Optimisation of high-temperature heat pumps for the efficient operation of direct air capture plants

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Abstract:
High-temperature heat pumps are seen as a promising solution to provide the large amount of thermal energy required for direct air capture plants in a sustainable way. However, while many studies on direct air capture propose the use of heat pumps, the optimal configuration and integration has not yet been studied in detail, and assumptions on the heat pump efficiency vary widely. In this paper, we use a heat pump optimisation model to analyse different systems in detail. Simple cycles, cycles with internal heat exchanger, and transcritical cycles are compared and different options of integrating them with the direct air capture plant are analysed. The overall best-performing solution uses a transcritical CO_2 cycle, as it can be well matched to the temperature profile of the heat sink. It reaches a COP of 3.18, which is a $62\,\%$ improvement compared to a simple heat pump cycle. Heat integration can further improve the efficiency of the process.

Keywords:
Flowsheet optimisation, Refrigeration cycle modelling, Supercritical CO_2 cycle, System integration, Waste heat.

1. Introduction

Direct air capture (DAC) describes the process of capturing carbon dioxide (CO_2) from the atmosphere and securely storing it, thus reducing the atmospheric CO_2 concentration and helping mitigate climate change. Although this process is still quite expensive and energy intensive, research interest and commercial investments into DAC technologies have recently increased significantly.
DAC is attractive due to its ability to address emissions "after it is already too late", i.e., after they have been emitted into the atmosphere. It does not require any changes to the emitting processes, can in principle be located anywhere, and can address the infamous "hard-to-abate" emissions [11]. Additionally, it can help reduce the atmospheric CO_2 concentration to acceptable levels after an initial overshoot, which is projected by many pathways due to insufficiently quick emission reduction action, despite the high risks that overshoot scenarios carry [1].
Despite the increase in atmospheric CO_2 concentrations, it is still quite dilute, with concentration values of around 420 to 430 ppm [2]. Thus, the minimum energy of separation, which constitutes the thermodynamic minimum energy demand, dictates that DAC must have a high energy demand. For example, even just capturing $50\,\%$ of the CO_2 at $50\,\%$ purity requires a minimum of $16.7\,\mathrm{kJ/mol}$, while the real energy requirement is many times higher [3].
DAC can only deliver climate benefits if the required energy is supplied in a low-carbon way to ensure that emissions related to running the plant are much lower than the amount of CO_2 captured and stored. Furthermore, the energy provision accounts for the largest share of operating costs and a significant share of overall costs of DAC. Therefore, an efficient provision of that energy in crucial to the successful deployment of DAC plants. High-temperature heat pumps appear to be the most promising option for widespread use in DAC plants, but have not yet been researched in any detail for this application yet, as explained in the following section.

1.1. Literature review

Academic research and commercial development mainly focusses on two archetypes of DAC: (i) high-temperature absorption processes, typically using aqueous potassium hydroxide as liquid solvent [4]; and (ii) low-temperature adsorption processes, typically based on amine-functionalised polymers as solid sorbent [5]. While the former requires heat supply at temperatures in excess of $900\,^{\circ}\mathrm{C}$ and must therefore be powered by natural gas, biogas, or hydrogen combustion, the latter only requires temperatures of about $80\,^{\circ}\mathrm{C}$ to $130\,^{\circ}\mathrm{C}$ [6]. The low-temperature DAC process has further advantages due to its flexibility and modularity, and it is currently the most-commonly used approach in pilot plants [7]. Therefore, it is the focus of the analysis presented here.

The most-commonly proposed ways to source the thermal energy required to run low-temperature DAC plants are utilising geothermal energy, waste heat, or heat pumps. Geothermal energy is attractive in regions with high availability. It powers the currently largest DAC facility worldwide, located in Iceland [8]. However, it limits DAC deployment to only a few regions in the world. Waste heat is also attractive, and co-locating DAC plants with industrial sites has been shown to reduce costs [9], but it hinges on the availability of suitable sources of waste heat, and competes with alternative uses of that energy. Heat pumps on the other hand are not limited by such constraints, such that they are emerging as an increasingly popular proposed solution to power DAC plants in the academic literature. They also offer potential synergies with DAC plants, such as utilising the heat of adsorption, and using the same fans to move air through both the adsorber and the heat pump evaporator.

The required temperatures of the low-temperature DAC process are attainable for high-temperature heat pumps. If powered by clean electricity, they offer a potentially attractive and efficient way to provide the required thermal energy without causing additional emissions that would be detrimental to the emission balance of the DAC plant. Even though other uses of that clean electricity, such as the decarbonisation of transportation and heating via electric vehicles and heat pumps, deliver higher emission savings per unit of electricity, DAC plants powered by heat pumps and clean electricity can deliver significant negative emissions [10].

