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Approaches to simplify industrial energy models for operational optimisation

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A B S T R A C T

Minimising energy consumption in today's industrial sector is a crucial objective for achieving established climate goals. One effective strategy to enhance efficiency is optimising energy system operations within industries. The initial step in establishing operational optimisation involves developing a comprehensive model of the energy system. This model necessitates a specific structure to meet optimisation requirements. However, creating a model from scratch incurs substantial effort. While numerous companies possess energy models, they often lack the requisite structure for optimisation. Consequently, simplifying existing models can significantly reduce the effort needed to implement operational optimisation.

This paper investigates the simplification of intricate industrial energy system models for optimisation purposes. The subsequent sections analyse two distinct approaches. One approach involves linearisation, while the other utilises neural networks. To facilitate a comparative analysis of these approaches, a reference model is developed. The assessment of these methodologies includes an investigation into optimisation robustness, computation time, accuracy concerning the reference model, and the effort required for developing and maintaining the simplified models. It proved that both approaches are suitable for operational optimisation. Linearisation exhibits superior computational efficiency compared to the neural network approach. The linearisation modelling approach together with the optimisation only required a few milliseconds for the calculation. The neural network approach needed 3 h for the calculation of the optimum with the genetic algorithm. The simulation of the neural network itself only required a few milliseconds. Hence, an improvement of the genetic algorithm is needed. However, the accuracy of linearisation falls short of that achieved by neural networks. The linearisation achieves a mean average percentage error from only 13%. In comparison the neural network's mean average error is 2.3%. Therefore, the linearisation must be improved. The impact using a piecewise linearisation on the results will be analysed in further research.

1. Introduction

Energy efficiency in the industry plays an essential part in reaching the climate goals for Europe. About a quarter of the overall energy consumption is related to the industry sector in Europe (Statistical Office of the European Communities, 2020). Therefore, a high potential for reducing emissions is given. The energy supply in industries gets more and more challenging. On the one hand side, the fluctuation of the energy supply is rising because renewable energy sources are gaining more share in the energy supply, which leads to highly volatile energy prices. And on the other hand, due to higher customer needs, flexibility in production increases, which leads to significant variations in the energy demand for the production. To avoid influences on production as good as possible, it is necessary to design and operate the company's energy system so that fluctuations in supply and demand can be balanced out in the best possible way.

One way to face the challenge of imbalance in supply and demand is to optimise the company's energy system. Herby, an operational optimisation is an instrument to find the most efficient way – according to

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Nomenclature

a	Area of the warm water volume
COP	Coefficient of performance
COP_{max}	Maximal reachable coefficient of performance
$e_{chiller}$	Electricity needed from chiller
e_{demand}	Electricity needed from production
EER	Energy efficiency ratio
e_{grid}	Electricity needed from grid
$e_{heat\ pump}$	Electricity needed from heat pump
e_{PV}	Electricity provided by PV
$e_{storage\ in}$	Electricity needed for charging electrical storage
$E_{storage\ out}$	Electricity provided by discharging electrical storage
f	Form factor
h	Height
h_{boiler}	Heat needed from boiler
$h_{charging}$	Logistic function for charging
h_{demand}	Heat needed from production
$h_{discharging}$	Logistic function for discharging
$h_{heat\ pump}$	Heat provided by heat pump
$h_{storage\ in}$	Heat needed for charging heat storage
$h_{storage\ out}$	Heat provided by discharging heat storage
$h_{waste\ heat\ chiller}$	Heat provided by chiller (waste heat)
l_f	Load factor
MAPE	Mean absolute percentage error
MILP	Mixed integer linear problem
m_{max}	Maximal mass for charging and discharging heat storage
oemof	Open energy modelling framework
$p_{charging}$	Power for charging
$p_{discharging}$	Power for discharging
p_{max}	Maximal power
q_V	Losses of the heat storage
r	Radius
ReLU	Rectified linear units
RSME	Root mean squared error
SOC	State of charge
T_C	Temperature heat source (cold)
T_{co}	Condensation temperature
T_e	Evaporation temperature
T_H	Temperature heat sink (hot)
u	Heat transition coefficient
$u_{e.s.in}$	Utilisation rate for the inflow of the electrical storage
$u_{e.s.out}$	Utilisation rate for the outflow of the electrical storage
$u_{h.s.in}$	Utilisation rate for the inflow of the heat storage
$u_{h.s.out}$	Utilisation rate for the outflow of the heat storage
u_{hp}	Utilisation rate of the heat pump
u_{PV}	Utilisation rate of the PV plant
u_{wh}	Utilisation rate of the waste heat from the chiller
VOFEN	Vision of Future Energy Networks
ΔT	Temperature difference
η_b	Efficiency of the condensing boiler
η_{HP}	Total energy efficiency of heat pump
$\eta_{useable\text{-}waste\text{-}heat\text{-}chiller}$	Efficiency of the useable waste heat from the chiller
ρ_{W80}	Density of water at 80 °C

the target function – to provide the energy (e.g. electricity, heat, cooling, pressurised air etc.) for the production. The target function can be the minimisation of the costs, increasing energy efficiency, reducing CO_2 emissions or a combination of them. Therefore, all relations, energy carriers, and connections between the inputs, outputs and convertors must be considered. Due to the complexity of the calculation and the dependency on several logistics parameters, the variation of the production program is difficult to implement and should therefore be researched separately. Hence, variation of the production program is not investigated in this work. To find the global optimum, a holistic approach is necessary where the whole energy system of the considered industrial plant is included. To optimise the energy system, future data is needed, like energy price or energy demand from the production.

In this work the non-energy intensive industry is inspected. Also, in the non-energy intensive industry, the operational optimisation of energy systems is highly interesting. Not only to reduce the energy costs but also customers insist more and more on CO_2-neutral production.

Before an operational optimisation can be developed, first a model of the energy system is needed. This model needs to fulfil the requirements according to the used optimisation method (e.g. a linear optimisation needs a model consisting of linear equations). Commonly energy models are built from scratch. This leads to a high effort for developing and maintaining the energy models. Therefore, a methodology is developed to simplify existing energy models so they fulfil all the requirements for the operational optimisation. Two different modelling approaches are investigated in this work. One is the linearisation approach which is used for a linear optimisation. The other is the neural network approach which is used for a genetic algorithm.

For the evaluation of the different modelling approaches in this paper the accuracy, computation time, robustness and the effort for setting up the model are investigated. The accuracy specifies the deviation of the original model and the model for the optimisation. Future data can change over time. To handle this changes in the future data the optimisation needs to calculate the results in a few minutes. This is measured with the computation time of the optimisation. The robustness describes how likely it is that the optimisation can find the global optimum. Also the effort which is needed for establishment and maintenance of the modelling approach and the optimisation is investigated. Because this is a decisive factor for the implementation in the industry.

To compare the two different approaches first a reference model was set up. This reference model represents the generated industrial energy system. Subsequently, this reference model is simplified according to the two approaches to meet the requirements of the respective optimisation. The optimisation is then executed for both approaches to observe their influence.

2. State of research

For modelling energy systems with different energy carriers on various levels in a defined system multi-energy systems (MES) are used. The reference model is built upon MES and the modelling approach has to simplify such models to use them for the operational optimisation. The MES is based on the energy hub approach. Therefore, the first section of this chapter introduces MES and energy hubs. Subsequently, ongoing research in modelling energy systems and the existing research gaps are discussed. Finally, a comparison between previous work and this study is presented, along with the research questions.

2.1. Multi-energy systems

A consistent definition of multi-energy systems has yet to be achieved. But in general, a multi-energy system requires a holistic consideration of the energy system and consists of different energy carriers (e.g. electricity, heat, cooling, natural gas) (Kriechbaum et al., 2018). In a holistic view their interaction must be considered. A multi-energy system may start by extracting and treating the different energy carriers and ends by supplying various energy demands. Mancarella et al. (Mancarella, 2014) define four categories to characterise multi-energy systems.

- Spatial
- Network
- Multi-service
- Multi-fuel

The spatial category describes the spatial resolution of a multi-energy system (e.g. buildings, cities, countries). The network is needed to interact with the energy supplier and customers. It connects the different components. Multi-service means that one energy supplier can provide multiple customers and multi-fuel that several suppliers can provide one customer.

2.1.1. Energy hubs

The approach of energy hubs is used to describe multi-energy systems, including multi-carrier energy networks and their specific physical characteristics in Geidl and Andersson (2007). The first time the energy hub concept was presented in the context of the project “A Vision of Future Energy Networks (VOFEN)” (Favre-Perrod, 2005). According to Geidl and Andersson (2008), Energy Hub provides the following basic elements.

- Inputs
- Outputs
- Converters
- Storages
- Buses

With these elements, it is possible to model multi-energy systems and their interconnections. Different resources like electricity from the grid, natural gas, solar energy, etc., can be defined as input. Possible outputs of the Energy Hub are electricity, heating, cooling, compressed air etc. The convertors describe the interlinking between the inputs and outputs. Storages are needed to shift the energy between different time steps or as buffer (e.g. a compressed air tank that is used to compensate fluctuations in production). To implement the network (which records the connections between inputs, outputs, converters and storages) buses are used in the Energy Hub approach. A bus represents an energy carrier or an energy form and describes how the other elements are connected to it. There can be several buses of the same type. E.g. if the PV-plant is only connected to the heat pump and to no other converter two electrical buses are needed to represent the energy system (c.f. Fig. 1 (d)). Buses are like nodes where the energy balance between inflowing and outflowing energy must always be zero. In Fig. 1, the five categories are shown how the separate components can be combined (Mohammadi et al., 2017).

Fig. 1 (a) shows the most straightforward way of an energy hub with a storage according to the definition from Favre-Perrod (2005). For a hybrid energy hub, different energy carriers have to be included, such as in Fig. 1 (b), where different demands are supplied by one energy carrier (like the multi-service in MES) or in Fig. 1 (c) where various energy carrier provide one supplier (like the multi-fuel in MES). But for a holistic approach, a multi-input and output system is needed to simulate the behaviour of a real system (HEMMES et al., 2007). An example of such a system provides Fig. 1 (d).

