<td>$v_W$</td>
<td>0.00159</td>
<td>1</td>
</tr>
</tbody>
</table>
The RMSE of the training data is 4.04 °C. The RMSE of the test data is 3.62 °C. There is almost no difference between the cylindrical and non-cylindrical form with the RMSE changing less than 1%. However, there are improvements for the internal temperatures, which are further discussed in Chapter 6.
6. Results, Comparison and Discussion

In this chapter, the results of the grey box models are described in detail. The grey box parameters are compared to the corresponding real-world parameters. An already existing white box model and an already existing neural network (NN) model are discussed. Finally, those three models are being compared and an overview of their advantages and disadvantages is given.

6.1 Grey Box Results

To gain more insight into the grey box models and their different results, the following models are discussed:

- Basic model, shown in Figure 6.1 (excluding the green parameters)
- Basic model with adapted heat loss, shown in Figure 6.1 (including the green parameters)
- Model with a wall, shown in Figure 6.2 (excluding the green temperature dependencies)
- Model with a wall and $c_{HS}(T)$, shown in Figure 6.2 (including the green temperature dependencies)
- Cylindrical model with a wall and $c_{HS}(T)$, shown in Figure 6.3
Results, Comparison and Discussion

Grey Box Results

Figure 6.1: Model structure of the basic model and the basic model with adapted heat loss (additional parameters are green)

Figure 6.2: Model structure of the model with a wall and model with a wall and $c_{HS}(T)$ (additional temperature dependencies are green)

Figure 6.3: Model structure of the cylindrical model with a wall and $c_{HS}(T)$
All discussed models are using the more robust heat transfer calculation described in Sub-
section 5.4.1. All models are trained using the training data shown in Section A.1 and 
tested using the test data shown in Section A.2. All models use a layer thickness of 1 cm, 
leading to 203 layers. Table 6.1 gives an overview of the different models and their results. 
All models are robust due to their model equations.

Table 6.1: Parameter comparison between different models

<table>
<thead>
<tr>
<th></th>
<th>Basic model</th>
<th>Adapted heat loss</th>
<th>Wall</th>
<th>Wall + $c_{HS}(T)$</th>
<th>Wall + $c_{HS}(T)$ + cylindrical</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{HSc}$</td>
<td>0.0461</td>
<td>0.0489</td>
<td>0.0502</td>
<td>0.0558</td>
<td>-</td>
<td>($m^3 s$)/kg</td>
</tr>
<tr>
<td>$c_{HSc1}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>27.9</td>
<td>s/kg</td>
</tr>
<tr>
<td>$c_{HST}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-3.69e-05</td>
<td>($m^3 s$)/(kgK)</td>
</tr>
<tr>
<td>$c_{HST1}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-0.0184</td>
<td>s/(kgK)</td>
</tr>
<tr>
<td>$c_{SW}$</td>
<td>-</td>
<td>-</td>
<td>4.36</td>
<td>4.65</td>
<td>4.62</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{HS}$</td>
<td>0.631</td>
<td>0.141</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_{SW}$</td>
<td>-</td>
<td>-</td>
<td>0.986</td>
<td>0.983</td>
<td>0.983</td>
<td>1</td>
</tr>
<tr>
<td>$v_{SM}$</td>
<td>3.97e-04</td>
<td>0.00167</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>$v_{W}$</td>
<td>-</td>
<td>-</td>
<td>0.00168</td>
<td>0.00160</td>
<td>0.00159</td>
<td>1</td>
</tr>
<tr>
<td>$v_{MA}$</td>
<td>-</td>
<td>-0.00114</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>$n$</td>
<td>-</td>
<td>191</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>CPU time</td>
<td>0.0833</td>
<td>3.065 1</td>
<td>0.1138</td>
<td>0.1371</td>
<td>0.1153</td>
<td>s</td>
</tr>
<tr>
<td>Training RMSE</td>
<td>9.56</td>
<td>6.60</td>
<td>6.03</td>
<td>4.08</td>
<td>4.04</td>
<td>°C</td>
</tr>
<tr>
<td>Test RMSE</td>
<td>7.28</td>
<td>5.40</td>
<td>5.17</td>
<td>3.66</td>
<td>3.62</td>
<td>°C</td>
</tr>
</tbody>
</table>

1 The higher computational effort is due to the inefficient recalculation of the sum of the previous 191 
time steps used for the adapted heat loss.