While many studies propose the use of heat pumps to power DAC plants, the heat pumps are typically not the focus of the analysis. They are modelled in a quite simplified way, and details on their design and operation as well as potential interactions with the DAC plant are not investigated. The most simplified heat pump modelling approaches simply assume a fixed coefficient of performance (COP) to calculate the electricity demand. For example, Breyer et al. [12] assume a COP of 3 as the global average, while in a related study Fasihi et al. [13] assume the COP to increase from 3 to 3.5 until 2050. On the other hand, Young et al. [14] and Sievert et al. [15] set the COP to 2, while Terlouw et al. [16] assume a value of 2.9.

More sophisticated heat pump modelling approaches estimate the COP based on the Carnot COP and the exergetic efficiency, η_{ex}, and the source and sink temperatures:

$$\mathrm{COP}_{\mathrm{real}} = \eta_{\mathrm{ex}}\mathrm{COP}_{\mathrm{Carnot}} = \eta_{\mathrm{ex}}\frac{T_{\mathrm{sink}}}{T_{\mathrm{sink}} - T_{\mathrm{source}}} \tag{1}$$

Using this approach and assuming an exergetic efficiency of $60\,\%$, Deutz and Bardow [17] estimate an average COP of 2.5 for a DAC plant located in Iceland. Sendi et al. [18] assume an exergetic efficiency of $50\,\%$ and a required supply temperature of $110\,^{\circ}\mathrm{C}$ while considering different climate conditions around the world to determine the source temperature. However, these studies also do not investigate details on the heat pump design and integration with the DAC plant.

Some papers specifically investigate the integration of heat pumps and DAC plants. Leonzio and Shah [19] analyse the possibility of integrating an air-source heat pump using transcritical CO_2, CO_2-R41, and CO_2-ethane cycles into a DAC plant. Ambient air first passes through the adsorber, where CO_2 is adsorbed, increasing the air temperature due to the heat of adsorption. The slightly warmer air then passes through the heat pump evaporator, cooling down in the process. The cold air is then used to cool the adsorber after the regeneration step, such that it can begin the next adsorption cycle.

Ge et al. [20] on the other hand propose splitting the refrigerant stream after the expansion valve. A share of the refrigerant is further expanded, then evaporated using the heat of adsorption, and finally compressed again, while the rest of the refrigerant follows a standard heat pump cycle. The authors also propose a system where steam is directly used to heat the adsorber, and energy from the steam is recovered in the heat pump cycle. Both studies find significant energy and cost reduction potentials.

1.2. Research gap and contributions

The design of efficient heat pumps for DAC processes is not trivial, and their integration requires careful engineering. Due to the high temperature lift from ambient conditions to $100\,^{\circ}\mathrm{C}$ and higher, standard heat pump cycle configurations struggle with low efficiencies, low heating capacities, and high compressor outlet temperatures. Advanced cycles including e.g., internal heat exchangers, vapour injection, transcritical process, or cascaded processes are likely more suitable [21], but details on the design on the heat pump cycles for DAC applications have not been studied in detail yet. Furthermore, the choice of refrigerant is an important question, especially due to tightening restrictions due to the F-gas and REACH regulations [22].

Further integration challenges arise due to the characteristics of the DAC process. Firstly, it is a batch process. In the temperature-vacuum-swing adsorption (TVSA) process, which is currently seen as the most suitable for DAC applications, each collector cycles through the following phases: (1) adsorption; (2) evacuation; (3) heating/desorption; (4) steam purge[1]; and (5) cooling [23]. The optimal integration of multiple adsorbers with a heat pump that is ideally running continuously has not yet been investigated. Furthermore, depending on the DAC process, the provision of hot water and steam is required, while the heat of adsorption and the energy from the cooling step can potentially be used in the process, resulting in multi-source multi-sink heat pump systems.

In this paper, we optimise and compare different heat pump configurations under the operating conditions required for DAC plants, and investigate different options to integrate the heat pump and DAC processes. Section 2. briefly introduces the methodology to model the DAC plant and the heat pump; Section 3. presents the results, focussing on the comparison of different heat pump flowsheets and options to integrate them with the DAC plant; and Section 4. concludes the paper.

2. Methodology

The analysis is based on data from a dynamic DAC model developed by Sendi et al. [18, 24], as well as the steady-state heat pump flowsheet optimisation tool *Crispy* [25]. Both are briefly introduced in the following sections, while for further details, readers are referred to the corresponding references.

