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Research Paper

Numerical investigation of a heat pump demonstrator for partial electrification of the steam supply for paper drying

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ABSTRACT

Industrial process heat is currently mostly generated by using fossil fuels. In order to reduce emissions, heat pumps have been identified as a key technology to electrify a wide range of industrial processes. For applications in the temperature range higher than 150 °C, there is a high demand of bringing technologies to market maturity. This is one of the main purposes of the EU-funded project SPIRIT. As a part of this project, a novel mechanical vapor recompression (MVR) system is integrated into the steam network of a paper mill producing high pressured steam with temperatures up to 180 °C using a prototype piston compressor. Application of heat pumps with very high temperatures exceed state of the art technology. For this reason, the demonstration in industrial environments is of high relevance and shows high research potential. Safe operation and minimal risk for disruption of currently installed supply systems are crucial for these demonstrators. This paper presents transient simulation studies of the MVR system in preparation for safe commissioning. A detailed model is introduced considering volume dynamics and thermal inertia. The model is generated in Modelica using the well-established library for thermal system simulations TIL. Component models are extended with part load characteristics and heat transfer capability. The focus of this work is the investigation of adaptive control concepts for the operating strategy during engine start-up, which is implemented by enabling automatic binary decisions to activate controllers based on system states. A strategy for the start-up procedure is proposed and it is found that the system can be heated up rapidly from initial ambient conditions to supply high pressure steam after a time span of 800 s. Steam is compressed from 2 bar total pressure at the compressor inlet to 6 bar at the outlet reaching a design pressure ratio of $\Pi_C = 3$. Furthermore, technical feasibility of the control concept to adaptively connect the MVR system to the steam supply network can be shown with stable and safe operation during all phases of the proposed start-up procedure. In addition to the overall engine control concept, a detailed study is performed to investigate controllers for optimal condensate injection. Feedforward controls with constant and adaptive gain as well as feedback controllers are compared. A regression based approach shows deviations of $\Delta T \approx \pm 3K$ while adapting to varying operating conditions. Feedforward concepts are easy to implement and are robust against disturbances. As a downside, the results indicate high sensitivity to changes in the inlet conditions of the compressor, which requires very accurate predictions of injected mass flows. A feedback controller is presented as an alternative reaching spot-on precision. It can be indicated that the model is able to accurately capture physical state changes. The relative value of condensate injection of 8%, which is specified by the manufacturer, is reproduced with satisfactory agreement.

1. Introduction

In the context of the urgency to reduce carbon emissions, the electrification of heat in industrial processes shows high potential to contribute in a significant way to reach climate goals [1,2]. Specifically in energy intensive industrial sectors like the production of pulp and paper, the contribution can be significant [3]. Because of this, the development of heat pumps with high sink temperatures and scaling to the capacity of industrial applications is an important task in research, as current technology operates only up to 150 °C [4,5]. There are many studies that come to the conclusion, that high temperature heat pumps

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Nomenclature

Abbreviations

DLR	German Aerospace Center
EU	European Union
MVR	Mechanical vapor recompression
SPIRIT	Project name
TIL	Modelica library for thermodynamic simulations
VLE	Vapor liquid equilibrium

Variables

$\dot{m}$	Mass flow [kg/s]
$\dot{Q}$	Heat flow rate [W]
A_s	Surface area [m^2]
C	Heat capacity [J/K]
h	Specific enthalpic [kg m^2/s^2]
k	Conductivity [kg m/(s^3 K)]
k_v	Eff. valve volume flow [m^3/s]
l_{fill}	Filling level [–]
l_{W}	Length [m]
m	Mass [kg]
n	Rotational speed [1/s]
p	Pressure [Pa]
R	Heat resistance [kg m^2/(s^3 K)]
T	Temperature [K]
t	Time [s]
V	Volume [m^3]

Greek symbols

α	Heat transfer coefficient [W/(m^2 K)]
ξ	Part load factor [–]
η	Isentropic efficiency [–]
λ_V	Volumetric efficiency [–]
ρ	Density [kg/(m^3)]

Superscripts and subscripts

C	Compressor
cond.	Conduction
conv.	Convection
d	Displacement
eff.	Effective
is	Isentropic
l	Liquid
nom	Nominal value
PL	Part load

are a crucial step to electrify process heat demands. Kosmadakis et al. evaluated the techno-economic potential and found feasible configurations up to sink temperatures of 150 °C [6]. There is a large variety of concepts with different working media and cycle architectures to adapt to a wide range of process requirements [7]. For this reason, the German Aerospace Center (DLR) focuses on innovative design methods and demonstration of various heat pump concepts with air and water as working medium. The reverse Brayton cycle is suitable for sensible heat transfer and high temperature lifts [8,9]. For latent heat transfer, heat pumps based on the Rankine cycle with multi-stage compression are in focus [10]. Additional to the design, the most suitable integration into the industrial process is an essential step [11]. Because of this, heat pump design and integration need to be experimentally investigated to bring these technologies further to market maturity. This is exactly what the EU funded project SPIRIT (https://spirit-heat.eu/) is aiming for: Three full-scale ($\dot{Q} \geq 0.7$ MWth) heat pump demonstrators are implemented into operational production facilities of a sugar company, a prawn processing plant and a paper mill. In addition to innovation in the technological developments, the economic performance of the three demonstrators will be evaluated so that potential users can estimate the investment costs and amortization period. The third demo-case focuses on electrified steam supply for paper drying by integrating a novel mechanical vapor recompression heat pump (MVR) into the steam network. This system will provide steam at temperatures of 180 °C, which exceeds the sink temperatures of established heat pump technologies. Heat pump demonstration on industrial sites serves various purposes: The application potential for users is increased with investigation of process integration, component development and testing as well as development of control concepts. Therefore, the project aims to test an innovative single stage 4-cylinder piston compressor in operation on site [12]. A small scaled compressor is fit into a standard container allowing for easier transport and installation with low risk to disruptively interfere with processes and installed supply systems. It is a prototype tested for serial production in future heat pump applications. The compressor operates for inlet pressures from 2 bar to 4 bar and is designed for pressure ratios of $\Pi_C = 3$. A large operating range with high part load efficiency is achieved. Condensate injection allows outlet temperatures up to 180 °C. All industrial demonstration cases are accompanied with digital twins (dynamic models) to investigate system behavior and develop control concepts for the operation on site, which is also the focus of this study.