The significant difference between the model parameters of the cone shaped model and 
its corresponding cylindrical model is due to the omission of $V_i$. With an average $V_i$ 
of 0.0020 $m^3$, the comparable values of the cylindrical model are 0.05582 ($m^3 s$)/kg for 
the parameter describing the heat capacity ratio between HTF and SM independent
of the temperature and $-3.6798e - 05 \, \text{m}^3/\text{s}/(\text{kgK})$ for the parameter describing the temperature dependent heat capacity ratio between HTF and SM. Those are almost identical to the model with a truncated cone shape with $c_{HS,c} = 0.05576 \, (\text{m}^3/\text{s})/\text{kg}$ and $c_{HST} = -3.685e - 05 \, (\text{m}^3/\text{s})/(\text{kgK})$.

Measured CPU times are applicable for simulating the packed bed regenerator (PBR) on a 10,000 min time window on an Intel Pentium CPU G3260 @ 3.30 GHz. So for example the cylindrical model with wall and $c_{HS}(T)$ would be able to simulate 86,730 time steps per minute.

Table 6.1 shows a continuous decline in the RMSE during the iterative implemented model changes. The improved RMSE of the models with a wall indicates, that some significant portion of the heat is stored in the wall and is partially recovered during the discharging cycle. We further recollect, that the basic model achieves better results with thicker layers of e.g. 7 cm, which underlines the insufficiency of the basic model structure.

To further compare the accuracy, Figure 6.4 shows a representative part of the test data to compare the different models. The graphs of the model with adapted heat loss and the model with a wall are basically identical. However, the model with a wall is slightly more accurate at low temperature outputs. Also, the model with a wall with $c_{HS}(T)$ and the corresponding model with a cylindrical form are nearly identical with respect to the output temperature. It is clearly visible that the basic model has the worst RMSE.

The main difference between the model with a wall with $c_{HS}(T)$ and the model with the additional cylindrical shape lies in the temperature distribution in the SM. The model with cylindrical shape has the same overall heat capacity ratio between SM and HTF. The lower layers of the cylindrical form are bigger than the lower layers of the truncated cone form. Therefore, the lower layers of the cylindrical form change their temperature more slowly. Inversely the higher layers of the cylindrical shape are smaller than the higher layers of the truncated cone shape. This effect can be seen in Figures 6.5 and 6.6.

The measured temperature values of $T_4$ are probably incorrect since the values are lagging the output temperature when they actually should be leading them. The cylindrical model fits the temperatures $T_1-T_4$ more accurately. This seems at first counter-intuitive because
Results, Comparison and Discussion

Grey Box Results

Figure 6.4: Comparison of the different grey box models

Figure 6.5: Temperature distribution of model with a wall, $c_{HS}(T)$ and truncated cone shape
the temperatures $T_1$-$T_4$ should be more accurately modeled by the actual truncated cone shape. However, the actual experimental setup shows a possible explanation. As seen in Figure 4.1, the storage vessel is supported by a steel table. The steel table may slow the temperature increase of the lower layers, as indirectly modeled by the model with cylindrical shape.