2.1. DAC process modelling

The parameters of the DAC process are taken from Sendi et al. [18], who developed a detailed dynamic DAC process model to evaluate the performance of DAC collectors under different climate conditions. The analysis is based on state-of-the-art DAC technology, using Lewatit VP OC 1065 as the sorbent, and a steam-assisted TVSA cycle for regeneration, as described in Section 1.2.. The required heat pump supply temperature is assumed to be $110\,^{\circ}\mathrm{C}$ [18].

For this preliminary analysis, we investigate the operation at an ambient temperature of $10\,^{\circ}\mathrm{C}$ and a relative humidity of $70\,\%$, representing an average day in central Europe. Under these conditions, the heat requirement of the DAC plant is approximately $3.1\,\mathrm{MWh_{th}/t_{CO_2}}$. The adsorption time is about $275\,\mathrm{min}$, the heating and desorption step takes about $200\,\mathrm{min}$, steam purging $12\,\mathrm{min}$, and cooling $30\,\mathrm{min}$. This means that adsorptions accounts for only just over half of the total time. The heating (and steam purging) to cooling time ratio, which will become important later on, is about 7 [18].

[1] This step is optional

2.2. Heat pump optimisation

The heat pump modelling and optimisation is performed using the *Crispy* tool, developed by Höges et al. [25]. The tool was designed to optimise the flowsheet and refrigerant of a heat pump for given design points, i.e., given operating conditions including heat source inlet and outlet temperatures as well as supply and return temperatures on the heat sink side. The objective is typically to maximise the seasonal COP (SCOP), which can be calculated for multiple operating points *i* as:

$$SCOP = \frac{\sum_{i=1}^{n} t_i \dot{Q}_i}{\sum_{i=1}^{n} t_i \frac{\dot{Q}_i}{COP_i}}, \tag{2}$$

where t_i is the time spent in each operating point, and $\dot{Q}_i$ the thermal power provided. About 20 different flowsheets are implemented in *Crispy*, ranging from a simple four-component heat pump cycle to vapour-injection cycles, cascaded cycles, and transcritical processes.

Crispy optimises process parameters such as the degrees of superheating and subcooling as well as the intermediate pressure and injection mass ratio for vapour-injection cycles. Simplified steady-state thermodynamic component models are used to estimate the performance of each configuration. Heat exchangers are assumed to be isobaric, and pressure losses from the pipes are neglected. Any heat losses to the environment are also neglected, leading to isenthalpic expansion valves. All fluid properties are obtained from *Refprop* [28].

The compressor performance is modelled via isentropic and volumetric efficiencies. For the sub-critical cycles using butane as working fluid (see Section 3.2.), polynomial efficiency maps fitted to experimental data obtained from a propane compressor are used [25]. The CO_2 compressors of the transcritical process on the other hand are modelled using the correlations developed by Okasha and Müller [27]. As the model contains no economic assessment, the heat exchangers are not modelled in detail. Instead, a minimum pinch point temperature difference of $2\,\mathrm{K}$ is used to ensure that the process is feasible. Additionally, the superheat at the compressor inlet is required to be at least $8\,\mathrm{K}$ to protect the compressor and ensure stable operation, i.e., avoid the oscillating behaviour that occurs if the superheat falls below the minimum stable superheat.

3. Results and discussion

In this section, results from the heat pump flowsheet optimisation are presented and several aspects of the integration of DAC plant and high-temperature heat pump are discussed. First, different options for the integration of DAC adsorber and heat pump evaporator are discussed. Then, different heat pump configurations, different options of thermal integration, and different methods for steam generation are analysed, before finally practical issues around the hydraulics and controls are discussed.

3.1. Integration of DAC adsorber and heat pump evaporator

The first point to be investigated is the integration of DAC adsorber and heat pump evaporator, as shown schematically in Figure 1. In Option A, ambient air first passes through the adsorber and then the evaporator, while in Option B the order is reversed. In either case, the same fan can be used to drive the air through both components, saving on investment costs compared to standalone DAC and air-source heat pump systems, even though the pressure loss and therefore the required fan power will be higher than that of just a DAC adsorber or a heat pump evaporator.

