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DYNAMIC SIMULATION AND EXPERIMENTAL VALIDATION OF A 35 MW HEAT PUMP BASED ON A TRANSCRITICAL CO₂ CYCLE

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ABSTRACT
Replacing the baseload providers on the energy market with decarbonized renewable solutions increases frequency dynamics on the grid. In order to handle the concomitant risks and chances linked with this change of paradigm between energy producers and consumers, complex dynamic models are required to optimize energy management strategies. Industrial transcritical carbon dioxide (CO₂) heat pumps, such as the one developed by MAN Energy Solutions Schweiz AG (MAN ES), offer a proven solution for the decarbonization of the district heating sector. Furthermore, they are associated with pathways to increase the usage of this solution for sector coupling applications. This work presents a detailed Modelica model of the high-temperature CO₂ heat pump, focusing on the thermodynamic states of the refrigerant during load variations of the system. In a consecutive step, the model is validated against testbed data of a heat pump from MAN ES with over 35 MW heat supply and a lift from 40 to 100 K. The model results match the testbed data with an accuracy of over 95 % and demonstrate a full coverage of the performance map minimum to maximum speed, providing water-side supply temperatures of 50 to 109 °C. Realistic dynamics in fast load balancing operation are demonstrated where power consumption was varied by 80 % compared to maximum power within 30 s. Models of this kind are essential for an accurate prediction how decarbonized energy networks react by linking electricity and heat supply together. These predictions are ultimately useful to upgrade or optimize complex control strategies.

1. INTRODUCTION
Three-quarters of the emissions that have pushed global average temperatures 1.1 ºC higher since the pre-industrial age stem from the energy sector [1]. Taking into consideration that the provision of heat for homes and industry accounted for more than half of the total energy consumption in 2021 [2], making it the largest energy end-use, throws into sharp relief the significance of sustainable heat supply for a transition towards a carbon-neutral future [3]. In this context, district heating networks receive particular attention from cities and communities which are leading the energy transition and are increasingly replacing conventional fossil-based heat plants with large-scale heat pumps [4]. Large-scale industrial heat pumps represent an emerging solution for future district energy networks and sector coupling, not only providing heat but also having the potential for cooling applications and ancillary services on the electric grid.

Heat pumps are usually classified according to their working fluid, heat source, temperature level, and physical working principle. Following the work from Lorentzen in 1994 [5], an increasing amount of work investigated CO₂ as a natural refrigerant with low global warming potential, flammability, and toxicity [6]. While large temperature glides in the heat source increase the potential ofzeotropic mixtures due to their non-isothermal phase change [7], the high transcritical temperature glide in the gas cooler makes CO₂ particularly suitable for large temperature differences in the heat sink, for example for domestic hot water heating [8]. Unlike ammonia (NH₃) based heat pumps, CO₂ heat pumps can easily achieve sink temperatures above 90 °C and up to more than 130 °C, ideally with heat sink inlet temperatures not too far above the relatively low critical temperature of 31 °C. Moreover, the high volumetric heat capacity of CO₂ allows the use of compact compressors and heat exchangers (HEX) [9]. Besides, using a natural refrigerant like CO₂ for large scale industrial systems reduces environmental and operating risks as well as capital costs compared to synthetic refrigerants or widely used NH₃.

As elaborated in a survey amongst 25 Danish operators and manufacturers of large-scale heat pumps [10], more than 25 %...
of the faults during operation are related to the compressor, accounting for the largest share overall and making it the most crucial component of the heat pump system. Additionally, the survey highlights that 38% of the considered heat pumps are already operating electricity price driven, as well as partly providing ancillary services based on agreements with the utilities.

In conclusion, the key design factors for a district heating heat pump are the selected working fluid and the compressor component. With a focus on these key factors, i) the demonstration of a large-scale system testing with ii) a suitable dynamic model for both, control system and energy management concept, is required. This work presents the dynamic simulation of an industrial high-temperature CO2 heat pump validated with latest full-scale testbed data from MAN ES.

1.1 Dynamic heat pump modeling

While the first dynamic modeling of heat pumps dating back to the 1980s was using lumped parameter models [11], distributed parameter models, for example, to investigate the dry evaporator for control purposes [12], emerged one decade later.

