

# Demonstration of Digital Twins for Heat Pumps

D6.3 - Case study III at Kredsløb





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# Demonstration of Digital Twins for Heat Pumps

**D6.3 - Case study III at Kredsløb  
Digital Twins for Large-Scale Heat Pump and Refrigeration Systems**



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## 2. Introduction

Large-scale heat pumps are a key-technology for decarbonizing industrial and residential heating demands. As the market share for heat pumps expands and heat pumps becomes a key component in future energy systems, the motivation for improving their long-term performance and to perform fault detection and diagnosis increases. This report summarizes the use case and the achievements in a case study of a large-scale heat pump located at Kredsløb in the Digital Twin project (Deliverable 6.3), which focuses on investigating such improvements.

For this use case a digital twin framework intended for continuous monitoring and set-point optimization was built and integrated with a graphical user interface (GUI) to easily provide the heat pump operator with insights from the digital twin. In this report the use case and data collection are first described, followed by a description of the modelling approach and a demonstration of selected digital twin-based services.

The overall concept diagram for the services, data collection, and model can be seen in. The data is here constantly being collected and feed in for new data analysis which in turn gives inputs to the services.

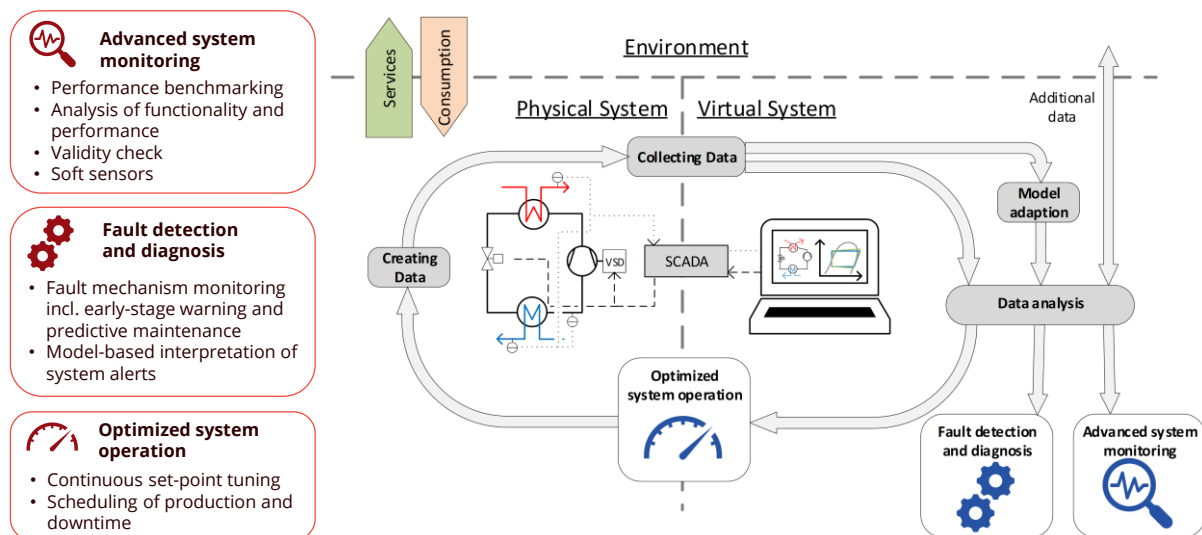


Figure 1: Concept diagram for digital twin-based services for heat pumps.



### 3. Case description

The large-scale heat pump system selected as a case study is managed by the Danish energy company Kredslob and located in "Maskinrummet" at Aarhus, Ø Denmark, see Figure 2.



Figure 2: Build at Århus Ø where the heat pumps are located [Kollision, 2020].

The system consists of two parallel systems installed by Johnson Controls Denmark. Each of the system has a nominal heating capacity of 1 MW and is designed in a two-stage cascade layout, as shown in Figure 3, where the system and its main control dependencies can be seen. The lower stage is a novel unit that uses seawater as a heat source and steam as a refrigerant. In this stage, a fraction of the seawater enters in the evaporator and evaporates under low pressure. The resulting steam undergoes compression in an axial multi-stage turbo compressor, which is then condensed in a separate vessel and transfers heat to the upper stage using ammonia as refrigerant.

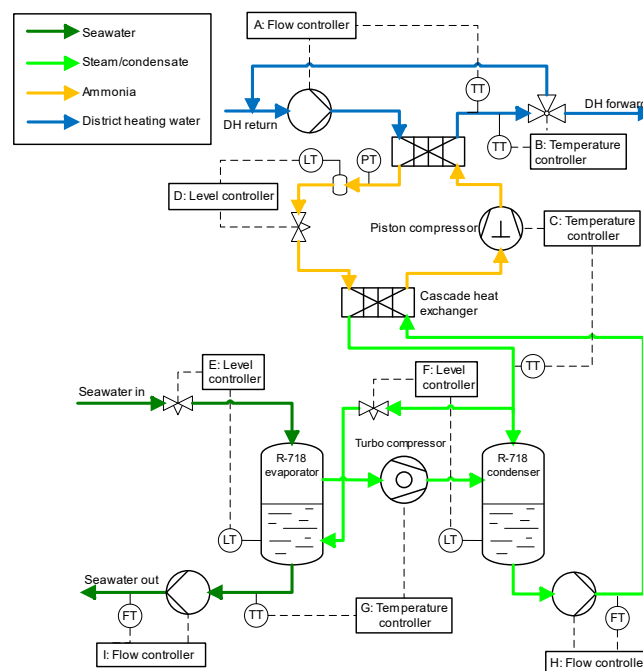


Figure 3: Layout of the heat pump and its main control dependencies.



The top cycle is a HeatPac 108S-V system with a piston compressor located on the top floor, while the water system in the bottom cycle is located on the lower level, see Figure 4.

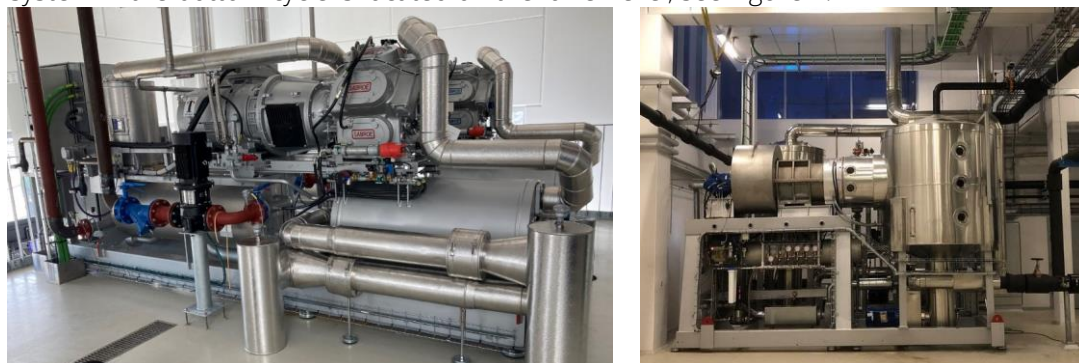


Figure 4: HeatPac 108S-V (left) and bottom cycle with turbo compressor (right).

