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Research Paper

Towards sustainable process heating at 250 °C: Modeling and optimization of an R1336mzz(Z) transcritical High-Temperature heat pump

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ABSTRACT

Fossil fuel boilers typically produce high-temperature process heating due to the impossibility of current renewable technologies. Vapour compression heat pump systems have been proposed up to 200 °C with subcritical cycles. To increase the heating production level, this paper proposes heating up to 250 °C through a transcritical high-temperature heat pump (THTHP) using R1336mzz(Z), which is not thermally degraded till this temperature, according to existing data. Computational models of a transcritical vapor compression cycle with and without an internal heat exchanger are developed for this work. The input cycle parameters, such as evaporation, production temperature, gas cooler output temperature, and the superheating degree, have been modified through iteration to consider possible scenarios in different industrial sectors. Moreover, the impact of using waste heat to increase evaporation temperature or superheating degree has been studied to optimize the cycle. The internal heat exchanger has also been considered for superheating the compressor suction. Other relevant parameters, such as compression ratio or volumetric mass flow rate, have also been assessed. The results show that a heat pump is feasible to reach 250 °C temperature using waste heat at 120 °C (evaporation at 100 °C and 20 °C of superheating degree), reaching a COP of 3.3. The variation of evaporator temperature from 80 °C to 140 °C increases COP from 2.5 to 5.9, while the increase of superheating degree from 20 °C to 100 °C increases COP from 3.2 to 7. Waste heat use optimization proves that it is more efficient to prioritize the increase of the evaporation temperature. If the industry requires lower production temperatures, the COP can reach a value of 7.0 at 180 °C. The decrease in gas cooler outlet temperature impacts less the COP than other input parameters. At baseline conditions, an optimum superheating degree with an internal heat exchanger of 45 K produces a maximum COP of 4.0. THTHP emissions are less than gas boilers for the same application, and in countries with greener electricity generation, these emissions can be 50 times lower.

1. Introduction

According to the International Energy Agency, industry accounts for approximately 24 % of global greenhouse gas (GHG) emissions, with the majority due to activities such as heat production in a wide range of processes, with temperatures up to hundreds of degrees Celsius (°C). Arpagaus et al. [1] listed process heat at different temperature ranges. They identified in the temperature range of 150 to 250 °C applications like wood glueing, textile colouring, plastic injection modelling, metal drying, chemicals distillation and compression, food and beverages, drying and evaporation, and paper drying and boiling.

Technological advances and the increasing availability of renewable energy sources drive the development of more efficient and sustainable heat production solutions for industrial processes [2]. High-temperature heat pumps (HTHP) offer a promising solution to this problem by offering higher energy efficiency and being environmentally friendly compared to traditional heating methods (Cao et al. [3]). Mota-Babiloni [4] highlights the relevance of HTHP in industrial decarbonization. However, implementing HTHP must be carried out with clean energy production (renewable electricity, waste heat, etc.) and sustainable working fluids [5].

Existing HTHP technologies have limitations, such as low efficiency, limited temperature range, and high installation costs [6]. So far, there are no commercial units for temperatures above 150 °C, and few researchers have published experimental results at this temperature with prototypes [7]. It is necessary to develop HTHP technology to generate heat at temperatures as high as possible, demonstrating an acceptable coefficient of performance (COP, ratio between heat capacity and electrical energy consumption) to replace fossil fuel boilers at a wide

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Nomenclature

CIF,β	Carbon intensity factor (gCO_2e)
CR	Compression ratio (-)
E_{annual}	Annual energy consumption (kWh year^{-1})
h	Enthalpy (kJ kg^{-1})
m	Refrigerant charge (kg)
$\dot{m}$	Mass flow rate (kg s^{-1})
n	system's lifetime period (years)
P	Pressure (MPa)
PBP	Payback period (years)
$\dot{Q}$	Heat transfer (kW)
T	Temperature (K)
TEWI	Total equivalent warming impact (gCO_2e)
$\dot{W}$	Power consumption (kW)
α	Recycling rate (%)
η	Efficiency (-)

Subscripts

cold	Cold fluid of heat exchanger
comp	Compressor
disc	Discharge
evap	Evaporator
gc	Gas cooler
hot	Hot fluid of heat exchanger
in	Inlet
is	Isentropic
out	Outlet
prod	production
ref	Refrigerant
suc	Suction

Abbreviations

ASHRAE	American Society of Heating, Refrigerating and Air-Conditioning Engineers
COP	Coefficient of performance
GHG	Greenhouse gas
GWP	IPCC AR5 100-yr global warming potential
HTHP	High-temperature heat pumps
IHX	Internal heat exchanger
ODP	Ozone depletion potential
ORC	Organic Rankine cycle
THTHP	Transcritical high-temperature heat pump

operational range and thus: 1) decarbonize, by practically reducing or eliminating GHG emissions, 2) electrify, the consumption of natural gas is replaced by electricity, 3) reduce the variability of operating costs.

Kosmadakis et al. [8] calculated the payback period (PBP) of a 500-kW HTHP. HTHP cost-effective solutions were found below 70 K, with the PBP between 3 and 4 years for a temperature lift of 20 K. The PBP depends mainly on the temperature lift, the refrigerant, and the configuration. According to Sun et al. [9], HTHP with a higher temperature lift and the heating temperature is of great significance in industrial steam, but temperature lift above 80 °C has been studied scarcely, mainly theoretically. They recommend further research to explore the cycle characteristics and application potential of HTHP in different temperature ranges.

For higher temperatures, Zühlsdorf et al. [10] exposed that HTHPs designed to reach up to 200 °C present several challenges. One is represented by the development of compressors at high temperatures (only five pilot-scale demonstration projects with heating capacity below 100 kW and a maximum temperature of 160 °C exist nowadays). The second is the working fluid. All current alternatives have limitations, and satisfying all the requirements (including thermal suitability, environmental compatibility, safety, efficiency, and availability) is still a significant challenge for developing HTHPs.

Some propositions for temperatures around 200 °C can be found. Researchers from the SINTEF (an independent research organization based in Norway) claimed they reached a heating temperature production of 180 °C [11]. The proposal is to use water and steam technology, with a rotary vane machine specially designed and built by Tocircle (Norwegian compressor manufacturer). Injected water in connection with steam lubricates the compressor moving parts in contact with the working medium and reduces the thermal stress on the system. Gómez-Hernández et al. [12] proposed CO_2 and acetone mixtures for 220 °C to cover the industrial process heat above 150 °C. It shows temperature glides below 50 K for CO_2 mass fractions up to 10 %. The highest HTHP performance mixture is the 5 % CO_2/95 % acetone in the mass fraction that obtains a 5.6 COP when the target outlet sink temperature is 200 °C. Ganesan and Eikevik [13] proposed CO_2/butane and CO_2/pentane mixtures, concluding that they can be reached 181 °C with a CO_2 composition of 20 %.

Currently, besides CO_2 in supermarket refrigeration and heat pump water heaters [14 15], working fluids are preferred to be used in subcritical operations. For instance, heat pump heating from 100 °C requires a working fluid with a critical temperature above 100 °C (plus a temperature difference of approximately 15–20 K to operate efficiently). Most fluids proposed for HTHP have a critical temperature between 130 and 196 °C, and few overcome 155 °C [16]: R1233zd(E), R1336mzz(Z), R514A (a mixture of R1336mzz(Z) and R1130(E) 74.7/25.3 by mass%) and R601 (critical temperature of 166.5, 171.4, 178 and 196.6 °C, respectively).