6.2 Grey Box Parameters vs. Physical Properties

The heat capacity ratio $c_{HS}$ of the grey box models can be compared to the actual heat capacity ratio of the SM and the HTF of the PBR. For this comparison, the model with a wall and $c_{HS}(T)$ is considered. The parameter $c_{HS_c}$ resembles the ratio of the heat capacity of the SM and HTF. The factual heat capacity of our SM equals 840 $J/kgK$ and the heat capacity of our HTF (dry air) equals 1010 $J/kgK$, [37]. With $c_{HS} = \frac{\Delta t c_{HTF}}{c_{SM} \rho_{SM}(1-\psi)}$ and $\Delta t = 60s$, $\rho_{SM} = 2590kg/m^3$ and $\psi = 0.375$ this results in a theoretical value of 0.0753 $(m^3s)/kg$. The grey box parameter $c_{HS}$ equals 0.0558 $(m^3s)/kg$, only 73% of the calculated heat capacity ratio. Further, the heat capacity ratio at higher temperatures can be compared. However, the exact composition of the SM is not known. The assumption
that the SM consists of quartz or SiO$_2$ would result in a heat capacity of 44.6 J/mol$K$ [38] or equal to 742 J/kg$K$ at 25 °C. This is not in accordance with [37], making the assumption of quartz inaccurate. However, the heat capacity at 600K for SiO$_2$ equals 64.4 J/mol$K$ or 1070 J/kg$K$. At 600 K the heat capacity of air equals 1050 J/kg$K$. This results in a heat capacity ratio of 0.0587. The grey box model parameter of the heat capacity at 600 K (326.85 °C) equals 0.0437, 74 % of the calculated heat capacity ratio. Even though the comparison is flawed it indicates that the temperature dependent heat capacity is plausible.

### 6.3 White Box Model of the PBR

The white box model of the PBR, created in course of the paper [5], is based solely on prior knowledge. The model structure consists of $n$-layers with 3 elements: SM, HTF, and wall. The insulation is not factored in as a layer but is factored in the heat flow resistance. The form of the elements is considered to be cylinders with the cone shape taken into account with different diameters for each layer. It is assumed that the air is dry, meaning that the humidity is neglected. The material parameters are considered constant for SM and wall and the material parameters of the HTF are taken from CoolProp, [39].
Figure 6.7 shows the effects that are modeled in the 1D-model. Non-convective heat transfer is indicated by red arrows. The heat transport between different materials is calculated using Newton’s law. The heat transport between wall and SM is calculated by the correlation of Schlünder, [14]. The heat transport between SM and HTF is calculated by the correlation of Gnielinski, [14]. The heat conduction is calculated using Fourier’s law and energy balance. The thermal conductivity between the 1D-layers is calculated via Krischer’s correlation by a combination of serial and parallel conduction of both materials, [14].

Convective heat transfer is indicated by the blue arrows in Figure 6.7. It is assumed that the mass flow has the same input and output value for each layer. The velocity across a cross-section is considered to be constant and can be calculated using the continuity equation. All used equations and a detailed model description can be found in [5].

6.4 Neural Network Model of a PBR

The neural network (NN) model, created in course of the paper [20], of the PBR is a recurrent NN. In contrast to a feed-forward NN, a recurrent NN has neurons that send inputs to neurons of its own layer or previous layers. A nonlinear autoregressive exogenous model network architecture has been chosen, which can enclose every network layer with a feedback connection. To achieve that only the state of the PBR is used as a renewed input, two output layers have been created: one output layer comprising the state variables, which is used as renewed input, and one output layer comprising the temperature $T_{out}$, which is only used as an output. The data sets used to train and test this NN were received during operation in the operating mode with counter current flow as described in Section 4.1.4.

The best-fitting model uses $\dot{m}^+$, $\dot{m}^-$ and $T_{in}$ as inputs. Since the direction of the air flow can be switched, $\dot{m}^+$ describes $\dot{m}$ while charging and $\dot{m}^-$ describes $\dot{m}$ while discharging. Accordingly, $T_{in}$ describes the temperature of the HTF at the top while charging and the temperature at the bottom while discharging. To achieve accurate model outputs, the RNN is trained in two different configurations. First, it is trained in a so-called open loop, in which the measured state values $T_1$ to $T_4$ are used as input for the NN. Second, it is trained
in a so-called closed loop, in which the state values of the NN are used as input for the NN. Those two training modes are used because the closed-loop training needs sufficiently good starting values. The best results have been achieved with a model that uses the fill level (consisting of the thermal energy stored in the PBR) as a state variable. Further details of the model and other model variations can be found in [20].