2.2. Research fields

The published literature on multi-energy systems and energy hubs has increased in the last few years. A thorough literature review on the Energy Hub concept was done in Mohammadi (Mohammadi et al., 2017). For multi-energy systems Geidl and Andersson (Kriechbaum et al., 2018), Kriechbaum et al. (Allegrini et al., 2015), and Mancarella et al. (Mancarella, 2014) provide a detailed overview. Geidl and Andersson (Kriechbaum et al., 2018) and Kriechbaum et al. (Allegrini et al., 2015) show that much research is ongoing in the field of grid-based multi-energy systems and on the district scale. These

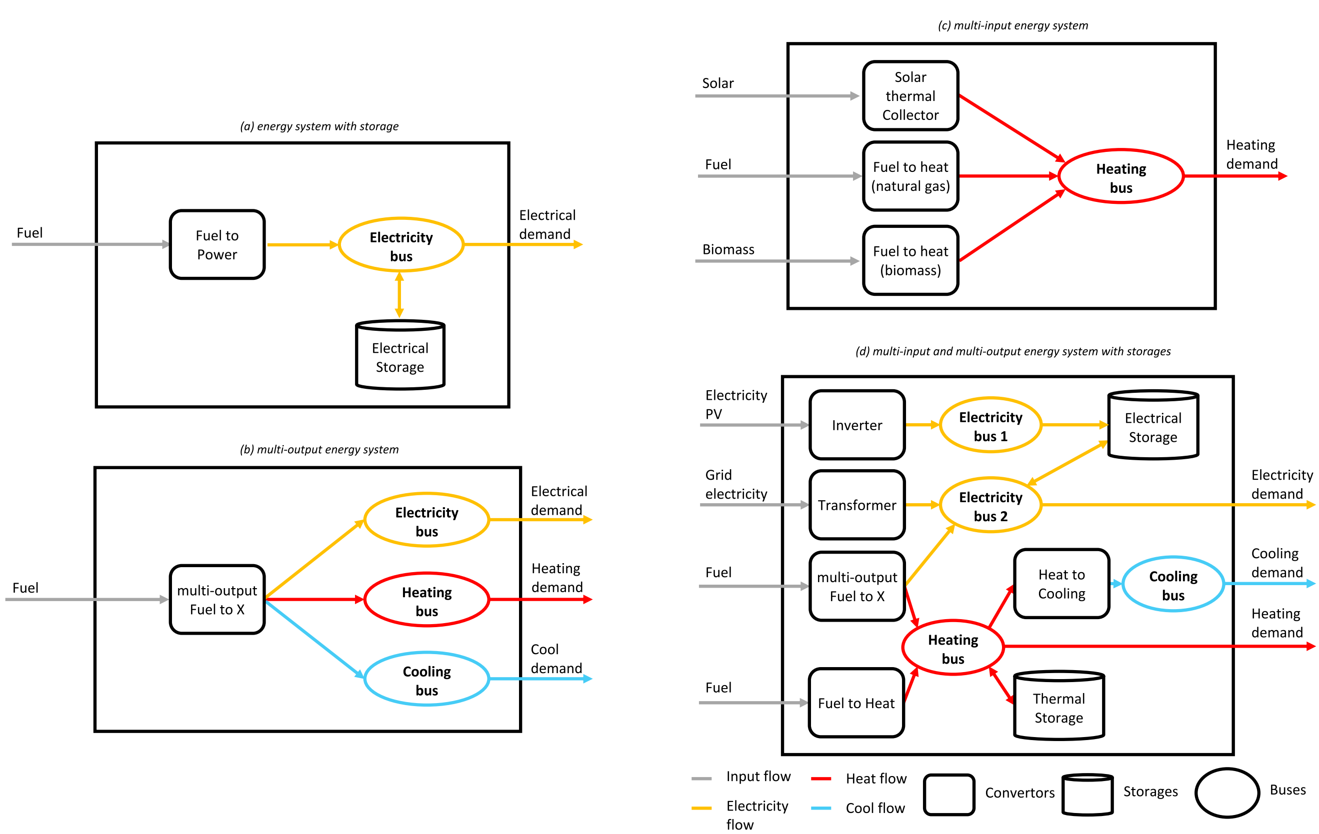

Fig. 1. Different energy hub systems

multi-energy systems have a high spatial resolution, and the transport losses in the network are of high interest. The energy system of an industrial site has a shallow spatial resolution, and the energy losses during transport can be neglected. So the network specifies only the structure and connections between the industrial energy system's inputs, outputs, convertors and storages. Although the industrial sector has a high potential for optimising energy systems, more work needs to be done in this field according to Mohammadi et al. (2018).

In Chang et al. (2021) and Prina et al. (2020), various energy system models, including those applicable to the industrial sector, were investigated. These papers emphasize trends, approaches, and challenges in energy system modelling. Prina et al. (2020) classified different approaches and identified the main challenges in this field. Four challenges revolve around the resolution theme: resolution in time, in space, in techno-economic detail, and in sector coupling. Additional challenges include transparency and uncertainty. Chang et al. (2021) provides an overview of the existing trends in energy system modelling.

2.2.1. Lack in multi energy carrier consideration

An approach for industrial energy hubs was made by Mohammadi et al. (Halmschlager and Hofmann, 2021). In this approach, the production program is optimised considering both the logistics and the energy requirements. But in this paper, the focus is on the optimisation of the energy supply. The production program is given. The main outputs of common energy hubs are electricity and heat (Mohammadi et al., 2017), but for the non-energy intensive energy industry also, cooling, compressed air and other energy carriers (depending on the production process) must be considered. Also, the converters like compressors, heat pumps and chillers are rarely used in energy hubs (Mohammadi et al., 2017).

2.2.2. Deeper consideration of operational optimisation requirements

A further consideration of the modelling approach from the industrial multi-energy system is to meet the needs of operational optimisation. Operational optimisation aims to find a solution to cover the energy demand most efficiently – according to the target function (Papageōrgiu et al., 2012). Based on the given energy demands at the output of the energy hub and available inputs, the optimal operation of the converters and storages is calculated by the operational optimisation for the next few days. Because the input parameters can change during time (e.g. electricity price changes every 15 min, energy demands can change when the production plan is reordered or machines break down), the optimisation must be recalculated in given time steps. Hence models with a low computation time are essential. Common modelling approaches do not fulfil this requirement.

2.3. Research needs and questions

The current research is focused on developing energy models from scratch. Chang et al. (2021) mention that building a tool capable of handling all aspects of modelling energy transitions is impossible. Instead, energy system models are customised to specific user needs (which fulfil a task within a defined scope), particularly in the industrial sector, where specific requirements (according to the user needs) are essential for an energy system model. Consequently, a unique model is developed for each specific need, leading to high efforts in maintenance and development. Usually also for the operational optimisation a unique

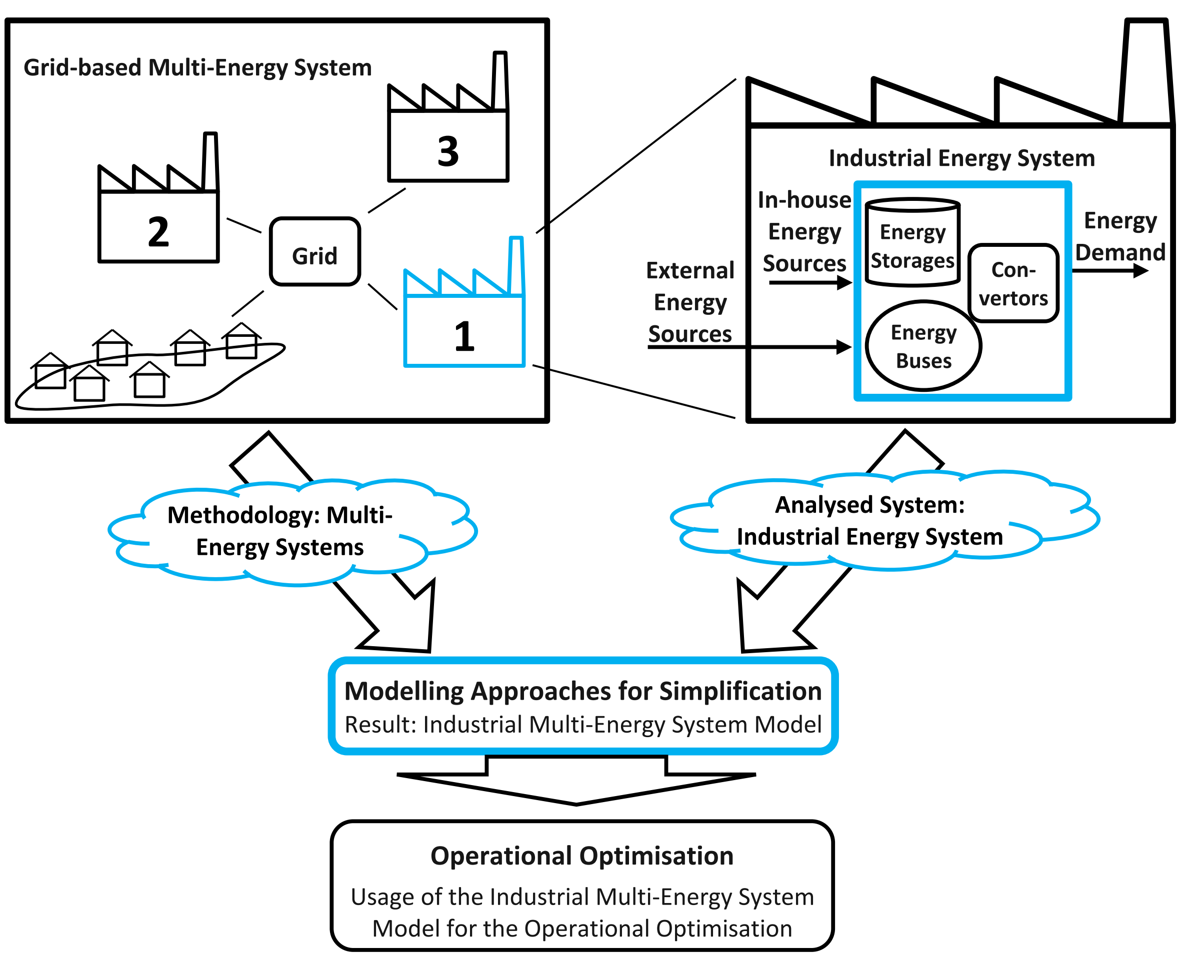

Fig. 2. Illustration of the inspected research field.

energy system is developed independent from the others. To address the challenge of reducing the modelling effort for energy systems, an approach is developed in this work to derive the model for operational optimisation from an existing model.

The system boundaries of this research are shown in Fig. 2. In contrast to the common grid-based multi-energy systems approach with a high spatial resolution the focus here is on an industrial energy system with a low spatial resolution. But it is crucial that the entire energy system of the site is inspected. The simulation horizon is limited to one week, segmented into 15-min time steps. Furthermore, the simplified model has to fulfil the requirements for the operation optimisation.

In this work, two approaches were analysed to investigate if they could be used for a simpler modelling of industrial energy systems. One approach is linearising existing models, and the other is training a neural network to represent the existing model. This paper investigates whether these approaches are suitable to model the multi-energy system of a non-energy intensive industry and how they affect the operational optimisation.