For HTHP applications, additional factors not considered in conventional refrigeration and heat pump systems must be considered besides thermodynamic, economic, environmental, and stability characteristics [7]. At high HTHP operation temperatures, attention should be paid to the refrigerant thermal degradation temperature. The working fluid can decompose when the temperature ruptures the weakest bond in the working fluid, forming the products of thermal degradation. The decomposition products will affect the system's performance, damage the components of the system, and cause safety problems (Huo et al. [17]). Juhasz and Simoni [18] measured the concentration of F – and Cl – anions in refrigerants after exposure to 200 °C and 250 °C for seven days to investigate the thermal stability. They measured a low degradation of R245fa at a temperature of 250 °C, but the degradation of R1233zd(E) was only acceptable below 200 °C. Perkins et al. [19] confirmed degradation above 180 °C and 15 bar for R1233zd(E), while Angelino & Invernizzi [20] recommended R245fa utilization up to 300 °C. According to Kontomaris [21], R1336mzz(Z) was stable in the presence of aluminium, copper, carbon steel, moisture, and air up to a maximum temperature of 250 °C. Majurin et al. [22] performed chemical stability tests considering the lubricant and materials of R123 chillers. The accelerated reaction study results indicate that R514A exhibited less than 0.1 % degradation under the same conditions (135 to 155 °C).

Allowing temperatures up to 250 °C without degradation, R1336mzz (Z) can be a solution to develop HTHP for temperatures higher than 200 °C. The critical temperature of R1336mzz(Z) is 171.4 °C. If we consider that a proper operation is 20 K below this value, the condensation temperature is limited to approx. 155 °C and it is necessary to work in transcritical cycles to reach 250 °C.

Giménez-Prades et al. [23] have studied the available information for simulating and predicting R1336mzz(Z) (and other molecules) performance. Accurate property measurements are necessary to build equations used in theoretical assessments and design the HTHP system components. In subcritical operation, Navarro-Esbrí and Mota-Babiloni [24] have published experimental results with R1336mzz(Z) and up to 158 °C heat production temperature. Similarly, Arpagaus and Bertsch [25] tested R1336mzz(Z) and other refrigerants in an HTHP prototype equipped with a piston reciprocating compressor and IHX (internal heat exchanger). The maximum production temperature was limited to 150 °C. They studied the influence of several operational parameters in the COP, obtaining promising results for commercial development. Other theoretical approaches are available in the literature, as found in [26] and [27].

Navarro-Esbrí et al. [28] used experimental results from medium and high-temperature heat pumps to accurately model a two-stage cascade-based R1336mzz(Z) HTHP and simulate its behavior with mixed-type refrigerants. Hu et al. [29] studied different refrigerants and mixtures and concluded by recommending R1234ze(E)/R1336mzz (0.3/0.7 by mass%). In the same line, Fernández-Moreno et al. [30] compared different binary and ternary mixtures, finding R601/1234ze(Z) (0.74/0.26) results in the highest COP.

A previous proposal for transcritical HPs was made by Verdnik and Rieberer [31], who experimented with subcritical (source temperature of 40 and 60 °C to supply temperatures of 110 °C) and transcritical (60 °C to supply 160 °C) operation using butane (R600) and measured a COP between 3.3 and 4.4, and 3.1, respectively. The transcritical CO_2 refrigeration sector has been developed, showing the possibility of working in transcritical mode [32]. Up to 200 °C, transcritical refrigerants were studied by Vieren et al. [33], concluding that R1336mzz (Z), R1234ze(Z) and R1233zd(E) have the best performance.

Reaching temperatures up to 250 °C is not possible with the technology developed nowadays. A few technologies have been proposed, such as reversed Brayton cycles or high-temperature heat pumps based on water as refrigerant [10]. However, these proposals are still far from commercialized and economically competitive with fossil fuel boilers. This work addresses the challenge of proposing a transcritical high-temperature heat pump that can reach the temperature of 250 °C, the next level targeted by the industry, once a 150 °C commercial high-temperature heat pump is progressively launched to the market.

The literature review shows that two issues must be solved before the first transcritical high-temperature heat pump (THTHP) is developed. First, the refrigerant R1336mzz(Z) is the most suitable option today because of the thermal degradation temperature and adequate safety and environmental characteristics. Another challenge is the extreme operational conditions that can damage components or materials used in the unit. To minimize the impact of operational conditions, offer flexibility in the design, and maximize the energy performance, the cycle can be modelled, and the impact of input parameters are studied [34]: evaporation temperature, total superheating degree, production temperature, or gas cooler outlet temperature.

No proposal for a transcritical high-temperature heat pump (THTHP) for 250 °C production temperature has been made before, and this work presents a pioneering approach to sustainable heating at high temperatures. The novelty of this work is proposing for the first time a cycle for reaching 250 °C, the thermodynamic analysis, and the optimization of an IHX. Also, it is novel to consider a transcritical cycle for those temperatures and the refrigerant R1336mzz(Z). This novel work can start a new research line in the heat pump and industrial heating sector, significantly reducing greenhouse gas emissions in the process. Other researchers could use the comprehensive study of the THTHP system to develop an experimental prototype in the future with the help of the conclusions of the work. Moreover, the energy performance of the cycle has been maximized by optimizing the superheating degree with an internal heat exchanger, so the potential of THTHPs is unlocked, and the feasibility and attractiveness of the proposed system are improved. An emissions analysis has been carried out considering different production temperatures to know how much CO_2 the cycle would emit according to its application. These emissions have been compared with the emissions of a gas boiler to verify the improvement.

2. Materials and methods

In this section, the THTHP model is explained with the assumptions, main parameters, and the characteristics of the refrigerant.

2.1. Modelling

The cycle calculated has the four principal components: evaporator, compressor, gas cooler, and expansion device from a heat pump for high temperatures.

For this model, a fixed isentropic compressor efficiency of 85 % has been used [35]. This specific assumption is due to the novelty of the model proposed application; there are still no compressors for these temperatures that allow the use of a more accurate correlation for the compressor efficiency. Other relevant assumptions are detailed in Table 1. These parameters are based on a scenario with process heat around 100 °C. This process heat will be heated up to 250 °C of the production temperature and, consequently, it will also be the gas cooler outlet temperature. The evaporator will absorb energy from a waste heat of 120 °C. However, the evaporator superheating degree must be set with a minimum of 20 K to avoid liquid in the compressor due to the slope of the refrigerant saturation lines [36], so the evaporation temperature will be 100 °C. These conditions will be modified and studied separately. The transcritical cycle at these fixed conditions is shown in Table 1. The thermal effectiveness of IHX is fixed at 85 % to maximize its effect on the system performance. The database for calculations with these refrigerants is from REFPROP v10.0 and NIST Standard Reference database 23. Python 3.10 has been used for the computational model. Fig. 1 shows the THTHP Ph diagram and the different input conditions modifications.

For a better understanding, Fig. 2 shows the flow diagram. The four baseline conditions are the first to assume and, subsequently, to study its influence; said value is modified from its minimum value to its maximum value step by step (+a). For the internal heat exchanger (IHX) optimization, the modified value is the superheating degree (+b), which will also affect the subcooling degree. Finally, a TEWI has been considered to evaluate the cycle emissions in function to carbon intensity factor value from minimum to maximum step by step (+c).