Already in 1995, Vargas et al. used a mathematical model for a heat pump operating with a variable-speed compressor in a transient regime to propose a closed-loop control (feedback control) instead of the traditional on-off control [13]. Since then, dynamic modeling of heat pumps and their control gained track, ranging from empirical compressor models in heat pumps [14] and performance maps for the entire heat pump [15] to various characteristic maps used to describe each compressor/expander stage individually [16]. However, the ability to provide ancillary services through load variation has only been tested with rapid dynamics on a small scale (kW-scale in seconds [17]) or with moderate dynamics on medium scale (100 s of kW in 1 to 3 minutes [18]).

A large variety of programming and modeling languages is generally used for dynamic modeling of heat pumps, such as Amesim [19], Fortran [9], TRNSYS [20], and Modelica/Dymola [21]. Recently, Modelica based object-oriented model libraries and their application come to the fore due to the availability of commercial simulation environments, with linearization remaining a numerically advantageous and required procedure [22]. Moreover, seminal approaches such as hardware-in-the-loop test benches [23] and reinforcement learning for control optimization [24] seem to have found their common ground in Modelica. Despite the latest advancements, current literature lacks validation on a large scale and for fast operational changes. Dynamic heat pump models are required to fill this gap and are crucial for accurate prediction and design of a variety of emerging application cases including the combination with cold [25] and/or hot [26] thermal storages that could even be used in a successive step for the reconversion to electricity [27].

Figure 1 offers an overview of a general methodology for model-based simulations with the steps presented in this work marked in red.

After the introduction in section 1, section 2 provides background on the heat pump unit (HPU) layout used for the experimental validation. The modeling part is elaborated on in section 3. Experimental data from a testbed is used to validate the dynamic model in section 4. A general conclusion and an outlook are given in section 5.

2. SYSTEM DESCRIPTION

2.1. HPU Design and Experimental Setup

The HPU layout investigated in this work is a CO2 transcritical heat pump cycle. Based on the schematic flow diagram in Figure 2, the main components employed and the thermodynamic cycle are illustrated in Figure 3. The multi-stage HOFIM™ radial turbo-compressor (A) brings the CO2 from a gaseous (1) to a supercritical state (2). In the hot heat exchanger (B), also referred to as the heat sink HEX, heat is transferred to the hot consumer. Still in a supercritical state (3), the CO2 enters either the turbo-expander (C) or the expander bypass valve (D) where it is expanded into a liquid state (4). A second expansion into the two-phase region takes place across the expansion valve (E). Exiting the expansion valve, the CO2 mixture at low temperatures (5) is evaporated by heat transfer with a cold consumer through the evaporator heat exchanger (F), also referred to as the heat source HEX.

The core component of the HPU is the high-speed, oil-free integrated motor HOFIM™ compressor which is more compact than conventional compressors, hermetically sealed, and equipped with magnetic bearings. The variable frequency drive allows continuous performance variation over a wide speed range without a gearbox. The motor is cooled with the process medium and reintegrates thermal motor losses into the process.

The selection of both HEXs is mainly determined by the external consumer circuits. The control valves D and E, however, have to be designed to match the turbo-expander. Both valves provide control flexibility to secure that the turbo-expander remains in a single-phase condition and within its pressure-ratio and flow limitations independent from the compressor operation.
In 2022, a full-scale HPU prototype was built by MAN ES and tested under various operating conditions. Table 1 gives an informative overview of the process parameters applicable for this kind of experimental setup. Test results have been used to validate the simulation model introduced in Section 4. A picture of the central part of the test setup with the HOFIM™ is shown in Figure 4. The heat sink was integrated using a full-scale printed circuit HEX unit [28] short-circuited with the heat source over several parallel shell-and-tube HEX connected to a water-glycol closed cooling loop. Any surplus of heat was extracted from the water-glycol loop with open air-to-water cooling tower. Redundant piping has been installed for high process flexibility for motor cooling gas flows and is more complex than Figure 2 shows.

For data acquisition, 256 industrial-grade sensors were integrated into the loop, including more than 200 temperature and pressure sensors. Each of the measurement points has been equipped redundantly with double or four-fold sensors to minimize measurement errors and risks of hardware failure. The process data is collected via OPC Unified Architecture [29] and is continuously recorded with a sample time of 0.5 Hz.