In course of the paper [5], the NN has been adapted to fit the continuous current flow. This adapted NN model is used for comparison since it is trained for the continuous current flow.

6.5 Comparison of Model Properties

To give a comparison the most relevant properties of the white box model, the grey box model with a wall, \( c_{HS}(T) \) and cylindrical shape, and the NN model are discussed. These properties comprise the accuracy of the output temperature, the accuracy of the internal temperatures, modeling effort, computational effort, robustness, and required resources.

6.5.1 Output Temperature Accuracy

The main attribute of a model is its ability to accurately simulate the output. The data used to compare the three models has not been used to train or test the grey box model. Therefore, it can be considered as a validation data set. Eight data sets are used to evaluate the white box, grey box, and NN model. Figures 6.8, 6.9 and 6.10 show representative profiles of the model output temperatures and the measured output temperature.

Table 6.2 shows the corresponding RMSEs. The RMSE only considers data starting from the 200th time step, because of inaccurate starting values.

The white box model has the worst RMSE in every data set. The grey box model has the second-best mean RMSE and the best RMSE for data set 5. The NN has the best mean RMSE of all other data sets. However, the NN has some sudden deviations from the output temperature, as seen for example in Figure 6.9 at the time steps 500 and 800.
Results, Comparison and Discussion

Comparison of Model Properties

Figure 6.8: 1st data set graph comparing white, grey and NN models

Figure 6.9: 3rd data set graph comparing white, grey and NN models
Results, Comparison and Discussion

Comparison of Model Properties

Figure 6.10: 5th data set graph comparing white, grey and NN models

Table 6.2: RMSE of different data sets

<table>
<thead>
<tr>
<th></th>
<th>White box</th>
<th>Grey box</th>
<th>NN</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE 1</td>
<td>12.94</td>
<td>8.53</td>
<td>3.43</td>
<td>°C</td>
</tr>
<tr>
<td>RMSE 3</td>
<td>10.89</td>
<td>5.41</td>
<td>3.39</td>
<td>°C</td>
</tr>
<tr>
<td>RMSE 5</td>
<td>12.66</td>
<td>3.55</td>
<td>4.26</td>
<td>°C</td>
</tr>
<tr>
<td>Mean RMSE (1-8)</td>
<td>10.98</td>
<td>4.77</td>
<td>3.44</td>
<td>°C</td>
</tr>
</tbody>
</table>

6.5.2 Internal Temperature Accuracy

The internal temperatures of the model influence the output temperature of the HTF and characterize how much heat is stored in a PBR. Therefore, they are an important part of the model. In the NN model, the internal temperatures are trained using the measured internal temperatures. In the grey box model, the internal temperatures are a result of the structure and parameter fitting of the model, whereby the measured internal temperatures are not used. The white box model is solely based on physical principles and not on measured data. Figure 6.11 gives an example of the measured internal temperatures used to train the NN.

The measured internal temperatures, which are used to train the NN, have anomalies. The
Comparison of Model Properties

Figure 6.11: Measured internal temperatures of data set 8

internal temperatures $T_3$ and $T_4$ achieve a higher measured temperature than the highest measured input temperature, which is not physically plausible. Further, during the charging cycle the temperature $T_2$ reaches higher temperatures than $T_1$ which is also physically not plausible. Due to the possible errors in the measured data, the NN model is not able to learn physically plausible internal temperatures. Therefore, the following Figures should be viewed with the necessary caution.

Figure 6.12 shows the modeled internal temperatures of the NN of the data set 4 in comparison with the measured data. Since the NN has been trained on the flawed data, it is only able to find and repeat the patterns. However, it can be stated that the internal temperatures sometimes sharply deviate from the measured temperatures. For example, at time step 330 $T_2$ and $T_3$ sharply decrease, just as the input temperature increases.