For each iteration, the cycle model is calculated. As the compressor discharge pressure is not determined, the discharge enthalpy is calculated using the target temperature and assuming an isentropic process in the compression as presented in Equation (1).

$$h_{disc,is} = f(T_{disc}, \eta_{is} = 100\%) \tag{1}$$

The discharge enthalpy is adjusted with Equation (2), which is the isentropic efficiency value.

$$h_{disc} = \frac{h_{disc,is} - h_{suc}}{\eta_{is}} + h_{suc} \tag{2}$$

The discharge pressure is a function of discharge enthalpy and target temperature as shown in Equation (3).

Table 1
Conditions assumed for the baseline condition (the blue cycle represents the baseline condition).

Parameter	Reference value	Modified cycle parameter in Fig. 1
Evaporation temperature	100 °C	Yellow
Evaporator superheating degree	20 K	Orange
Compressor discharge temperature (production)	250 °C	Green
Gas cooler outlet temperature	100 °C	Red
Thermal power	100 kW	Not visible

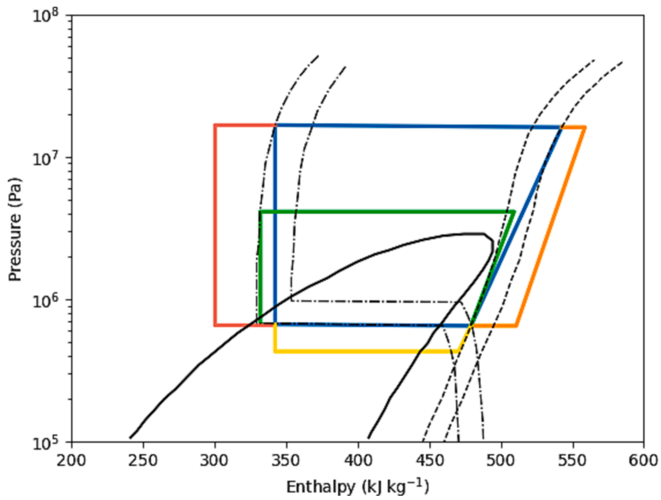

Fig. 1. Pressure-enthalpy diagram of R1336mzz(Z) transcritical cycle.

$$P_{disc} = f(T_{disc}, h_{disc}) \tag{3}$$

Compressor power consumption is calculated with Equation (4) as a product of the mass flow rate and the enthalpy difference between the discharge and suction.

$$\dot{W}_{comp} = \dot{m}_{ref}\ (h_{disc} - h_{suc}) \tag{4}$$

Equation (5) of the gas cooler is necessary for the mass flow rate. Gas cooler outlet conditions are the function of gas cooler outlet temperature and pressure, calculated with the compressor outlet point.

$$\dot{Q}_{gc} = \dot{m}_{ref}\ \left(h_{in,gc} - h_{out,gc}\right) \tag{5}$$

The gas cooler outlet enthalpy is calculated with the gas cooler outlet temperature and pressure, Equation (6).

$$h_{out,gc} = f(T_{out,gc}, P_{gc}) \tag{6}$$

An isenthalpic process in the expansion allows for calculating evaporator inlet conditions, and then it is used to determine the cooling capacity or the heat exchanged in the evaporator, Equation (7).

$$\dot{Q}_{evap} = \dot{m}_{ref}\ \left(h_{in,evap} - h_{out,evap}\right) \tag{7}$$

The energy performance of the cycle is calculated with the coefficient of performance (COP), which is the ratio of the heating capacity and the compressor power consumption, Equation (8).

$$COP = \frac{\dot{Q}_{gc}}{\dot{W}_{comp}} \tag{8}$$

The compression ratio, an essential parameter for analysing the operational and energy performance in vapour compression systems, is the relationship between discharge and suction pressure, Equation (9).

$$CR = \frac{P_{disc}}{P_{suc}} \tag{9}$$

An IHX has been proposed to optimize the superheating degree depending on the gas cooler outlet temperature. Its operation is defined by Equations (10) and (11).

$$\eta_{IHX} = \frac{T_{out,cold} - T_{out,cold}}{T_{in,hot} - T_{in,cold}} \tag{10}$$

$$\dot{m}_{ref}\ \left(h_{out,hot} - h_{in,hot}\right) = \dot{m}_{ref}\ \left(h_{in,cold} - h_{out,cold}\right) \tag{11}$$

2.2. Refrigerant characteristics and suitability

The refrigerant (term used for designating the working fluid) for this THTHP is R1336mzz(Z), as it has been exposed in Section 1. As aforementioned, this refrigerant allows temperatures up to 250 °C without degradation. Table 2 shows the main characteristics of R1336mzz(Z).

2.3. TEWI and gas boiler characteristics

In addition to thermodynamic analysis, a comparison of CO_2e emissions with a gas boiler has been made. To obtain the emissions of the THTHP, a Total Equivalent Warming Impact (TEWI) calculation has been made, which indicates the sum of the equivalent carbon dioxide emissions for the heat pump's lifetime. TEWI considers direct and indirect emissions, including leakages, recycling, and producing electricity emissions, Eq. (12).

$$TEWI = GWP\ m\ L_{annual}\ n + GWP\ m\ (1-\alpha) + (E_{annual}\ \beta\ n) \tag{12}$$

All cycles inevitably lose a percentage of their charge throughout their useful life, and the greater the amount of refrigerant (m), the more charge will be lost. 5 % has been considered for the annual refrigerant leakage rate (L_{annual}), a common assumption in the refrigeration and heat pump industry. The refrigerant charge has been determined based on the available literature. Peter et al. [38] needed 1.6 kg to optimize a 20 kW heat pump. Arpagaus et al. [39] used a 10 kW experimental HTHP with an R1336mzz(Z) charge of 4.2 kg. Arpagaus and Bertsch [25] used 4.1 kg of R1336mzz(Z) in another HTHP. Also, Arpagaus et al. [40] used 3.6 kg for another 10 kW experimental HTHP. Considering the published papers, 42 kg has been considered for the system charge for a 100 kW HTHP. Since the refrigerant leakage are provided in an annual basis, the system's lifetime period in years (n) of the system must be considered. For this parameter, 15 years of operation has been considered. The global warming potential (GWP) depends on the specific refrigerant. At the end of the system lifetime, part of the refrigerant can be extracted and recycled. A recycling rate (α) of 85 % has been considered based on data from the International Institute of Refrigeration [41]. Finally, the indirect emissions are regarding the annual energy consumption of the system expressed in kilowatt-hours (E_{annual}). It is also considered the carbon intensity factor (β, which is the amount of carbon dioxide released by electricity production. In this case, the factor of the European Environment Agency is considered [42], 0.238 $kgCO_2e\ kWh^{-1}$.

For the gas boiler, an efficiency of 90 % has been considered [43 44]. Also, for the CO_2e emissions, Arpagaus et al. [44] proposed factor has been considered (0.265 $kgCO_2e\ kWh^{-1}$).

3. Results and discussion

This section presents the main results of the proposed alternative technology for producing 250 °C renewable heating. The results focus on the energy performance of the R1336mzz(Z) THTHP in combination with other relevant parameters at different input parameters and operational conditions. In this section, the baseline conditions are first presented, and then, the impact of the input parameters on energy performance is studied.