In the top cycle ammonia (R-717) is circulated through a combined de-superheater, condenser, and sub-cooler in a plate and shell heat exchanger which heats up district heating water, typically to 65 °C in forward temperature. A level measurement is controlling the expansion valve which returns the ammonia to the cascade heat exchanger where it is evaporated. The cascade heat exchanger is also a plate and shell heat exchanger. On the district heating water side, a booster pump and three-way valve is installed which can be used to control the forward temperature.

#### 4. Establishment of data infrastructure

A data infrastructure system was set up for this project. This was made in order for the project group to access and continuously collect the operating data from the heat pump the digital twin in a secure way, which required new hardware to be installed. A review of all data points was made which resulted in the selection of 120 operating parameters which continuously were sent to a secure SQL database. For this data the name, type, tag number, address, unit, value, and number of decimals were identified. The data were collected from three different PLC's, where it was collected and processed with a Python script that were connected to the read-only SQL database. The data were protected by a firewall, but pre-allowed IP addresses could access with a password, see the database server in Figure 5. Further details are confidential.



Figure 5: Database PC server with a firewall setup for the project.



## 5. Modelling

The detailed simulation model was built in the programming language Modelica by using the software Dymola and the TIL Suite library, see Figure 6.

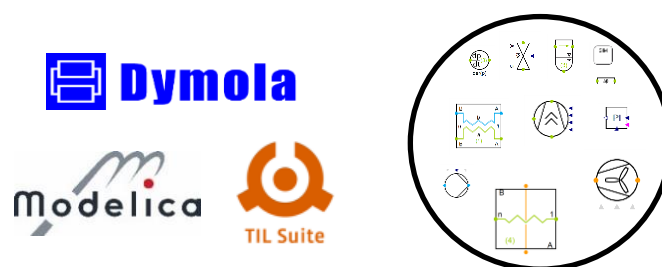


Figure 6: Programs used for modelling.

### 5.1. Heat exchangers

All the heat exchangers in the system were represented by modified plate heat exchanger models available in the TIL Suite library. The exception to this was the evaporator, which was modelled by a vessel that separated the seawater in the heat source stream into gas and liquid. The modelling approach for the evaporator plate-and-shell heat exchanger was to use a plate heat exchanger which evaporates the liquid part of the working fluid after the expansion valve by using a separator where the liquid part was pumped to the heat exchanger. The superheating of the working fluid was modelled as tubes with constant UA-values. The combined de-superheater, condenser, and sub-cooler plate and shell heat exchanger was modelled as 3 separate corrugated plate heat exchangers, each discretised into 5 control volumes where the mass and energy balances were calculated.

The pressure drop in each heat exchangers was assumed to have a linear dependency to the mass flow. The number of plates and outer size of the heat exchanger were known from the available datasheets, while the exact thickness of the plates and details of the pattern for the corrugated plates were not known. For the ammonia working fluid the heat transfer correlations included in the TIL Library from Shah Chen [1], Shah [2], and Gnielinski Dittus Boelter [3] were used. For the district heating water the correlation for VDI plate alpha for one phase fluid was used [4].

In order to parametrise the heat transfer models to the operating data from the heat pump system correction factors for the overall UA values, calculated by the heat transfer models and its submodels, were fitted to match the heat transfer for each heat exchanger. The correction factors were fitted in a number of different operating points. The tool used for this was ModelFitter version 2.1, which is a software tool that can be used for automated fitting of model parameters to data by using the Levenberg-Marquard algorithm with the use of models in the Functional Mock-up Interface (FMI) standard [5]. Figure 7 shows a comparison of the simulation results for the given parameters and the dependent variable after fitting.