The main question in this work is how existing industrial energy system models can be simplified to use them for operational optimisation. For this purpose, the advantages and disadvantages of the linearisation and neural network approach were examined. In the validation of the two approaches, the following points need to be considered.

- What is the accuracy of the simplified models compared to the reference model?
- Is the computation time of the optimisation within the boundaries?
- How robust is the optimisation result?
- How high is the effort for setting up and maintaining the simplified model?
- Is the simplified model suitable for further usage in operational optimisation?

3. The reference model

In the first step, a model of the energy system of a generic industrial plant (containing typical elements of heating, - cooling-, and electricity supply) is established. This model is referred to as the reference model in the further work. The reference model comprises literature data and industrial data, presenting a simple yet sufficiently complex representation to capture all necessary behaviours.

The reference model only simulates the behaviour of the energy system and does not optimise it. The simulation has a resolution of 15 min. The horizon of the simulation can be varied and depends on the input data. During this work always a time horizon of one week is investigated. This leads to 672 time steps for one run. How the reference model can be converted for the optimisation purpose is examined in chapter 5. To determine the accuracy, computation time, robustness and effort for creating the simplified models in section 5 the reference model was elaborated first.

3.1. Modelling concept of the reference model

To model the reference model, the energy hub approach was chosen. Fig. 3 shows the general structure of it. As mentioned it depicts the energy system of a generic industrial production side in non-energy intensive industry. The five components (inputs, outputs, connectors, storages and buses) of the energy hub approach can be retrieved in this figure.

3.1.1. Inputs and outputs

The Inputs can be separated into two groups, the energy sources from outside and the in-house energy sources. External energy sources like electricity and gas from the grid are imported into the energy system. These parameters have time resolved costs or specific CO_2 emissions which have a direct impact on the optimisation targets. These are the parameters, the optimisation wants to improve (e.g. absolute energy costs, total CO_2 emissions etc.). Therefore, the related time series (e.g. energy price for each time step, CO_2 emissions, etc.) are needed. Depending on the parametrisation of the energy system, the reference model calculates different results for the external energy resources. The in-house energy resources are produced on-site, e.g. electricity from a PV plant or the waste heat from processes.

The outputs represent the different time resolved energy demands of the processes, also given as model-exogenic parameters. The most common are electricity and heat, but also cooling, pressurised air and water are essential energy demands in the non-energy intensive industry. Further energy demands can also be implemented.

The inputs and outputs are given parameters which can origin from forecasts or are results from the simulation of the energy system. The optimisation cannot change them.

3.1.2. Convertors and storages

Convertors are machines or aggregates which transform energy from

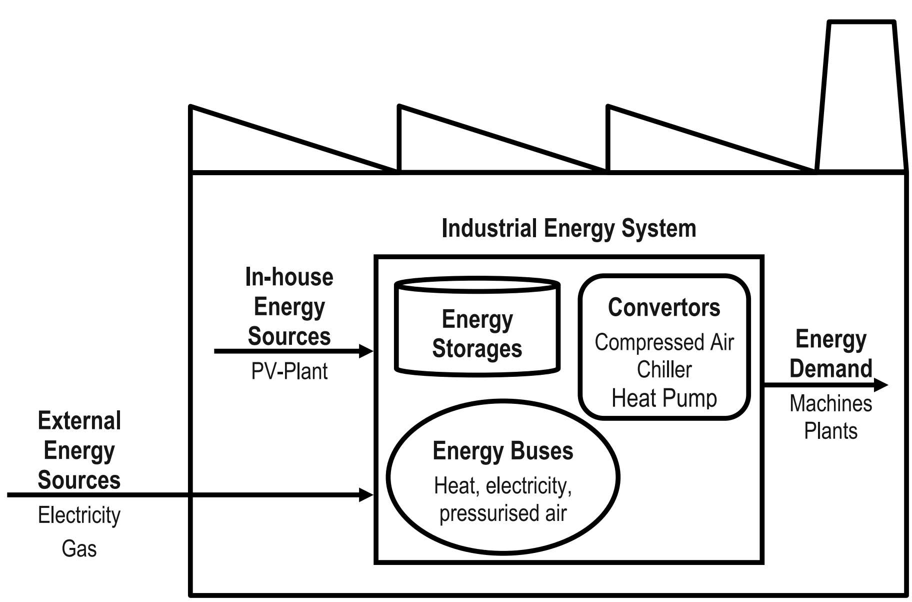

Fig. 3. General illustration of the energy system of a non-energy intensive company.

a given energy form into another energy form (e.g. Power-to-Heat, Heat-to-Power, Power-to-Power). Storages can store various energy forms. Electricity, heat, pressurised air, H_2 and other types of storages are possible. The operation of the convertors and storages can be changed in the model. These model-endogenic parameters of the operation are the variables which can be changed by the optimisation. The optimisation calculates the best combination of these variables which leads to the ideal result defined by the target function and the constraints.

3.1.3. Network and busses

Besides the components inputs, outputs, connectors and storages the network is also an essential part of the energy system model. The network describes how the different components are connected. E.g. if heat pump one is only connected to machines A and B but not to machine C. So it is impossible to cover the heat demand from machine C with heat pump one. Machine C must be supplied by another source. In industrial energy systems it is very common that a source cannot supply all demands. For the integration of the network in the energy system buses are used as described in section 3.1.1.

3.2. Description of the reference model

The reference model represents the fundamental behaviour of the real system. In Fig. 4, the structure of the reference model is illustrated.

The reference model is used to verify the different simplification approaches in Section 5. It simulates the behaviour of a generic industrial energy system. The energy models from non-energy intensive industries can consist of very accurate models (e.g. thermodynamic model) to very simple ones (e.g. characteristic curve) – depending on the needs of the company. Therefore, the reference model has parts with different levels of complexity. It was decided to develop the reference model in Dymola (2023), based on OpenModelica (Pop and Fritzson, 2006), to easily integrate already existing sub-models.

The different components of the reference model are listed in Table 1. They are assigned to the five categories of the energy hub system (section 3.1.1).

Utilizing the reference model, the energy system can be simulated over a defined time horizon. The reference model calculates the required electricity and gas procurement from the grid. The calculation needs the time series from the electricity produced by the PV plant and the time series from the electricity, heat, and cooling demand from the production process. The subsequent sections describe the behaviour of converters and energy storages. Using this information, the required electricity from the grid (e_{grid}) and the heat demand for the boiler (h_{boiler}) can be determined (see equations (1) and (2)). To calculate the gas required from the grid based on the heat demand from the boiler, equation (13) is employed.

$$e_{grid} = e_{demand} + e_{heat\ pump} + e_{chiller} - e_{PV} + e_{storage\ in} - e_{storage\ out} \tag{1}$$

$$h_{boiler} = h_{demand} - h_{heat\ pump} - h_{waste\ heat\ chiller} + h_{storage\ in} - h_{storage\ out} \tag{2}$$

For the simulation of the reference model also the control of the energy system is important. For controlling the energy system, the following parameters are used.

- inflow of the electricity storage ($u_{e.s.in}$)
- outflow of the electricity storage ($u_{e.s.out}$)
- inflow of the heat storage ($u_{h.s.in}$)
- outflow of the heat storage ($u_{h.s.out}$)
- usage of the PV (u_{PV})

Table 1
Components of the reference model.

Inputs	electricity grid, natural gas grid, PV production
Outputs	electricity demand, heat demand, cooling demand
Convertors	heat pump, chiller, condensing boiler
Storages	heat storage, electricity storage
Buses	electricity, heating, cooling, natural gas

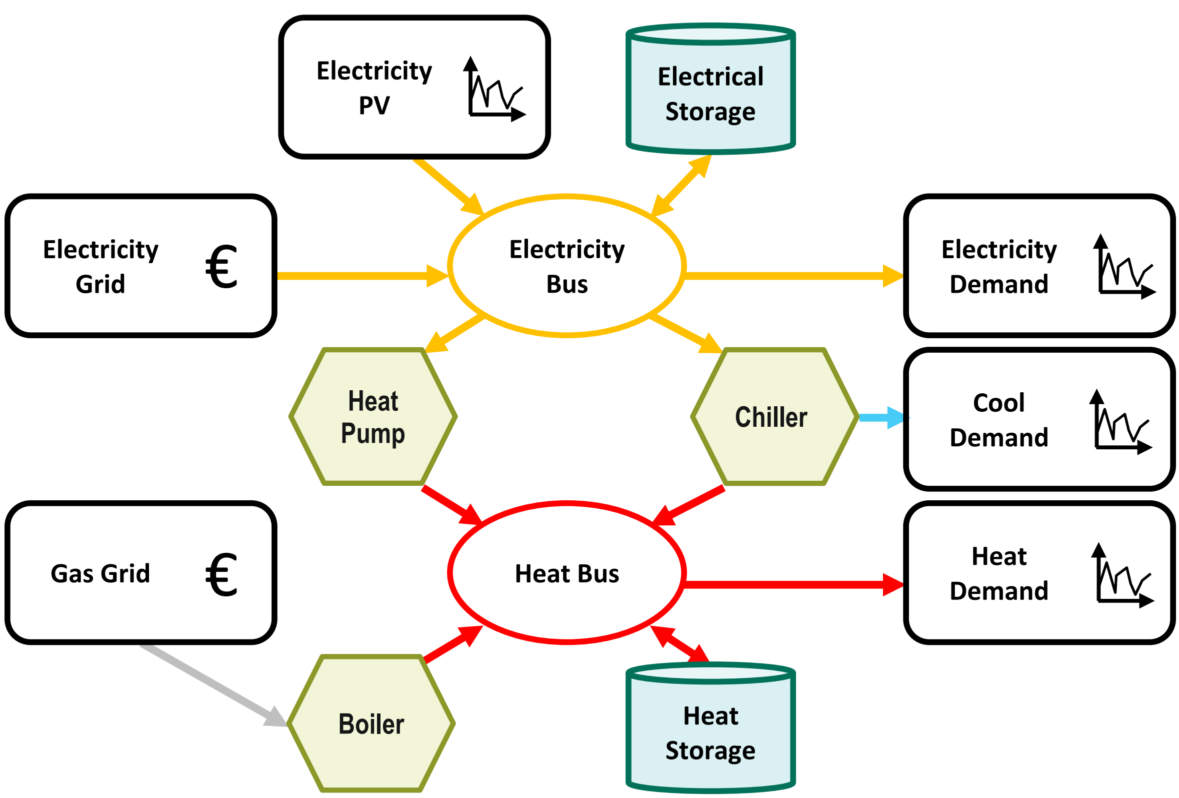

Fig. 4. Schematic representation of the reference model.