2.2. Figures of Merit

Turbomachines are described by their characteristic performance maps. This work uses the pressure ratio \( \Pi = \frac{p_{\text{outlet}}}{p_{\text{inlet}}} \) as the work coefficient and the volumetric flow \( \dot{v} \) as the flow coefficient spanning a map shown in Figure 6. The performance of both, the compressor and expander, can be expressed in a single point each in their respective characteristic, yielding a compressed comparative value pair containing information on the process conditions at points 1, 2, 3, and 4 of Figure 3 combined. The turbomachine characteristics in this work are based on volume flow instead of reduced mass flow since the compressor is a volumetric machine.

![Figure 2: Flow diagram of the HPU. (A) turbo-compressor; (B) hot HEX; (C) turbo-expander; (D) expander bypass valve; (E) expansion valve; (F) evaporator HEX; (G) variable frequency drive.](image2)

![Figure 3: State diagram of CO\(_2\): (1) Superheated gas at compressor suction; (2) hot supercritical state at compressor discharge; (3) cooled supercritical CO\(_2\) at expander inlet; (4) liquid state at expander outlet; (5) subcooled liquid and gas mixture (two-phase) at evaporator inlet.](image3)

![Figure 4: Picture of the turbomachinery part of the testbed setup in MAN ES facility, incl. scale.](image4)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Max. Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Motor Active Power</td>
<td>MW(_{\text{el}})</td>
<td>10.5</td>
</tr>
<tr>
<td>Heating Duty</td>
<td>MW(_{\text{th}})</td>
<td>35</td>
</tr>
<tr>
<td>Cooling Duty</td>
<td>MW(_{\text{th}})</td>
<td>25</td>
</tr>
<tr>
<td>CO(_2) Pressure</td>
<td>bar</td>
<td>140</td>
</tr>
<tr>
<td>CO(_2) Temperature</td>
<td>°C</td>
<td>130</td>
</tr>
<tr>
<td>Min. CO(_2) Evaporation Temperature</td>
<td>°C</td>
<td>-2</td>
</tr>
</tbody>
</table>

Table 1: HPU testbed process parameters.
Figure 6: Exemplary characteristic map of a compressor with different lines of constant speed spanning between the choke and surge limit.

Nevertheless, the pressures and temperatures, before and after the compressor, as well as the mass flows at the compressor suction and the motor active power – which is the actual shaft power after the VFD - are more suitable to identify dynamics and shall be referred to as evaluation parameters.

The coefficient of performance (COP) is defined based on Figure 3 as

\[ \text{COP} = \frac{Q_{\text{Out}}}{W_{\text{In}} - W_{\text{Out}}}. \]

The values in Table 1 indicate that the approximate COP of the investigated system is roughly 3.3.

For each measured and calculated testbed value, an uncertainty analysis has been performed in order to evaluate the reliability of data and maximum achievable validation accuracy. The acquired data with a sampling time of 0.5 Hz has been grouped and analyzed in sets of one minute. Within this minute, the standard deviation based on mean, minimum, and maximum has been computed and a relative uncertainty to the average data value was calculated. For each test operation, the maximum relative uncertainty of the related minutely datasets has been selected as a maximum confidence interval.

3. MODELLING

3.1. Language and environment

According to the classification by [30], the HPU model is categorized as a non-causal, object-oriented, dynamic, physical-based system simulation, see Figure 5.

The applied object-oriented programming language Modelica is widely used for modeling physical systems. The system components are described by differential-algebraic equations and stored in libraries. The result of the translation is an equation system that is solved by a selected algorithm. One main advantage of Modelica is the multi-domain modeling allowing for the simultaneous modeling and simulation of electric, thermal, mechanic, hydraulic, and pneumatic components. The process-relevant parameters like pressure, temperature, or composition are transferred by connectors between objects. In this context, the acausality of Modelica is worth mentioning. Compared to signal flow oriented software systems like Matlab/Simulink, system circuits are generated faster and in a clear manner. However, some circuit rules need to be considered [31].

