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DECARBONISATION THROUGH INNOVATION

Carbon-neutral steam supply for a chemical plant: Thermo-economic analysis of the integration of a thermal storage unit to a high-temperature heat pump using CO_2

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Abstract

Ensuring a CO_2-neutral supply of process heat is critical for advancing the energy transition in industrial sectors. A promising approach is the integration of high-temperature heat pumps, powered by renewable electricity, to generate process steam at elevated pressure levels, which is widely used in the chemical industry. An ultra-high temperature heat pump concept with supercritical CO_2 as the working medium, designed for the supply of a generic chemical plant, was developed as part of the project CO2NEICHEM.

At this stage, the inclusion of a thermal storage unit, consisting of one hot and one cold tank, and its effect on the part load behaviour of the heat pump is to be investigated. The heat pump represents a transcritical reverse Brayton cycle with an internal heat exchanger and an expansion turbine. For the analysis of the part load behaviour, characteristic curves are used for the turbomachinery and the heat exchangers, while the part load itself is controlled by the heat flow at the heat source side. Within this study, it is shown that a high relative COP ($COP_{PartLoad}/COP_{Design}$) can be maintained with and without the inclusion of the storage unit, with a corresponding shift in the pressure levels at inlet and outlet of the compressor. Moreover, it is shown how different part load operation conditions and a variation of the design point influence the results and technical limitations.

The storage unit is integrated to be able to decouple the electricity consumption from the heat generation, so the effect of high electricity prices and the peak load demands can be moderated. To investigate the economic benefit, a thermo-economic evaluation is performed based on the LCOH to later allow the integration of the system in different configurations into an energy system analysis with the determination of relevant parameters like operational and capital costs of the overall system.

Keywords: Carbon Dioxide, High-Temperature Heat Pump, COP, Thermal Storage, LCOH

1. Introduction

Reducing CO_2 emissions is a crucial step to achieve climate goals aiming at a net-zero society in the future. One important aspect is the decarbonization of process heat production, since process heat accounts for around 66 % of the final energy consumption in Europe [1] and is still mainly generated by burning fossil fuels [2]. Especially high-temperature process heat is considered a hard-to-abate sector. While there are different alternatives to produce process heat, the use of heat pumps is widely considered one of the most promising ones [3], [4], [5]. Numerous studies considered the technical feasibility of industrial heat pumps to deliver the required process heat conditions of different industrial sectors [6], [7], [8], [9]. Moreover, many techno-economic approaches investigate the economic competitiveness of heat pumps in comparison to current

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technologies like gas boilers or future alternatives like electric boilers or hydrogen solutions with many studies coming to the result that heat pumps are a cost-effective solution, especially for applications with a small temperature lift [10], [11], [12]. One challenge of heat pump integration can be the requirement of steady heat production even at times of high electricity costs. A solution that decouples electricity consumption and heat production is the usage of a thermal energy storage (TES). Here, the number of studies is significantly smaller, even though this is also suggested as an economic option [4], [13], [14]. In this paper, the ideal-typical utility infrastructure of a chemical plant is investigated as it offers a detailed description of the process heat requirements in terms of physical properties of this process heat and the course of the demand over the year [15]. A heat pump system designed to cover the different process heat demands has already been described but is now to be extended with a thermal storage system [16], [17]. The technical operation in different load points and the limitations as well as the efficiency are to be described in detail in this paper. Afterwards, a techno-economic investigation in terms of Levelized Costs of Heat is performed to evaluate the competitiveness of the storage system in comparison to a regular heat pump.