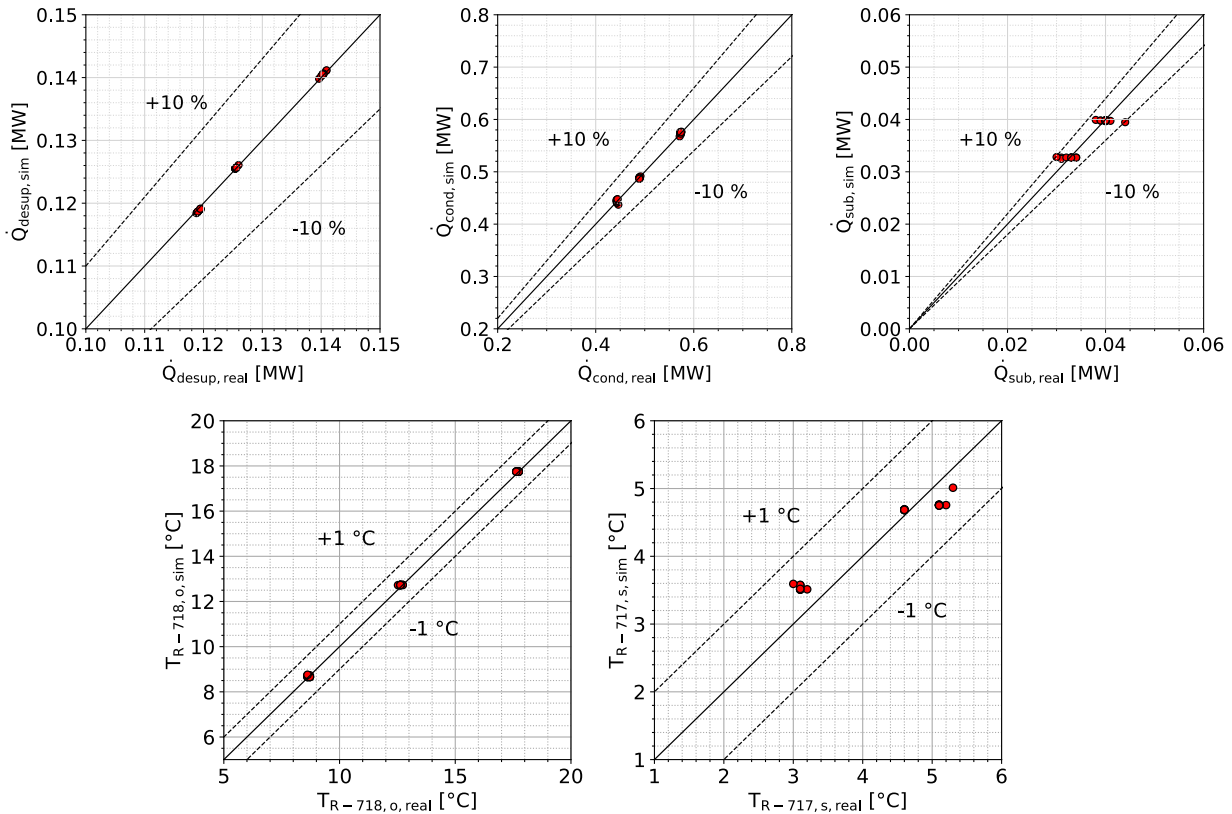


Figure 7: Comparison of simulation and measured variables in fitting of top cycle heat exchangers.

## 5.2. Top cycle – piston compressor

The reciprocating compressor model was based on linear regression polynomials for the isentropic and volumetric efficiency, which were derived from experimental data provided by the compressor manufacturer. In addition to that a heat loss from the compressor to the surrounding environment was assumed. After a sensitivity analysis the polynomials were made as a function of the evaporation temperature, condensation temperature and the speed of the compressor. Figure 8 shows the volumetric and isentropic efficiency at different operating conditions for the compressor.



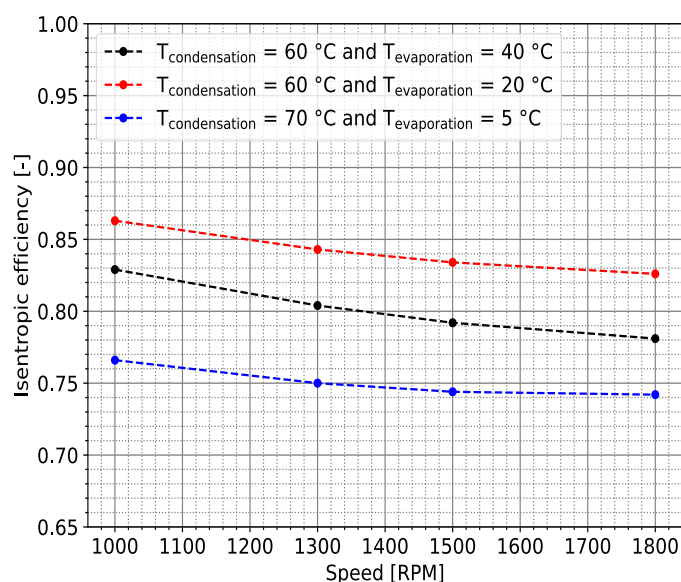


Figure 8 : Volumetric and isentropic efficiency at different operating conditions for the piston compressor.

### 5.3. Bottom cycle – turbo compressor

The model for the turbo compressor used in the water cycle was made from a table-based interpolation map derived from experimental data from previous measurements done on the compressor [8]. The interpolation was made with the TLK software “DataMap Creator” [9]. These measurements provide the dependency between volume flow, pressure ratio (PR), efficiency, and compressor speeds. Figure 9 shows the dependency between pressure ratio and the relative volume flow rate for different compressor speed curves varying from minimum to maximum.

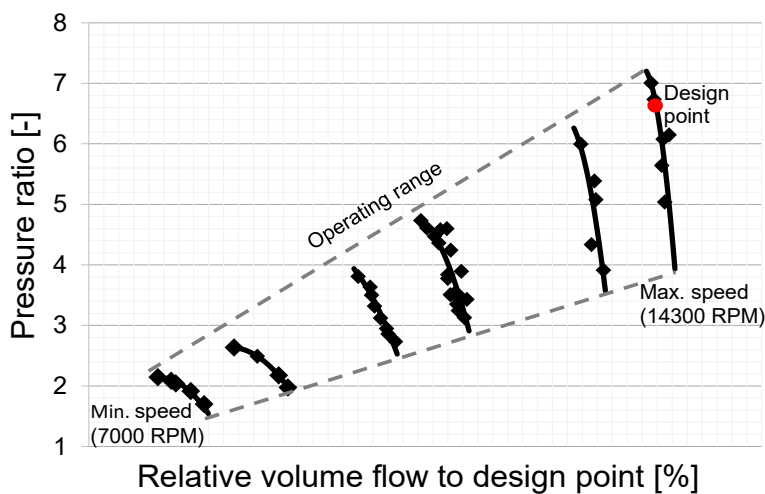


Figure 9: Turbocompressor operating dependency.



## 5.4. Control dependencies

A graphical interface for dynamic model of the heat pump system can be seen in Figure 10. Here all the various components are connected, including the various system controllers in the cascade system. All the controllers in the system were modelled by proportional integer (PI) controllers available in the TIL Suite library.