In contrast to the programming language Modelica, the simulation environment Modelon Impact used in this work is not open source. In addition to the Modelica Standard Library [32], the modeling in this work is supported by the commercial libraries VaporCycle, ThermalPower, and ThermoFluidPro from Modelon [33].

3.2. Implementation

In preparation for modeling the full HPU, all single components have been validated individually against available datasheets from manufacturers. The full-loop HPU has been composed of the described models in a structure as displayed in Figure 7. Table 2 lists the auxiliary models used, including their underlying physics and associated limitations or advantages, while the main components are explained below.
3.2.1. Medium Model

The medium model is based on a spline-based table lookup (SBTL) method. The simulation is much faster compared to the Helmholtz approach which calculates the medium properties from equations of state. Especially the stability along the transition between single- and two-phase regions gives the advantage to the table-based approach. Increased speed is achieved by fast access to pre-calculated properties defined in the spline coefficient tables computed with the REFPROP database [34]. Spline coefficient tables are loaded as external objects at the initialization of a simulation. In general, property functions from SBTL (as well as their first derivatives and inverse functions) are continuous and numerically consistent with each other, hence used for various computationally extensive process simulations whenever conventional multi-parameter equations of state are unsuitable due to their computing time consumption, as extensively described by Kunick [35].

3.2.2. Turbomachine Model

The main focus lies on the implementation of the turbomachine as it is the core of the heat pump system. Since the compressor, expander, and motor are physically one unit, there is an individual model for the whole unit. This allows a simple exchange of the turbomachine from the heat pump model and separate validation and testing of the high-speed machine model. As can be seen on the right-hand side close-up in Figure 7, the compressor and expander stream are strictly separated. The compressor is separated into two sections representing different numbers of stages. Each of the turbo machines is described by a table of polytropic efficiency and a flow table. Based on the polytropic head over the model and the impeller tip speed relative to the medium's Mach number, mass flow, torque, and efficiency are computed from 2D tables. While the expander has no leakage streams, the compressor side respects extraction of motor cooling gas over a control valve from between the compressor stages as well as a leakage stream from the high-pressure side into the motor. Motor losses are calculated with a given motor efficiency from the accumulated total shaft power and transferred into the motor cooling stream by a heat flow source.

3.2.3. Heat Exchanger Models

The heat exchangers have been modeled based on the generic model of the Modelon Thermal Power library for two-phase media. It basically represents a pipe-wall-pipe system where pipes can be arbitrarily multiplied and discretized. The heat sink model is discretized into 10 segments, while the heat source model has only 3 segments. The pressure drop over the heat exchangers is calculated based on the friction of a nominal operating point. The heat exchanger model can be fine-tuned with correction factors for both pressure drop and heat transfer. For the hot heat exchanger, the heat transfer correlation of Shah [36] and Akers [37] was used for CO₂.

Figure 7: Overview of the HPU in Modelon Impact. The illustrated models correspond to the models described in Subsection 3.2 and Table 2. Please note that detailed piping, control components and cooling gas streams are excluded from this figure.
3.2.4 Pipe Models

The pipe models of Modelon's VaporCycle library have been manipulated to include a pipe wall and an optional insulation layer as well as an additional flow resistance accounting for all pipe fittings which are not modeled in detail. Pipe elements between major components are represented as straight pipes of constant diameter with a two-phase correlation for friction as proposed by [38] and confirmed for CO\textsubscript{2} by [39]. Additional losses due to fittings such as bends and reductions are summed up into a theoretical resistance factor $\zeta$ which imposes

$$dp = \zeta \left( \frac{\rho v^2}{2} \right).$$

Geostatic height differences between the inflow and outflow of the pipe section are also respected in this model. Heat losses to the environment are included by a constant heat transfer coefficient over the pipe surface to a constant ambient temperature. Pipe models have been parameterized for sections of similar pipe diameter, which results in two consecutive pipe elements at the compressor suction. Short pipe sections such as the framing of the expander bypass valve have been neglected for simplification.

4. VALIDATION

The validity of the dynamic model is tested for the full range of achievable operating conditions which are predominantly defined by the compressor map, see Figure 6. Since the main operational changes in order to move the operating point within the compressor map are identified as the rotational speed of the compressor and the loop resistance, subsection 4.1 and 4.2 compare the model and testbed HPU behavior for large individual changes of these two inputs. While subsection 4.3 validates the simultaneous change of both inputs, the main observations are discussed in subsection 4.4.