3.1. Baseline conditions

First, the operation and energy performance of the R1336mzz(Z) THTHP cycle at the reference conditions (Table 1) is studied. From an operational point of view, the conditions do not present any inconvenience in the compressor suction at R1336mzz(Z) THTHP reference conditions. Also, there is no risk of two-phase compression because of the relatively high suction superheating degree, as proved by Mateu-Royo et al. [36]. This consideration is particularly critical for R1336mzz(Z), attending to the saturation line slope and comparing it

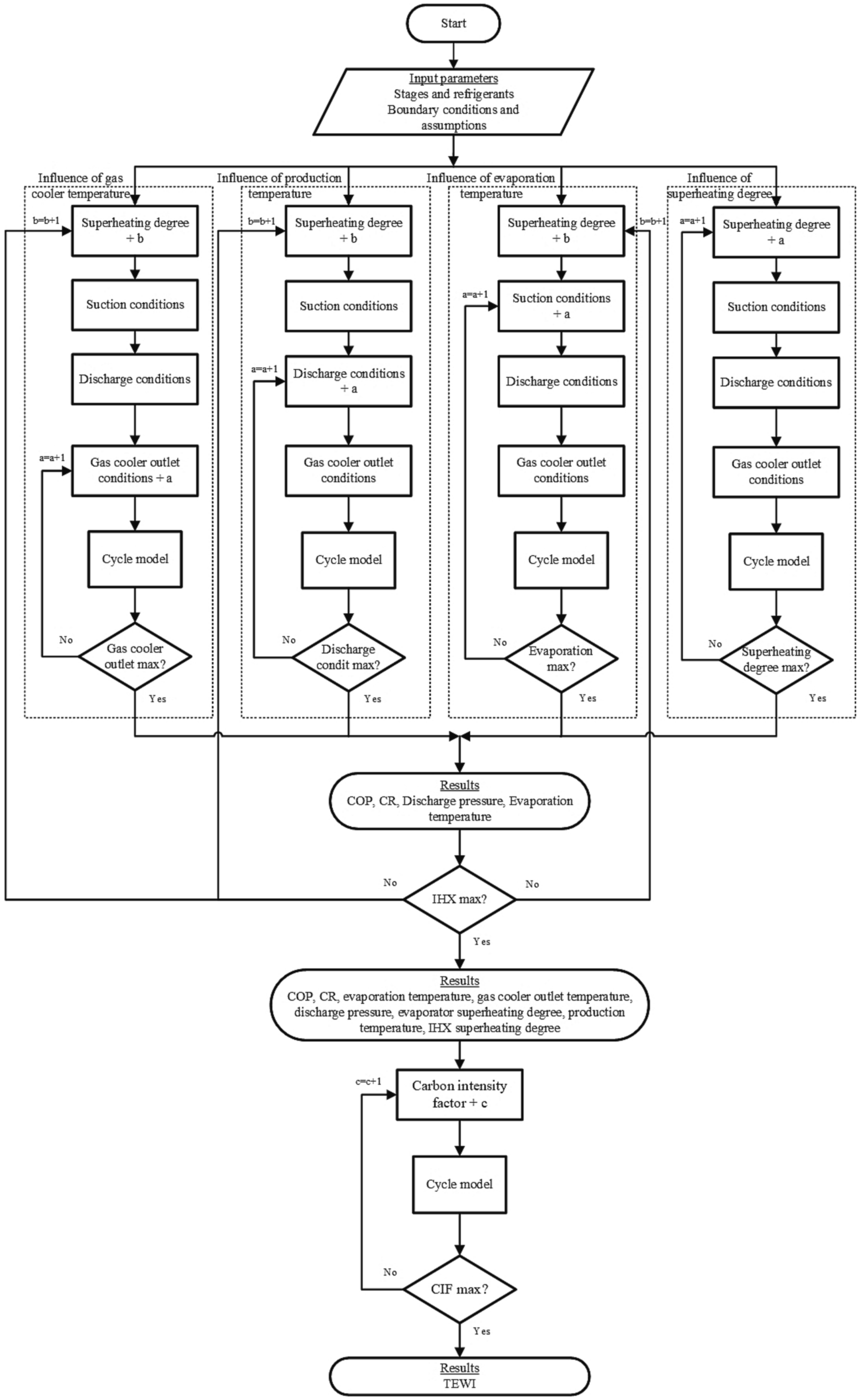

Fig. 2. Methods flow diagram.

Table 2
Refrigerant main characteristics [37].

Characteristic	Value
Refrigerant designation	R1336mzz(Z)
Chemical formula	*cis*-CF3CH=CHCF3
CAS Number	692–49-9
Molecular weight	164.06 g mol^{-1}
Normal boiling point	33.45 °C
Critical temperature	171.35 °C
Critical pressure	2.906 MPa
ASHRAE Std 34 classification	A1
$GWP_{100\text{-yr}}$	2
ODP	0
Thermal degradation temperature	250 °C

with other high-temperature and conventional working fluids.

For the baseline conditions, the COP obtained is 3.3, which means that the system's energy performance is acceptable for being a green alternative to fossil fuel boilers. Remember that the higher the COP, the lower the electricity the heat pump consumes for the same heating capacity. Moreover, higher COP values promote the consideration of heat pumps as renewable heating systems besides the financial benefits and avoiding the emission of larger quantities of CO_2e into the atmosphere.

At an intermediate superheating degree, the discharge pressure to reach the 250 °C production temperature is around 12 MPa, a relatively high pressure compared to standard heat pump applications (maximum operational pressure with R410A heat pumps is approximately 3.5 MPa). Still, it could be technologically feasible by attending to the recent technological advancements for transcritical CO_2. However, the difference is that the R1336mzz(Z) suction pressure is relatively lower (0.7 MPa) and causes a high compression ratio (17.1), contrary to standard CO_2 refrigeration and heat pump cycles [45].

The compression ratio reduction can be achieved through different methods. For instance, the compression process could be split into different compressors, considering compressors in series, several stage configurations, or modifying the basic cycle configuration. From a cycle design perspective, the compression ratio reduction for a fixed production temperature could be achieved by increasing the evaporation temperature or superheating degree. This proposal would require a higher temperature of the waste heat current (heat source or secondary fluid), and it reduces the range of applications that could be considered, or even requires another different cooling method. It is essential to consider that the operational conditions depend on the targeted industry's requirements, so studying the impact of each THTHP condition on the rest of the operational parameters and energy performance is of interest.

3.2. Influence of compressor suction conditions

The compressor suction temperature can be determined by modifying the evaporation temperature or the superheating degree. First, the evaporation temperature has been modified, keeping the superheating degree at the baseline condition of 20 K. Then, the superheating degree has been modified, keeping the evaporation temperature at the baseline condition of 100 °C.