1.1. High temperature heat pumps for electrification of process heat

Heat pumps for applications in the area of domestic heating are widely demonstrated. For high temperature applications in industrial use cases with high energy demands there is a very high potential for further development of technological concepts. There are a wide range of process requirements with regard to sink temperatures, available heat sources and temperature lifts. Consequently, the best candidate for a heat pump concept is very case specific. In general, heat pumps are classified in open cycle and closed cycle approaches. Bless et al. investigated different heat pump types for steam generation, which is a typical heat carrier in several industries [13]. They compared closed cycles with different working media, a reversed Brayton cycle and MVR concepts to generate steam at 150 °C. The impact of the cycle concept was clearly shown, whereby an open cycle heat pump similar to the system in this work shows a promising performance. The number of demonstration projects to advance technological developments in this area increases. Prototype systems have been installed in different industrial applications. The project Dryficiency investigates heat pump concepts in the brick and tile industry. Open and closed cycle heat pumps have been demonstrated for steam generation and brick drying [14]. A steam producing heat pump that reaches 180 °C was installed at AstraZeneca [15]. It can be concluded, that heat pumps will be applicable to various industrial processes with advancements made by demonstration of the technology. Subject to this paper is a paper production facility, which is a typical use case with high potential for electrification.

In paper production there is a high demand for process heat and a large fraction is needed for paper drying. The solid paper material is transported on the outside of rotating cylinders while vapor condenses on the inside, thus transferring heat. There are several options to improve energy efficiency of steam supply through heat recovery as well as potential concepts for decarbonization. These include mainly electrification using heat pumps and electric boilers or making use of regenerative fuels [16,17]. Energy efficiency can be further improved by optimizing the operation of supply systems like cogeneration

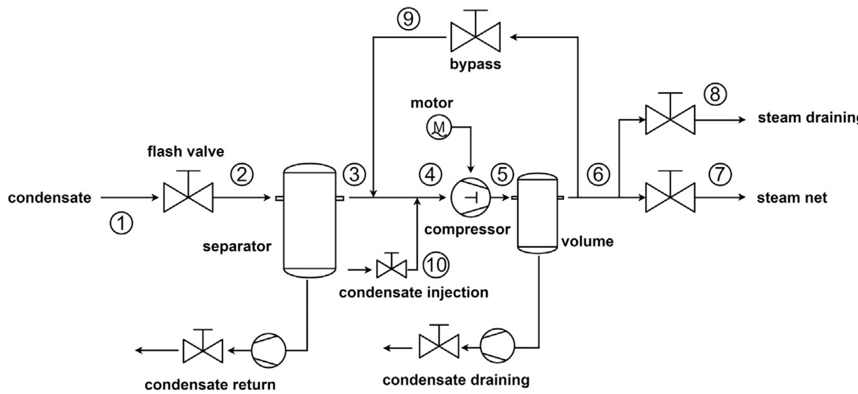


Fig. 1. Simplified system layout of MVR and its connection to the steam supply network.

Table 1
Main data of the systems stations.

Parameter	Value
$p_{1,l}$	5.5 bar
$T_{1,l}$	155 °C
$p_{2,\mathrm{flash}}$	2 bar
$p_{6,\mathrm{steam}}$	6.1 bar
$T_{6,\mathrm{steam}}$	180 °C
$\dot{m}_{3,\mathrm{flash}}$	[0, 0.24] kg/s
$\dot{m}_{5,\mathrm{C}}$	[0, 0.2916] kg/s

plants [18,19], increase the amount of recoverable heat e.g. with heat pumps [20] or integration of thermal storages [21]. A virtual battery concept with consideration of fluctuating renewables has been introduced by Zauner et al. [22] and evaluated with regard to energetic, environmental and techno-economic aspects. Detailed studies on the integration of heat pumps in the overall paper production process have been performed by Bakhtiari et al. [23], where two concepts of heat pumps are investigated for hot water supply. Different heat pump systems for paper drying are compared by Abrahamsson et al. [24]. This is also what the project SPIRIT aims for, although in the present use case of this paper, the focus is more on the demonstration aspect with a simple system layout enabling high accessibility for the technology users and on-site testing. The concept of the integrated MVR system is introduced in the following section.

1.2. Demo case: Mechanical vapor recompression heat pump

The basic idea behind the integration approach of the MVR heat pump is to apply a simple concept using electrical energy to generate part of the required high-pressure steam. Fig. 1 shows the system layout of the MVR system. Condensate returning from the drying cylinders of the plant is flashed to mixed flow (1 → 2) and then separated in liquid and gaseous phase (2 → 3). A piston compressor is used to compress the saturated steam (4 → 5) to be fed back to the high-pressure steam network (6 → 7). Upstream of the compressor, condensate is injected (10 → 4) to lower the outlet temperature. During start-up of the system, the steam draining valve (8) is opened until the pre-heating phase is finished. Then, the draining valve is closed and pressure builds up rapidly in the volume downstream of the compressor, until a threshold is reached which activates valve 7 and the connection to the steam net is opened. Accordingly, this valve also functions as a non-return flap valve, as it is closed as soon as the pressure drops in this part of the system below the target value. For testing purposes, the mass flow of the compressor can be maximized by using the bypass (6 → 9). This allows to increase the mass flow in the compressor to reach its nominal operating point, which cannot be achieved with the flashed steam for this demonstration case.

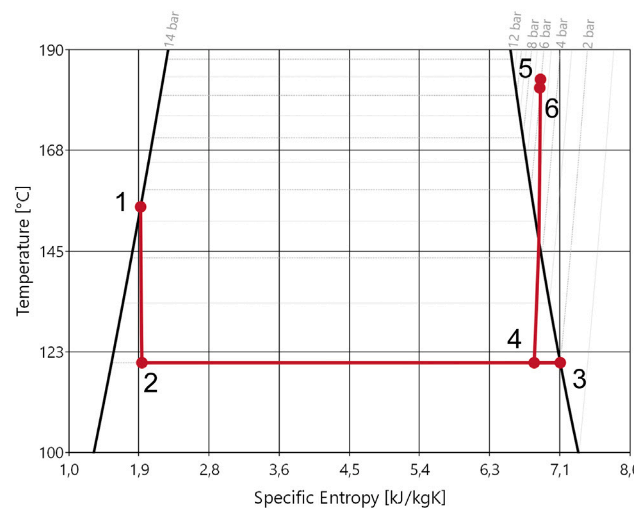


Fig. 2. Simulation of thermodynamic state changes plotted in $T-s$ diagram.