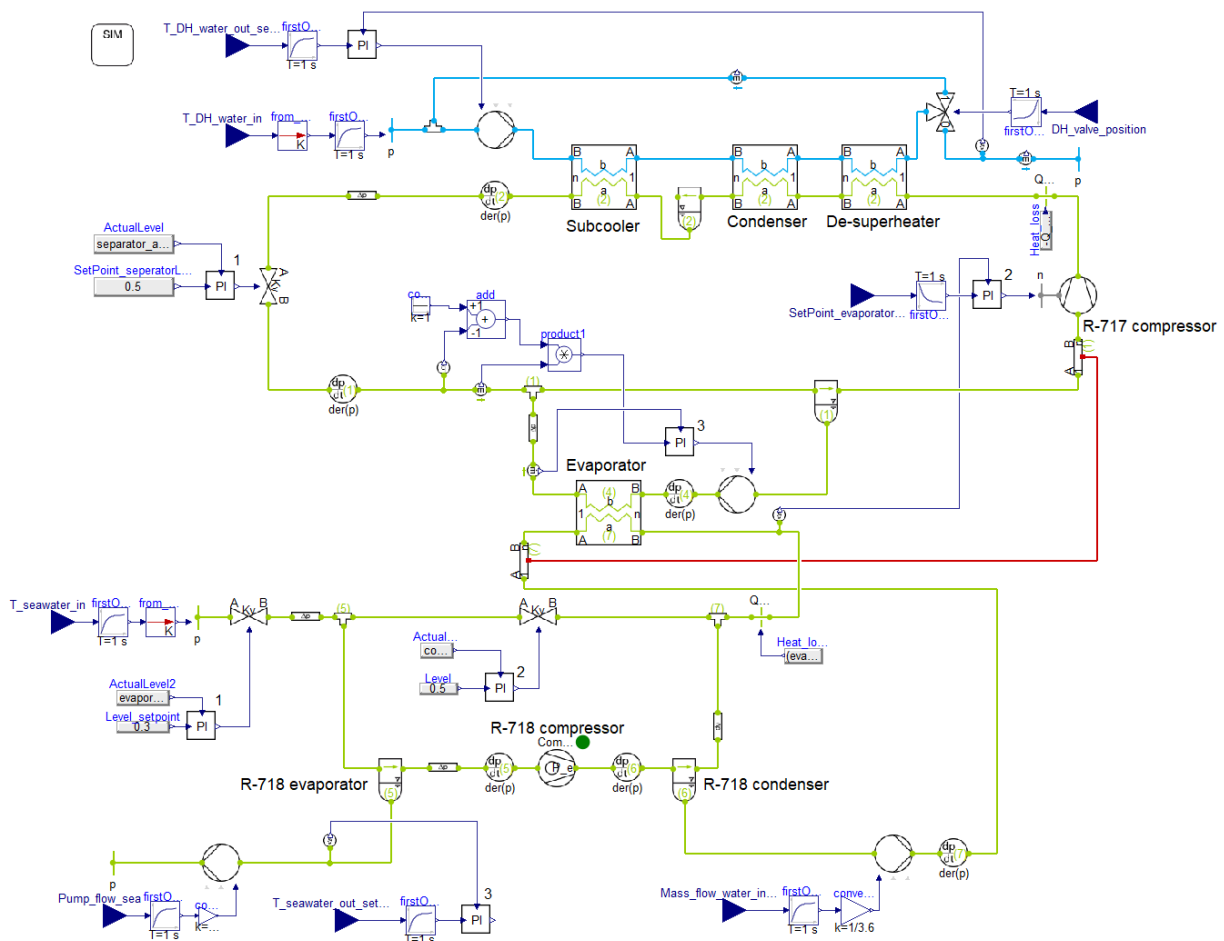


Figure 10: Graphical interface for dynamic model of the heat pump system.

The top cycle was controlled with four PI controllers, and the bottom cycle with three. Both the proportional gain and time constant in these controllers were tuned according to tuning rules to fit with measurement data. The four control parameters in the top cycle were:

1. Expansion valve: Controlled according to a level sensor in a reservoir in the outlet of the condenser heat exchanger providing heat for the district heating water.



2. Speed of the reciprocating compressor: Controlled according to the outlet temperature of the cascade heat exchanger for the R-718 cycle.
3. Mass flow for evaporator: Controlled according to equation (1), where the mass flow for the evaporator ( $\dot{m}_{\text{evap}}$ ) was calculated as function of the mass flow ( $\dot{m}_{\text{a,exp}}$ ) and quality ( $x_{\text{a,exp}}$ ) after the expansion valve.

$$\dot{m}_{\text{evap}} = \dot{m}_{\text{a,exp}} \cdot (1 - x_{\text{a,exp}}) \quad (1)$$

4. Mass flow of district heating water: Controlled according to the forward temperature of district heating water.

The bottom cycle was controlled with 3 PI controllers:

1. Seawater inlet valve: Controlled according to the level in the R-718 evaporator in deep vacuum conditions.
2. Control valve for flow of seawater between R-718 evaporator and condenser side. Flow is controlled according to level in R-718 condenser.
3. Speed of the turbo compressor: Controlled according to the outlet temperature from the R-718 evaporator. In some cases, the speed of the turbocompressor was also directly set.

## 5.5. Optimization framework

In order to investigate the potential of using the dynamic simulation model for set-point optimization the simulation model was converted to a Functional Mock-up Unit (FMU) by using the FMI standard [10]. The resulting FMU was simulated using the software environment Python (version 3.9.5) with historic transient boundary conditions as inputs, e.g. varying temperatures of the inlet flow for seawater and district heating.

An optimization framework were then developed which aimed at enhancing the energy performance of the case study by characterizing and adjusting its operation. This framework was comprised of the data management setup, the detailed dynamic simulation model of the system, and a control optimization routine. Due to security reasons, it was not possible during the project to directly modify the conventional operation of the system, instead a “human-in-the-loop” approach were planned, where the Digital Twin were to continuously collect data which in turn could provide insights and suggestions to the operation of the heat pump.

The optimization process uses an optimization function from the SciPy package in Python to find a local optimum in the given bounded interval with the simulation model. One of the possible optimization procedures was to calculate the set points for the “process out temperature” which influences the evaporation source temperature ( $T_{\text{source,sp}}$ ) in the water and ammonia cycles and maximized the COP of the system, as shown in Equation 2. This process was performed for single-time steps of operation, maintaining the boundary conditions of the system fixed during the optimization. As a result of the



optimization, the speed of the compressor in the water cycles was reduced, decreasing the total power intake of the system.

$$\max \text{COP}(T_{\text{source,sp}}) = \max \left( \frac{\sum_{i=1}^n \dot{Q}_{\text{sink},i}}{\sum_{i=1}^n \dot{W}_{\text{total},i}} \right) \quad (2)$$

The overall procedure for changing set points in order to optimize a given parameter is shown in Figure 11. The procedure started with obtaining inputs for the measurement data at a given time step for the historic data. Based on the given new inputs for the given time step, the resulting system operation was calculated by using the function “fmu.doStep” in Python which also takes the historic operation of the system at previous time steps into account. This loop ran until a specified time step counter ran a sub-routine for optimization. For the optimization sub-routine, the FMU of the model was run in a period which ensures steady state calculations with the inputs in the given time step. Simulation results were investigated in the sub-routine where the simulations were made with pre-determined allowed changing inputs combined with inputs for the boundary conditions at the given time step. This allowed the sub-routine to e.g. change the parameter for the turbo compressor speed in a predetermined allowed interval in order to investigate the simulation results for the COP, or other parameters that could be of interest to optimize.