- usage of the heat pump (u_{hp})
- usage of the waste heat (u_{wh})

These parameters must be also given as time series for the reference model to simulate it. They can reach from 0 to 1 (0%–100%). In the optimisation these parameters can be changed to find the best control of the energy system. So equations (1) and (2) are adapted to:

$$e_{grid} = e_{demand} + e_{heat\ pump} * u_{hp} + e_{chiller} - e_{PV} * u_{PV} + e_{storage\ in} * u_{e.s.in} - e_{storage\ out} * u_{e.s.out} \quad (3)$$

$$h_{boiler} = h_{demand} - h_{heat\ pump} * u_{hp} - h_{waste\ heat\ chiller} * u_{wh} + h_{storage\ in} * u_{h.s.in} - h_{storage\ out} * u_{h.s.out} \quad (4)$$

Based on the needed electricity and gas from the grid it was possible to calculate also the costs for them.

The time series for heating, cooling, and electricity demand to supply the industrial production processes was provided by the considered company. For the calculation of the electricity price and gas price, the guidance of E-Control (E-Control, 2022) was used as a reference. The source for the market price was the EXAA (EXAA, 2022). The model from Staffell and Pfenninger (Pfenninger and Staffell, 2016; Renewables.ninja, 2022) was used to generate the PV plant's electricity production profile.

3.2.1. Convertors

Three types of converters (heat pump, chiller and boiler) are implemented in the reference model. In this section the detailed behaviour of the converters is described.

3.2.1.1. Heat pump. The behaviour of the heat pump in the reference model is represented by the coefficient of performance (COP). Is the heat demand given it is possible to calculate the needed electricity with the COP.

$$heat\ demand_{heat\ pump} = electricity_{heat\ pump} * COP \quad (5)$$

The COP_{max} is the theoretical maximal COP, which is reachable. To calculate the real COP, the COP_{max} has to be multiplied by the total energy efficiency (η_{HP}). The equation for the COP is:

$$COP = COP_{max} * \eta_{HP} \quad (6)$$

Heat pumps' total energy efficiency lies between 0.4 and 0.6 (Dott, 2018). For the reference model, 0.5 as η_{HP} was used. The COP_{max} depends on the temperature of the heat source (T_C) and the heat sink (T_H). The target temperature for the heat supply is 50 °C, so this constant value was used as the temperature for the sink. For the source, the measured (time-resolved) air temperature was used.

$$COP_{max} = \frac{T_H}{T_H - T_C} \quad (7)$$

3.2.1.2. Chiller. Data on the chillers from the investigated production site was provided as time series. With these measured data points, it was possible to establish a function to calculate the energy efficiency ratio (EER). This was done with a simple curve-fitting in Excel. The EER from the approximated function has a mean absolute percentage error (MAPE) of 1.5% and a root mean squared error (RSME) of 0.073 compared to the EER from the production site. The most influencing parameters for this function are the evaporation temperature (T_e), the condensation temperature (T_{co}) and the load factor (l_f).

$$EER = -0.000054110 * l_f^2 + 0.005446 * l_f - 0.1121 * T_{co} + 0.06803 * T_e + 7.5892 \quad (8)$$

The evaporation temperature can change between 7 °C and 10 °C and the condensation temperature between 28 °C and 48 °C. The load factor can vary from 0% to 100%.

With the EER the electricity can be calculated which is needed to produce the specified cooling demand. The maximum available waste heat can also be calculated with the EER.

$$cooling\ demand_{chiller} = electricity_{chiller} * EER \quad (9)$$

$$max.\ waste\ heat_{chiller} = electricity_{chiller} + cooling\ demand_{chiller} \quad (10)$$

Not all of the maximal available waste heat can be used. The investigation of the chillers in the inspected company have shown that the efficiency ($\eta_{useable\text{-}waste\text{-}heat\text{-}chiller}$) for the useable waste heat is only 75%.

$$usable\ waste\ heat_{chiller} = max.\ waste\ heat_{chiller} * \eta_{useable-waste-heat-chiller} \quad (11)$$

3.2.1.3. Condensing boiler. In the reference model, a condensing boiler generates low temperature heat from natural gas. The data for modelling this condensing boiler was taken from (Wolf GmbH). In Fig. 5 the comparison between the condensing boiler from (Wolf GmbH) and the linear one used in the reference model is shown. The linearisation was done to represent components of different complexity in the reference model.

Based on (Wolf GmbH) a linear function for the boiler's efficiency (η_b) was calculated. The two points for the calculation are chosen at 10% load factor (efficiency = 108%) and 100% load factor (efficiency = 96%).

$$\eta_b = -0,1333 * l_f * 100 + 109,333 \quad (12)$$

In the last step, 11,1% has to be subtracted from η_b to convert the lower heating value into the higher heating value. So the equation for the needed natural gas to cover the heat demand is:

$$heat\ demand_{condensing\ boiler} = natural\ gas_{condensing\ boiler} * (\eta_b - 0.111) \quad (13)$$

The MAPE of the linear equation is 0.699% and the RSME is 0.825.

3.2.2. Storages

Energy storages provide good flexibility for energy systems. Therefore, different storages are implemented in the reference model. The behaviour of the storages can differ strongly from each other (Sterner and Stadler, 2014). Losses can occur while charging and discharging and also during the storage period. In the reference model, a heat storage and an electrical storage are integrated.

In this section the detailed behaviour of the storages is described. During optimisation the behaviour of the storages cannot be changed. The optimiser only decides the inflow and outflow rate of the storages.

3.2.2.1. Electrical storage. For more flexibility, a lithium-ion battery is implemented in the reference model. The maximum capacity of the storage is 3000 kWh. In each time step (15 min), 600 kWh can be loaded or unloaded from the storage (p_{max}). According to Kurzweil and

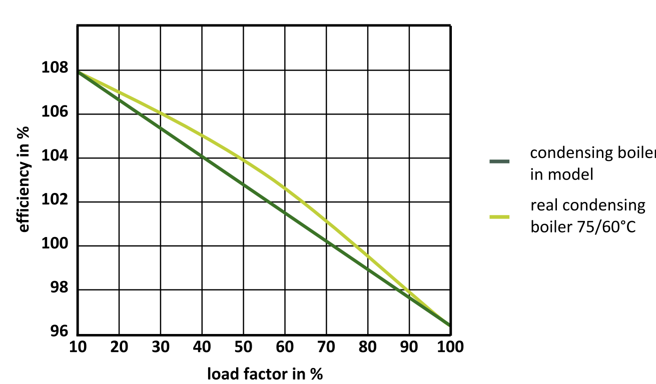

Fig. 5. Efficiency of boilers according to (Wolf GmbH).

Dietlmeier (2015) the losses of a lithium-ion battery can be classified into the losses for charging/discharging and the losses from self-discharge. Due to the low self-discharge rate of lithium-ion batteries (Korthauer, 2013) and the inspected time period of only one week the losses for self-discharge are neglected in the model. For charging and discharging, losses of 3.5% each occur (Korthauer, 2013). This means when 1 kWh is stored, only 0.931225 kWh is discharged.

For the lithium-ion battery, care must be taken not to discharge or charge it too deep or too high. The battery is charged or discharged exponentially in the last 20% to avoid this. So the charging and discharging capacity depend on the state of charge (SOC) (Jossen and Weydanz, 2021; Julia Vopava, 2021):

$$p_{charging} = \begin{cases} SOC < 80\% : p_{charging} = p_{max} \\ SOC > 80\% : p_{charging} = p_{max}\, e^{\frac{0.8-SOC}{f}} \end{cases} \tag{14}$$

$$p_{discharging} = \begin{cases} SOC > 20\% : p_{charging} = p_{max} \\ SOC < 20\% : p_{charging} = p_{max}\, e^{\frac{-0.2+SOC}{f}} \end{cases} \tag{15}$$

The form factor f was used to adjust the curve's shape.

For the usage in the reference model the equation needs to be adapted. First, a logistic function was used to switch between the two sections ($h_{charging}$, $h_{discharging}$).

$$h_{charging} = \frac{1}{e^{\frac{SOC-0.8}{0.00001}}+1} \tag{16}$$

$$h_{discharging} = \frac{1}{e^{\frac{SOC-0.2}{0.00001}}+1} \tag{17}$$

Next, the two section are added together and the exponential part is simplified. The behaviour of the storage is shown in Fig. 11 and in equations (18) and (19).

$$p_{charging} = p_{max} * h_{charging} + \left(\frac{p_{max}}{1-0.8} - \frac{p_{max}}{1-0.8} * SOC\right) * \left(1 - h_{charging}\right) \tag{18}$$

$$p_{discharging} = -p_{max} * \left(1 - h_{discharging}\right) - \left(\frac{p_{max}}{1-0.8} * SOC\right) * \left(h_{discharging}\right) \tag{19}$$

3.2.2.2. Heat storage. A hot water storage is used in the reference model to store heat. The maximum capacity of the storage is 2000 kWh, and the extraction and filling volume is limited to 5000 kg water (m_{max}) per time step (15 min). The feed water temperature is 20 °C. This water is heated up and leaves the storage with 80 °C. As model framework, the water in the storage is divided into a region with water of 20 °C (cold water) and one with 80 °C (warm water). During loading the volume of the warm water increases. The volume of the cold water decreases by the same amount the warm water increases. For unloading it is the other way round.