2. Methods

2.1. Description of the heat pump system

The heat pump configuration which is investigated is based on a transcritical Reversed-Brayton cycle that has already been described before [17]. It consists of a compressor, three heat exchangers in series on the heat sink side (denoted as Heat Sink 1, see Figure 1), a turbine for expansion and heat exchangers at the heat source side. Additionally, a bypass around the economizer feeds an internal heat exchanger to reduce the temperature differences in the economizer and this internal heat exchanger (in contrast to adding it at the outlet of the economizer) to improve the COP of the system. The internal heat exchanger is hereby crucial to keep the required pressure ratio at a reasonable level and the turbine recovers a part of the energy demand of the motor. The expansion into the two-phase region still needs some investigation, but since the density ratio between the saturated liquid and vapor phase for CO_2 at this pressure level is much smaller than, for example, for water in a steam turbine expansion, this assumption is made here. This heat pump system was already analyzed in detail in design and part-load mode and is now to be investigated expanded by a thermal storage system. To achieve this, the system is expanded with another high-temperature heat exchanger, which is connected to the outlet of the compressor and transfers heat to a heat storage medium upstream of the internal heat exchanger. The hot storage medium is connected to the hot storage tank, where it remains until the storage is to be discharged. A heat loss equivalent to a temperature decrease of 5 K is assumed between charging and discharging as a very conservative scenario. During discharge, the medium passes through three heat exchangers in series to preheat, evaporate and superheat the process steam as an additional heat sink (see Figure 1). This second evaporation chain downstream the storage unit is termed Heat Sink 2. Afterwards it remains in the cold storage tank until heat has to be stored again. The inclusion of the storage unit adds two additional degrees of freedom to the design of the complete system, since the heat pump unit itself and the storage unit can be designed and operated for various heat demands. This leads to operational limits of the heat demand being able to be covered by Heat Sink 2, which will later be analyzed. They occur, since the mass flow in the heat exchangers have to be within certain limits regarding the design point, as well as minimum temperature differences, that have to be fulfilled also in part load.

The process steam conditions are the same as for heat supply by the heat pump directly and align with the medium pressure steam demand of the utility infrastructure of the chemical plant (31 bar, 300 °C) [15]. A block scheme diagram including the main boundary conditions during the design and part-load operation phase, process parameters and pinch point temperature differences in the heat exchangers is given in Figure 1. The isentropic efficiency of the turbine is calculated with a design efficiency from a first turbomachinery design approach, which is based on the CO2OLHEAT project [18] and a relative efficiency based on the relative volume flow. The compressor efficiency is also derived from a design value and a compressor characteristics map, which uses the relative volume flow and the flap position to calculate the relative efficiency and the according pressure ratio. The heat storage medium was chosen to be Therminol 66, since it combines a high energy density, low specific costs and a large operation temperature range from the maximum process temperature down to −9 °C to avoid anti-freeze mechanisms.

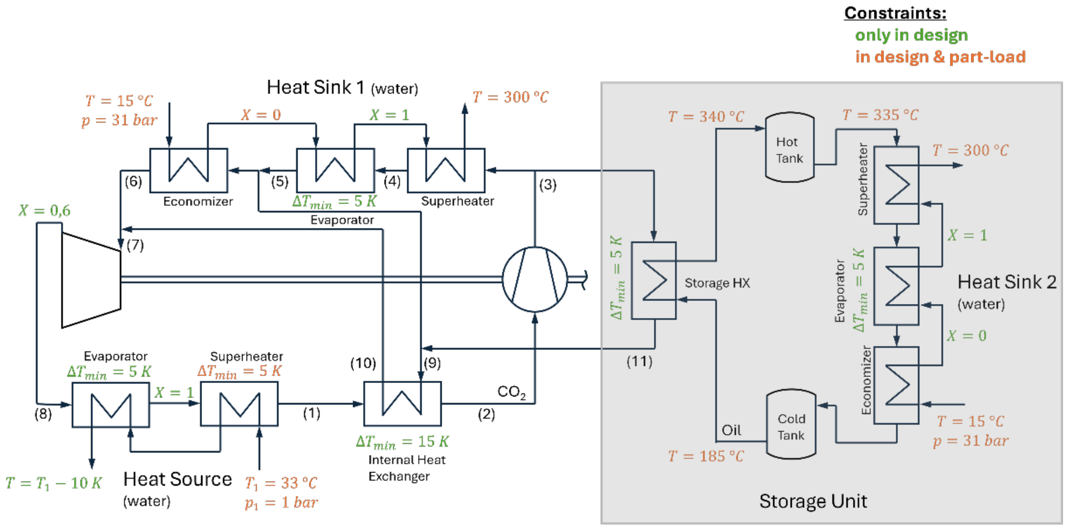

Figure 1: Scheme of the heat pump system including the storage unit

2.2. Economic methodology

To evaluate the economic benefits of the storage system, a reasonable scenario for the process-heat demand is necessary. This is based on the demand curve of Bauer et al. [15], which offered a publicly available ideal-typical utility infrastructure of a chemical plant including its process heat demand. The process steam conditions of the presented heat pump application are based on the demands specified in this publication. Since no clear pattern of the demand data could be identified over a day or week, an idealized demand profile was created. This demand profile is represented by a sinusoidal function to represent the daily demand variation with five periods (so five minima and maxima) per day, while the amplitude of the idealized function was chosen to fit 90 % of the deviation of the original data to its mean value. The actual trend is, naturally, less uniform, but shows a similar trend, why it is used here. The mean value of this idealized function is 84.5 MW which enables the supply of the complete heat demand within one very large machine.