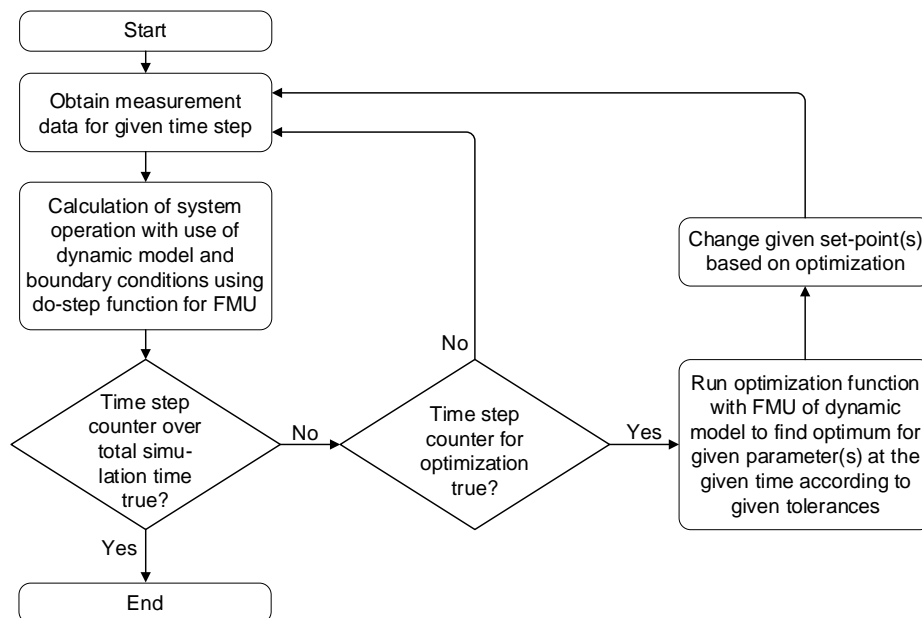


Figure 11: Flowdiagram for optimization framework.

When running the optimization calculations the function “minimize\_scalar” from the module “scipy.optimize” was imported to the Python environment. This function uses the Brent method to find a local



minimum in the given bounded interval, and uses an algorithm for inverse parabolic interpolation when possible to speed up convergence of the golden section method as described in [11].

## 6. Validation of model

The model were validated with various historic operation data of the heat pump. Figure 12 shows a TQ diagram for the top cycle, together with the district heating water (red) and the heat extracted from the bottom cycle (blue) for both the model results and the operating data.

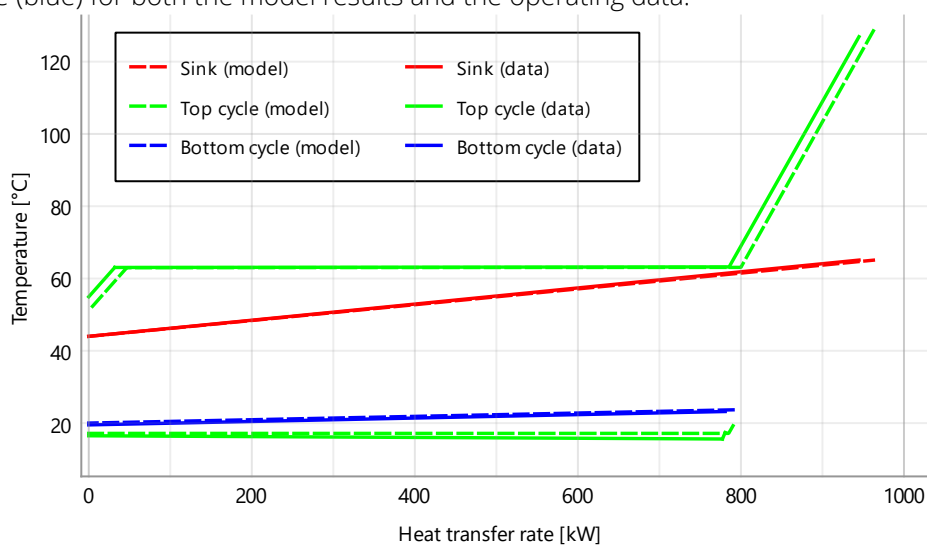


Figure 12: Comparison between the model and operating data in a TQ-diagram.

Figure 13 (temperatures) and Figure 14 (heat transfer rates) show two hours of operation, where there after 1 hour of operation is made an increase of 150 RPM of the speed of the turbocompressor. Again the model and the data can be compared.

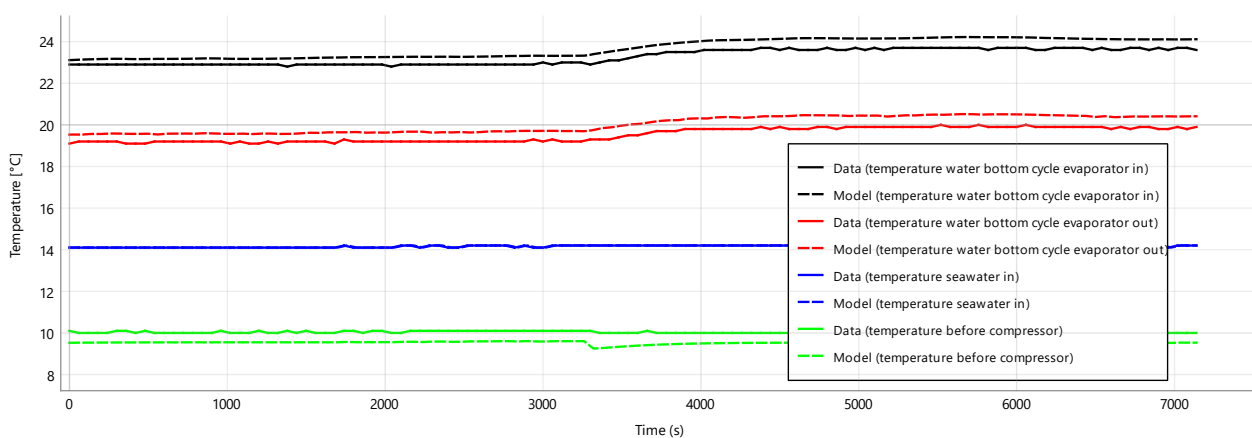


Figure 13: Comparison of temperatures during 2 hours of operation.