Option A represents the system proposed by Leonzio and Shah [19]. Ambient air first passes through the adsorber and is heated due to the heat of adsorption, thus increasing the heat pump source temperature, resulting in a higher heat pump efficiency. However, this effect is marginal due to the low CO_2 concentration in the air. Assuming a CO_2 concentration of 430 ppm and considering molecular weights of $44.01\,\mathrm{g/mol_{CO_2}}$ and $28.96\,\mathrm{g/mol_{air}}$, a stream of $1\,\mathrm{kg/s}$ air only contains $0.000\,65\,\mathrm{kg/s}$ CO_2 that can be adsorbed. In the most optimistic case, assuming that all CO_2 is adsorbed, and with a heat of adsorption of $70\,\mathrm{kJ/mol}$ = $1591\,\mathrm{kJ/kg}$ [18], this results in a thermal power of $1.03\,\mathrm{kW}$ to

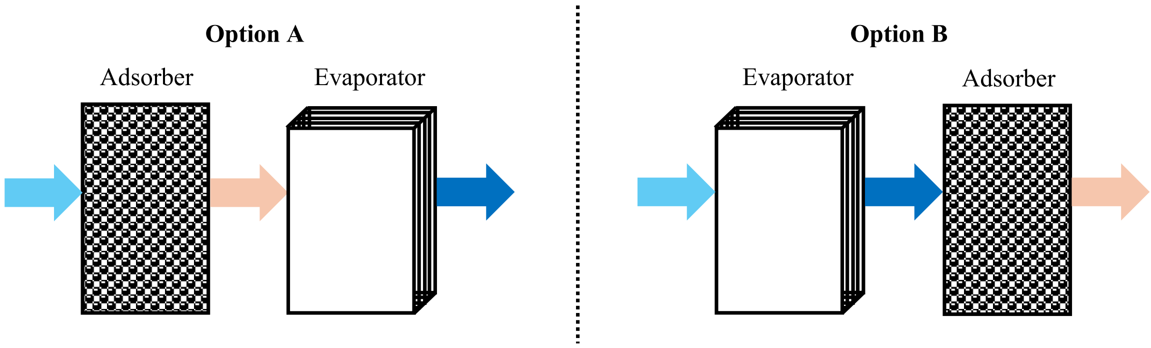

Figure 1: Options for the integration of DAC adsorber and heat pump evaporator.

heat up the stream of $1\,\mathrm{kg/s}$ of air. Consequently, given that the isobaric heat capacity of air is approximately $1\,\mathrm{kJ/(kg\,K)}$, in this most-optimistic case, the air is heated up by about $1\,\mathrm{K}$. Assuming the process parameters presented in Section 2.2., the Carnot COP increases from 3.83 to 3.87. Therefore, for an exergetic efficiency of $50\,\%$, this "preheating" of the air results in an increase of the COP of 0.02, corresponding to a $1\,\%$ increase compared to the case without "preheating".

Option B does not offer this benefit of "preheating" the air, but it potentially offers advantages for the DAC process. The working capacity of the adsorber, i.e., the difference in CO_2 loading between adsorption and desorption, depends on the temperature difference. Elfving et al. [26] modelled the equilibrium working capacity depending on air temperature and regeneration temperature. Under dry conditions, an air temperature of $10\,^{\circ}\mathrm{C}$ and a regeneration temperature of $90\,^{\circ}\mathrm{C}$ results in a working capacity of about $0.6\,\mathrm{mmol_{CO_2}/g_{Sorbent}}$. If the feed temperature is reduced to $0\,^{\circ}\mathrm{C}$, for example by cooling it in the heat pump evaporator, the working capacity increases to about $0.7\,\mathrm{mmol_{CO_2}/g_{Sorbent}}$, corresponding to a $17\,\%$ increase. In other words, by cooling down the air feed, the amount of CO_2 captured per cycle can potentially be significantly increased. However, it is important to note that this analysis is only valid for dry air. In reality, the relative humidity of the air will increase as it is cooled down, leading to more water adsorption and consequently less CO_2 adsorption. Furthermore, the time to heat up the collector for regeneration will increase if the collector is colder, increasing the cycle length and reducing the time the collector is productive. More detailed investigations of both Option A and Option B are necessary to draw conclusions on the best setup.

3.2. Comparison of different heat pump configurations

As a baseline, we consider a standard four-component heat pump cycle. Based on the temperature levels, we select butane (R600) as the working fluid, as it is a natural refrigerant with a low global warming potential and no ozone depletion potential that remains subcritical even at the high temperatures required here. However, the first challenge is that it evaporates at pressures below $1\,\mathrm{bar}$ at the lower temperature level, which is undesirable as it can lead to ambient air leaking into the refrigeration cycle. Furthermore, the COP of the optimised system is only 1.96, corresponding to a modest exergetic efficiency of $31\,\%$. The T-h diagram, shown in Figure 2(a), indicates some of the reasons for the poor performance. Firstly, the high temperature lift and corresponding high pressure ratio leads to a low Carnot COP. This is defined by the operating conditions and will be the case for every heat pump cycle. Secondly, however, the large difference between inlet and outlet temperature on the heat sink side leads to a high temperature difference between the primary and secondary side in the condenser, thus a high entropy production and a low exergetic efficiency.