4.1 Loop resistance variation

For the validation of system behavior along the plant characteristic, the valve openings have been varied while keeping a constant speed. This variation was performed at the minimum speed (Figures 8, 9, 10) as well as at nominal speed (Figures 9, 11, 12).

![Figure 8](image-url)

*Figure 8: System inputs during the loop resistance variation at low speed by closing the expansion valve; simulated (- -) and testbed data (—).*
Figure 8 shows the system inputs. The turbomachine speed was constant at the minimum allowed rotation of 60% of the nominal speed. The operation starts at the low loop resistance A1 with the expansion valve and expander bypass valve open at 80 and 62%, respectively. Successively, the valves are shut to a medium resistance point A2 and finally to a high resistance point A3. These three operating points cover most of the compressor’s characteristic maps speed line as depicted in Figure 9. Since the characteristic map is composed of multiple stages, it varies with changing suction condition, the indicated surge and choke line can only serve as an orientation, not exact values.

Figure 9: Characteristic compressor map during the low- (A) and high-speed (B) loop resistance variation; simulated (---) and testbed data (—-).

Figure 10 compares the main physical quantities of the simulation and testbed data. The simulated compressor performance, temperatures, and mass flow are more than 95% accurate (based on the system inputs from Figure 8).

For nominal speed, the allowed resistance variation was limited due to testbed restrictions of the cooling water system. The valve variation is therefore constrained to a slight closing of the expansion valve as shown in Figure 11 and results in only a small movement in the theoretical characteristic map from Figure 9. The agreement between simulation and testbed results in Figure 12 is consistently satisfactory over every parameter with an accuracy of 95%. The testbed data uncertainty during these rather slow dynamics is below 2% throughout all data points.

Figure 10: Physical quantities during the low-speed loop resistance variation; simulated (---) and testbed data (—-) with a confidence interval (■) as defined in subsection 2.2. Results of adding a time delay on the simulation output of the temperature are plotted in green.

Figure 11: System inputs during the loop resistance variation at high speed by closing the expansion valve; simulated (---) and testbed data (—-).
4.2 Rotational speed variation

In order to validate the system behavior along the compressor characteristic (see Figure 6), the speed was varied rapidly while keeping all other parameters (e.g. valves, water temperatures) constant, imitating a primary frequency reserve operation on European markets [40]. In Figure 13, the speed as input in the simulation and testbed procedure is shown. From nominal speed, at 100 %, the rotation of the turbomachine shaft was reduced to 60 % within 30 s and restored after a settle-out period of 50 s. Similarly, a speed variation increasing from nominal to 105 % was performed.

While the transient dynamics demonstrate high accuracy, the visualization in the characteristic compressor map in Figure 14 suffers mainly from the smallest deviations in absolute pressure measurements. Both curves resemble an 8-shape where the larger, lower loop is related to the speed decrease operation 100 %–60 %–100 % and the much smaller, upper loop is caused by the speed increase operation 100 %–105 %–100 %.

Figure 13: System inputs during the high-speed loop resistance variation; simulated (---) and testbed data (—)

The power consumption of the HPU – as a result – falls to 26 % of the nominal duty. The transient dynamics are in good agreement between the simulation and testbed system, showing only a small deviation when settling after the large speed increase from 60 % to nominal. A similar agreement can be found in the fluid state measurements as presented in Figure 15. The transient behavior is captured well in absolute numbers and dynamics. A larger deviation is found in the temperature, where the dynamics of the simulation are much quicker than what testbed data shows. Adding a first-order transfer function with a delay of 15 s to the simulation temperature data yields the green result and much better agreement with the testbed measurements.

Figure 14: Characteristic compressor map during the speed variation; simulated (---) and testbed data (—).
The testbed measurements show a high uncertainty of up to 20% for mass flow and temperatures during these fast dynamics. Generally, it is concluded that the simulation results show a good qualitative agreement with the testbed data. Over wide ranges, especially during steady states, the quantitative values also reach a high accuracy of more than 95%. Several result deviations are discussed in subsection 4.4.