3.2.1. Influence of evaporation temperature

As mentioned, the relatively high compression ratio due to high compressor discharge pressure is challenging for designing compressors and, therefore, THTHP prototypes. For a fixed production temperature, the temperature lift (difference between compressor discharge and evaporation temperatures) can be reduced at higher evaporation temperatures. Fig. 3 shows the impact of the evaporation temperature on the compression ratio and discharge pressure. Also, lower evaporation temperatures have been included in the figure to analyse the viability of THTHPs at additional temperature ranges and applications. The rest of

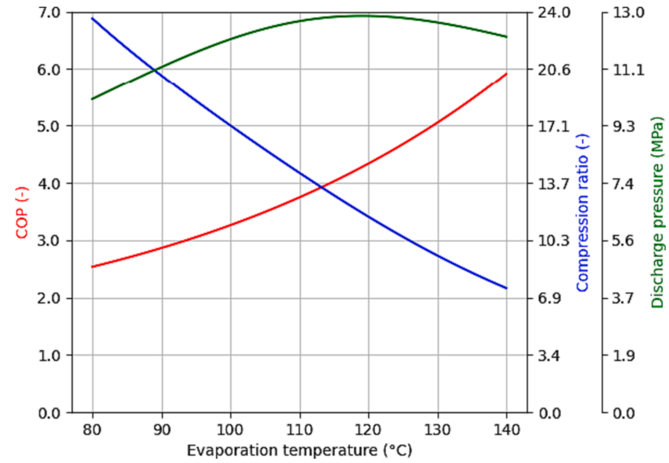

Fig. 3. Evaporation temperature versus main operational parameters.

the conditions (input parameters) remain as in Table 1.

The COP varies between 2.5 and 5.9, considering that the higher the evaporation temperature, the higher the COP. Also, the compression ratio is reduced from 25.3 to 7.4 when increasing the evaporation temperature from 80 to 140 °C. This could be considered a significant reduction, but the industrial process applicability is also reduced. This variation indicates that if relatively high-temperature waste heat were available, the increase in energy performance and the decrease in compression ratio would be very pronounced, reducing the challenge of designing and developing the THTHP. Another critical aspect of the cycle viability is the volumetric mass flow. In this case (100 kW), the highest value reached is 0.018 m^3/s, an acceptable value for a heat pump compressor. The pressure ranges between approximately 10 and 13 MPa with a slight decrease over 120 °C due to the inherent thermodynamic properties of the refrigerant (shape of the 250 °C isothermal curve in transcritical conditions).

3.2.2. Influence of superheating degree

The second way to reduce the compression ratio is by using part of the waste heat to increase the evaporator superheating degree. Therefore, instead of setting the evaporation temperature at 140 °C as proposed in the previous section, the evaporation temperature can be kept at 100 °C (baseline conditions) and the refrigerant superheated at the evaporator to 140 °C (superheating degree of 40 K). Fig. 4 shows the results of the variation of superheating degree.

By superheating the R1336mzz(Z) refrigerant in the evaporator, a higher temperature in compressor suction is obtained, allowing a lower

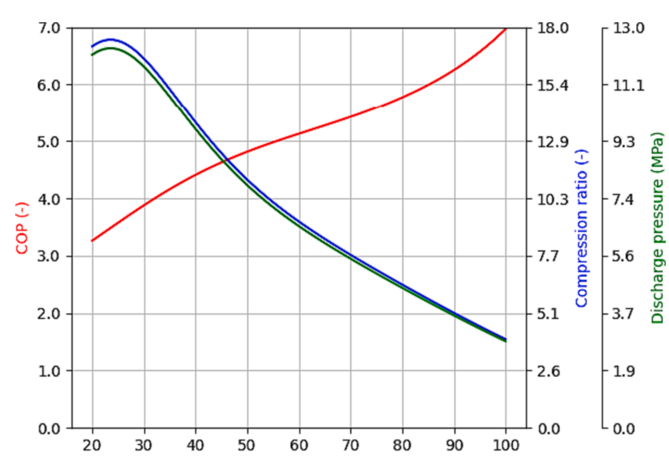

Fig. 4. Evaporator superheating degree versus main operational parameters.

compression ratio and higher COP (an increase from 3.2 to 7.0) for obtaining the same discharge temperature (also assumed as the heating production temperature in this work). There is a maximum compression ratio and discharge pressure at an initial 24 K evaporator superheating degree. Then, like in the previous section, the reduction of compression ratio and compressor discharge pressure is significant for a relatively small superheating degree increment, being the minimum values at 3.9 of compression ratio and 2.8 MPa of discharge pressure for 100 K evaporator superheating degree.

On the other hand, comparing the COP presented in the previous section (impact of evaporation temperature), if a waste heat source is available at 160 °C, it can be concluded that it is better to use it for increasing the THTHP evaporation temperature close to 160 °C (depending on the pinch point) than increasing the evaporator superheating degree at 60 K and 100 °C evaporation temperature. For 160 °C (previous section) evaporation temperature and 20 °C superheating degree, the COP is 5.9, and the compression ratio is 7.4. In contrast, for 100 °C evaporation temperature and 60 K superheating degree, the COP is 5.1, and the compression ratio is 9.

3.3. Influence of production temperature

Another option to decrease the THTHP compression ratio is reducing the production temperature (determined by the compressor discharge temperature). The interaction of these parameters and the COP is shown in Fig. 5.

Production temperature mainly depends on the industrial process requirements for installing the THTHP. For instance, metal drying only requires temperatures up to 200 °C, but plastic injection modeling can require temperatures up to 300 °C (more examples can be consulted in Arpagaus et al. [1]).

The results show that considering a production temperature from 180 °C to 250 °C (less restrictive than the baseline scenario), the THTHP COP decreases from 7 to 3.3. Therefore, a significant decrease in COP can be highlighted, which indicates how detrimental it is to require higher temperature production. Moreover, the higher the production temperature, the higher the compressor discharge pressure and, consequently, the compression ratio, which varies from 4.2 to 17.1. Note that the production temperature required for the same heating process could be slightly reduced by a better design of the heat exchanger at the gas cooler.

3.4. Influence of gas cooler outlet temperature

The last parameter individually analysed in this paper is the gas cooler outlet temperature (expansion valve inlet in ideal conditions). Besides the high pressure of the THTHP cycle (discharge or gas cooler pressure and pressure drops), this parameter depends on the temperature at which the secondary fluid enters the THTHP gas cooler (process heat or heat sink inlet temperature). This section analyses the impact of this parameter on the rest of the parameters when it is varied from an ambient temperature of 25 °C to matching the baseline evaporation temperature of 100 °C. Fig. 6 presents the influence of the gas cooler outlet temperature on the COP. Unlike previous sections, discharge pressure and compression ratio are not displayed in the figure because they would remain at the same level.

The variation of the COP for different gas cooler outlet temperatures is not as significant as that observed in previous sections, where the impact of other input parameters was analyzed. The COP decreases from 4.7 to 3.3 with increased gas cooler outlet temperature from 25 to 100 °C. This improvement is mainly due to the decrease in the mass flow rate of the cycle, which consequently allows the power consumption provided by the compressor to be reduced.

3.5. Combined effect of input parameters

After analysing the influence of input parameters separately, the combined effect of these parameters facilitates the assessment of the THTHP operational behaviour and provides insight for further system optimization.

3.5.1. Combined effect of evaporation and production temperature

First, the combined impact of evaporation and production temperatures on energy performance is analysed. Fig. 7 shows the results in a contour plot.

The COP results vary between 2.5 and 11, so at a lower temperature difference between both parameters, the COP increases. It is, therefore, benefitted from a lower temperature lift or compression ratio. Even though the overall results are relatively low, the minimum COP is still valid to replace fossil fuel boilers. Then, the COP is above 4.5 in most situations, a value generally considered the maximum in refrigeration systems (considering their cooling COP).

