# Concept study for industrial heat pumps up to 250°C heat sink temperature using radial turbo compressors

(5) Dekarbonisierung: Industriesektor

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### Abstract:

Today, compression heat pumps are well known as the solution for sustainable and energy efficient industrial heat supply up to 130°C. Various projects with prototype plants on TRL7 show the technical feasibility of utilization temperatures up to about 155°C. However, increasing the sink temperatures further up to 200°C and above leads to problems regarding compressor technology (oil-free), refrigerant and circuit design. Within simulations, a heat-pump based on a two-stage turbo compressor using several natural and synthetic refrigerants and mixtures is investigated. At sink temperatures above 200°C, many refrigerants must be operated in the transcritical regime. It was found out that pentane, cyclopentane and R1233zd(E) should be preferred for 200°C sink temperature with 110°C lift. However, the pressure ratio is a limit for the radial turbo compressor, which is a strong argument against cyclopentane, which has the highest COP.

Keywords: Heat pump, High-temperature, Radial compressor, Refrigerant

# 1 Introduction

Driven by decarbonization targets and recent developments in the gas market, the interest in heat pumps for utilizing industrial waste heat is increasing worldwide. However, in contrast to domestic systems, industrial processes require significantly higher sink temperatures and heat loads. Operating temperatures above 130°C lead to novel application areas for high-temperature heat pumps and a much larger sales market than what was previously common for manufacturers [1][2].

However, to meet these requirements the manufacturers have to overcome technological barriers which come with higher temperatures. Nearly all industrial heat pumps are using piston and screw compressors which are heavily depending on the stability of lubricating oil [3][4] that is tending to change its properties and decompose with rising temperatures. Therefore, it is necessary to go for oil-free solutions if targeting sink temperatures above 180°C. One of these solutions can be the use of a radial turbo compressor, which is presently only used for high thermal power (>5MW<sub>th</sub>) e.g. district heating systems. Therefore, the Austrian Institute of Technology (AIT) – Center for Energy together with TU Wien - Institute of Energy Systems and

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Thermodynamics are working within the framework of the FFG-Project "NERO" on a concept of industrial heat pumps using radial turbo compressors for heat sink temperatures up to 250°C and heating capacities in the 1  $MW_{th}$  area.

Previously published publications [3][4] showed already the feasibility of the concept and discussed refrigerant selection and transcritical heat pump cycle configurations. However, an optimization of the COP by means of a variation of the high-pressure level especially under consideration of the performance of refrigerant blends is still missing and should be targeted in this publication.

## 2 Heat pump

### 2.1 Refrigerants

Table 1 contains a pre-selection of natural and synthetic refrigerants as well as certain mixtures, which are described by their physical and thermodynamic parameters. For the first evaluation, the critical temperature, the ODP value, the GWP value and the safety class are used. This is already simplified as the volumetric heating capacity and the required system pressure should also be taken into account or at least checked afterwards. Although water (R718) as a refrigerant generally has good properties in terms of thermodynamic, safety and environmental aspects, for the desired temperature range the advantages of the other refrigerants are valued higher as already discussed in [3]. Moreover, it was completely excluded based on the high critical point and its inability for mixing with hydrocarbons due to its strong hydrogen bonds. The same goes for ammonia (R717) which is basically known for its good performance as a refrigerant in terms of a high volumetric capacity, but the high pressure which is needed for temperatures above 100°C makes it infeasible if costs for equipment such as valves and vessels are taken into account.

Both mixtures, which are shown in Table 1, are based on the fact that R601 (Pentane) showed the best performance in preliminary calculations [4] with the downside of a high pressure ratio for the compressor. The components and exact fractions are based on Fernández-Moreno et al. [5] who were investigating the possibility of various mixtures but for a designed sink temperature of 140°C. However, the results are checked in accordance with preliminary calculations and expected performance of the blends, whereas two of those mixtures were identified as promising for the desired temperature range.