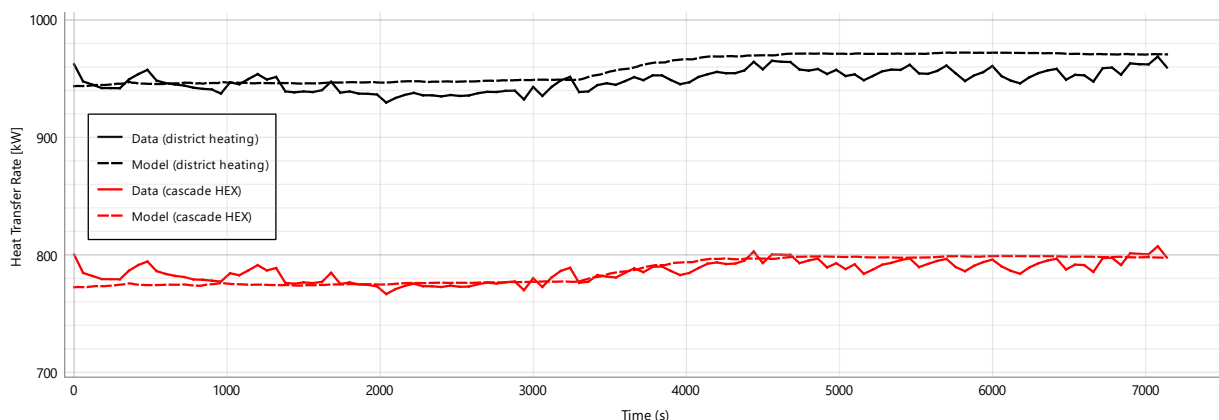


Figure 14: Comparison of heat transfer rates during 2 hours of operation

In general the comparison between measurements and simulation results indicated that the simulation model provides a suitable description of the operation of the system, both in steady-state mode (off-sets) and during dynamic changes of the system.

## 7. GUI for digital twin

A software tool was developed for creating a graphical-user-interface (GUI) in order to easily monitor and optimize the operation of the large-scale heat pump system. This is shown in Figure 15. The development of this tool was directed to Kredsløb who is responsible for the operation of the system. The tool was shared as an .exe file and made with QT designer and Python, and uses a setup with an interface, which is able to show the layout of the system, along with operational variables of the system in real-time and their comparison with the results from the simulation model.

The program uses Python scripts for operating data pre/post-processing, and links the user interface with operating data and the simulating model (FMU).

Moreover, the tool enables to test different hypothetical scenarios. In this context, control set points as well as other relevant system parameters that can be modified, and the resulting performance of the system is estimated through the simulation model.

Comparison of the operating data and simulation data are shown, and predefined plots of  $\log(P)$ - $h$  diagrams and  $T$ - $Q$  diagrams are included. A dedicated fan is made for each of the services *System monitoring*, *Set-point optimization*, and *Steady state analysis*.

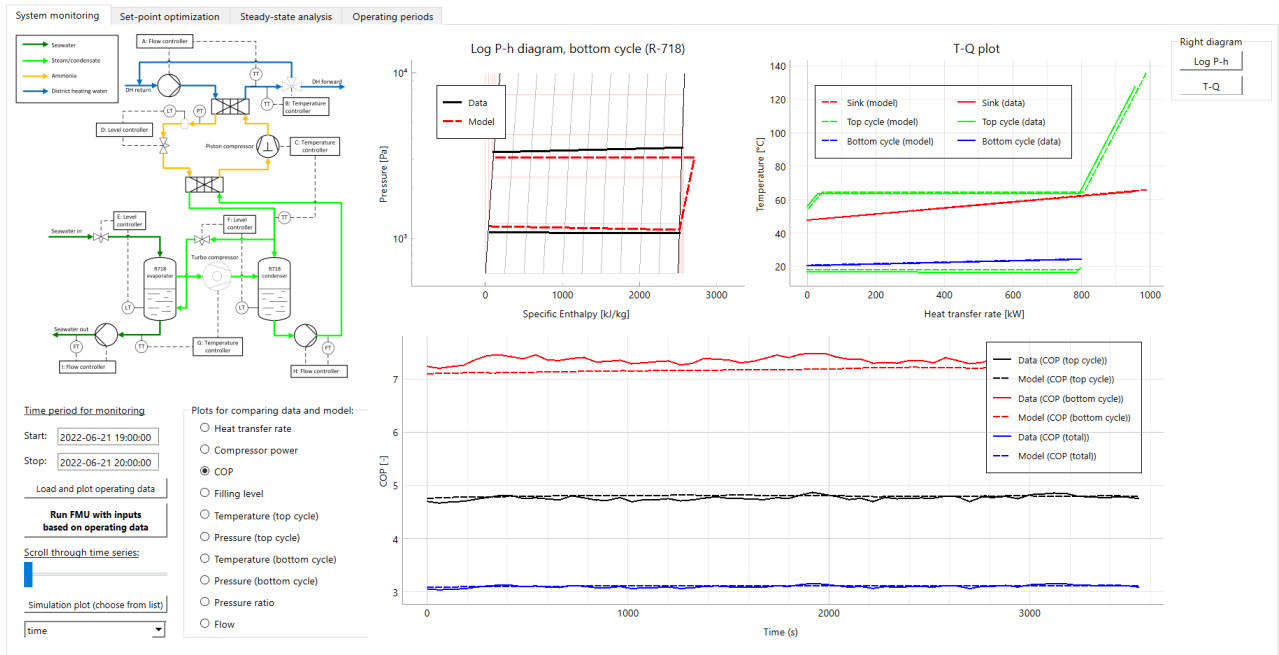


Figure 15: Interface of the GUI software developed for monitoring and optimizing the operation of the large-scale heat pump system used as case study.

## 8. Demonstration results of digital twin-based services through GUI

After setup of the dataflow and the validation of the model an overhaul in a longer period was made on the heat pump system, which caused the demonstration and investigation of the potential of the digital twin to be made on the basis of historical data, and hence not with live data in a continuous loop. Besides to possibilities with system monitoring, where deviations between the model and the heat pump operation data can be followed (as seen in Figure 15) possibilities for steady state analysis and set point optimization were investigated as described in the following two sections.

### 8.1. Steady-state analysis

An option were made possible for the user to be able to change a series of inputs variables to the model in order to perform manual investigations of the expected performance in different modes and boundary conditions, e.g. the expected difference in performance for COP and heat transfer rate during summer and winter. The tab for this service in the program is show in Figure 16, where the inputs needs to be entered in the boxes on the left-hand side, and the outputs and diagrams are shown on the right-hand side.