Figure 15: Physical quantities during the speed variation; simulated (- -) and testbed data (—) with a confidence interval (■) as defined in subsection 2.2. Results of adding a time delay on the simulation output of the temperature are plotted in green.

4.3 Combined variation of rotational speed and loop resistance

After the validation of transient operation with a single input variation, the response of a simultaneous change of both, speed and valve position, is investigated. A fast load-balancing operation is performed, reducing the speed by 60% within 30 s and at the same time opening both valves, expansion and expander bypass, as given in Figure 16.

Figure 16: System inputs during the speed as well as loop resistance variation; simulated (- -) and testbed data (—).

Figure 17 shows the transition in the characteristic map. The operating point moves diagonally from a high-speed point at high resistance to a minimum speed closer to the choke line. A slight offset of the simulation is present again, but the shape of the path is in good agreement between experimental data and simulation.

The power consumption of the testbed HPU falls by over 80% within 45 s and is well matched by the simulation. Also, compressor pressures, temperatures, and mass flow remain in agreement with the experimental data in highly dynamic transitions as shown in Figure 18. As seen above, the hot temperature measurement on the compressor discharge is delayed on the testbed but can be compensated with an imposed time delay to the simulation output.
4.4 Discussion of the results

The most relevant observations during the validation, together with their root and potential measures, are summarized in Table 3 as well as elaborated in the following subsections.

4.4.1 Pressure drift for slow dynamics

In Figure 10, a strong pressure drift, defined as a gradual, unintended deviation of the process from the expected performance, can be observed. This unsteady drift can be linked to challenges in manually adjusting the cooling water flow in the testbeds interlinked heat sink and source. Balancing the thermal energy of the testbed loop is complex and results in a thermal shift on the evaporator. This directly influences the evaporation pressure and can project to all of the closed-loop states. Further, this limitation of the interlinked heat sink and source also restricts the loop resistance variation at high speeds, resulting in the rather short path in Figure 9.

4.4.2 Loop resistance uncertainties

Another major discrepancy between the simulation and testbed is the overall loop resistance, visible in the deviating valve positions throughout all validation cases in Figures 8, 11, 13, and 16. A fundamental cause lies in the simplifications of pipe modeling. Additional pipes and armatures on the testbed as well as varying surface conditions on different pipe elements and a high number of flange connections are difficult to model accurately. On top of this comes the poor quality of the valve characteristics. In ever-changing fluid properties from liquid to multiphase to supercritical and even gaseous states, the correlation between opening, $C_v$, and actual resistance is non-trivial. The choice of a simple linear valve model in correspondence with the manufacturer is a conscious decision to allow for tuning flexibility on the loop resistance. While a fitting valve opening can be easily found based on measurement data, it limits the control application of the model at this stage to qualitative use only.

Table 3: Summary of the most relevant observations together with potential causes as well as proposed measures.

<table>
<thead>
<tr>
<th>Observation (corresponding subsection)</th>
<th>Root</th>
<th>Measure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure drift for slow dynamics (4.4.1)</td>
<td>Thermal shift on the water-glycol loop impacts the evaporation pressure</td>
<td>None – physical testbed limitation</td>
</tr>
<tr>
<td>Loop resistance uncertainties (4.4.2)</td>
<td>Simplified pipe modeling, challenging valve characteristics</td>
<td>Linear valve model based on testbed or improved manufacturer data</td>
</tr>
<tr>
<td>Elevated testbed path in the characteristic compressor map (4.4.3)</td>
<td>Overperformance of the manufactured compressor (conservative compressor model)</td>
<td>Regenerate compressor maps based on testbed measurements</td>
</tr>
<tr>
<td>Temperature deviations (4.4.4)</td>
<td>Thermal inertia of temperature sensors</td>
<td>Implementation of first-order transfer function(s)</td>
</tr>
<tr>
<td>High sensitivity to total CO$_2$ mass (4.4.5)</td>
<td>Inaccurate mass balance measurement on the testbed</td>
<td>None – physical testbed limitation</td>
</tr>
</tbody>
</table>

Figure 18: Physical quantities during the speed as well as loop resistance variation; simulated (--) and testbed data (—) with a confidence interval (≡) as defined in subsection 2.2. Results of adding a time delay on the simulation output of the temperature are plotted in green.
4.4.3 Elevated testbed path in the compressor map