As in the previous sections, other parameters like compression ratio and the volumetric mass flow rate are also relevant for the analysis of the THTHP operation. Fig. 8 shows the impact of evaporation and production temperatures on compression ratio and volumetric mass flow rate. The compression ratio increases from 2.5 to 24 following the increment of temperature difference. This indicates that different compressors in series would be necessary for specific conditions to reach the required high compression rate. In the case of the volumetric mass flow rate, this is higher than the evaporation temperature but always in acceptable

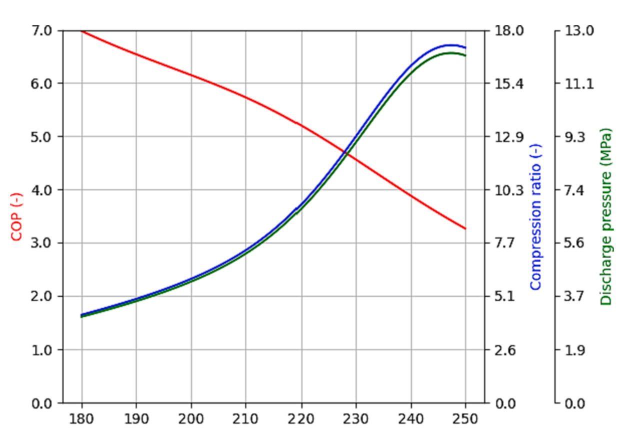

Fig. 5. Production temperature versus main operational parameters.

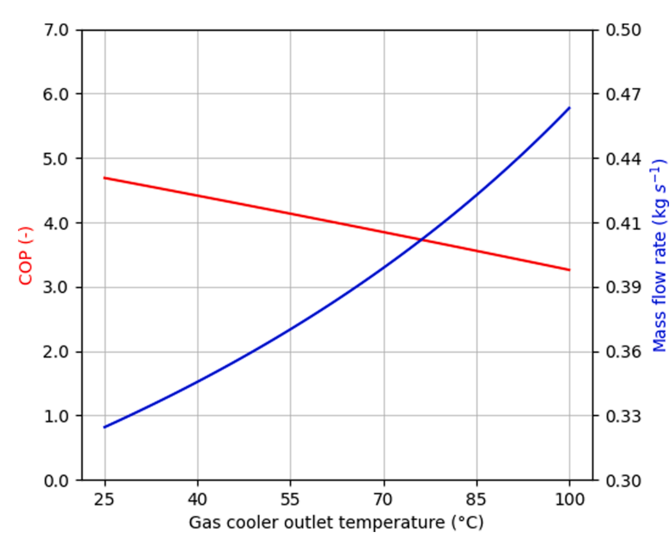

Fig. 6. Gas cooler outlet temperature versus COP and mass flow rate.

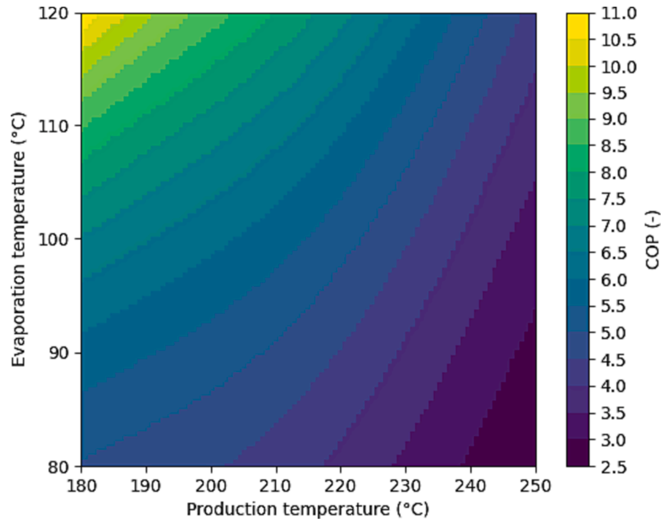

Fig. 7. COP with evaporation and production temperature variation.

values and can be adapted to different compressor technologies (from reciprocating to screw, and for higher heating capacities than considered in this work, centrifugal models).

3.5.2. Combined effect of evaporation and gas cooler outlet temperature

The combined effect of evaporation and gas cooler outlet temperatures on energy performance is also assessed. Fig. 9 shows the results in a contour plot.

In this case, if a production temperature of 250 °C is required, the maximum COP reached is 6.2 with a gas cooler outlet temperature of 25 °C and an evaporation temperature of 120 °C. The results are similar to before; the COP benefits from a lower temperature lift or compression ratio. Higher waste heat allows higher evaporation temperatures and, consequently, higher COP. Similarly, the low process heat temperature allows for lower gas cooler outlet temperature and, consequently, higher COP.

3.6. COP maximization through an IHX

The superheating degree can be increased with an IHX (also known as liquid-to-suction heat exchanger), transferring heat from the liquid (between the gas cooler outlet and the expansion valve inlet) to the suction line (between the evaporator outlet and the compressor suction). The superheating degree depends on the gas cooler outlet temperature.

The higher the heat exchanged at the IHX, defined by the inlet temperatures and the heat exchange effectiveness, the higher the resulting superheating degree at the compressor inlet. The compressor discharge temperature can be maximized at high total superheating degrees for a lower discharge or gas cooler pressure. Because superheating degree and gas cooler pressure influence compression ratio and COP, a system operation optimization can be proposed to maximize the COP. In this way, Fig. 10 shows the gas cooler outlet temperature impact on compressor suction superheating degree, COP and compression ratio.

The results confirm a maximum COP for a specific gas cooler outlet temperature. The IHX causes that at 150 °C gas cooler outlet temperature (keeping the rest of the parameters as specified in Table 1), the COP reaches the maximum value of 4. At the same time, the THTHP produces 250 °C heating and requires a heat source at only 120 °C. The COP presents values of 4.0 at 40 K superheating degree but is reduced at 3.2 at 75 K. Therefore, if the IHX operation is not adequately designed, the energy performance can decrease to 20 %. In conclusion, it can be observed that R1336mzz(Z) THTHP are benefitted mainly from the inclusion of IHX.

The production temperature also influences the efficiency of the cycle with IHX. Therefore, it is also necessary to add this parameter to observe the behavior of the COP of the cycle. Fig. 11 shows the COP

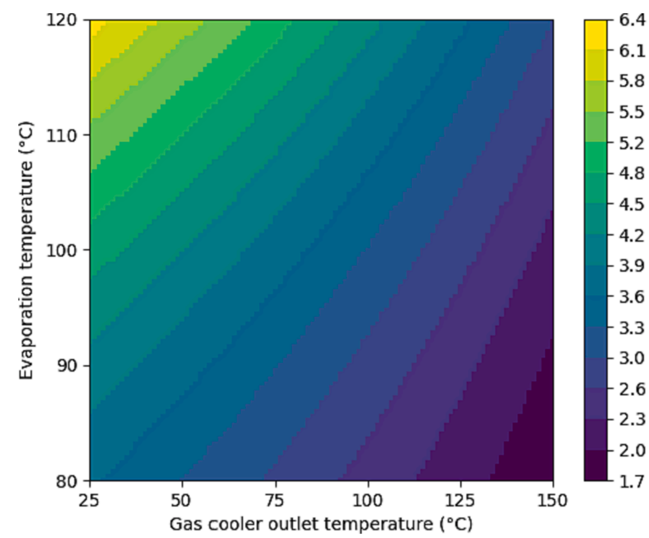

Fig. 9. COP with evaporation and gas cooler outlet temperature variation.