In order to compare the economic performance of the system with and without a storage unit, the concept of Levelized Costs of Heat (LCOH) is employed, incorporating the cost categories capital expenditures I, electricity costs E and operation and maintenance (O&M) costs M as well as the heat generation H. The LCOH is calculated as follows:

$$LCOH = \frac{\sum_{t=1}^{N} \frac{(I_t + M_t + E_t)}{(1+r)^t}}{\sum_{t=1}^{N} \frac{H_t}{(1+r)^t}}$$

The lifetime of the system N is assumed to be 20 years and the common assumptions are made for the discount rate *r [19]*, which results in 9.6 %. The capital expenditures are calculated through cost equations for supercritical CO_2 components for the standalone heat pump system from Weiland *et al.* [20], while the costs for the storage system are taken from Kolb *et al.* [21] and for the heat exchangers in the storage cycle from Guo-Yan *et al.* [22]. All cost assumptions are summarized in the appendix. Since future electricity prices are hard to predict, day-ahead electricity prices for Germany of the year 2024 have been used in this analysis. Since the course of the price trend over the day is very decisive for energy storage, the hourly values have been averaged for each hour across all days of the year, aiming to find a representative daily price curve. Finally, the O&M costs are derived from equations directly depending on the capital costs for the heat pump cycle components and depending on the size of the storage system. Since these differing cost equations are often developed in different years, the Chemical Engineering Plant Cost Index (CEPCI) was used to bring all cost functions to the same base year of 2023.

3. Results

3.1. Technical implications

First, the technical consequences of the integration of the storage system are explained. Depending on the design of both the storage system and the standalone heat pump, certain limitations of the operating range come into play. As an exemplary case, the heat pump part has a capacity to cover 100 % of the mean process heat demand directly in the first heat sink and the storage unit is designed to cover 20 % of this process heat demand. For these conditions, the technical operational limits are visualized in Figure 2. Here, the storage capacity (so the amount of energy stored) is not yet considered.

The lower charging limit (visualized in green in Figure 2) is a consequence of the minimum temperature difference in the storage heat exchanger falling below 2 K. By contrast, the upper charging limits (orange, pink) are attributable to maximum relative mass flows in the heat exchangers when compared to the design case. This is further compounded by the fact that the lower pressure level of the system increases with higher overall mass flows in the cycle, and at one point exceeds the critical pressure of the fluid (blue). It is important to acknowledge that own-chosen assumptions influence the specific locations of these operation limits, but their existence must be taken into account when designing the heat pump system with the storage unit.