Table 1 gives an overview of the main data of the introduced MVR system. The condensate returned from drying cylinders is flashed from $p1 = 5.5\,\mathrm{bar}$ to $p_2 = 2\,\mathrm{bar}$ total pressure. At nominal operation conditions, the compressor delivers steam at $p_6 = 6.1$ bar and $T_6 = 180\,°\mathrm{C}$. For all investigations, the initial state of the system is set to ambient conditions. Further details of the thermodynamic states at each station throughout all operating points are discussed in the result section below. The mass flow of flashed steam is limited to a maximum value of $\dot{m} \approx 0.24\,\mathrm{kg/s}$. The bypass allows for an increase of the maximum compressor mass flow to $\dot{m}_{5,C} \approx 0.29\,\mathrm{kg/s}$, which enables experiments with nominal rotational speed of the piston compressor.

The thermodynamic system states under nominal operating conditions are shown in the $T-s$-diagram in Fig. 2. The positions of highlighted points are the results computed for a specific point of time during transient simulation, when the system reaches steady state operation. The first step of condensate flashing from 5.5 bar to 2 bar mixed flow (1 → 2) can bee seen in the almost vertical line on the left side. Steam is separated from the liquid phase (2 → 3) and led together with injected condensate to the piston compressor inlet (3 → 4). These thermodynamic state changes are indicated by the bottom horizontal line. Now, the pressure is raised to $p_5 = 6.1\,\mathrm{bar}$ (4 → 5) to reach the superheated steam condition as required in the steam network, which is connected at position 6. The minor temperature drop downstream of the compressor (5 → 6) is caused by heat losses in volumes and piping. To reach the target temperature of $T_6 = 180\,°\mathrm{C}$, the amount of condensate injection upstream of the compressor has to be additionally controlled.

1.3. Research objectives and state of the art: Transient operation of heat pump systems

Demonstration projects with innovative technology using prototype components are a key factor to advance heat pump application in industry. At the same time, a seamless integration and safe operation on site needs to be guaranteed minimizing the risk to disrupt the processes. To achieve this, detailed models or digital twins are applied for design, operation and maintenance of such systems. This is the motivation for the studies performed in this paper. The present work focuses on the investigation of system controls with transient simulations using a detailed model considering part load and heat transfer. A controller setup for safe and energy efficient operation is proposed. A preliminary start-up strategy is introduced with control of compressor speed and logically activated valves. Three concepts for the control of the supply temperature of the MVR system are compared. At the time of publishing this paper no experimental data is available, which will be used later on in the project for validation and model tuning during commissioning. The following research questions are addressed in this paper:

- Does the proposed controller setup ensure secure system start-up and stable dynamic operation?
- How does the system respond to control inputs, and what are the associated time scales for transitions between operating points and thermal ramp-up?
- Are feedforward controllers with constant or adaptive gain suitable to control the supply temperature?

Similar studies have been performed by Qiao et al. [25] with investigation of start-up transients and development of control strategies. Their detailed modeling approach for a flash tank vapor injection heat pump is described and transient results for simulations of start-up and shutdown are presented. The model is validated with experimental data and is able to approximate the impact of key system parameters. Start-up and shutdown with dynamic models have also been studied by Li et al. [26] with a dynamic model of a vapor compression cycle in Matlab/Simulink. Their focus was on heat exchanger modeling switching between different modes. It was shown with experimental validation that the model is able to give accurate predictions of transient manoeuvres. A general overview of heat pump controls is given by Goyal et al. [27]. Research goals for system controls with steady-state and transient modeling are discussed. They highlight that transient models are crucial to develop advanced control systems. The difference between conventional controls, advanced controls and intelligent controls is discussed. In conclusion, the important link between detailed models and the development of control strategies is underlined.

2. Methodology: Transient modeling of the MVR system

The system is modeled using the object-oriented language Modelica [28]. Dymola is used as the simulation environment and the TIL library is applied and extended to model the components [29, 30]. The TIL suite is developed by TLK Energy for the simulation of thermodynamic systems. The library mainly consists of the TIL model library with various component classes and secondly TIL Media. In this work, the VLEFluidComponents (VLE = vapor liquid equilibrium) are applied to model the MVR system considering phase change, volume dynamics and thermal inertia. The modeling concept for the main components is introduced including extensions of existing models as well as the creation of new classes aiming to meet the requirements to simulate system start-up. Beyond that, compressor and valve controls are proposed, which are partly logically activated in response to the system state.

2.1. Extended compressor model

The piston compressor is the key component of the MVR system. The TIL library contains different classes for compressor approximation ranging from basic efficiency-based compressor to complex models with physics-based correlations for friction induced losses in the cylinders. In this work, the efficiency-based compressor class is extended to match the requirements of approximating part-load rotational speed and modeling heat transfer to the casing.

$$\dot{m} = \lambda_V \ \rho \ n_C \ V_d \tag{1}$$

The mass flow is calculated as shown in Eq. (1) using the piston frequency n, the displacement volume V_d and volumetric efficiency λ_V. Displacement volume and volumetric efficiency are set according to the geometrical specifications of the compressor developed by the project partner Spilling that specializes in steam compression.

$$n_{\text{rel, PL}} = \frac{n}{n_{\text{nom}}} \tag{2}$$

The base class in TIL calculates the state changes based on a constant isentropic efficiency. To include variable part-load performance, a characteristic line for the efficiency as a function of the rotational speed is integrated as the first modification to the compressor class. In the extended class, a user defined nominal speed parameter is set as shown in Eq. (2), which allows to compute the relative rotational speed $n_{rel,PL}$, which indicates part-load operation.

$$\eta_{\text{is}} = \eta_{\text{is, nom}} \ \xi_{\text{PL}} \tag{3}$$

$$\text{with} \quad \xi_{\text{PL}} = f(n_{\text{rel, PL}}) \tag{4}$$

With Eqs. (3) and (4) the newly introduced part-load factor ζ_{PL} is calculated to correct the isentropic efficiency for operating points that deviate from nominal rotational speed. The function for ζ_{PL} is defined as a polynomial and can be derived with linear regression from known operating points.

$$h_5 = (h_{5,is} - h_4)/\eta_{is} + h_4 + \frac{\dot{Q}_C}{\dot{m}} \tag{5}$$

The second important modification for this work is the consideration of heat transfer to the metal casing of the compressor. This is a requirement to control the start-up, which identifies if the system is in the pre-heating phase depending on the surface temperature of the compressor casing. In order to include this aspect, heat flow between the fluid side and the metal casing needs to be considered. A heat port is added and the equation for energy balance is modified to now include the source term for $Q = \dot{Q}c/\dot{m}$ as shown in Eq. (5). An additional class to approximate heat transfer mechanisms is then connected to this heat port, which is introduced in the following section.