The losses of the storage (qV) depend on the temperature difference (ΔT), heat transition coefficient (u) and the area of the warm water (80 °C) volume (a):

$$q_V = u * a * \Delta T \tag{20}$$

The temperature of the environment is assumed to be constant at 20 °C. So the temperature difference is 60 °C, and the transition coefficient of the storage is assumed to be 0,00035 kW/m^{2}K (Sterner and Stadler, 2014). The state of charge (SOC) and the density of water at 80 °C ($\rho_{W80} = 971.79$ kg/m^{3}) are needed to calculate the hot water area. Furthermore, warm water storage is expected to have a cylinder shape where the radius (r) is three-quarters of its height (h). Then the area can be calculated:

$$a = r^2 * \pi + 2 * r * \pi * h \tag{21}$$

$$h = \frac{4}{3} r \tag{22}$$

$$a = r^2 * \pi * \left(1 + \frac{8}{3}\right) \tag{23}$$

$$V = r^2 * \pi * h \tag{24}$$

$$V = m_{max} * \rho_{W80} * SOC \tag{25}$$

$$r = \sqrt[3]{\frac{3 * m_{max} * \rho_{W80} * SOC}{4 * \pi * h}} \tag{26}$$

$$a = \left(\frac{3 * m_{max} * \rho_{W80} * SOC}{4 * \pi * h}\right)^{\frac{2}{3}} * \pi * \left(1 + \frac{8}{3}\right) \tag{27}$$

If the storage is full, also the bottom area of the cylinder has to be considered. Therefore, the area changes to:

$$a = \left(\frac{3 * m_{max} * \rho_{W80} * SOC}{4 * \pi * h}\right)^{\frac{2}{3}} * \pi * \left(1 + \frac{16}{3}\right) \tag{28}$$

The equation for charging and discharging of the electrical storage was also used for the heat storage. Instead of 80% and 20% in the electrical storage, 98% and 2% were used in the heat storage.

$$h_{charging} = \frac{1}{e^{\frac{SOC-0.98}{0.00001}}+1} \tag{29}$$

$$h_{discharging} = \frac{1}{e^{\frac{SOC-0.02}{0.00001}}+1} \tag{30}$$

$$p_{charging} = p_{max} * h_{charging} + \left(\frac{p_{max}}{1-0.98} - \frac{p_{max}}{1-0.98} * SOC\right) * \left(1 - h_{charging}\right) \tag{31}$$

$$p_{discharging} = -p_{max} * \left(1 - h_{discharging}\right) - \left(\frac{p_{max}}{1-0.98} * SOC\right) * \left(h_{discharging}\right) \tag{32}$$

3.2.3. Overview components

Here the components of the reference model are summarised. In Table 2 the convertors and storages are shown. For each of them the connection to the buses, the maximal capacity, the relation between input and output, the losses and the source is presented. The maximal capacity of the heat pump is limited by the electricity. The maximal heat production depends on the ambient temperature. For the chiller and the condensing boiler, the maximal capacity is specified for cooling and heating production. Losses only occur in the storages. The row "source" indicates the origin of the data, where "industry" signifies that the data is derived from the analysed industry. The sizes of the components were specifically selected to match the energy system of a non-energy-intensive industry.

Also the details for the inputs and outputs of the reference model are summarised in Table 3.

4. Simplification of the reference model for the operational optimisation

The reference model described in section 4 represents the behaviour of a generic energy system in non-energy intensive industry with components of different complexity. It is assumed that the reference model accurately represents the reality. But the reference model is unsuitable for an operational optimisation. Either the structure of the reference model does not align with the requirements for executing linear optimisation, or the computation time is too high to use a genetic algorithm. Therefore, it is necessary to investigate how this model can be adjusted to use it for operational optimisation. Fig. 6 summarises the problems encountered when using the reference model for the optimisation methods, along with the solution approaches and requirements.

Table 2
Convertors and storages of the reference model.

	heat pump	chiller	condensing boiler	electrical storage	heat storage
input	electricity bus	electricity bus	gas bus	electricity bus	heat bus
output	heat bus	heat bus cooling bus	heat bus	electricity bus	heat bus
max capacity	60 kW	4000 kW	3320 kW	size: 3000 kWh charge: 2400 kW	size: 2000 kWh charge: 20000 kg/h
relation input & output	equation 5	equations (9) and (11)	equation 13	equations (18) and (19)	equation (31) and (32)
losses	–	–	–	3.5% for charging and discharging	equation 20
source	Dott (2018)	industry	(Wolf GmbH)	(Jossen and Weydanz, 2021; Julia Vopava, 2021; Korthauer, 2013; Kurzweil and Dietlmeier, 2015; Sterner and Stadler, 2014)	Sterner and Stadler (2014)

Table 3
Inputs and outputs from the reference model.

	electricity grid	natural gas grid	PV production	electrical demand	heat demand	cooling demand
Input	–	–	–	electricity bus	heat bus	cooling bus
Output	electricity bus	natural gas bus	electricity bus	–	–	–
max capacity	unlimited	unlimited	3000 kW	8000 kW	4000 kW	4000 kW
source	(E-Control, 2022; EXAA, 2022)	(E-Control, 2022; EXAA, 2022)	(Pfenninger and Staffell, 2016; Renewables.ninja, 2022)	industry	industry	industry

reference model	**linear optimisation**	**genetic algorithm**
- Components with different complexity (linear function, quadratic function, exponential function) - Accurate representation of the reality - Long simulation time	**Problem:** The model of the energy system may only consist of linear functions **Solution:** Conversion of the reference model into a linear model consisting only of components with linear functions	**Problem:** The genetic algorithm is not able to reach the optimum in a reasonable time, because the simulation time of the reference model is to high **Solution:** Usage of a neural network which replicates the behaviour of the reference model but simulates the energy system much faster
	Requirements: - High accuracy of the energy system model - Low computation time of the optimisation - Robust optimisation results - Low effort for setting up and maintaining the energy system models	

Fig. 6. Problems, solutions, and requirements for the optimisation approaches compared to the reference model.

Two approaches were analysed for the simplification of the reference model. The first approach is to reproduce the reference model as a linear model to prepare it for mixed integer linear problem (MILP) optimisation. The second approach is to train a neural network. Which is used for a genetic algorithm which optimises the energy system. In the section methodology it is explained how the simplification of the reference model was done and how it was implemented in the optimisation. In the section model structure, the simplified models are described in detail.

For the validation the data points where divided in three categories.

- Input parameters
- Optimised variables
- Output parameters

Beware that these don't match with the definition of the inputs and outputs from the energy hub approach. Here the relation to the model and the optimisation is in focus. The input parameters are those data points which are needed to simulate the model. They are fixed and will not be changed during the optimisation. But the input parameters can be changed within the limits before the optimisation to simulate different behaviours and scenarios. The optimised variables are the data points which can be changed by the optimisation to find the best possible values according to the target function. The output parameters are the results of the simulation. In Table 4 all input parameters and output parameters with their properties are listed. For the output parameters only the most important ones are listed and not all possible ones.

In the section validation the accuracy of the simplified models compared to the reference model is investigated. For this comparison 1000 different time series are used. Each time series has 672 time steps. This represents one week with a resolution of 15 min. The input parameters which have been changed for the comparison are the energy demands (electricity, heat, cooling). These parameters are set randomly for each time series in the specified range (see Table 4). The other parameters stayed the same or are calculated for each time series.

Afterwards the discussion of the results from the validation follows. Further the computation time of the optimisation and the robustness of the results from the optimisation are analysed in this section. Also the effort for setting up and maintaining the simplified models is addressed.

4.1. Linearised modell

During linearisation, the reference model is re-modelled in a simplified way. Then the models are implemented in the tool: open energy modelling framework (oemof – python package). With oemof, a mixed integer linear optimisation can be carried out based on the modelling.

4.1.1. Methodology

For the development of the linear optimisation model, the following steps were carried out, which are illustrated in Fig. 7 and subsequently described in more detail.

1. Create linearised model from the reference model
2. Establishment of the optimisation model
3. Comparison of the reference model and linear model (validation)

4.1.1.1. Create linearised model from the reference model. Based on the reference model, a linear model was created in the optimisation tool oemof (Hilpert et al., 2018). For this purpose, the reference model was reconstructed piece by piece with linear components. The oemof model was constantly brought closer to the reference model in an iterative process. The extent to which the individual components influence the results was also determined.

Every single component has to be adapted for the linearised model – every convertor and storage, all the inputs and outputs and all the connections between them have to be defined. This needs a lot of effort until the linearised model approximates to the reference model. Finding mistakes in the linearised model during the simplification is also very time consuming.

4.1.1.2. Establishment of the optimisation model. To compare the reference model with the linear model, the linear optimisation model was given the exogenic input parameters. With this information the linear optimisation can calculate the lowest costs by varying the endogenic variables. The linear model is also able to show all the energy flows within the energy system. The costs and the energy flows are summarised in the output.

4.1.1.3. Comparison of the reference model and linear model (validation). The exogenic input parameters and the optimised variables are transferred to the reference model. Then the results of the simulation from the reference model are compared with the output from the linear model. This allows to calculate the accuracy of the linear model. For the validation every time series was considered.

Table 4
Data points for validation.

	Data points	min	max
Input parameters	Electricity demand	100 kWh	2000 kWh
	Heat demand	0 kWh	1000 kWh
	Cooling demand	0 kWh	1000 kWh
	PV production	0 kWh	750 kWh
	Electricity price	unlimited	unlimited
	Natural gas price	unlimited	unlimited
	Electricity storage level (start)	0%	100%
	Heat storage level (start)	0%	100%
Optimised variables	inflow of the electricity storage	0%	100%
	outflow of the electricity storage	0%	100%
	inflow of the heat storage	0%	100%
	outflow of the heat storage	0%	100%
	usage of the PV	0%	100%
	usage of the heat pump	0%	100%
	usage of the waste heat	0%	100%
Output parameters	Electricity from grid	0 kWh	unlimited
	Natural gas from grid	0 kWh	unlimited
	Costs	0 €	unlimited
	Electricity storage level (end)	0%	100%
	Heat storage level (end)	0%	100%

4.1.2. Model structure

The oemof model is structured like the reference model and also based on the energy hub principle. In oemof, there are predefined components for modelling, such as sources, sinks, transformers, storage and buses. Sources and sinks correspond to the inputs and outputs of energy hubs. The transformers are the same as the converters. The buses have in both systems the same function.

The reference model was reconstructed with the predefined components from oemof. The basis was the schematic of Fig. 4 from Section 4. In addition to the reference model, two sinks for unused heat and electricity were added to oemof. These additional sinks are needed to correctly balance the surplus waste heat from the cooler or the surplus electricity from the PV system in the busses. To use oemof, it is necessary to adjust the converters and storages of the reference model to the predefined components from oemof. The structure for converters are shown in Fig. 8 and for storages in Fig. 9.

For the oemof component transformer the following parameters have to be defined.

- label: name of the transformer
- inputs: the bus where the inflow of the transformer is connected to with the maximal allowed inflow rate (nominal_value)
- outputs: the bus where the outflow of the transformer is connected to with the maximal allowed outflow rate (nominal_value)
- conversion_factors: represents the relation between input and output – can be compared with the efficiency of the transformer

For the oemof component storage the following parameters have to be defined.