An alternative is using a cycle with internal heat exchanger, as shown in Figure 2(b). This leads to a lower condensation temperature and a larger share of sensitive heat transfer, thus smaller temperature differences in the condenser. As a result, the COP increases to 2.57, corresponding to an exergetic efficiency of $41\,\%$. The internal heat exchanger results in an over $30\,\%$ higher COP compared to the simple cycle, but also leads to an increase in compressor outlet temperature by over $25\,\mathrm{K}$, which can be detrimental to the operation and lifetime of the compressor.

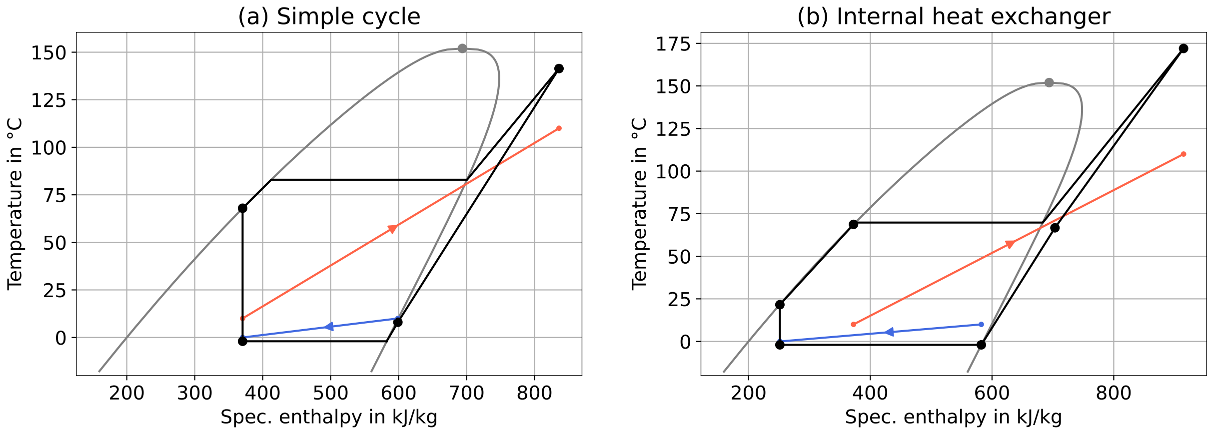

Figure 2: T-h diagrams of the optimised heat pump cycle using: (a) a simple four-component cycle; and (b) a cycle with internal heat exchanger. The heat source is shown in blue, while the heat sink is shown in red colour.

The large temperature difference of the secondary fluid in the condenser is potentially attractive for transcritical processes, as the transcritical isobars can be better matched to the temperature profile of the secondary fluid than the isothermal heat transfer in the two-phase region. This is shown in Figure 3 for a transcritical cycle using CO_2 as working fluid. The plot highlights that the temperature difference between primary and secondary side in the "condenser", which becomes a gas cooler in the transcritical cycle, is much smaller. Consequently the entropy production is smaller, leading to a COP of 3.18, which corresponds to an exergetic efficiency of $50\,\%$.

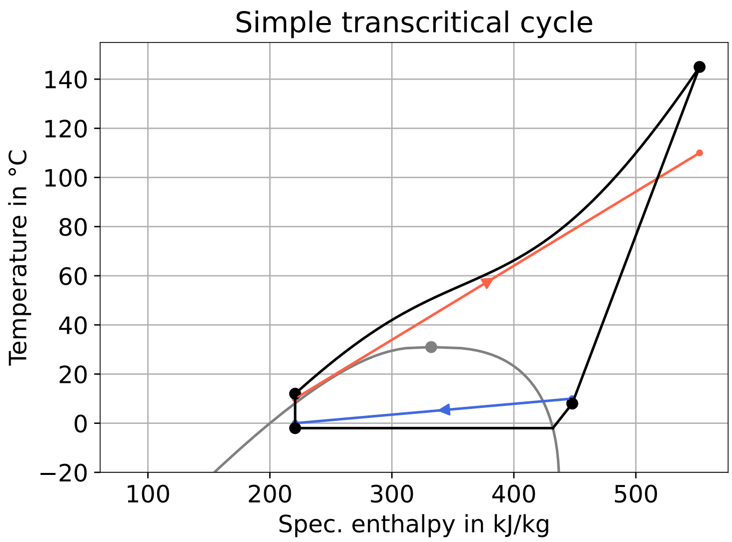

Figure 3: T-h diagram of the optimised simple transcritical heat pump cycle using CO_2 as working fluid. The heat source is shown in blue, while the heat sink is shown in red colour.