A simplified setup for controlling the compressor operation is shown in Fig. 3. The mass flow of the steam is controlled by setting the rotational speed. A PI-controller is used to adapt the rotational speed n according to a target mass flow rate to be reached. In order to set the desired pressure ratio, a second PI-controller adjusts the opening of a downstream valve. In this way, the flow resistance is controlled to raise the measured pressure at the compressor outlet to a target value. The last aspect of the compressor model is condensate injection, which is not visualized here. This is considered by injection of condensate upstream of the inlet. The injected mass flow is set as a specified fraction of the primary steam mass flow and is adapted depending on the flow conditions with a performance curve approach. In this way, the outlet conditions of the high-pressure steam can be controlled and high temperatures, that could potentially lead to damage e.g. of the sealing, are avoided.

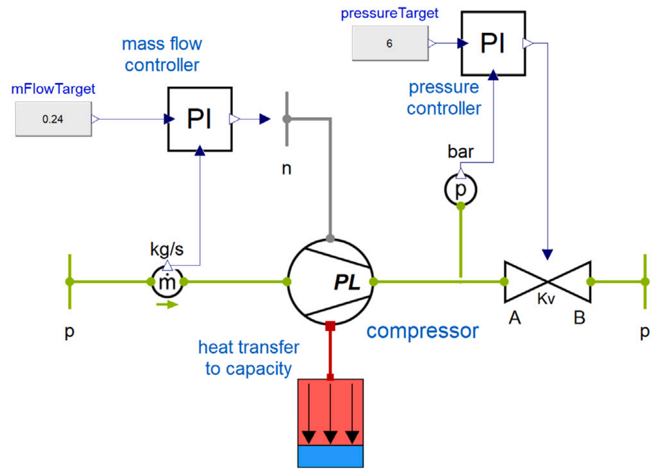


Fig. 3. General setup of compressor controls without injection cooling. Model is extended with regard to part-load capability and energy balance considering heat transfer to the casing, which is considered as a capacitor.

2.2. Heat transfer class

The main requirement for the models in this work is to investigate transient system response during start-up. Starting from initial ambient conditions, the heat transfer from the fluid to solid bodies and convective losses to the environment have to be modeled to approximate thermal inertia. This is important for the metal parts like the separator tank, the compressor and other volumes as well as piping.

To meet this requirement, a heat transfer class based on thermal resistances R_i and capacitors is introduced. In the overall system model, the heat transfer class can be identified by the boxes in red and blue, as can be seen in the lower center of Fig. 3. The basic structure of the class is shown in Fig. 4. It accounts for the heat transfer mechanisms of convection from fluid to metal, heat conduction within the solid body and free convection to the environment, which is set by using a temperature boundary. A heat port connects the class to compute energy balances of attached models and the ambient temperature is set as a boundary condition, as can be seen on the left side of the figure.

$$Q = \frac{T_{\text{out}} - T_{\text{in}}}{R} \tag{6}$$

In general, the transferred heat based on a thermal resistance is calculated as shown in Eq. (6). It is dependent on the temperature difference and the magnitude of R, which is specified according to geometric and material properties.

$$R_{\text{conv}} = \frac{1}{A_s\ \alpha_{\text{conv}}} \tag{7}$$

For convection, the resistance is calculated according to Eq. (7) by setting the heat transfer surface area A_s and the heat transfer coefficient α_{conv}.

$$R_{\text{cond}} = \frac{l_W}{A_s\ k_{\text{cond}}} \tag{8}$$

For conduction of heat, the resistance is calculated in a similar way, also considering the surface area and in this case a material specific value for thermal conductivity k_{cond}.

$$\dot{Q} = C\frac{dT}{dt} = m\ c_p\ \frac{dT}{dt} \tag{9}$$

The heat flow rate and the temperature change in the solid material can then be computed as shown in Eq. (9). The capacitor C is the product of the specific heat capacity c_p and the mass of the component. High masses and materials with large heat capacities potentially invoke significant thermal inertia, meaning that heat is absorbed according to temperature gradients between fluid and solid bodies. This is an important aspect to consider when transient operation and load changes need to be investigated. In the MVR system model, heat transfer is considered at three position: The separator flash tank, the compressor and the volume downstream of the compressor. So, heat transfer is simplified by lumping individual parts like piping and vessels into a smaller number of solid bodies.

2.3. Valves

Valves are used in several positions in the MVR system to control pressure levels or mass flows. The OrificeValve model is used from the TIL library, which calculates the mass flow according to the equation of Bernoulli:

$$\dot{m} = A_{\text{eff}}\sqrt{\Delta p 2 \rho_{\text{in}}} \tag{10}$$

With a given mass flow e.g. set by the compressor speed, the pressure change is determined by the opening of the valve. This also works the other way around, so that mass flows can be set for a specified pressure drop. In both approaches, the desired effective flow area is varied by using the parameter k_v, which is chosen to be set by the controllers in this work:

$$A_{\text{eff}} = k_V\sqrt{\frac{1000\ (\text{kg/s})}{2 \cdot 1\ \text{bar}}} \tag{11}$$

The k_v parameter is an equivalent value for the effective volume flow occurring at a pressure drop of 1 bar. Pressure controllers are used for the flash valve ($1 \rightarrow 2$), the steam draining valve ($6 \rightarrow 7$) and the connection to the steam network ($6 \rightarrow 8$). In case of the condensate injection (10) and the bypass ($6 \rightarrow 9$), the mass flow is controlled by setting the k_v value with the controllers, as pressure levels on both sides are defined by the system.