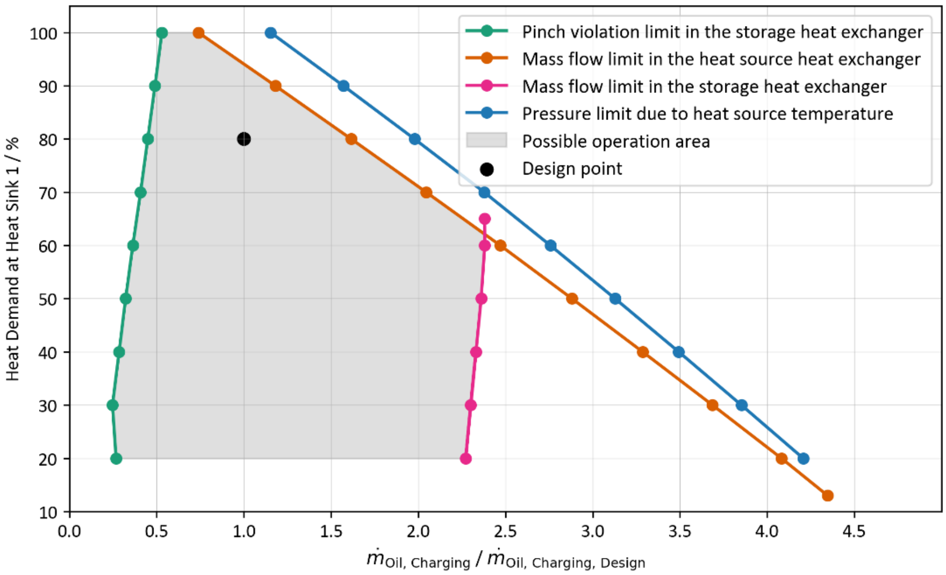

Figure 2: Technical operational limitations of the heat pump storage system

Moreover, the influence of the storage unit on the relative COP is to be analyzed. For the standalone heat pump, the relative COP for the operation in part-load is easy to define as the ratio of the COP in part-load by the one in design mode. If the storage unit is integrated, the COP in part-load or storage operation includes the heat which is charging the storage unit $\dot{Q}_{\text{Storage}}$, while P_{Net} is the necessary work of the system.

$$COP_{\text{ Storage Mode}} = \frac{\dot{Q}_{\text{sink}} + \dot{Q}_{\text{Storage}}}{P_{\text{Net}}}$$

To evaluate this value, it is important to establish the boundary conditions, since there are several degrees of freedom in this configuration. Both the capacity (in MW) of the standalone heat pump system as well as the storage unit can be designed individually and then cover a specific load. In this case, the relative COP is shown, when the standalone heat pump part is always able to cover the maximum process heat demand in design mode and the storage system is able to store 20 % of the mean heating demand additionally. For this case, the relative COP for the standalone heat pump in part-load is shown in Figure 3 a) for a relative heat demand of less than 1. Moreover, the relative COP for the inclusion of the storage system for different amounts of process heat being covered in the original heat pump system is shown in Figure 3 b). The efficiency in part-load is high, as the relative COP loss is only about 4 % for 50 % process heat demand. Generally, the relative COP decreases when the storage system is used, which is due to the less efficient utilization of the working fluid in the storage cycle than in the standalone heat pump. The storage cycle provides a lower temperature stream to the bypass than the evaporator, reducing the internal heat exchanger inlet temperature. As a result, the effective temperature difference in this component is decreasing, causing the heat transfer and thus the COP to decrease. This effect is valid for differing amounts of the steam demand at heat sink 1 in the original heat pump system, even though the amount of heat that can be stored is much larger, if the other part runs in part-load, as it can be seen in Figure 3 b). Also, the relative COP decreases less rapidly, if the demand in the direct heat delivering system decreases. This overall trend shows that the storage unit does not yield energetic advantages but can only be beneficial though an economic evaluation.

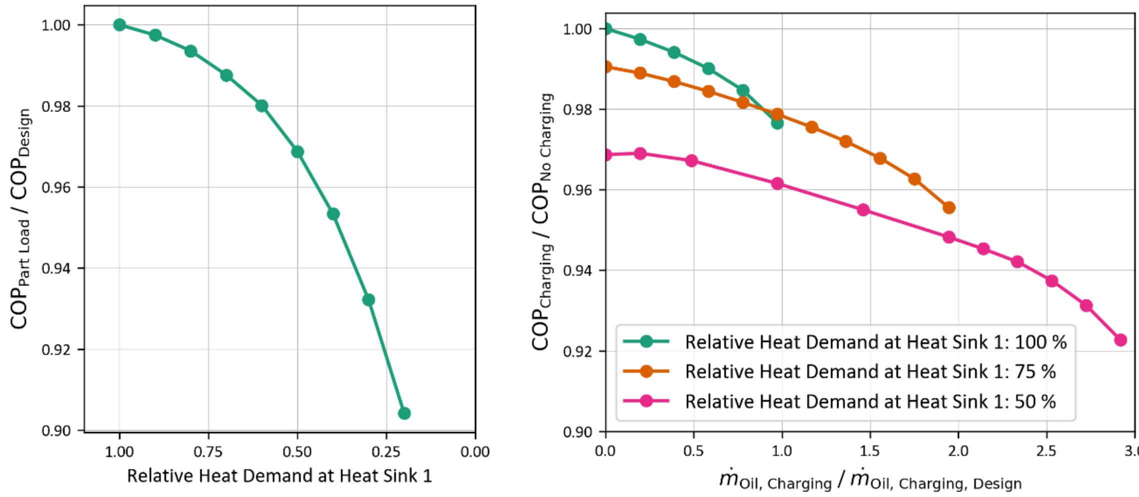

Figure 3: a) Relative COP of the original heat pump cycle in part-load
b) Relative COP of the storage-heat pump system for different load factors of the original heat pump cycle

3.2. Economic evaluation

To analyze the benefit of this system, a comparison of the LCOH of the standalone heat pump system against the system including the storage unit is to be performed for a specific case of boundary conditions. The general process of the evaluation of the system is described in the block scheme in Figure 4. It is based on a charging and discharging concept, already describing the amount of heat that is produced in the original heat pump part and the amount that is delivered through the storage unit over time, therefore, predefining the capacity of heat pump and storage unit.