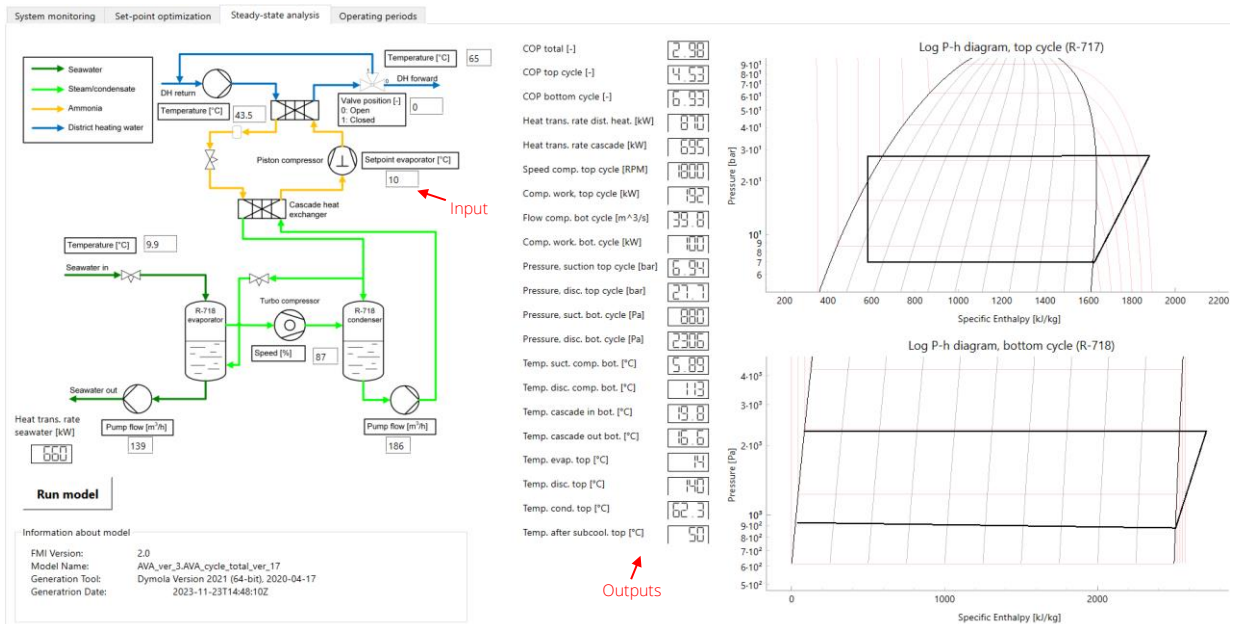


Figure 16: Steady state analysis of the heat pump system.

## 8.2. Set-point optimization

The program were also used for set-points optimization, please refer to Figure 17 on the next page. Here the optimization procedure can be initiated after choosing the following inputs:

- Parameter to optimize, chosen in a drop-down list
- Parameter to vary, chosen in a drop-down list
- Lower limit for parameter to vary
- Upper limit for parameter to vary
- The time interval for executing the optimization algorithm, and get a suggestion for a change in set-point adjustment.

Besides this, trend curves with key data over time, and the characteristics of the optimization are shown in the discretized boundary interval chosen. This enables the user to look for any local optimization points.





Menu

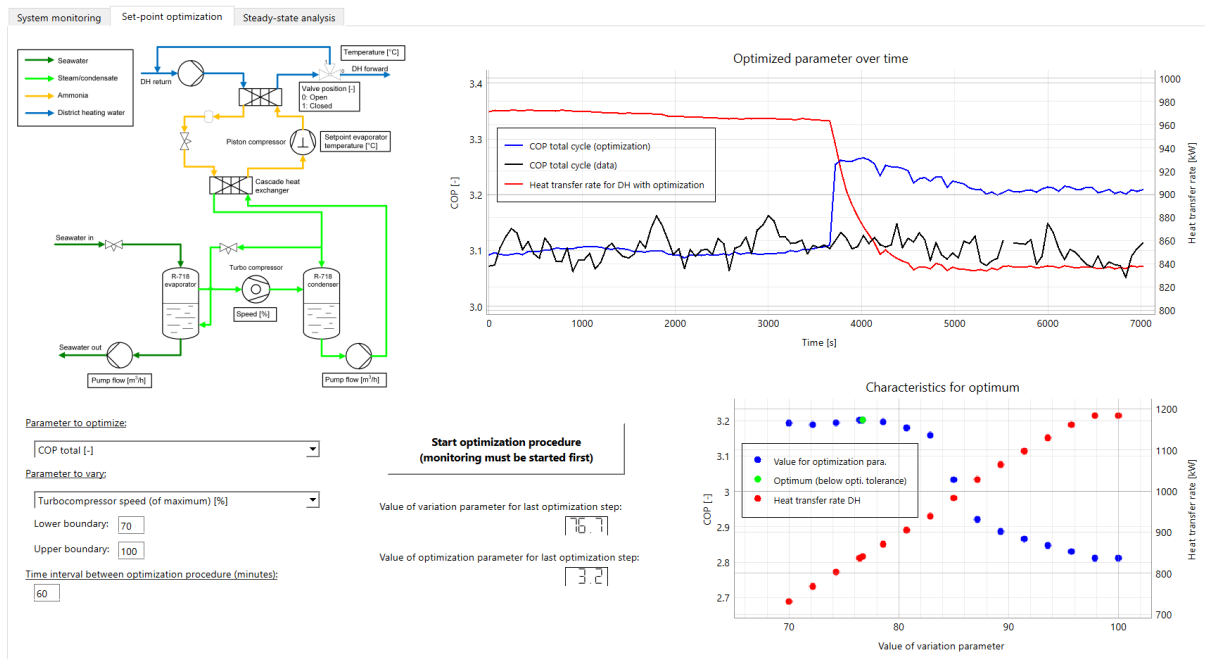


Figure 17: Program with services for set-point optimization.

The potential for such optimizations were investigated with regards to controlling the speed of the compressors in the system, aiming to maximize its energy efficiency (COP). This is illustrated in Figure 18 and Figure 19. Figure 18 shows the relation between the speed of the turbo compressor in the water cycle and the COP as well as the heat output of the system, whereas Figure 19 presents the same relation for the ammonia cycle. These findings facilitated the identification of optimal controller set points, represented by specific compressor speeds for each cycle, which maximized the COP of the system.