2.4. Flow separator volumes

For the MVR system, a flash valve is used to expand condensate to mixed flow, which needs to be separated in a downstream flash tank. This tank is modeled with the TIL-Separator class. The separator has an inlet port for mixed flow and separates the fluid to individual outlet ports for gas and liquid phase. It is based on ideally mixed volume and calculated with a transient energy balance. The model also contains a heat port, so that heat transfer can be considered by connecting the heat transfer class as introduced above. An important parameter to control the tank is the filling level:

$$l_{\text{fill}} = \frac{V_l}{V} \tag{12}$$

This parameter is controlled by pumping out liquid water if a user defined threshold value is reached. For this, a hysteresis control is applied, which periodically activates the pumps if a threshold filling level is exceeded. Two separators are used in the system model. The first one is the flash tank of the system, where the vapor phase is separated from liquid water to supply steam for the compressor. The second one is used to approximate all volumes downstream of the compressor. Volume and heat transfer dynamics are considered in this way and condensate can be collected and removed, which occurs during start-up.

The modeling approach in this work is based on well-established methods that have proven to be of high accuracy in similar work. In general, Modelica models are widely used in different disciplines. Their capability to produce accurate results for the modeling of thermofluid systems like heat pumps is widely studied [31]. Graeber et al. performed simulations with the TIL library for a CO2 heat pump system in a residential application [32]. The results are validated with experimental data. A thermoelectric heat exchanger was modeled with TIL by Junior et al. and also shows good agreement with experimental results [33]. For the piston compressor, there are several modeling approaches similar to this work calculating mass flows, losses and state changes [34]. These studies indicate the feasibility of the results in this paper.

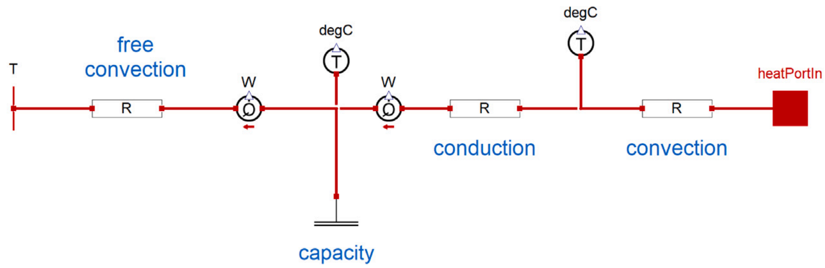


Fig. 4. Heat transfer class: Heat transfer mechanisms convection, conduction and free surface convection are modeled using heat resistances R_i. Masses and material properties are considered using a heat capacity.

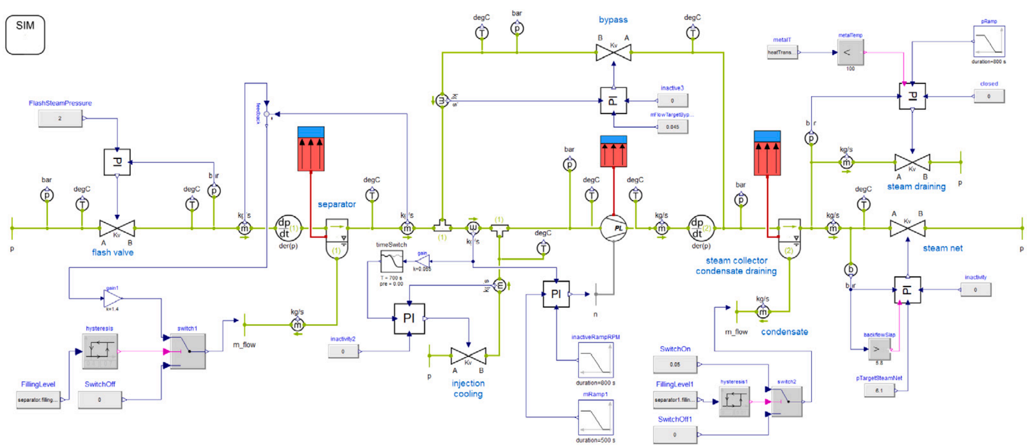


Fig. 5. System model and controller setup in Dymola using TIL library components and extended classes.

2.5. Controller setup

An overview of the system model and the controller setup can be seen in Fig. 5. Feedback controllers (PI-controllers) are used to set valve openings and compressor speed with constant or ramp target values. For each controller, the lower and upper bounds of outputs have to be set, as well as the initial value. The proportional gain and time constant are chosen according to the dynamic characteristics of the system. TIL provides features, so that the controllers can be activated at a specific time or switched on and off during the simulation using a boolean input. This is used to conditionally activate or deactivate controllers depending on system states. As an example of this, the valve that provides the connection to the steam network opens automatically if a certain pressure level is reached. If this is not the case, the valve remains closed to prevent the occurrence of reverse flow, which is realized by setting an if-statement in the model, which is the boolean input to activate this valve. If activated, outlet pressure of the compressor is controlled to reach the desired value. As described above, this combines the non-return flap and the pressure control valve in a single model. Additionally, hysteresis controls are used to control filling levels of the separators. To model the start-up behavior, ramp inputs and smoothing functions are additionally applied to set mass flows or pressure rise during transient operation within user defined time spans. Condensate injection upstream of the compressor is controlled with a feedforward approach, setting the mass flow as a specified fraction of the mass flow of flashed steam. This is considered as a baseline setup. To investigate suitable concepts to precisely control the outlet temperature of the compressor, adaptive feedforward control based on a map input is implemented. As a last step, the feedforward controllers are replaced with a PI controller. Its performance and potential interaction with the remaining controller setup during changes of operating conditions is investigated in the result section.

2.6. Numerical setup and simulation performance

The model is assembled using the component classes introduced above with the TIL library and the described extensions. In Modelica, a system of differential–algebraic equations (DAEs) is derived. Steady-state initialization is used to provide a robust starting point for dynamic simulations. The DASSL (Differential/Algebraic System Solver) [35] algorithm is employed as the numerical solver, configured with a relative tolerance of 1e−5 and a maximum simulation time interval of 5000 s. The resulting DAE system consists of 3809 equations. The computational performance of the simulation is efficient, with a total integration time of approximately 2.4 s. The model demonstrates stable performance with inputs including ramp functions and logically activated controllers, confirming the reliability and robustness of the implementation. The model performance is well suited to perform set-point or trajectory optimizations in dynamic control problems of future studies. Furthermore, rapid computation of detailed dynamic models will allow for software-in-the-loop integration to apply advanced optimization based real-time control strategies.

3. Dynamic simulation of MVR operation

A transient system model is created in Dymola applying the main components as described in the previous section. For this work, the model is used to simulate a preliminary system start-up with all components initialized with ambient pressure and temperature. The impact of thermal inertia and volume dynamics can be studied in order to validate the start-up strategy for the real-world demonstrator. The component performance characteristics and geometrical data are partly based on assumptions at this point and will be updated once the commissioning of the system starts and experimental data is available.