- nominal_storage_capacity: maximal capacity of the storage
- label: name of the storage
- inputs: the bus where the inflow of the storage is connected to with the maximal allowed inflow rate (nominal_value) – can be compared with maximal charging capacity of the storage
- outputs: the bus where the outflow of the storage is connected to with the maximal allowed outflow rate (nominal_value) – can be compared with maximal discharging capacity of the storage

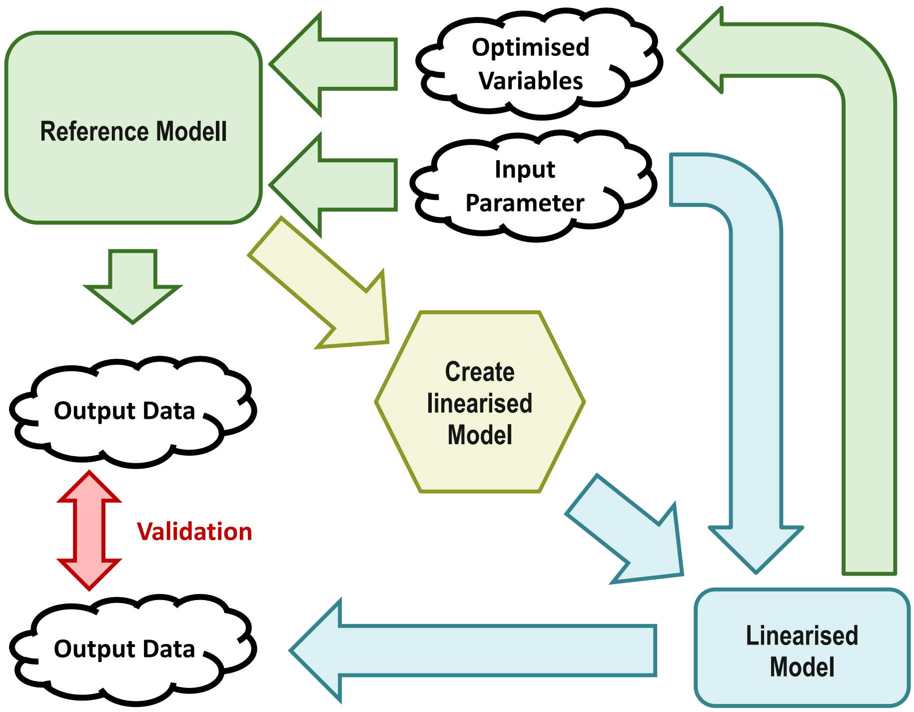

Fig. 7. Methodology for the development and validation of the linearised model.

```
transformer_xxx = solph.components.Transformer(
    label="xxx",
    inputs={bus_xxx: solph.Flow(nominal_value=xxx)},
    outputs={bus_xxx: solph.Flow(nominal_value=xxx)},
    conversion_factors={bus_xxx: xxx})
```

Fig. 8. Transformer from oemof.

```
storage_xxx = solph.components.GenericStorage(
    nominal_storage_capacity=xxx,
    label="xxx",
    inputs={bus_xxx: solph.Flow(nominal_value=xxx)},
    outputs={bus_xxx: solph.Flow(nominal_value=xxx)},
    loss_rate=xxx,
    initial_storage_level=xxx,
    inflow_conversion_factor=xxx,
    outflow_conversion_factor=xxx,
    )
```

Fig. 9. Storage from oemof.

- loss_rate: losses per time step
- initial_storage_level: storage level at the start of the simulation
- inflow_conversion_factor: losses during charging
- outflow_conversion_factor: losses during discharging

4.1.2.1. Linearisation of the heat pump. An adaption is not required for the heat pump. As described above, the heat pump was modelled so that its efficiency (COP) only depends on the outdoor temperature and the temperature to be provided. These temperatures must be transferred to the model beforehand, as exogenic input parameters. The efficiency can then be calculated based on these. This means the efficiency can already be calculated for each time step before the optimisation is executed. This allows the efficiency to be transferred to the optimisation as a time series and does not have to be considered in the optimisation.

```
my_energysystem.add(solph.components.Transformer(
    label="heat_pump",
    inputs={bus_el: solph.Flow(nominal_value=40)},
    outputs={bus_heat: solph.Flow()},
    conversion_factors={bus_heat: 4.971538}))
```

Fig. 10. Parametrisation of the heat pump in oemof.

In Fig. 10 the parametrisation of the heat pump in oemof is shown. For the conversion_factors only a fixed value is insert for the visualisation. This fixed value must be exchanged with the described time series for each time step. The nominal_value at inputs limits the heat pump.

4.1.2.2. Linearisation of the storages. In oemof it is not possible to make the maximum charging capacity or the maximum discharging capacity dependent on the SOC. Only a constant value can be set for it. So the ramp up part above 80% or below 20% was neglected for the electrical storage and above 95% or below 5% for the heat storage (c.f. Eqs. (18), (19), (31) and (32) in section 4.2.2). The simplification for the electrical storage is illustrated in Fig. 11.

The losses of 3.5% for charging and discharging the electrical storage can be copied from the reference model. The losses from the heat storage had to be adjusted for oemof. As average 0.01% loss per time step is used.

Figs. 12 and 13 show how the parameterisation was implemented in oemof. For the heat storage very low losses are needed for the inflow_conversion_factor and outflow_conversion_factor. Otherwise the oemof simulates the energy system not correctly. But the small losses have a negligible effect at the result compared to the reference model.

4.1.2.3. Linearisation of the condensing boiler. For the condensing boiler the same problem as for the charging and discharging of the storages occurred. Also here oemof is not able to make the efficiency of the boiler

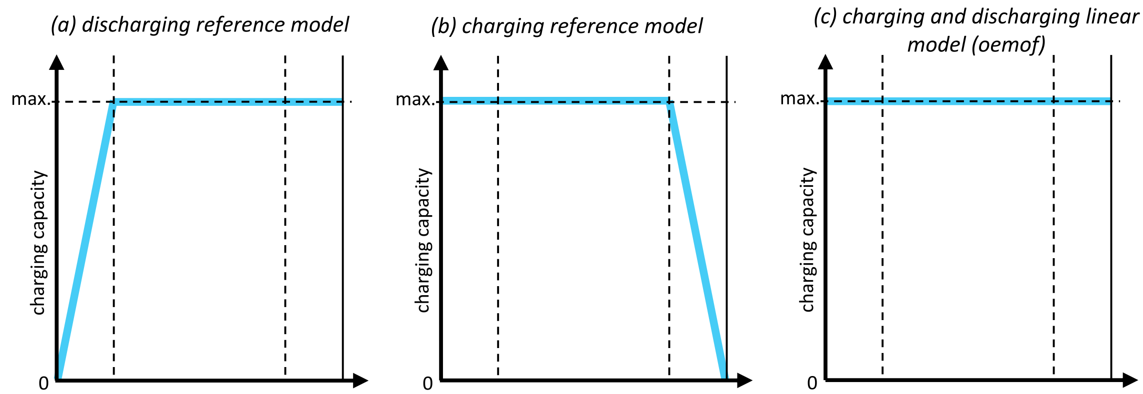

Fig. 11. Charging and discharging behaviour of the electrical storage.

```
el_storage = solph.components.GenericStorage(
    nominal_storage_capacity=3000,
    label="electrical_storage",
    inputs={bus_el: solph.Flow(nominal_value=2400)},
    outputs={bus_el: solph.Flow(nominal_value=2400)},
    loss_rate=0.0,
    initial_storage_level=0.5,
    inflow_conversion_factor=0.965,
    outflow_conversion_factor=0.965,)
```

Fig. 12. Parametrisation of the electrical storage in oemof.

```
heat_storage = solph.components.GenericStorage(
    nominal_storage_capacity=4000,
    label="heat_storage",
    inputs={bus_heat: solph.Flow(nominal_value=1396.67)},
    outputs={bus_heat: solph.Flow(nominal_value=1396.67)},
    loss_rate=0.0001,
    initial_storage_level=0.5,
    inflow_conversion_factor=0.99999,
    outflow_conversion_factor=0.99999,)
```

Fig. 13. Parametrisation of the heat storage in oemof.

```
my_energysystem.add(solph.components.Transformer(
    label="gas_boiler",
    inputs={bus_gas: solph.Flow(nominal_value=1000000)},
    outputs={bus_heat: solph.Flow(nominal_value=1000000)},
    conversion_factors={bus_heat: 0.9}))
```

Fig. 14. Parametrisation of the condensing boiler in oemof.

dependent on the load factor. So 90% was used as constant value for the efficiency of the condensing boiler (see Fig. 14). The nominal_value for the input and output was set in oemof very high because the boiler must always be able to cover the heat demand.

4.1.2.4. Linearisation of the chiller. The chiller had to be adapted for the linear model. Instead of equation (8) in section 4.2.1 for the EER a constant factor of 2.8 is used. The useable waste heat is always 75% of the maximum available waste heat (c.f. Eq. (11)) which can be insert as fixed value in oemof (see Fig. 15).

```
my_energysystem.add(solph.components.Transformer(
    label="Chiller",
    inputs={bus_el: solph.Flow()},
    outputs={bus_cool: solph.Flow(nominal_value=4000),
             bus_heat: solph.Flow(nominal_value=4000)},
    conversion_factors={bus_cool: 2.8, bus_heat: 2.85}))
```

Fig. 15. Parametrisation of the chiller in oemof.

4.1.3. Validation

For the validation of the linear model on the reference model, in addition to the total costs, the 15-min time-resolve energy profiles of electricity and natural gas from the grid are of particular interest. The total costs are calculated based on these profiles. Analysing these profiles makes the influences of them on the energy system more recognisable than in a simple analysis of total costs alone. To verify the deviation between the linear model and the reference model, 1000 time series are compared, with a specific focus on the electricity demand from the grid, as it significantly influences total costs. For all 1000 time series, the difference in electricity demand between the linear model and the reference model was calculated for each time step. This resulted in 672000 time steps that were considered and visualised in Fig. 16.

In Fig. 16, the differences between the two models are given in percent and divided into the respective error categories. In addition, the amount of electricity required from the grid was marked in colour. The figure shows that over 50% of the time steps have a deviation of less than 1%. For the error categories above 5% the share of time steps with high electricity amount is decreasing. That means the absolute failure for time steps with a low electricity amount is smaller than for those with a high electricity amount. So the categories with a bigger error doesn't affect the results strongly due to the fact that the absolute errors are not so high. Therefore, it can be deduced that overall the linear model represents the reference model well.

During identifying the cause for the deviation between linear- and reference model, it turned out that the storages are the decisive factor for the difference between them. In this regard, the difference in the electricity demand of the two models was examined for all 672000 time steps and the storage level as well as their difference (reference-minus linear model) were determined and illustrated in Fig. 17.