Figure 6.13 shows the modeled internal temperatures of the grey box model of the data set 4 in comparison to the measured data. The internal temperatures of the grey box model seem plausible, but with the data available it is not possible to know how accurate they are.
RESULTS, COMPARISON AND DISCUSSION

Comparison of Model Properties

Figure 6.12: Internal temperatures of the NN of data set 4

Figure 6.13: Internal temperatures of the grey box model of data set 4
Results, Comparison and Discussion

Comparison of Model Properties

Figure 6.14: Internal temperatures of the white box model of data set 4

Figure 6.14 shows the modeled internal temperatures of the white box model of the data set 4 in comparison to the measured data. The internal temperatures of the white box model also seem plausible, but due to the lack of accurate data, an exact comparison is not possible.

6.5.3 Other Aspects

Table 6.3 gives an overview of further properties of the different models. The modeling effort for the grey box model is a lengthy process due to its iterative characteristics. However, the first basic model already has an RMSE of 8 °C in the validation data, compared to the white box RMSE of 11 °C. Further, the effort needed for any kind of adaption of the grey box model, due to changes of the PBR or usage for a different PBR, is small, because for most changes of the PBR the grey box model should be able to adapt to the changed PBR by optimizing the parameters based on new data.
Table 6.3: Comparison between white box and NN model, following [5], with addition of the grey box model.

<table>
<thead>
<tr>
<th></th>
<th>White box</th>
<th>Grey box</th>
<th>NN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modeling effort</td>
<td>↑</td>
<td>↑</td>
<td>↓</td>
</tr>
<tr>
<td>Computational effort</td>
<td>↑</td>
<td>↓</td>
<td>↓</td>
</tr>
<tr>
<td>Robustness</td>
<td>robust</td>
<td>robust</td>
<td>limited robustness</td>
</tr>
<tr>
<td>Accuracy</td>
<td>↓</td>
<td>↑</td>
<td>↑</td>
</tr>
<tr>
<td>Required knowledge</td>
<td>detailed</td>
<td>advanced</td>
<td>basic</td>
</tr>
<tr>
<td>process knowledge</td>
<td></td>
<td>process knowledge</td>
<td>process knowledge</td>
</tr>
<tr>
<td>Required resources</td>
<td>numerical software</td>
<td>numerical software</td>
<td>numerical software</td>
</tr>
<tr>
<td>validation data</td>
<td>small data sets</td>
<td>large data sets</td>
<td></td>
</tr>
</tbody>
</table>

6.6 Discussion

The white box model considered the PBR in detail. Physically derived model equations and known parameters of the materials of the PBR were used. Therefore, it is the only model that allows for simulation of the PBR without training data. The used model equations and material properties robustly predict the behavior of the PBR. However, it is the least accurate of the three models and is computationally intensive.

The NN was trained using data, but also physical information was considered to create the model structure of the NN as it uses feedback state variables. The NN seems to be the most accurate of the three models based on the RMSE. However, sudden and physically not explainable changes in the output temperature question its accuracy for input data sets that it was not trained for. This is due to the many weights and biases which are adapted based on the results and not derived from physical insights. Further, it was partly trained on the validation data set. Hence, it received better training data than the grey box model. Due to its NN structure, its computations are faster than the white box model and it can be easily retrained for changes of the PBR or a different PBR.