The preliminary start-up procedure investigated with the present model is shown in Fig. 6. The MVR system is initially set to 15 °C and 1 bar pressure. When the flash valve is opened and the compressor is

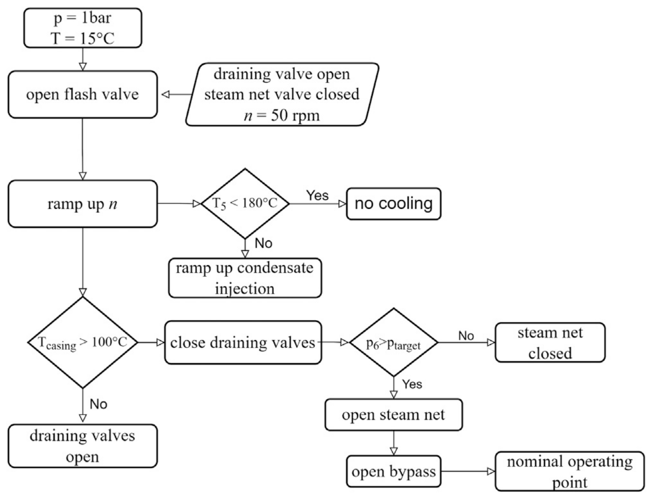


Fig. 6. Flowchart of the proposed strategy for system start-up.

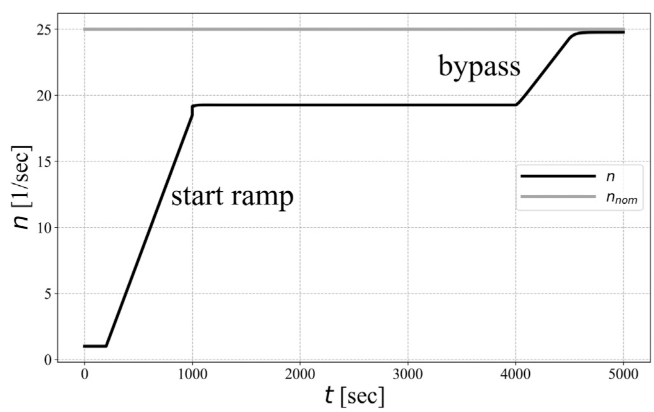


Fig. 7. Compressor rotational speed $n_C(t)$.

put into rotation, the system is flooded with saturated steam and is starting to heat up. For this pre-heating phase, the draining valve is open while the connection to the steam net is initially closed. For the first period of time, the compressor is driven at low rotational speed, which is ramped up after that. This invokes the pressure to rise in the system. When the metal temperature on the outside of the compressor reaches a temperature of approx. 100 °C, the draining valves are fully closed. The system is now a closed volume, which has the effect that the pressure jumps to the target level and the connecting valve (non-return flap) to the steam net is opened. When the outlet temperature of the compressor exceeds 180 °C, the injection cooling is activated to prevent high temperatures, that could potentially cause damage. As a last step, the bypass valve is opened to move a fraction of the steam in the inner cycle, which allows the compressor to reach its nominal mass flow. With this step, the start-up procedure is complete. The functionality of this strategy is evaluated with the execution of transient simulations and their results are discussed in the following section.

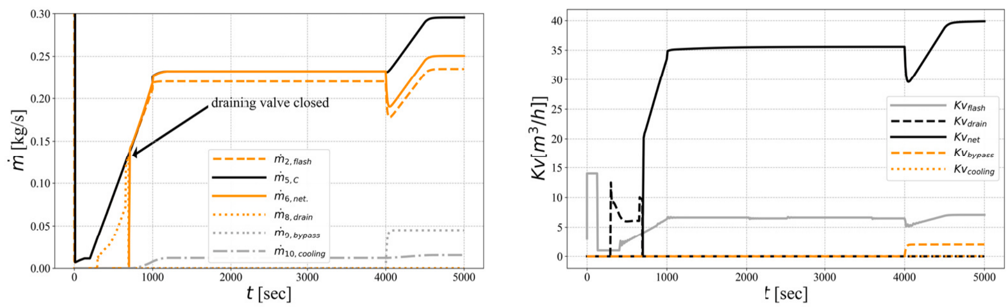
3.1. Simulation of system start-up

Fig. 7 shows the compressor speed control during the start-up procedure. Initially, the compressor is kept at low speed and then accelerated until the mass flow target of flashed steam is reached. The system is kept in this state for a period of time until almost steady-state operation is achieved and after 4000 s the bypass is activated. This allows to further increase the mass flow and the compressor speed is ramped up to its nominal value.

Fig. 8 shows the mass flows as they occur during system start together with the valve openings as a result if the control concept. The dashed orange line is the mass flow of flashed saturated steam. For the first 1000 s when the compressor speed is ramped up, this mass flow is identical to the compressor mass flow (solid black line). The dotted orange line indicates the flow through the draining valve. This valve remains closed for the initial flooding of the system and is then opened until pre-heating of the system is complete. The deviation to the compressor mass flow is due to volume dynamics and condensation downstream of the compressor. After approx. 700 s, this valve is closed and the connecting valve to the steam net is opened. This flow is represented by the solid orange line. The mass flow is slightly higher compared to the flashed steam, as condensate is injected into the compressor. That can be seen by the dash-dotted gray line at the bottom. As indicated by the dashed gray line starting at 4000 s, the bypass is activated. As the compressor speed is again ramped up for a period of time at this point, the flashed mass flow and steam net mass flow first decrease and then rise again with higher rotational speed until the final system state is reached. The compressor runs now at nominal speed and testing is complete. Fig. 8(b) shows the valve openings as set by the controllers and ramp functions. In general, the smooth trajectories indicate stable operation and no instabilities or overshooting are detected. In the starting period, only the flash valve is opened to flood the system. A transition is visible after 800 s, when the draining valve is closed (dashed black line) and the connection to the steam net is opened, as indicated by the solid black line. This valve also controls the flow resistance downstream of the compressor and sets the pressure ratio. The dent after 4000 s is caused by the bypass (dashed orange line) that splits the flow while the compressor speed is ramped up. This first decreases the flow through this valve, which is why the opening is smaller to uphold flow resistance. When the compressor reaches its nominal speed, the overall mass flow is increased and the valve opening is narrowed again.