Designation	Composition (mole fraction)	Critical Temperature (°C)	ODP	GWP	Safety class	Decomposition Temperature (°C)
R1233zd(E)	1	166,4	≈0	1	A1	277
R1336mzz(Z)	1	171,3	0	2	A1	>250
R1336mzz(E)	1	137.7	0	18	A1	>250
R601 (Pentane)	1	196,5	0	5	A3	376

Table 1: Properties of Refrigerants and Mixtures [5][6][7][8]

Cyclopentane	1	238,5	0	5	A3	275
R600 (n-Butane)	1	152,0	0	4	A3	302
R601/1234ze(Z)	0.74/0.26	180.8	0	5.6	A3	n.a.
R1233zd(E)/601/152a	0.65/0.25/0.1	165.5	0	14.4	A2L	n.a.

## 2.2 Design

As already mentioned in previous publications [3][4], the investigated refrigeration circuits are based on a two-stage centrifugal compressor which restricts the pressure ratio per compression stage to keep the efficiency high. At first the pressure ratio has to be the same for both compressors, in consequence, the medium pressure level is set to

$$p_M = \sqrt{\frac{p_H}{p_{evap}}} * p_{evap} \tag{1}$$

This also preserves the possibility of intermediate injection, which can be performed from an economizer or intermediate pressure vessel (flash tank). However, it was shown in a previous publication that the so-called Reference Cycle (see Figure 1) had the best performance [4]. This fact is caused by the need to limit the transferred heat in the IHEX to retain the opportunity of an intermediate injection, which needs a certain fraction of gaseous refrigerant. The advantage of the flash tank on the medium pressure level is therefore neglected by the thermodynamical restrictions. Intermediate injection at medium pressure level between the compressor stages thus proves as a suboptimal solution for the investigated refrigerants.

However, a refrigerant regulating component such as a refrigerant accumulator will be necessary for the circuit design to react to varying evaporation or high-pressures. It ensures that in part-load operation the optimal operating point (high-pressure, refrigerant mass flow) can still be applied.

The solution to this problem is the Intermediate Pressure Expansion Cycle shown in Figure 3 (a). With the introduction of a flash tank and an additional expansion valve, which is expanding the gas phase of the refrigerant in the flash tank to evaporation pressure, controllability of the system is achieved. A comparison between the Reference Cycle and the thermodynamical nearly identical Intermediate Pressure Expansion Cycle is shown in Figure 2. As can be seen in the log(p)-h-diagram (Figure 2), the pressure in the introduced flash tank is not matching the medium pressure between the compressors. Thereby, a complete utilization of the maximum capacity of the IHEX in order to achieve the highest possible compressor outlet temperature is possible.



Figure 1: Reference cycle



Figure 2: Comparison between Reference cycle(black) and Intermediate Pressure Expansion Cycle (green) by means of the log(p)-h-diagram for the refrigerant R1233zd(E)

An even better alternative is to design the evaporator of the refrigeration circuit as a flooded tube bundle heat exchanger or trickle film evaporator, see Figure 3 (b). When using oil-lubricated compressors, flooded evaporators should be avoided due to the risk of oil deposits. However, with oil-free compression, this criterion does not apply any longer, and it is possible to implement an accumulator capability with such evaporator types. As a result, the expansion valve doesn't control the suction gas superheat but ensures that the high-pressure is controlled. In further consequence, not superheated but saturated refrigerant is sucked into the IHEX and superheated by that before entering the compressor. Since the superheat control in the simulations is set to 0.1 K, this implementation variant shows hardly any differences from a thermodynamic point of view compared to the Reference Cycle. Compared to the Intermediate Pressure Expansion Cycle there are less expensive parts, like valves and vessels, needed. However, the flooded tube bundle or trickle film heat exchangers are subject to different regulations and so it is expected that at least this component is more expensive.



Figure 3: Flash tank cycle (a) and solution with flooded evaporator (b)

# 3 Simulation

## 3.1 Model and Setup

The heat pump cycles, including the required components (e.g. compressors, vessels), were modeled using the object-oriented, acausal, equation-based open-source modeling language Modelica. As simulation environment Dymola 2022x is used. Basic components (heat exchanger, expansion valve, separator) from the commercial library TIL 3.10.0 [11] developed by TLK Thermo GmbH [9] are used for the system simulations. To simulate the thermophysical properties of the working media, the fluid database TILMedia included in the library was used and the missing material data was supplemented with the help of the tool REFPROP [10]. The mixtures are modelled with splines to ensure numerical stability and speed up the calculations. The maximum error is around 3% near the critical point and in most points even a power of ten beneath.