The grey box model is created to overcome the disadvantages of the NN (sudden changes in the output temperature, unreliable for input data it was not trained for, and physically implausible internal temperatures) and the white box model (inaccurate model results). Therefore, the grey box model equations are based on physical insights and data is used to optimize its parameters. Creating the first basic grey box model is achieved quickly and
already leads to more accurate results than the white box model. However, many different models are tested to find the final grey box model, which is time-consuming. The final grey box model, trained on a different data set, is almost as accurate as the NN - but its output is predictable and robust. The output temperature and internal temperatures are physically based and plausible due to the used model equations. The small number of equations leads to the highest computational efficiency of the three models. Further, it allows for fast adaption to a wide variety of PBRs by retraining its optimization parameters even when little data are available. All those model properties, but especially the reliability and accuracy due to few and comprehensible equations, recommend the grey box model for industrial applications.
7. Summary and Outlook

An accurate grey box model with fast computational time for the packed bed regenerator (PBR) situated at the TU Wien has been created and compared with previous models of the same PBR. During the modeling process, different models have been created and compared. The best modeling approaches have been combined to achieve the final grey box model. The grey box model has been compared to an already existing white box model and an already existing neural network model of the PBR. The grey box model is substantially more accurate than the white box model and almost as accurate as the neural network model. The grey box model is more robust than the neural network model. The grey box model allows for insight into the temperature distribution of the PBR. Further, the grey box model needs only a small amount of data to accurately predict the behavior of the PBR. Those model properties allow for the implementation of the grey box model to optimize PBRs in industrial applications.

There is still potential for improvement by adding or changing parts of the model. However, the potential benefits are limited. More complex models may be more accurate but add complexity. Of interest could be to test the forecasting ability of the grey box model. Therefore, the SM could be changed to a material with a different heat capacity and adapting the model parameter $c_{HS}$ accordingly. Also, the filling height of the PBR could be changed. With corresponding changes to the grey box model, its forecasting ability could be further tested.
Bibliography


A. Data

A.1 Training Data

Figure A.1: Training data set 1
Figure A.2: Training data set 2

Figure A.3: Training data set 3
Figure A.4: Training data set 4

Figure A.5: Training data set 5
A.2 Test Data

Figure A.6: Test data set 1
Figure A.7: Test data set 2

Figure A.8: Test data set 3
Figure A.9: Test data set 4

Figure A.10: Test data set 5
Figure A.11: Test data set 6
A.3 Validation Data

Figure A.12: Validation data set 1
Figure A.13: Validation data set 2

Figure A.14: Validation data set 3
Figure A.15: Validation data set 4

Figure A.16: Validation data set 5
Figure A.17: Validation data set 6

Figure A.18: Validation data set 7
Figure A.19: Validation data set 8
B. Scientific Publication

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

Published in Energies in collaboration with Verena Halmschlager and René Hofmann

In this paper, the development of three different grey box models for a packed bed regenerator is discussed. In particular, the model equations and parameters of the models are outlined. The results of the three models are compared to previously created models, a white box model and a neural network model. Especially the extended model II with 5 equations and 6 parameters shows favourable results, due to its high accuracy and robustness.

My contribution: Conceptualization, Methodology, Formal Analysis, Investigation, Data Curation, Writing - Original Draft Preparation, Writing - Review and Editing, Visualization.


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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 stand 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

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, Häichen 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, e.g., in Barton [29] for the storage of solar thermal energy. Furthermore, numerical modeling is used in Odenthal et al. [30] 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 $T_{\text{in}}$, the HTF outlet temperature $T_{\text{out}}$, an average temperature for every horizontal layer of the vessel $T_1$–$T_4$, 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].

![Picture of the insulated PBR](image1)

![Illustration of the PBR](image2)

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 $T_{\text{in}}$ 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 $T_{\text{out}}$ 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.