With the transcritical CO_2 heat pump cycle, we are able to achieve significantly performance, increasing the COP by $24\,\%$ compared to the subcritical cycle with internal heat exchanger, and by $62\,\%$ compared to the simple cycle. One of the challenges of the transcritical CO_2 cycle is the high pressure level. The evaporation pressure is about $33\,\mathrm{bar}$, while the pressure at the compressor outlet and in the gas cooler reaches $125\,\mathrm{bar}$. Thus, highly pressure-resistant components and pipes with thick walls are required. On the other hand, the CO_2 captured by the DAC plant is typically compressed to about $150\,\mathrm{bar}$ for transport and storage [18], such that the planners and operators of DAC plants should be well equipped to handle CO_2 at such high pressures.

3.3. Opportunities for thermal integration

Step 5 of the TVSA cycle, the cooling step, involves cooling down the adsorber bed from the regeneration temperature of about $95\,°C$ to below $60\,°C$ before starting with the adsorption step to avoid oxidation of the adsorbing material. This thermal energy is available to be integrated into the process to avoid wasting it. However, as noted in Section 2.2., the ratio of heating to cooling duration is about 7 to 1, meaning that for every 7 collectors being heated at any given time there is only 1 being cooled. With the simplified assumption of constant heating and cooling rates[2], this means that approximately $14\,\%$ of the energy demand of the process can be covered by the waste heat. Additionally, the steam used during the steam purging step, step 4 of the TVSA cycle, must be condensed to separate the CO_2 from the water. Under the operating conditions specified in Section 2.2., steam generation accounts for about $10\,\%$ of the total thermal energy demand [18].

The first option is to use this available energy directly to heat other collectors, meaning that the heat output of the heat pump can be reduced by approximately $24\,\%$. Based on this, an "equivalent COP" can be calculated as:

$$COP_{\text{eq}} = \frac{\dot{Q}_{\text{DAC}}}{P_{\text{el,new}}} = \frac{\dot{Q}_{\text{DAC}}}{\frac{\dot{Q}_{\text{HP,new}}}{COP}} = \frac{\dot{Q}_{\text{DAC}} * COP}{\dot{Q}_{\text{DAC}} * (1 - 0.24)} = \frac{COP}{0.76} = 4.18 \tag{3}$$

Alternatively, the waste heat can be integrated into the heat pump cycle as shown in the T-h diagram in Figure 4. This setup approximately corresponds to the S-DAC configuration proposed by Ge et al. [20]. The refrigerant stream is divided after the gas heater outlet. Part of it is evaporated using the available waste heat, while the rest is expanded, evaporated using thermal energy from the ambient air, and then compressed. The two streams are then mixed and compressed slightly further, before then entering the gas heater again. However, since the temperature of the waste heat is sufficiently high to be used directly, this option performs worse, reaching only a COP of 3.78. A simple supercritical CO_2 cycle and direct heat integration should be preferred over a setup like this.

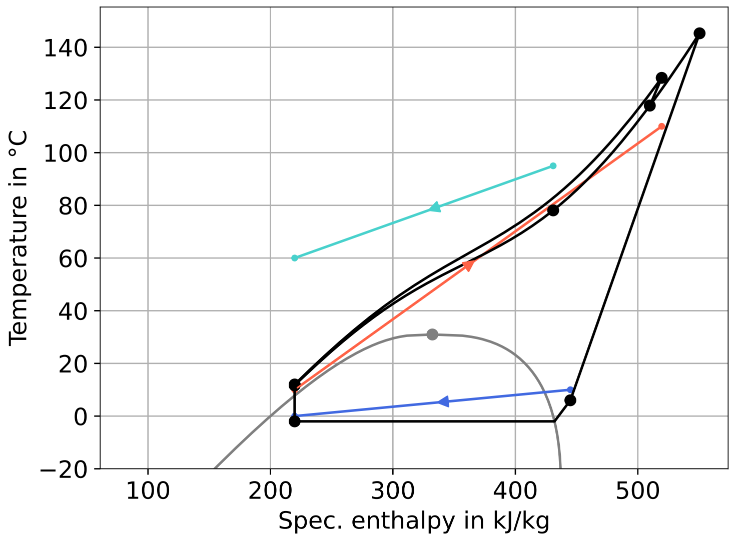

Figure 4: T-h diagram of the optimised heat-integrated transcritical heat pump cycle using CO_2 as working fluid, similar to the S-DAC configuration proposed by Ge et al. [20]. The heat source is shown in blue, the waste heat source in turquoise, and the heat sink is shown in red colour.