The pressure levels of the system are plotted in Fig. 9. With the initial flooding of the system, the pressure drops due to condensation in the closed volume downstream of the compressor. This is partly related to the fact, that the working fluid is water for all time steps in the simulation. In the real world demonstrator, the engine will be initially filled with air that is drained during start up. With increasing compressor speed and control of the flow resistance by the setting the opening of the draining valve, the pressure is raised until the draining valves are closed at approx. 700 s. This has the effect, that the pressure jumps to the target value. The engine is now effectively a closed volume and as mass is flooding in, the pressure rises quickly. At this point of time, the connecting valve to the steam net is opened and pressure is controlled afterwards to stay at the desired level. Controllers for flashed steam as well as for the pressure ratio of the compressor invoke smooth curves, which indicates stable operation and the functionality of the start-up approach.

The temperature curves of fluid flows and solid bodies of the system are visualized in Fig. 10. The solid black line is the outlet temperature of the compressor. When steam compression leads to high temperatures $T_5 \geq 200\,°\mathrm{C}$, the condensate injection is activated to control the temperature of the steam fed to the supply net. The thermal inertia can be seen by the time delay between fluid and solid body temperatures. The temperature of the compressor casing is used to indicate the time when the pre-heating phase of the system is finished and the condensate draining valves are closed. This is reached after 700 s and the surface temperature of the compressor exceeds $T_C \geq 100\,°\mathrm{C}$. As discussed above, the input parameters remain unchanged until almost steady state operation is reached. The temperature rise after 4000 s is caused by the activation of the bypass. In the starting procedure used for this work, the condensate injection is only slightly adapted with a fractional value of the primary mass flow, which invokes higher outlet temperatures of the compressor when the bypass is open, due to higher energy at the inlet. In conclusion, it can be stated that the proposed



(a) set-point temperature at the compressor outlet

(b) k_V values of controlled valves

Fig. 8. Trajectories for mass flows as a result of valve control.

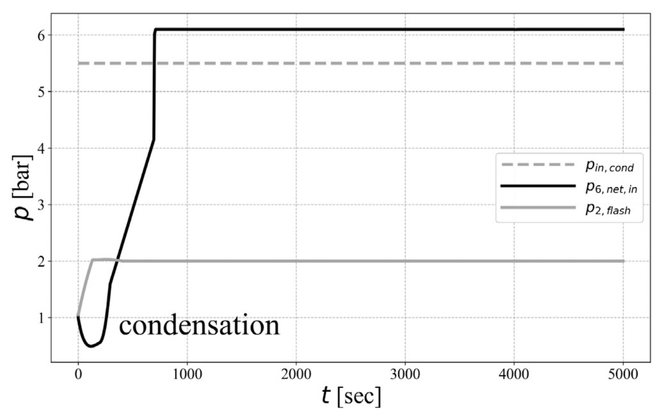


Fig. 9. System pressures during start-up. Pressure upstream of connection valve to steam net: Solid black line.

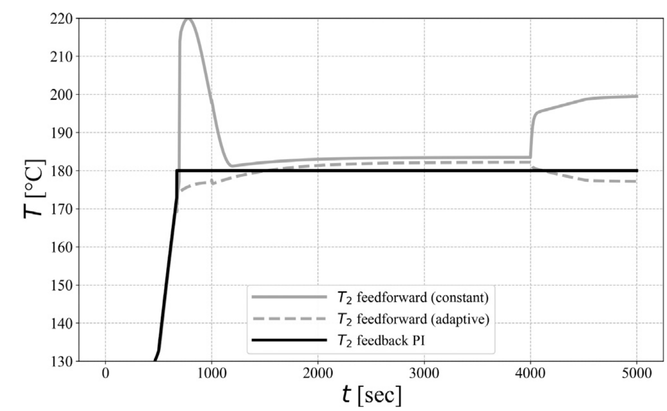


Fig. 11. Control concepts for condensate injection: Set-point temperature at the compressor outlet.

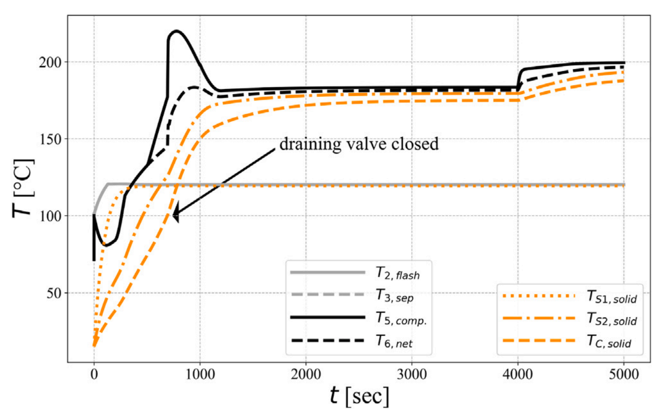


Fig. 10. System temperatures during start-up. Fluid temperatures in gray and black. Solid body temperatures in orange.

start-up strategy and the controller setup enable to perform the system start in a rather short time span and reach stable operation at all time steps. The input parameters like the compressor rotational speed can be further adapted in the future, so that load changes can potentially be performed even faster.

3.2. Control concepts for condensate injection

The temperature of the steam produced by heat pumps is an important set-point so that process demands can be accurately met. In the present study, one key parameter to control the outlet temperature of the compressor is the amount of injected condensate. There are several control concepts to determine the correct mass flow to be injected. The goal here is to set a constant temperature of compressed steam while too high temperatures that could potentially lead to damage have to be avoided at all times. In this study, three concepts are investigated. First, a feedforward control which sets the condensate mass flow as a constant fraction of the inlet mass flow, which is directly proportional to the compressor rotational speed. This value is kept constant independent of the inlet temperature. A second concept replaces that constant with an adaptive gain which is calculated with map based characteristics. The data for this is simulated beforehand and a polynomial regression is performed to predict the optimal condensate mass flow: $\dot{m}_{cond.} = f(T_{in}, \dot{m}_{in})$. These feedforward controls are known to be very robust and are functional for a wide range of control problems. For this reason, they are currently the preferred choice of the compressor supplier in the project. As a third option, a feedback controller is applied.