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

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).

\[ Q_{SM}^{i,k} = (T_{eq}^{i,k} - T_{SM}^{i,k})/\rho_{SM} (1 - \varphi) V \]  

(1)

\[ Q_{HTF}^{i,k} = (\rho_{HTF}^{i,k} - T_{HTF}^{i,k-1})/(\Delta k \, \rho_{HTF}) \]  

(2)

\[ (T_{eq}^{i,k} - T_{SM}^{i,k})/(\rho_{SM} (1 - \varphi) V) = -(T_{eq}^{i,k} - T_{HTF}^{i,k})/(\Delta k \, \rho_{HTF}) \]  

(3)

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

\[ \beta_{SH} = \frac{\Delta k \, c_{HTF}}{c_{SM} \, \rho_{SM} (1 - \varphi) V} \]  

(4)

\[ T_{eq}^{i,k} = \frac{\beta_{SH} \, m \, T_{HTF}^{i,k-1} + T_{SM}^{i,k-1}}{\beta_{SH} \, m + 1} \]  

(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 $\delta_{SH}$ is introduced that describes the share of heat exchange between HTF and SM. $\delta_{SH} = 0$ stands for a complete heat exchange and $\delta_{SH} = 1$ 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 $\delta_{SH}$ 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 $k$.

\[ T_{HTF}^{i,k} = T_{eq}^{i,k} - (T_{eq}^{i,k} - T_{HTF}^{i,k-1}) \, \delta_{SH} \]  

(6)

\[ T_{SM}^{i,k} = T_{eq}^{i,k} - (T_{eq}^{i,k} - T_{SM}^{i,k-1}) \, \delta_{SH} \]  

(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 $\nu_{SM}$ 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).

\[ T_{SM}^{i,k} = T_{eq}^{i,k} - (T_{eq}^{i,k} - T_{SM}^{i,k-1}) \, \delta_{SH} - \nu_{SM} \, (T_{SM}^{i,k-1} - T_{sur}) \]  

(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—$\delta_{SH}$, $\beta_{SH}$, and $\nu_{SM}$—that aggregate or estimate relevant characteristics of the heat transfer between HTF and SM, and heat loss. $\beta_{SH}$ describes the relation of heat capacity between HTF and SM according to Equation (4) and the two empirical parameters $\delta_{SH}$ and $\nu_{SM}$ 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 $\beta_{SW}$ and $\gamma$ are introduced. $\beta_{SW}$ describes the weighting of the moving average and $\gamma$ 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).

$$T_{SM}^{k,j} = T_{SM}^{eq,j} - (T_{SW}^{eq,j} - T_{SM}^{eq,j - 1}) a_{SW} - \nu_{SW}(T_{SM}^{eq,j - 1} - T_{sur}) - \frac{\nu_{MA}}{\gamma} \sum_{j=1}^{\gamma} (T_{SM}^{k,j} - T_{SM}^{eq,j})$$

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 $a_{SW}$, $\beta_{SH}$, and $\nu_{SW}$, and the new parameters $\beta_{MA}$ and $\gamma$.

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 and the auxiliary parameter $m$ and the auxiliary parameter $\alpha$ described in the basic model, $\alpha_{SW}$ that describes the heat exchange between SM and W. In accordance with Equation (4)—a parameter $\beta_{SW}$ 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 $m_{W}$, being the mass of the wall in one layer.

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

$$T_{SM}^{eq,j} = \frac{\beta_{SW} T_{SM}^{j} + T_{W}^{j}}{\beta_{SW} + 1}$$

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 $a_{SW}$ that describes the share of heat exchange between SM and W. In accordance with $a_{SW}$ described in the basic model, $a_{SW} = 0$ stands for a complete heat exchange and $a_{SW} = 1$ for no heat exchange.

$$T_{SM}^{k,j} = T_{SM}^{eq,j} - (T_{SM}^{eq,j} - T_{SM}^{eq,j - 1}) a_{SW}$$

$$T_{W}^{eq,j} = T_{W}^{eq,j} - (T_{W}^{eq,j} - T_{W}^{eq,j - 1}) a_{SW}$$

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 $\nu_{W}$ that describes the heat loss of the wall, leading to Equation (14) for the calculation of the wall temperature in one layer.

$$T_{W}^{k,j} = T_{W}^{eq,j} - (T_{W}^{eq,j} - T_{W}^{eq,j - 1}) a_{SW} - \nu_{W}(T_{SM}^{eq,j - 1} - T_{sur})$$
In addition in this extended model, the parameter $\beta_{SH}$—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 $\beta_{SHT}$ and includes the parameters for the constant $\beta_{SH}$ and temperature dependent $\beta_{SHt}$ heat capacity ratio, according to Equation (15).

$$\beta_{SHT} = \beta_{SH} + \frac{T_{iSM}}{1 + \beta_{SHt}}$$

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

### 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, $T_{out}$ the measured outlet temperature, and $k$ the index for the time.