The paths of the testbed and the simulation data in the characteristic map for the load-balancing operation are slightly shifted. The data translation into pressure ratio emphasizes small deviations and measurement inertia on the testbed projects onto the volume flow. In Figure 14 the simulation gives a nearly ideal path, while the path of the testbed data appears morphed. On one hand, this is caused by a fast pressure measurement and a comparably low temperature sensor which results in a temporarily wrong combination of data points. The dominating shift of the experimental data to higher pressure ratios is explained by a conservative compressor model. The manufactured compressor wheels reach higher pressures than designed for a given volume flow. The compressor look-up tables should be recalculated and updated based on the testbed experience.

4.4.4 Temperature deviations

The dynamic response of the temperature differs significantly between the simulation results in the dotted gray and the testbed results in solid black as described in section 4.2 and is visible in Figure 15 and Figure 18. By adding a first-order transfer function with a time constant of 15 s to the temperature output of the simulation, the resulting temperature curve in dotted green is in much better agreement. This could be explained by the thermal inertia of the temperature sensors, which had not been in direct contact with the medium but placed in an insertion sleeve, leading to a delay. The impact of measurement inertia is non-negligible and contributes to the systematic validation uncertainty. Especially computed values from the testbed such as volume flow, enthalpy and ultimately COP propagate this error and inhibit a higher uncertainty during transient operation.

4.4.5 Total refrigerant charge

It is challenging to accurately monitor the total mass of refrigerant present in the test loop. Therefore, it can only be roughly estimated based on weight inventory measurements during the charging procedure. Moreover, some refrigerant was added or removed during the multiple days of testing, resulting in significant uncertainties of the refrigerant charge at a certain time. The actual refrigerant mass varied in the range between 5.5 to 6.5 tons. This relatively large uncertainty creates, however, a degree of freedom for the simulation which can have an impact on the results.

5. CONCLUSION

Large-scale industrial heat pumps are crucial solutions for the decarbonization of district energy networks or process heat applications. An optimal integration in complex operating frameworks must take into consideration the system dynamics. Hence, transient simulation is one of the key tools to provide accurate predictions of future heat pump operation. More specifically, application services such as seasonal load planning, day-to-day heat balancing, and highly dynamic grid services can be supported by the concept and tool elaborated in this work. The presented model improves on the current state-of-the-art by its validation with full-scale experimental testing results. For fast self-induced operational changes, the major results can be summarized as follows:

- The developed Modelica HPU model matches the testbed measurements with an accuracy of 95 % in the discussed physical quantities (with few exceptions as discussed).
- Fast dynamic changes of the power consumption up to 80 % within 30-45 s by varying the loop resistance and the speed have been validated both, individually and combined.
- The validated HPU model is qualified to predict transient plant operation and control responses.

As the next step of development, the integration of elaborated valve characteristics can provide dynamic models for even more accurate system predictions. Besides ensuring the scalability of such models, future studies should investigate control strategies on different time scales. A validated dynamic model as presented here can serve as the foundation for more complex energy management systems connecting long-term resource planning with fast dynamics of ancillary services on an industrial scale.

NOMENCLATURE

- CO₂: Carbon Dioxide
- COP: Coefficient of Performance
- Cv: Valve Flow Coefficient
- ρ: Density [kg/m³]
- dp: Pressure Loss [Pa]
- HEX: Heat Exchanger
- HPU: Heat Pump Unit
- IEC: International Electrotechnical Commission
- ISA: International Society of Automation
- MAN ES: MAN Energy Solutions Schweiz AG
- NH₃: Ammonia
- SBTL: Spline-based Table Lookup
- Qln/out: Specific Heat [J/kg]
- v: Median Flow Velocity [m/s]
- Wln/out: Specific Work [J/kg]
- ζ: Flow Resistance Factor [-]

CREDIT AUTHOR STATEMENT

Leonhard Wolscht Conceptualization, Data curation, Software, Model, Writing, Visualization Kai Knobloch Conceptualization, Data curation, Software, Writing, Visualization, Funding acquisition Emmanuel Jacquemoud Resources, Supervision, Writing - Review Philipp Jenny Writing - Review.
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