Each time step represents a point in Fig. 17. The darker the area, the more points overlap. Hardly any deviations between 20% and 80% SOC can be seen, as the electrical storage behaves linearly in this range. Above 80% and below 20%, two distinctive lines appear. With one line, the error remains relatively small, and with the second line, the error increases strongly due to the exponential behaviour of the storage. The two lines are since the exponential behaviour only occurs during charging or discharging and never both simultaneously. In the range

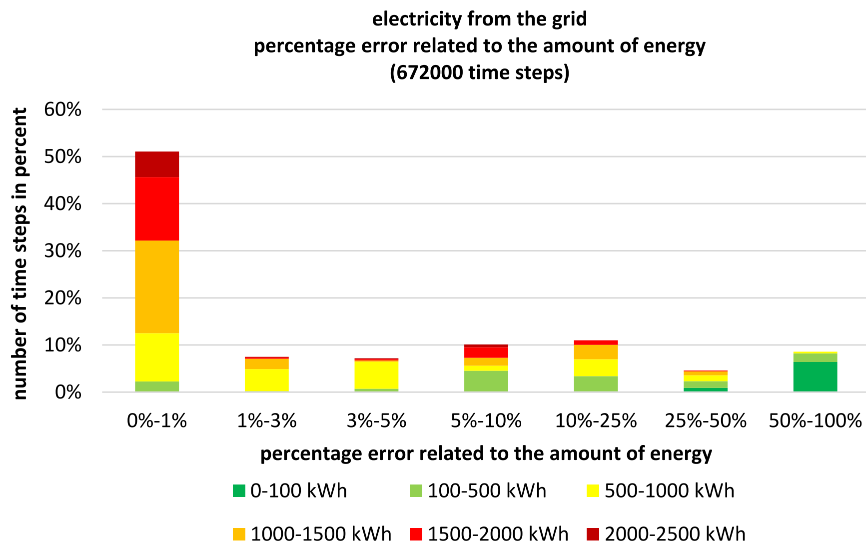

Fig. 16. Comparison reference model and linearised model – for all time steps, the error of the electricity from the grid between the two models is assigned to one of the seven categories of percentage error.

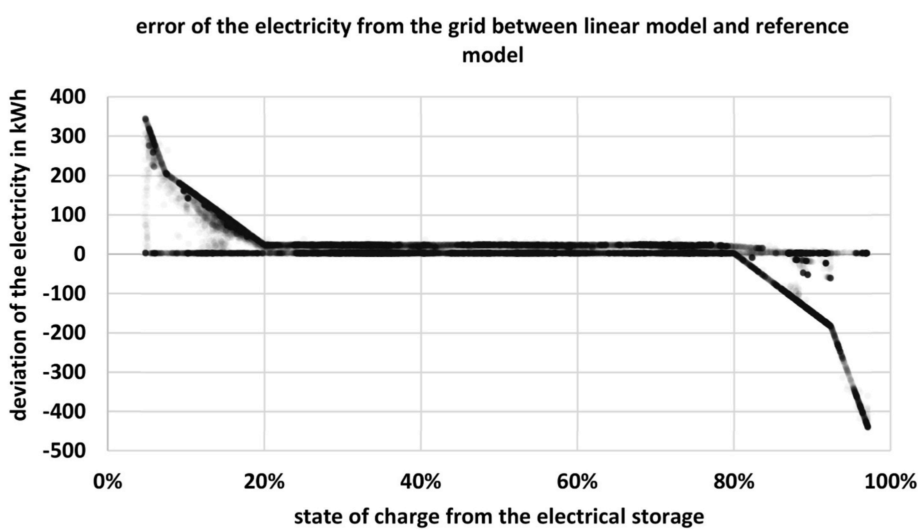

Fig. 17. Deviation of the electricity from the grid between the reference model and the linearised model related to the storage level of the electrical storage (darker area shows higher data density).

below 20%, the behaviour of the storage is linear for charging but exponential for discharging. The opposite is the case for the range above 80%. The points between the two lines are caused by the complete charging or discharging power not being used. The kink, in line with the higher deviation in the two ranges, is caused by the heat storage. The non-linear behaviour of the heat storage leads to this kink. The figure also shows that the storage level of the electric storage is never wholly filled or emptied. This is because the reference model's exponential behaviour means less power is available than in the linear model. Suppose the charging and discharging programme of the electric storage is transferred from the linear model to the reference model. In that case, the reference model needs more time steps for the complete discharging or charging of the storage.

After validating the individual time steps, the costs for an entire time series were compared between the two models. In the first test, only the energy price was considered for calculating the costs. This resulted in an error between the two models of approximately 1%. When the capacity price costs were added, the average error increased to over 10% (see Table 5). For a few time steps, the error was even over 20%. The slight deviation in consideration of the energy price can be explained by the fact that, as shown in Fig. 16, the average error in the individual time steps is small. In addition, negative and positive deviations can balance each other out. For the capacity price calculation, only a single point in time (the one with the highest energy consumption) is used to calculate the costs. This means that a single incorrect time step significantly impacts the overall result. As shown in Fig. 16, for energy demands between 500kWh and 2000kWh, the probability of a deviation between 3% and 50% is about 20%. Looking at one week, the share of the energy price is about 20% of the total costs. Thus, the capacity price influences

Table 5
Accuracy of the linear model.

	MAPE	RMSE
without capacity price	0.782%	4497
with capacity price	13.01%	36004

the total price much more than the energy price, and its errors have a more significant impact.

4.1.4. Discussion

The results from the validation are used in this section to discuss if the linearisation approach is suitable for the operational optimisation.

4.1.4.1. Accuracy. During the development of the linear model, it turned out that not all parts of the energy system need to be linearised and that some have a more influence on the accuracy of the model than other. Parts whose behaviour can already be calculated before optimisation do not need to be linearised—for example, the heat pump. The COP only depends on the outdoor temperature and the temperature to be provided. Since these parameters are already known before the optimisation, the COP can be transferred to the optimisation as a time series. The storages had the most significant influence on the result.

As already explained in section 5.1.3 errors increase from 1% to 10% when the capacity price is considered. Even though the accuracy of the linear model is not very high, the linear optimisation approach was able to find good results compared to the neural network approach.

4.1.4.2. Computation time and robustness. The linear model offers the advantage that a linear optimisation system can be used to perform operational optimisation. The results could be calculated in a few seconds using linear optimisation. Linear optimisation guarantees that a global optimum can always be found.

4.1.4.3. Effort. The development of the linear model took a lot of work. All energy system parts had to be investigated and transitioned into the linear system. This requires a good understanding of the already existing model to be linearised. Linearisation is even more complicated if the reference model is only available as a black box model. Automation of linearisation is a challenge that still needs investigation to see whether this is possible. However, due to the exact mapping during linearisation, it is possible to consider intermediate results or interrelationships of the energy system also in the linear model and not only in the reference model.

4.2. Neural network

In the second approach, a neural network was trained from the reference model in cooperation with ENEXSA (ENEXSA, 2023). First the simplified model (the neural network) was developed and afterwards this model was used in a genetic algorithm to perform the operational optimisation.

4.2.1. Methodology

The method for training and validating the neural network is shown in Fig. 18. During the development of the neural network approach, the following steps were executed.

1. Generate input and output data
2. Training of the neural network
3. Validation of the neural network
4. Implementation of the neural network in the genetic algorithm

In contrast to the linearisation approach the neural network doesn't need to adapt every single component. The neural network replicates the hole reference model by using input and output data.

4.2.1.1. Generate input and output data. The first step before training the neural network is to generate the input and output data from the reference model. These parameters must be defined. It is crucial to choose the parameters so that the parameter space to be investigated is as small as possible. Otherwise too much input and output parameter sets are needed and it becomes more challenging to train the neural network. After the input and output parameters have been generated, they can be used to train the neural network.

4.2.1.2. Training of the neural network. The training of the neural network uses the input and output data to train the neural network. The trained neural network can then reproduce the behaviour of the reference model. The training of the neural network needs a high amount of computation time but the simulation time of the trained neural network is then much lower compared to reference model.

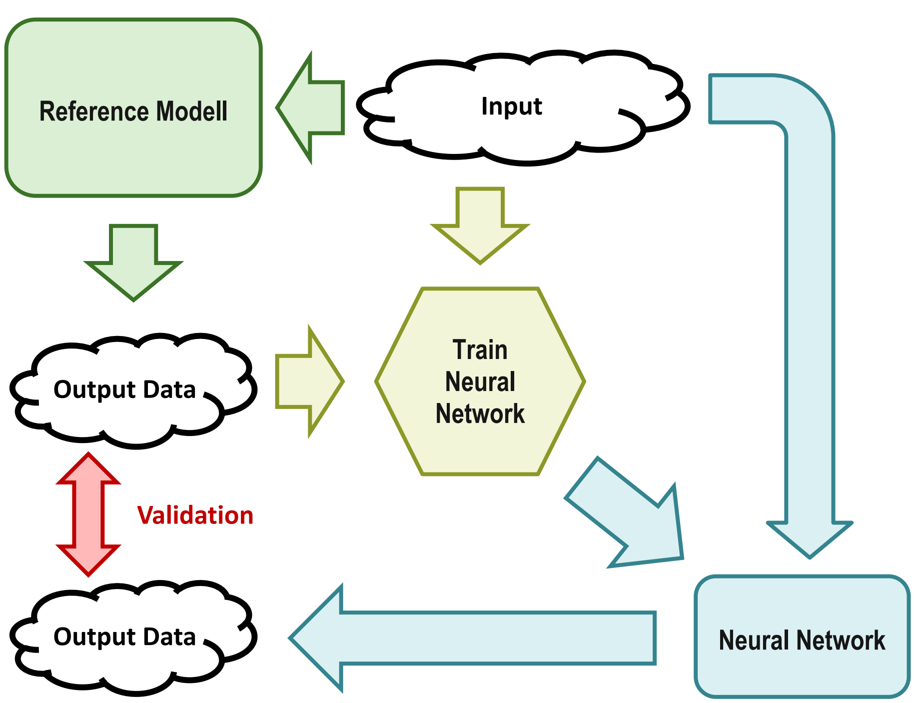

Fig. 18. Methodology for the development and validation of the neural network.

4.2.1.3. Validation of the neural network. It must be evaluated whether the trained neural network fits with the reference model. For this purpose, different randomly generated input parameters are used to calculate the output with the reference model and the neural network. The outputs from the reference model and the neural network can then be compared.

4.2.1.4. Implementation of the neural network in the genetic algorithm. After validation, the neural network can be used for operational optimisation. Since using a linear optimisation method with the neural network is impossible, another optimisation method must be used. In this work, a genetic algorithm was used for this purpose.

4.2.2. Model structure

For the neural network approach first the input and output for training the neural network are determined. Then the training of the neural network is described and in the end the setup of the neural network model is explained.

4.2.2.1. Determination of inputs and outputs. The input for the neural network is based on the input parameters and optimised variables from Table 4 except the electricity price and natural gas price.