To keep the simulations as simple and comparable as possible, the following simplifications are made in the calculations:

- No pressure losses in the pipes and heat exchangers
- No thermal losses to the environment
- Constant superheat of 0.1°C at the outlet of the evaporator
- Constant isentropic efficiency of the two compressors
- Oversized heat exchangers to minimize the influence of heat transfer and heat transfer coefficients

The operating parameters of the heat pump, which are the same for all refrigerants, are summarized in Table 2.

Designation	Abbreviation	Value
Thermal power	$\dot{Q_H}$	200 kW <sub>th</sub>
Sink temperature (outlet)	$T_{sink}^{out}$	200 ° <i>C</i>
Sink temperature spread	$\Delta T_{sink}$	40 <i>K</i>
Source temperature (inlet)	$T_{source}^{in}$	95 ° <i>C</i>
Source temperature spread	$\Delta T_{source}$	5 <i>K</i>
Evaporation temperature *	$T_{evap}$	90 ° <i>C</i>
Isentropic efficiency	$\eta_{is}$	0,76

#### Table 2: Operating parameters

\* for the mixture a temperature glide of around 5 °C in the evaporator is emerged

### 3.2 Results

For all refrigerants except Pentane and Cyclopentane, the heat pump operates transcritically. Therefore, the condenser is a gas cooler with a temperature glide. As a result, the high-pressure level does not depend on the two-phase equilibrium and can be chosen individually,

given a compressor outlet temperature high enough. With a falling high-pressure level, the mass flow has to be increased to ensure that the same thermal power output is delivered. If the high-pressure level is increased, the electrical power input raises. However, there is a certain pressure level where the coefficient of performance

$$COP = \frac{\dot{Q_H}}{P_{el}} \tag{1}$$

reaches its maximum.

Besides the level of the high-pressure the size of the IHEX has a large impact on the COP. In these calculations, the transferred heat in the IHEX is varied by setting different temperature spreads in the IHEX, whereby a smaller temperature spread is leading to a larger IHEX transferring more heat.



Figure 4: COP depending on high-pressure level and temperature spread in the IHEX for different refrigerants

In **Error! Reference source not found.** the COP depending on the high-pressure level for each refrigerant is seen. Three different temperature spreads in the IHEX are analyzed and depicted in different colors. It can be noticed that the COP is higher if more heat is transferred in the IHEX. In case of conventional heat pumps, the compressor outlet temperature is limited by the properties of the oil, but this restriction doesn't apply for a compressor which is free of oil. In general, for a heat pump using a turbo compressor a larger IHEX is advantageous.

Pressures exceeding 40 bar<sub>a</sub> will go along with a significant increase of the piping, component, and vessel costs, as for instance Pachai et. al. [9] mention. Based on this fact and the comparatively low COP, R1336mzz(E) and R600 (butane) reveal to be disadvantageous.

Besides the absolute pressure level, the pressure ratio between the evaporator pressure and the high-pressure is important for the efficiency of the turbo compressor. Furthermore, for a turbo compressor the pressure ratio per stage is limited. Based on the high-pressure level, the evaporation pressure and a two-stage compressor, the pressure ratio per stage is calculated. Figure 5 shows the COP depending on the pressure ratio per stage for each refrigerant applying a temperature spread of 15°C in the IHEX. Even if cyclopentane achieves the highest efficiency with a COP above 3.1 it is disadvantages because of the high pressure ratio of around 2.7 per stage. This would lead to very high compressor speeds, fatigue problems and poorer compressor efficiencies. A solution to this problem could be to use a third stage, but with the huge disadvantages of increasing costs of around 50% for the compressor. Pentane (R601) has the second highest COP with around 2.9 but is also critical in terms of the pressure ratio. The safe option would be to go for the third highest COP using R1233zd(E). The optimal pressure ratio is beneath 2.4 with a COP of at least 2.7. The refrigerant blends which were designed to enhance the performance of Pentane (R601) and R1233zd(E) didn't rise to the expectations. The first one with R601 as main component leads to a lower pressure ratio but with an even greater drop in COP, so that it cannot match R1233zd(E) anymore. The second mixture with R1233zd(E) as main component showed a lower COP than the pure fluid corresponding to a similar pressure ratio.