[2]For a detailed calculation of the heating energy required and cooling energy available, CO_2 and water co-adsorption behaviour must be modelled in detail to determine the mass of water and CO_2 adsorbed. Based on the heat capacities of adsorbing material, water and CO_2 as well as the heat of adsorption, the energy requirements can then be calculated. Such an approach should be used in future work to refine the assumption of constant heating and cooling rates.

3.4. Steam generation

As discussed in Section 1.2., the DAC process requires both hot water and steam. Following Sendi et al. [18], so far the analysis was based on the assumption that the heat pump constantly generates heat at $110\,^{\circ}\mathrm{C}$, sufficient to generate steam at ambient pressure. However, there is potential to optimise the process for heat pump use. One option is to use a cascaded cycle, with the main heat pump only providing thermal energy at the $95\,^{\circ}\mathrm{C}$ required for the hot water, and a smaller booster heat pump increasing the temperature to $110\,^{\circ}\mathrm{C}$. However, since the adsorber is evacuated during the regeneration process, this is not necessary. Instead, steam can simply be generated at below-ambient pressure, as it will still be at a higher pressure than the adsorber, which is evacuated at the beginning of the regeneration step.

The COP of the simple transcritical CO_2 cycle increases to 3.41 when reducing the required supply temperature to $95\,^{\circ}\mathrm{C}$, which corresponds to a $7\,\%$ increase compared to a supply temperature of $110\,^{\circ}\mathrm{C}$. However, this comes at the cost of the heating step taking longer, as the temperature difference between hot water and adsorber is reduced. There is a complex trade-off between: (i) the impact of the supply temperature on the heat pump efficiency; (ii) the impact of the supply temperature on the duration of a TVSA cycle; and (iii) the impact of the final regeneration temperature on the working capacity of the adsorber. Detailed dynamic modelling is required to find the overall optimum setup.

3.5. Hydraulic setup, scheduling, and control algorithm

One of the big challenges of the integrated heat pump and DAC systems analysed in this work are the hydraulic setup and the scheduling and control algorithm. Large-scale DAC plants will consist of hundreds or thousands of individual collectors, each running the TVSA batch process, while the heat pump is ideally a centralised asset running continuously.

The analysis presented so far assumed the heating water to have a constant inlet temperature of $10\,^{\circ}\mathrm{C}$ and a constant outlet temperature $110\,^{\circ}\mathrm{C}$. The implicit assumption is that it first passes through an adsorber near the end of the heating step, i.e., having a high temperature. Then it passes through colder and colder adsorbers, until finally it passes through an adsorber that is only just at the beginning of the heating step, i.e., it is still at ambient temperature. As the adsorber temperatures are constantly changing, the order in which the heating water is flowing through them has to change often, as illustrated in a schematic way in Figure 5. The thermal integration and the steam purging step (not shown in Figure 5) add additional layers of complexity.

3.6. Limitations

The analysis presented in this work is based on a steady-state heat pump model and data for one single operating point obtained from a dynamic DAC model. The models are not coupled. Integrated dynamic models should be used to expand the analysis and investigate the dynamic interactions between the two systems in more detail. Especially the analysis of the thermal integration potential would benefit from more detailed modelling of the adsorption processes. Furthermore, the analysis is only performed for one set of operating conditions (temperature and relative humidity as well as supply and return temperature), leading to a single COP value. For a more robust comparison of different heat pump configurations, SCOP values should be estimated, either from an annual simulation or at least using different operating points and weighing them as detailed in Equation 2.