The amount of energy was chosen as the output parameter and not the energy costs to keep the number of parameters low. This saves energy costs as input parameters and reduces the complexity of the neural network. The energy costs were calculated afterwards. Other output parameters are the storage level for the electrical storage and the heat storage at the end of the time step.

The reference model was used to generate 15 million data points of the described inputs and outputs before. Therefore, the randomly created input was used for the simulation of the reference model to get the corresponding output. The input parameters are in uniform distribution between the minimum and maximum values of any parameter. The minimum and maximum values can be taken from Table 4.

4.2.2.2. Training of neural network. For training the neural network the generated input and output data was split into train (80%) and test data (20%). The neural network was created with tensorflow. It consists of four layers, including a normalisation layer at the input and an output layer. The remaining two layers are dense layers of 1024 and 512 neurons, respectively. The dense layers use rectified linear units (ReLU) as activation function.

4.2.2.3. Explanation of neural network model. Only a single time step was trained to reduce the effort required to train the neural network, not the entire time series. This has the following advantages.

- The data space is kept smaller. Fewer input and output parameters are necessary, making the neural network easier to train. This improves the accuracy of the neural network considerably.
- The time series length can be varied and is not limited to 672 time steps.
- The data for the individual time steps are also available and not only the final result.

The neural network must be executed several times in series to calculate the required energy from the grid for the entire time series. The individual time steps are calculated one after the other. The input parameters are transferred to the neural network in the corresponding time step. The storage level the neural network outputted in the previous time step is used as input for the storage levels. A predefined start value is to be used for the first time step. After the neural network has been executed for all time steps, the energy costs for the entire time series can be calculated.

4.2.3. Validation

The validation of the neural network approach is split into two parts. First the deviation between the simplified model (neural network) and the reference model are investigated and afterwards the performance of the genetic algorithm in combination with the neural network is analysed.

4.2.3.1. Deviations between the models. For the comparison of the neural network with the reference model, the 1000 time series were used. Here, too, the focus is on the electricity supply from the grid for each time step. The 672000 time steps are shown in Fig. 19 in the same way as in Fig. 16. Here, the differences between the electricity from the grid of the reference model and those of the neural network are compared.

Fig. 19 clearly shows that the deviations of the neural network from the reference model are more minor than those of the linear model. Especially in the ranges between 1% and 5% and 25% and 100%, the neural network behaves better than the linear model. This is mainly because the neural network represents the storages better. The errors of the linear model, which mainly occur in the range below 20% and above 80% of the SOC, are more minor within the neural network.

When calculating the total costs for a time series, only the energy price was considered first, and the capacity price was added in the next step. However, no big differences were found in the deviation for the two calculation types (see Table 6). In both cases, the majority of the deviations were below 3%. Only in some cases was the deviation higher and reached a value of up to 6%. The remarkable thing about the deviation of the neural network is that they were all negative. This means that the costs calculated by the neural network are within the limit. In comparison, the costs calculated by the linear model can be significantly higher.

4.2.3.2. Analysis of the genetic algorithm. To evaluate the calculation time and the robustness of the genetic algorithm it is compared to the linear optimisation. Therefore, it was analysed how long the genetic algorithm needs to reach the same result as the linear optimisation. The duration fluctuates during the different runs but it can be ensured that after 3 h the result from the genetic algorithm is as good as from the linear optimisation.

4.2.4. Discussion

The results from the validation are used in this section to discuss if the neural network approach is suitable for the operational optimisation.

4.2.4.1. Accuracy. The validation of the neural network has shown that it agrees well with the reference model and only shows minor deviations. In addition, the results from the reference model are always better than those from the neural network when the same input is used. This guarantees that the results calculated by the genetic algorithm don't get worse when the simulation is done in the reference model.

4.2.4.2. Computation time and robustness. When using the neural network, no linear optimisation procedure can be used for the optimisation. Instead, a genetic algorithm has been investigated here. A computing time of about 3 h is necessary to obtain the same results with the genetic algorithm as with linear optimisation. When programming the genetic algorithm, the runtime has yet to be optimised, and parallelisation has yet to be carried out. If this is implemented, it can be assumed that the genetic algorithm can deliver the results in a suitable time. The simulation time of the neural network itself has only a few milliseconds.

4.2.4.3. Effort. For training the neural network, it has been determined that it does not make sense to train the entire time series but only one time step. This allows a variable design of the time series length and

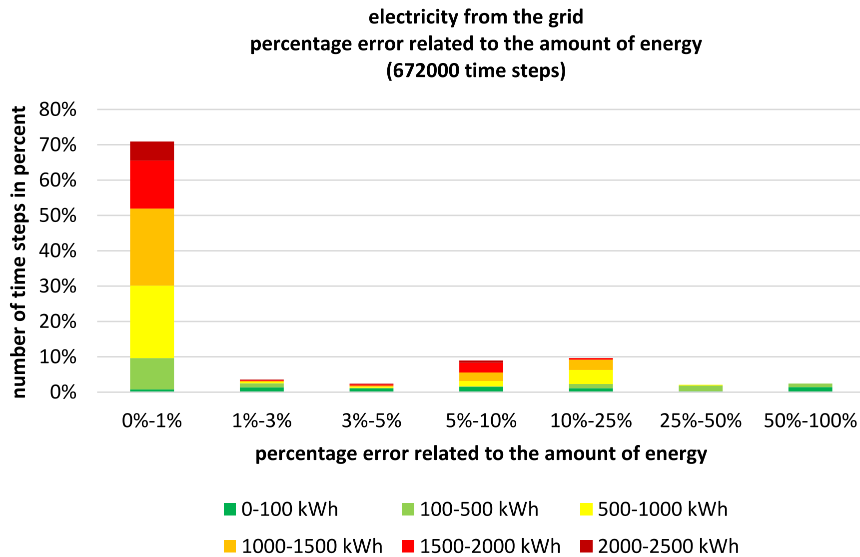

Fig. 19. Comparison reference model and neural network – for all time steps, the error of the electricity from the grid between the two models is assigned to one of the seven categories.

Table 6
Accuracy of the neural network.

	MAPE	RMSE
without capacity price	2.095%	9350
with capacity price	2.295%	8874

reduces the effort for training the neural network. Thus, the accuracy of the neural network can be increased. A further simplification for training the neural network was to return the required electricity from the grid as output, not the costs. The cost can be easily calculated from the required energy afterwards.

It is crucial to generate enough data from the reference model and to parameterise the neural network correctly for the training of the neural network. Although the training of the neural network takes several hours to days, the calculations of the trained neural network can be carried out much faster than with the reference model. Hardly any knowledge of the energy system is required to train the neural network. As long as the data can be generated from the reference model and the range in which the data is generated can be defined, the neural network can also be trained with a black box model. After the parameterisation of the neural network, even automation for the training of the neural network can be considered.

5. Conclusion

The work has shown that both modelling approaches are generally suitable for simplifying energy systems and their usage in operational optimisation. However, both approaches still have weaknesses that need to be investigated in more detail in future work. The linearisation approach lacks in accuracy and it is laborious to develop the linear model. For the neuronal network approach, the genetic algorithm needs too long for the calculation of the optimum.

The most significant disadvantages of the linear model are the high effort and the necessary expertise required for its creation and the deviation from the reference model that arises when the capacity costs are considered. The establishment of the linear model requires good knowledge of the existing model to be able to derive a linear model from it. For this, the individual components of the energy system must be considered and adapted, which is associated with effort and requires the necessary expertise in mathematics for linearisation and in the used programming tool. This is particularly difficult when models are only available as a black box. To apply linearisation in industrial operations, it is essential to investigate how linearisation can be automated or at least to create a guideline on how to proceed with linearisation. To avoid the high inaccuracy of the linear model, whether a piecewise linearisation improves the model should be investigated. In addition, the effects of linearisation on the computation time must be considered. The advantage of the linear model is that a linear optimisation method can be used for operational optimisation. The linear optimisation method guarantees that the global optimum is always found. Furthermore, calculating the optimum takes only a few seconds and provides good results despite the deviation of the linear model.

In contrast to the linear model, the neural network model has a high degree of accuracy compared to the reference model. Another speciality is that the results from the reference model tend to be better than those from the neural network when the same input is used. That means, the likelihood is very low that the results from the genetic algorithm getting worse when simulated in reference model. Automation for the neural network development is also easier to implement than for the linear model. Automated model creation would guarantee easier handling in the industry, and the energy system can then be adapted more quickly to changes. Based on this, the neural network model would be preferable to a linear model. The problem with the neural network is that this model cannot be used for linear optimisation. Therefore, a heuristic, e.g. the genetic algorithm, may be used for the optimisation. This has the disadvantage that it does not necessarily finds the global optimum and can deliver different results for the same input parameters due to the heuristic behaviour. If the runtime is long enough, a stable result is achieved. In the case of a genetic algorithm used, it has been shown that the same quality of results can be reached after about 3 h as with the linear model in a few seconds. However, the performance of the genetic algorithm can still be improved significantly because some code elements still need to be optimised. A wise selection of the starting population is necessary to obtain a good result with the genetic algorithm. How this can be better selected will be investigated in more detail in future work. This should lead to better and more stable optimisation results.

In addition, it should be mentioned that a better understanding of the model is possible with the linear model than with the neural network.

With the linear model, energy flows between the individual components of the energy system can be considered. In contrast, the neural network only outputs the final results, and intermediate steps cannot be considered. To create the linear model, knowing the individual intermediate steps was essential. From this, it could be determined where the deviations from the reference model originate. The neural network did not show such strong deviations as the linear model. Therefore, a closer inspection of the model is mandatory. The deviation of the neural network was satisfactory and did not need further investigation.

For industrial operation, in addition to the challenges already mentioned, the implementation in a real energy system and the stability of the optimisation results in the presence of changing input parameters must be investigated. Since the input parameters (such as energy demand of production, electricity prices, etc.) are based on forecasts, they can change constantly. The effects of these changes on the optimisation result have yet to be discovered. According to initial assessments, the two optimisation methods investigated are also suitable for more extensive and real energy systems. Another issue with real energy systems is that they can change over time. Here, methods still need to be developed on how changes in the energy system can be systematically integrated into the existing models. If the models can be extended easily, it is possible to simulate future energy systems. Combined with operational optimisation, a wide range of variants for the energy system can be tested, and the optimal design or expansion of the energy system can be determined.

CRediT authorship contribution statement

Thomas Kurz: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Philipp Gradl:** Software. **Lukas Kriechbaum:** Software, Data curation. **Gernot Solic:** Software, Data curation. **Kerstin Pfleger-Schopf:** Writing – review & editing. **Thomas Kienberger:** Writing – review & editing, Supervision.

Declaration of competing interest

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

Data availability

The data that has been used is confidential.

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