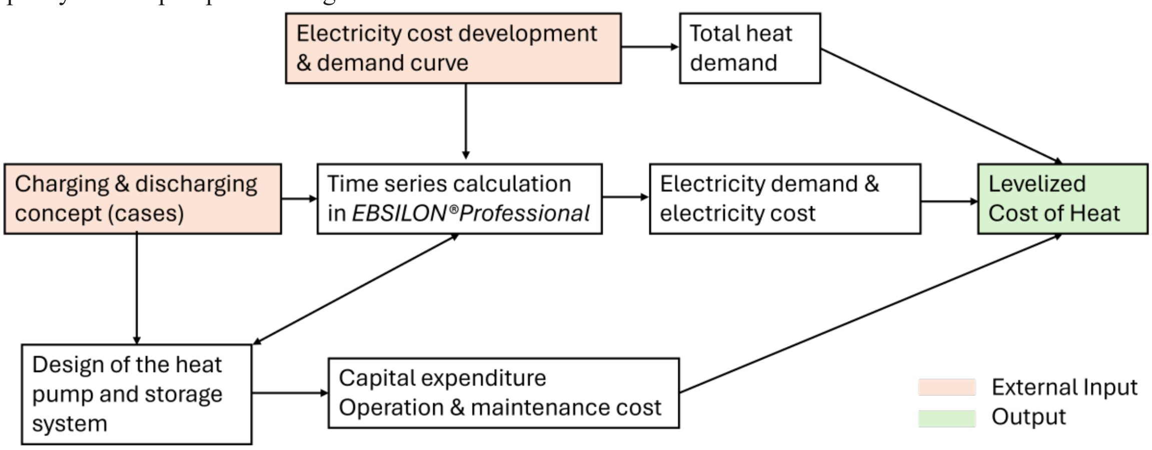

Figure 4: Process scheme of the LCOH calculation

Since the heat demand curve is represented by an idealized sinusoidal function with five daily periods while the electricity price curve has two minima and maxima per day, there are different options for the charging and discharging concept. The first concept is price driven and aims to utilize the low electricity prices by charging the storage unit during those periods and avoiding high electricity prices by discharging. This concept should produce savings in electricity costs, even though the efficiency of the heat pump will decrease since it frequently runs outside of the design operation and more total heat is required because of the losses caused by the storage unit.

The second concept is demand driven and utilizes the uniform course of the heat demand by charging the storage unit in times of low heat demand and discharging during the load peaks. This allows the design of a smaller heat pump and therefore savings in investment costs, while also reducing losses due to less part-load operation. In both cases these savings need to outweigh the costs for the additional storage unit. In the third case, these two concepts are combined, which leads to a more complex operation, which is illustrated in Figure 5. To fully define those concepts, upper and lower boundaries for the heat demand and electricity price have to be defined. Besides, to simplify operation during those periods, some cases include a constant charging or discharging demand. In all concepts, the minimal storage capacity is calculated to find the capital investment costs, while the heat demand is always just considered the heat flow at the specific time.