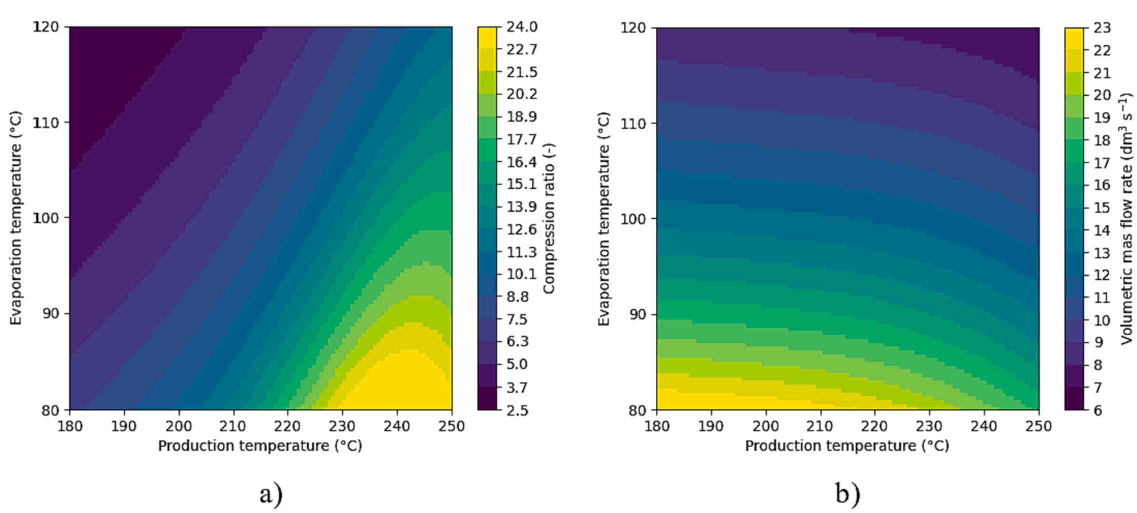

Fig. 8. Influence of production and evaporation temperature on: a) compression ratio and b) volumetric mass flow rate.

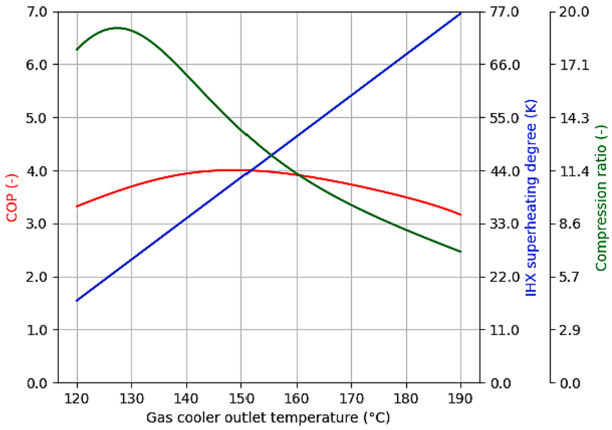

Fig. 10. Internal heat exchanger optimization.

variation depending on the gas cooler outlet, evaporation, and production temperatures.

The COP varies significantly with each parameter. A higher gas cooler outlet temperature generally decreases COP, as explained before. This decrease is more significant at lower production temperatures because, following 225 °C and 200 °C points in Fig. 11, the lowest COP is between 5 and 6 times lower than the highest COP. The behavior can be explained at a thermodynamic level, given that the difference between the outlet temperature of the gas cooler and the production temperature sets the heating capacity provided to the fluid to be heated. If the temperature difference is very low, the heating capacity transferred also is, and consequently, the COP. Regarding evaporation temperature, the higher evaporation temperatures allow higher COPs. In this case, due to compressor power consumption, low evaporation temperatures cause the pressure drop to be more significant, and consequently, power consumption will be greater as the compression ratio.

3.7. Equivalent CO_2 emissions comparison

Natural gas boilers are the most common systems for high-temperature heating, but they emit a significant amount of CO_2e globally. Because of this, a comparison between the proposed cycle and a gas boiler is necessary to complete the assessment. As Udroiu et al. [46] demonstrated, the principal contributor to CO_2e emissions of vapour compression cycles with low GWP refrigerants is the indirect emissions (caused by electricity generation). Because of that, the carbon intensity factor is a very relevant parameter. This carbon intensity factor is external to the cycle because it depends on what each country uses to generate electricity. Fig. 12 shows the CO_2e emissions depending on the carbon intensity factor and production temperature.

The CO_2e emissions depend also on the cycle efficiency, as indicated in the previous figure. The higher the production temperature, the lower the efficiency will be, as seen in previous sections, and consequently, the emissions will also be higher. Furthermore, this difference becomes more pronounced at a higher carbon intensity factor. At low carbon intensity factor, the cycle can reach much higher production temperatures cleanly in countries that generate their electricity in cleaner ways,

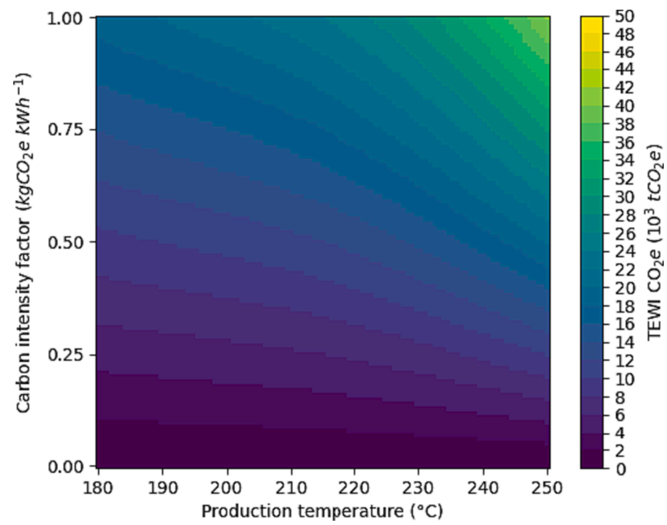

Fig. 12. CO_2e emissions according to production temperature and carbon intensity factor.

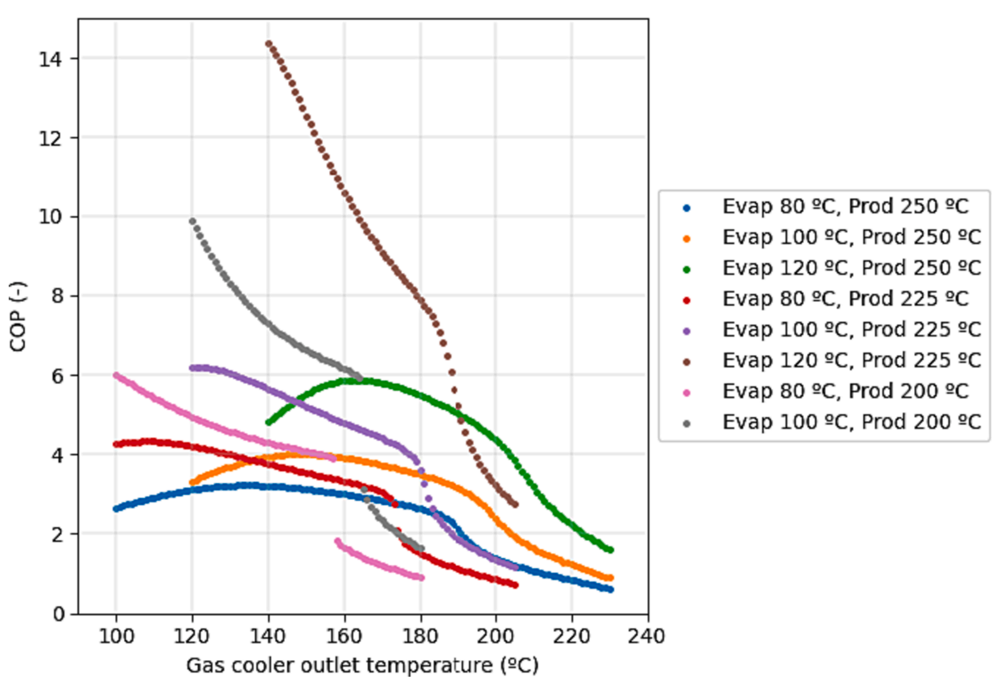

Fig. 11. COP with evaporation, production, and gas cooler outlet temperature variation.