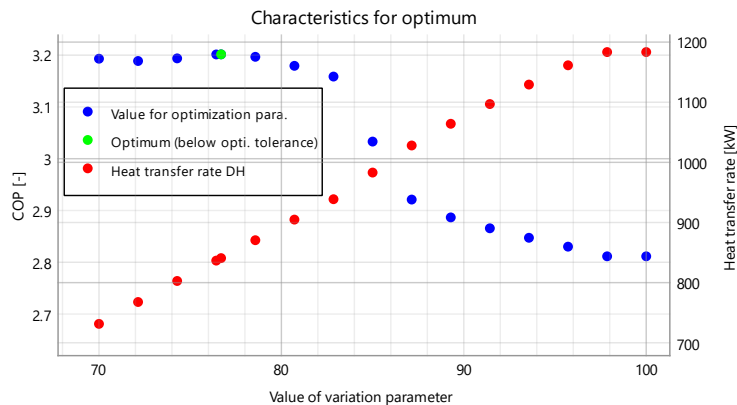


Figure 18: COP and heat output of the system as a result of a variation of the water compressor speed, where the energy-optimal value for this speed is shown in green (around 76 % of max. speed).



In the water cycle, the optimal compressor speed resulted in a reduction in heat output to the district heating water compared to higher speeds, while for the ammonia cycle, the optimal (and maximal) compressor speed did not lead to a reduction in heat output compared to higher speeds. In this context, the detailed simulation model enabled the characterization of the trade-off between energy performance and the net output of the system resulting from set point variations. Although the focus of this study was on defining energy-optimal set points, the results from the proposed framework could also be applied to adjust the balance between the heat output of a system and its energy performance.

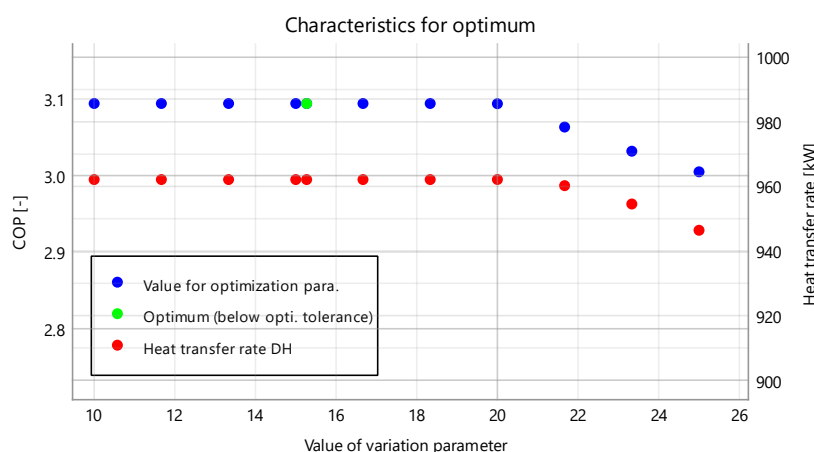


Figure 19: COP and heat output of the system as a result of a variation of the ammonia compressor speed (which is a function and the process out temperature shown here as the "value of variation parameter", where the energy-optimal value found for this speed is shown in green).

Figure 20 shows the transient response of the optimization with the set point for the turbo compressor in the water cycle adjusted after one hour of operation (at time = 3600 seconds). Here the calculated simulation model and the results (blue curve) can be compared with the measurements from the system if no optimization were made (black curve).

This information could be used for adjusting the operation of other components supplying or storing heat in the same network as the heat pump system. The results showed that the optimal set point after around 30 min increased the COP of the system by around 3 % compared to how the system was running before, while the heat transfer rate decreased from 960 kW to 840 kW. These findings underscored the potential of using the proposed set point optimization framework for enhancing the energy performance of the system used as a case study, and that the framework can be used to find best compromise between COP and heat transfer rate depending on the prices for power and district heating.

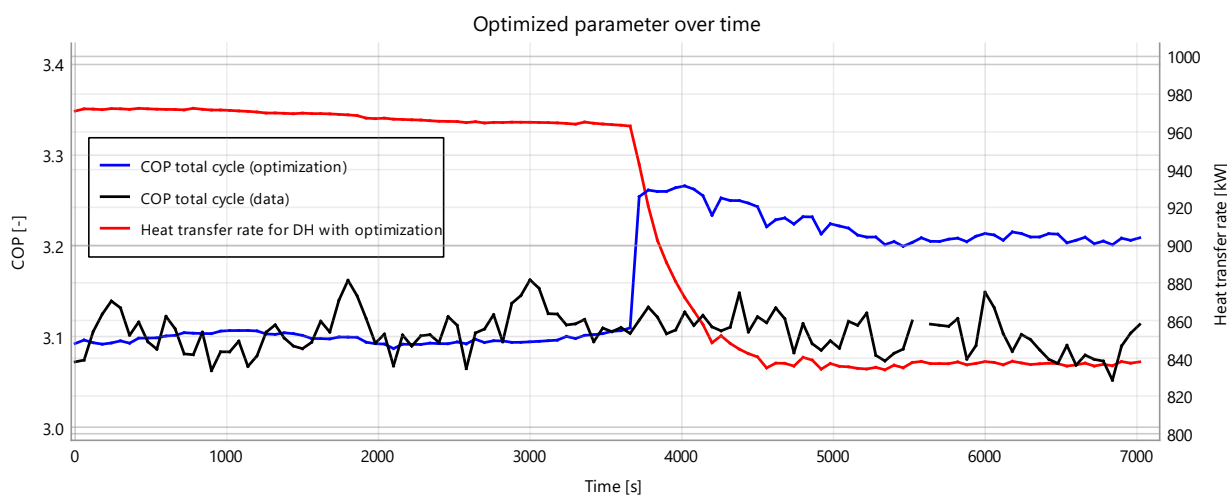


Figure 20: COP and heat output of the system resulting from the implementation of the energy-optimal speed of the water compressor.

## 9. Conclusion

A model-based framework was proposed for optimizing the energy efficiency of a large-scale district heating heat pump system using seawater as a heat source. The framework comprised a data management system, a detailed heat pump simulation model, a data-driven optimization method, and an GUI for the operator. The optimization aimed at determining energy-optimal set points for controlling the speed of the compressors in the system. The simulation results showed that the simulation model used was able to provide a suitable representation of the operation of the system. This showed the potential for using the simulation model as a performance benchmark for the physical heat pump system, where the expected COP of the system is obtained through simulations. The model complemented with the optimization enabled to characterize the trade-off between enhancing the energy efficiency and heat production of the system derived from adjusting the speed of the compressors.

Overall, the findings from the implementation of the framework in the case study highlighted its potential for optimizing the operation of the system in real time. The framework was found to be a promising approach for the further future development of digital twin-based services, and hence energy efficient operation of large-scale heat pump systems. The framework can adapted be used on other heat pump systems, where a higher degree of changing boundary conditions increases the potential for this service further.



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