Figure 5: COP depending on the pressure ratio for different refrigerants



Figure 6: Condenser QT-Diagram for cyclopentane

For Pentane (R601) the heat dissipation takes place just slightly below the critical point. Therefore, the characteristics of the transcritical operation (temperature glide in the gas cooler and a selectable high pressure) are still fulfilled. In contrast to all the other investigated refrigerants, with cyclopentane clearly a subcritical operation arises from its high critical point. As can be seen in Figure 5, using cyclopentane leads to a significantly higher COP but with the downside of very high pressure ratios. With the given boundary condition of heating water from 160°C to 200°C and an evaporation temperature of 90°C, lower pressure ratios are not possible due to a pinch point issue. Depending on the transferred heat in the condenser, the temperature curve of cyclopentane at 23 bar and water is shown in Figure 6. Caused by the two-phase equilibrium, a lower pressure would result in a lower condensing temperature, which is not possible due to the water temperature.

Refrigerant	Evaporation Pressure (bar)	High pressure (bar)	Pressure ratio per stage (-)	COP (-)	Volumetric heating capacity (MJ/m <sup>3</sup> )
R1233zd(E)	8.33	46	2.35	2.73	7.0
R1336mzz(Z)	5.55	37	2.58	2.71	5.0
R1336mzz(E)	12.3	69	2.37	2.31	9.6
R601 (Pentane)	4.70	30	2.53	2.90	4.3
Cyclopentane	3.26	23	2.67	3.12	3.3
R600 (n-Butane)	12.5	60	2.19	2.55	9.2
R601/1234ze(Z)	6.61	39	2.43	2.72	5.5
R1233zd(E)/601/152a	8.80	48	2.34	2.67	7.1

Table 3: Main results for 15°C temperature spread in the IHEX and the highest COP

In Table 3, the main results for each refrigerant for the operating conditions presented in Table 2 and the high-pressure, which is corresponding to the best COP, are summarized. Values, which are in a problematic range or disadvantageous, are highlighted in light red and results, which are especially beneficious, are highlighted in light green. The volumetric heating capacity is an indicator for the size and the space requirements of the heat pump. A higher volumetric heating capacity reduces the size of the parts of the heat pump and therefore also its investment costs, which applies especially to the compressor.

## 4 Conclusion

A study on the optimal operation conditions for different refrigerants with desired sink temperatures of 200°C was conducted. All considered refrigerants are technical feasible, but R1336mzz(E) and n-Butane (R600) require relatively high upper pressure levels of 72 bara and 62 bar<sub>a</sub>, respectively. This leads to higher costs and no further advantage as the COP is even lower as for most other refrigerants. The best COP is achieved using Pentane (R601) or even better cyclopentane. However, also the pressure ratio is guite high with more than 2.5 per stage which challenges the compressor design in terms of performance and fatigue strength quite heavily. Especially for the use of cyclopentane the authors would suggest a third stage, which would be a huge blow in terms of costs. The most promising pure refrigerant candidate is R1233zd(E) with the third highest COP and a pressure ratio beneath 2.5. The refrigerant blend using R1233zd(E) as main component performed in terms of COP a little bit worse than the pure fluid. Although the mixture using R601 as main component achieved a lower pressure ratio, the COP went down to around 2.7, which is quite the same as for R1233zd(E). Therefore, the two tested blends didn't show a significant performance advantage over the considered pure fluids. As cyclopentane showed a COP of 3.1 compared to 2.7 achieved by R1233zd(E) with the drawback of an unbearable pressure ratio, it should be investigated whether a specific blend using it as main component could be advantageous. Moreover, as R1233zd(E) seems to be the best fit for the desired operational conditions a radial compressor design is needed to evaluate the performance of the heat pump in part-load and to assess its feasibility further.

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