such as renewable or nuclear energy. Considering some specific values, in 2022, the carbon intensity factor of Iceland was 0.028 $kgCO_2e\ kWh^{-1}$, and for Germany was 0.473 $kgCO_2e\ kWh^{-1}$ [47]. For Iceland, the total emissions for 15 years of use of the THTHP at 180 °C are $37.65{\cdot}10^3$ tCO_2e. The emissions are $884.78{\cdot}10^3$ tCO_2e for the same conditions in Germany. Instead, for the same 15 years at 250 °C, the emissions in Iceland would increase only to $80.60{\cdot}10^3$ tCO_2e, while for Germany, emissions would increase to $1894.11{\cdot}10^3$ tCO_2e. To better exemplify these differences, Fig. 13 shows the ratio between CO_2e emitted by the gas boiler and the CO_2e emitted by the THTHP.

As can be seen, a significant difference in CO_2e emissions clarifies the importance of having an electrical system with clean energy. Considering a high carbon intensity factor like Germany, the THTHP are superior to gas boilers, with 2 and 4 times less CO_2e emissions. However, with a low carbon intensity factor, the THTHP is significantly superior to gas boilers in emissions, emitting 50 or even 100 times less CO_2e.

4. Conclusions

This work proposes a vapour compression system to achieve temperatures of 250 °C using R1336mzz(Z) refrigerant and under transcritical operation. This working fluid is used to take advantage of the fact that it can operate at 250 °C without thermal degradation. Therefore, the system proposed is a transcritical high-temperature heat pump (THTHP). The impact of different parameters on the operational and energy performance of the system has been assessed, and the system has been optimized to maximize the COP.

The results confirm that the THTHP proposal is promising according to different perspectives. If the parameters are carefully selected, the energy performance can be increased and the operation less challenging despite working at high pressures and temperatures. The COP can reach the value of 3.3 under a temperature lift of 150 °C and keep a minimum superheating degree of 20 °C to protect the compressor from liquid strokes. The discharge compressor pressure, the highest pressure of the vapour compression cycle, reaches values of 12 MPa. A challenge would be the compression ratio of 17 at the reference conditions. This situation would require technological advancements or solutions in the cycle itself. A solution could be compressors in series, reducing the individual compression ratio. Another solution could be modifying the external cycle conditions considering the heat sink and source temperatures. It should be noted that these temperatures depend on the industry's requirements in which the heat pump is installed.

Evaporation temperatures can be modified by altering the waste heat temperature, which is the fluid exchanging heat with the evaporator. From 80 °C and 140 °C, the COP of the cycle varies between 2.5 and 5.9, and the compression ratio from 25.3 to 7.4. In the case of the superheating degree, instead of modifying the evaporation temperature, a variation in COP from 3.2 to 7 is observed with a superheating degree from 20 °C to 100 °C. These superheating degree values can be reached using part of the energy of the secondary fluid for superheating instead of evaporating or with an alternative cooling system. Also, it is observed that it is more efficient to use the energy of the secondary fluid to increase the evaporation temperature at the same conditions. For example, a secondary fluid entering at 160 °C can be used in a cycle that evaporates at 140 °C and 20 °C superheating degree (the COP is 5.9) or evaporating at 100 °C and superheating degree of 60 °C (the COP is 5.1).

Considering the parameters in the high-pressure section, the cycle conditions can also be modified. Increasing the production temperature from 180 °C to 250 °C decreases the COP from 7 to 3.3. The gas cooler outlet temperature is not a parameter that substantially influences the cycle performance. A gas cooler outlet temperature of 25 °C increases the COP to 4.7 instead of 3.3, as in the case of 100 °C.

The optimization of the superheating degree at the compressor suction with an internal heat exchanger reduces the gas cooler outlet, and the maximum COP is reached at 150 °C of the gas cooler outlet pressure with a COP of 4.

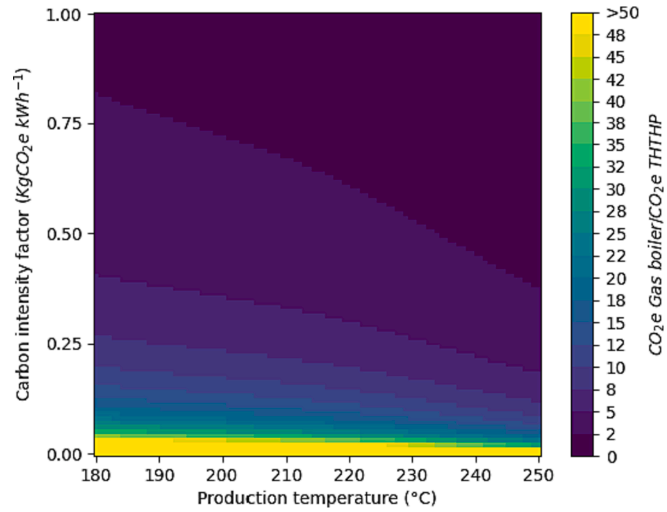

Fig. 13. Emission ratio between a gas boiler and THTHP.

THTHP emissions depend significantly on their location and how electricity is obtained. However, even in countries with very high carbon emissions, the THTHP emits less CO_2e than a boiler gas used today. THTHP can emit between 50 and 100 times less CO_2e in countries with a very low carbon emission factor.

This paper demonstrates that theoretically, reaching the temperature of 250 °C with a vapour compression cycle is technically possible and attractive from an energy point of view (COP of 3.3 at baseline conditions). The selection of the operating parameters should be carefully followed. Still, some challenges should be addressed before this proposal is brought into practice, and this paper proposes ideas that can be solved using different compressors in series or modifying the system. Also, the compressors and lubricants for these high temperatures and pressures are subject to future research.

CRediT authorship contribution statement

Cosmin-Mihai Udroiu: Data curation, Investigation, Software, Visualization, Conceptualization, Methodology, Writing – original draft, Writing – review & editing, Formal analysis. **Joaquín Navarro-Esbrí:** Data curation, Investigation, Software, Visualization, Writing – review & editing, Formal analysis. **Pau Giménez-Prades:** Data curation, Investigation, Software, Visualization. **Adrián Mota-Babiloni:** Conceptualization, Funding acquisition, Methodology, Project administration, Supervision, Writing – original draft, Writing – review & editing, Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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