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

For the three developed grey-box models, different parameters are optimized with this approach, which are all dimensionless. The basic model optimizes $\alpha_{SH}$, $\beta_{SH}$, and $\nu_{SM}$. The extended model with heat loss dependency adds two parameters $\nu_{MA}$ and $\gamma$. In the extended model with the wall and non-constant heat capacity, the parameters $\alpha_{SH}$, $\alpha_{SW}$, $\nu_{W}$, $\beta_{SW}$, $\beta_{SH}$ and $\beta_{SHt}$ 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 $T_{in}$ 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 $T_{1}$–$T_{4}$ 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.

<table>
<thead>
<tr>
<th>Type of Model</th>
<th>Basic Model</th>
<th>Ext. I Heat Loss</th>
<th>Ext. II Wall + β_SHT</th>
</tr>
</thead>
<tbody>
<tr>
<td>α_SH</td>
<td>0.722</td>
<td>0.155</td>
<td>0</td>
</tr>
<tr>
<td>α_SW</td>
<td>-</td>
<td>-</td>
<td>0.99</td>
</tr>
<tr>
<td>β_SH</td>
<td>22.0</td>
<td>23.6</td>
<td>27.2</td>
</tr>
<tr>
<td>β_SHt</td>
<td>-</td>
<td>-</td>
<td>-0.0197</td>
</tr>
<tr>
<td>β_SW</td>
<td>-</td>
<td>-</td>
<td>4.75</td>
</tr>
<tr>
<td>ν_MA</td>
<td>-</td>
<td>0.00117</td>
<td>-</td>
</tr>
<tr>
<td>ν_SM</td>
<td>0.000459</td>
<td>0.00174</td>
<td>0.00135</td>
</tr>
<tr>
<td>ν_W</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>γ</td>
<td>166</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

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 $T_1$–$T_4$ 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 $T_1$ to $T_4$ while charging, physically correct behavior is displayed. Although it therefore seems evident to use the temperatures $T_1$–$T_4$ as additional model outputs, these measurements show inaccuracies ($T_3$ and $T_4$ 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 $T_1$–$T_4$ could further improve the models’ accuracy.

For the basic grey-box model, the measured and predicted outlet temperature and two of the internal temperatures, $T_1$ and $T_3$, 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 $T_1$ to $T_3$ to $T_{out}$) in contrast to the evidently inaccurate experimental data that shows higher values for $T_3$ than $T_1$. 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.
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.

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 $T_{1\text{wall}}$ and $T_{3\text{wall}}$ 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 $\beta_{SHt}$ in Table 2, which indicates a relatively low temperature dependence of $\beta_{SHt}$.

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 $\approx3$, 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 $T_3$ than $T_1$.

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.

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.

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

<table>
<thead>
<tr>
<th>Modeling Approach</th>
<th>Grey-Box Model</th>
<th>Physical Model</th>
<th>NN Model</th>
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<tr>
<td>Accuracy</td>
<td>↑</td>
<td>↓</td>
<td>↑</td>
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<tr>
<td>Modeling Effort</td>
<td>↑↓</td>
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<tr>
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<td>Effort for Small Adaptations</td>
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<tr>
<td>Required Knowledge</td>
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<tr>
<td>Required Resources</td>
<td>Numerical Software + Optimization Tools, Test &amp; Training Data</td>
<td>Numerical Software, Validation Data</td>
<td>Numerical Software + ML Toolbox, Large Data Sets</td>
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</table>

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 robustly, 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 work’s 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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