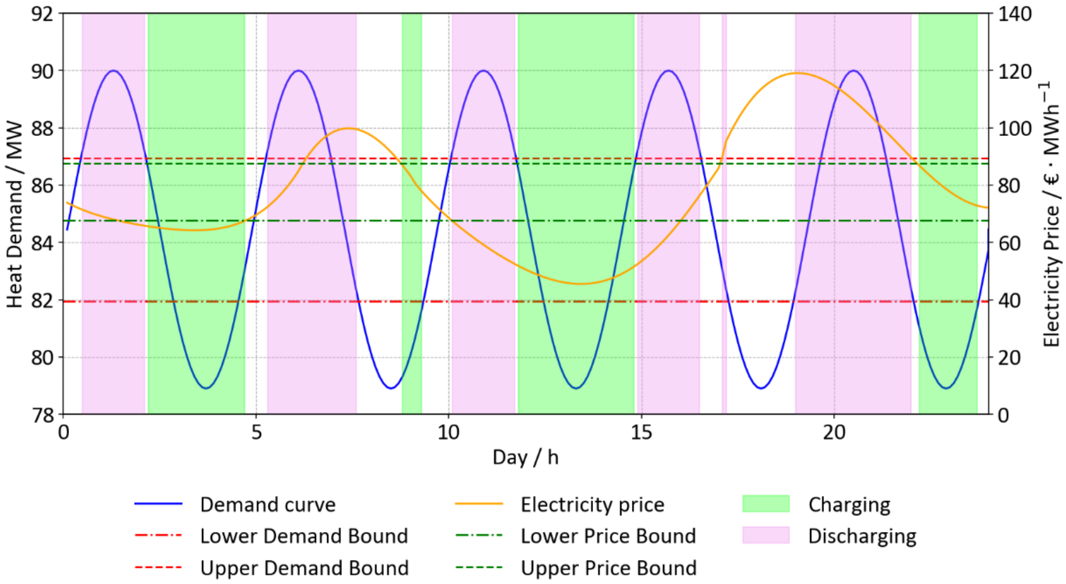

Figure 5: Visualization of the charging and discharging times for the combination concept

The two individual concepts (price-driven and demand-driven) as well as the combination case have been analyzed with the combination presenting the most promising option, since it brings together the advantages of both concepts. The resulting LCOH of this combination case and the reference heat pump without a storage system with the shares resulting from investment costs, electricity costs and O&M costs are shown in Figure 6. The difference between the standalone heat pump and the system including the storage unit are only marginal. With the assumed boundary conditions, no competitive economic case can be shown. The total capex costs have been reduced by only 1.28 %, with the smaller heat pump itself accounting for a decrease of around 4 %, but the extra investment into the storage unit largely compensates this effect. The mean electricity procurement cost decrease by only 0.16 %, which is a hint that this combination case is mostly dominated by the peak shaving of the second concept presented and the electricity price driven operation is only secondary. Also, since the storage system leads to extra O&M costs, this share increases by around 4.28 %. It is notable that the capacity of the heat flow is always relatively small in contrast to the overall energy transferred by the system.

To understand the influence of the upper and lower boundaries of the electricity price and heat demand of this concept, these values are varied, which affects the time of charging and discharging and therefore the amount of energy stored. Here, the demand threshold (difference between lower and upper boundary) has a strong influence on the LCOH. A minimum occurs between 1 MW and 2 MW. The influence of the price threshold is less prominent, since times rarely occur, in which the system is charging because of this limit (see Figure 5). Nonetheless, an optimal operation point for this scenario can be found for a price threshold of 15 €/MWh. This is the best operating point, for which the LCOH are visualized in Figure 6.

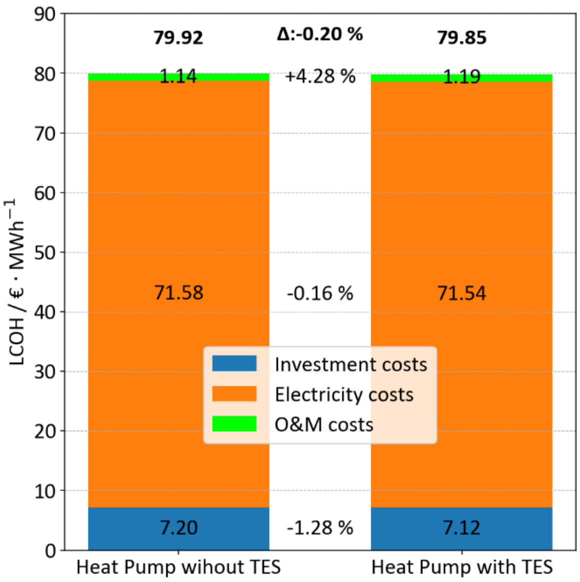

Figure 6: LCOH comparison between the heat pump without storage and the system including the thermal-energy storage (TES) unit