Fig. 11 shows these three approaches and their effect on the outlet temperature of the compressor. As seen in the results before, setting the condensate injection as a constant fraction of the main mass flow leads to varying temperatures. This is due to the fact, that during start-up the inlet conditions of steam flow are not constant. When the bypass is opened, temperatures are increased. This is clearly represented by the solid gray line. Constant gain might not be a desired control concept in industrial environments where the temperatures are usually precisely set. The map based approach with an adaptive gain leads to better results. The desired temperature is met after the initial pre-heating phase but there are clearly some deviations. This is because the inlet parameters are quite sensitive to the output and the database for the regression is kept low for this study. A design of experiments (DoE) with full factorial sampling is applied resulting in a database of 9 samples. If the map based approach is further pursued, a more precise prediction

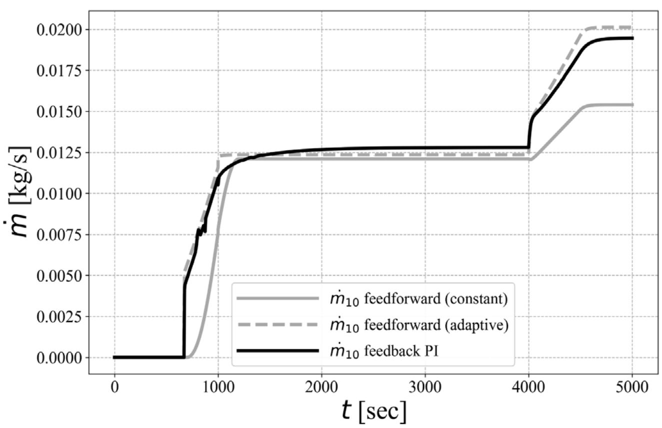


Fig. 12. Control concepts for condensate injection: Controlled mass flow of condensate.

should be ensured. Another downside is, that feedforward approaches hardly account for dynamic effects like heat loss that also contributes to cooling effects. The solid black line shows the best results. This is expected, as the applied PI-controller continuously adapts the mass flow which leads to a very even temperature profile for the entire trajectory.

Fig. 12 shows the trajectories of the injected condensate mass flows for all three approaches. The feedforward controller with adaptive gain and the mass flow set by the feedback controller are very similar. Although there are only minor differences, its impact on the outlet temperature is significant and results in deviations of several Kelvin. This also shows the sensitivity of this parameter. The solid gray line of the constant feedforward concept deviates during initialization of the injection and after the bypass is opened. Condensate injection is ramped up too slowly leading to a temperature peak near 800 s. The increased energy at the compressor inlet induced by the bypass is also not compensated as well as with the adaptive concepts. This results in a temperature rise up to 200 °C, which should be avoided.

In summary it can be stated, that the correct choice of the control concept for the MVR heat pump is a major factor for its operation under variable inlet conditions. An interpolated map or regression based approach with feedforward control is easy to implement and shows promising results. But if measurement uncertainty, dynamic heat loss or component wear are taken into consideration, the prediction of the optimal condensate injection might be imprecise. This is especially relevant in industrial environments. A feedback controller is the best alternative to precisely meet the target temperature. As a downside, feedback controllers require tuning and may lead to instabilities in the presence of disturbances or interactive effects. The results of these simulations highlight the relevance of dynamic models to investigate preliminary control concepts in order to guarantee efficient and safe operation. The compressor manufacturer names an approximated value of $\dot{m}_{cond}/\dot{m}_{in} \approx 8\%$ in the nominal operating point. Aerodynamic loss mechanisms and heat losses over the compressor have a high impact on the temperature rise and are represented by simplified parameters in this study. The model predicts a relative value of $\approx 7\%$, which is a satisfactory agreement and indicates that physical state changes and heat losses are accurately captured.

4. Conclusions and outlook

This study presents a concept for demonstration of a novel high-temperature mechanical vapor recompression (MVR) system within the steam network of a paper mill, showing its potential for reducing emissions in industrial process heat supply. These demonstration cases for industrial heat pumps are highly relevant to increase market potential and enable user acceptance by proving the functionality directly on site. Several challenges occur in this process, which are addressed by this study: The integration concept aims for retrofitting into an existing supply systems with a non-disruptive plug and play installation of the compressor module. Additionally, development and testing of innovative components can be performed. A prototype 4-cylinder piston compressor for efficient steam compression is investigated in an industrial use case. For this reason, detailed transient models and concepts for system controls are introduced. Simulation studies for the start-up have proven the systems ability to safely and rapidly heat up from ambient conditions, reaching the required high-pressure steam compression within 800 s. With an inlet pressure of 2 bar, flashed steam is compressed and the target conditions are reached with a pressure ratio of $\Pi_C = 3$ under nominal operating conditions. A start-up procedure is proposed together with a control strategy that includes logic based activation of controllers based on boolean decisions depending on system states. The results underline that stable operation throughout all phases of engine start-up is ensured. Furthermore, the detailed evaluation of three control methods for optimal condensate injection reveals that feedforward control strategies are sensitive to compressor inlet conditions. It can be derived that accurate predictions are required to set the optimal injection flow in order to achieve a constant temperature of 180 °C for varying inlet conditions of the compressor. Using feedback control instead offers a viable alternative for temperature control, which is potentially beneficial when measurement uncertainties are also taken into account. Those are not compensated with adaptive feedforward, which relies on the accuracy of its preliminary generated database and prediction quality. The system model uses well established component classes and it can be indicated that physical state changes are accurately captured. A satisfactory agreement with the value of 8% relative condensate injection under nominal operating conditions supports the feasibility of the simulations. With additional tuning of the model parameters when experimental data is available, a high level of accuracy is expected. The presented results are valuable to gain an understanding of system response and its time scales for safe and efficient operation. These findings contribute to highlight the application of detailed transient models to support the development of efficient, safe, and adaptable control strategies for high-temperature heat pumps in industrial applications. Projects with technology demonstration will accelerate the path to electrify industrial process heat demand.

Parameters of component performance and geometrical data will be updated once the commissioning is starting. Experimental data will be used to validate and further calibrate the model accordingly. In a last step, it will be used to perform set-point optimizations for energy efficient operation. Future heat pump concepts for paper drying can built up on the presented results. Based on this, scaled versions and more complex heat pump designs can be integrated in steam generation making use of available heat sources to improve energy efficiency while offering a significant potential for electrification of process heat.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Jens Gollasch reports financial support was provided by Horizon Europe. Maximilian Kriese reports financial support was provided by Horizon Europe. Nancy Kabat reports financial support was provided by Horizon Europe. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

Data will be made available on request.

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