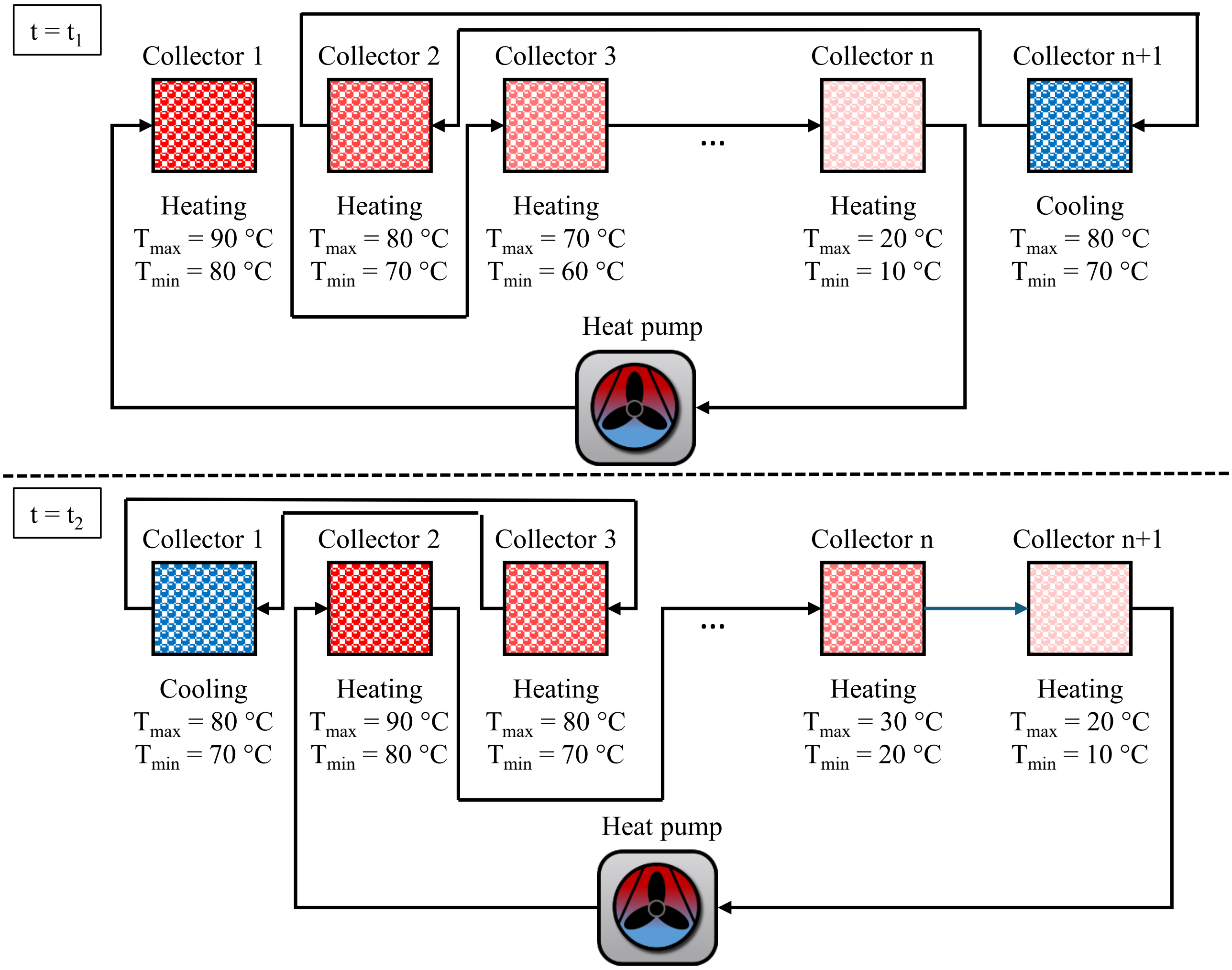

Figure 5: Schematic of the required changes in hydraulic configurations over time.

4. Conclusions

In this paper, we have investigated high-temperature heat pumps for direct air capture (DAC) plants, analysing different heat pump configurations and different ways of integrating the heat pump and DAC processes. From this preliminary analysis, we can draw the following conclusions:

- Using the heat of adsorption to "preheat" the air leads to only marginal increases of the COP, about 1 % in the best case. An alternative is "precooling" the air in the heat pump evaporator before passing through the adsorber. This leads to an increase in adsorber working capacity of about 17 %, but will also increase water adsorption and the length of the heating step, which both leads to a decrease in collector productivity.
- Using an internal heat exchanger leads to an over 30 % higher COP compared to a simple cycle when considering subcritical processes with butane as working fluid. However, the best-performing cycle is a transcritical CO_2 cycle, which reaches a COP of 3.18.
- Direct utilisation of the available waste heat appears to be more effective than integrating it into the heat pump process. In both cases, the hydraulic setup and controls are challenging due to the number of adsorbers and the batch process they perform.
- Reducing the supply temperature is possible, as steam can be generated at below-ambient pressure since the collector is evacuated during regeneration. Lower supply temperatures lead to a higher COP, but also longer cycle times, such that there is a trade-off between both.

Future work should integrate DAC and heat pump models to capture dynamic interactions better, and more different operating points should be considered.

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We would like to thank Dr. Marwan Sendi for very helpful discussions and providing detailed information on the DAC process and how he modelled it.

Nomenclature

Abbreviations

COP Coefficient of performance

DAC Direct air capture

SCOP Seasonal coefficient of performance

TVSA Temperature-vacuum-swing adsorption

Latin symbols

h Specific enthalpy, $\mathrm{J/kg}$

P_{el} Electrical power, W

$\dot{Q}$ Thermal power, W

t Time, s

T Temperature, K

Greek symbols

η_{ex} Exergetic efficiency

Subscripts and superscripts

a Air

eq Equivalent

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