When trying to compare these results to other studies investigating the LCOH of heat pumps systems including a storage unit, it is important to notice that they are significantly influenced by the electricity price as well as the heat sink conditions of the heat pump, which influence the COP, and the storage concept. Nevertheless, Markussen et al. [4] found in their study for a HTHP with a free store and COPs in the region of this work LCOH between 40 and 120 €/MWh, depending on the electricity price and the hours of heating demand in the year, so this aligns well with the preformed calculations. Moreover, they saw a reduction in the LCOH for the inclusion of a storage unit for relatively low hours of heating demand of 4000 h. For 8000 h, only marginal LCOH reduction could be observed, which also aligns with this work, where a heating demand is present for all hours of the year, just with a fluctuating level. Furthermore, it must be addressed that the heat demand can be only covered carbon neutral with carbon neutral electricity, but the specific CO_2 emission can be reduced with this system even for current conditions. With the combined COP of the system for the combination case, even with the mean emission factor for electricity for Germany for the year 2024 of 0,363 t_{CO2}/MWh_{el}, a reduction of more than 10 % compared with the usage of a gas boiler (η = 90 %, Emission factor of natural gas = 0,202 t_{CO2}/MWh_{NCV}), can be achieved [15]. This would also increase in the coming years, when the emission factor for electricity is decreasing, even though the reduction in comparison to the stand-alone heat pump is neglectable, as it could be seen in the economic evaluation.

4. Conclusion

In this paper, a novel heat pump system using CO_2 as the working fluid as a Reversed-Brayton cycle and including a thermal-energy storage unit was introduced, as it presents an opportunity to decouple the electricity consumption and the process heat demand of the utility infrastructure of a large industrial plant. The storage unit is linked through a heat exchanger, whose inlet is connected to the outlet of the compressor, while the outlet is fed directly to the internal heat exchanger of the original heat pump cycle. The storage unit consists of two tanks, one at high and one at low temperature. First, the technical limitations of this system for a specific case of the capacities of the direct heat pump and the storage system are explained, with the main message that the storage unit must be included in detail in the design as the operating range is very limited otherwise. This is due to too small pinch temperature differences in the heat exchangers. Moreover, an economic comparison of the system on the basis of the LCOH against a standalone heat pump is performed for defined charging and discharging concepts, which includes a varying, but repetitive process heat demand as well as a fluctuating electricity price. The investigated concepts utilize price arbitrage, peak shaving and a combination of both. Nonetheless, only a very small decrease of the LCOH could be observed for the most competitive scenario, which is mainly since the mean electricity procurement costs could not be reduced as much as aspired. The small reduction of the capital investment costs of the heat pump is counterbalanced by increasing costs for the storage unit and rising O&M costs. However, the presented analysis is based on averaged electricity price fluctuations of the German day-ahead market 2024. Under these conditions, inclusion of a TES unit is at least no commercial disadvantage. With future price spreads and variability increasing, the economic benefit of a system with TES will increase. Moreover, an adjustment of the charging and discharging concepts, for example by forcing an enlargement of the storage unit to a capacity that allows to drastically reduce electricity consumption at high prices, is worth further investigations.

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Appendix

Table 1: Financial Boundary Conditions [19]

Parameter	Value
Amount of Equity	40%
Amount of Debt	60%
Cost of Equity	12%
Cost of Debt	8%

Table 2: Costs equations for the heat pump system [20], [22]

Component	Cost equation
Turbine	$C_{t,ax} = 182{,}600 * P_t^{0.5561} * f_T$ $f_T = \begin{cases} 1 & if\ T_{max} < 550°C \\ 1 + 1.106 * 10^{-4}(T_{max} - 550°C)^2 & if\ T_{max} \geq 550°C \end{cases}$
Compressor	$C_{comp} = 1.123.000 * P_{comp}^{0.3992}$

Open drip-proof motor	$C_{Motor} = 399.400 * P_{Motor}^{0.6062}$
Heat Exchanger with CO_2 in contact	$C_{HX} = 49.45 * UA^{0.7544} * f_{HX}$ $f_{HX} = \begin{cases} 1 & if\ T_{max} < 550°C \\ 1 + 0.2141(T_{max} - 550°C) & if\ T_{max} \geq 550°C \end{cases}$
Heat Exchanger without CO_2 in contact	$C_{HX,storage} = 2769 * A^{0.573}$

Table 3: Specific Costs for sensible TES [21]

Item	Cost / $[\$/kWh]$
Tanks	6
Foundations	0.85
Piping & Small Support Pumps	0.6
Controls and Instrument	0.3
Spare Parts and Other Directs	0.95
Contingency	3.5