How to Choose the Best Refrigerant in Heat Pumps from an Ecologic Perspective? Analyzing the Influence of the Evaluation Method

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Abstract:

Heat pumps are one of the key technologies to reduce CO_2-emissions and reach a net zero building stock. However, heat pumps still induce CO_2-emissions, which split up into direct and indirect emissions. Direct emissions result from leakages on site and indirect emissions mainly relate to the power consumption. In particular, the refrigerant choice influences both direct emissions due to its global warming potential, and indirect emissions due to the efficiency of the heat pump. Thus, the refrigerant choice is crucial to minimize the overall emissions of heat pumps. When selecting a proper refrigerant, several evaluation methods exist in the state of the art. In this work, we analyze the influence of the evaluation method on optimal fluid selection. Four methods are employed: Efficiency-based method using the seasonal coefficient of performance (*SCOP*), Total Equivalent Warming Impact (*TEWI*), Life Cycle Climate Performance (*LCCP*), and Life Cycle Assessment (LCA). The study includes ten refrigerants. For method comparison, the study includes refrigerants with either a high GWP or an ODP greater zero also to account for the sensitivity with respect to the evaluation method. The investigation shows only minor differences between the studied refrigerants when comparing the results of *SCOP*, *TEWI* and *LCCP*. The refrigerant ranking is not influenced by the assessment method. Main reason is the high share of the indirect emissions and thus, the dependency on *SCOP*. Using the LCA, the main difference occurs for refrigerants with an ODP. Using current regulations (zero ODP, GWP < 150), we conclude, *SCOP* comparison is a sufficient evaluation criterion when selecting refrigerants.

Keywords:

Fluid selection; TEWI; LCCP; LCA; low-GWP refrigerants.

1. Introduction

In the context of climate change, global greenhouse gas (GHG) emissions have to be reduced in all sectors. In the building sector, the provision of heating and cooling in the building sector is responsible for approximately 19 % of global CO_2-emissions [1]. To achieve the goal of a CO_2-neutral building stock, heat pumps are considered a key technology to replace conventional technologies. Typically, heat pumps use electricity to upgrade ambient heat and thus provide useful heat for heating purposes. Thereby, the emissions of heat pumps are divided into indirect and direct emissions [2]. Indirect emissions are related to the energy demand to operate the system. Most heat pumps use mechanical energy to lift the temperature level and match heat supply and demand. In Germany, the necessary energy is mostly provided by power plants that emit CO_2 and thus, leads to emissions not at the place of the heat pump but at the power plant. For a user-specific heating demand, the emissions depend on electric power demand and thus, on the cycle efficiency of the heat pump. Direct emission originates to refrigerant leakages on site. All currently used refrigerant have a non-zero global warming potential (GWP). Therefore, their leakage supports the greenhouse effect. The main contributor to direct emissions is the used refrigerant, its charge, and its respective GWP. To reduce the overall emissions of heat pumps, direct and indirect emissions need to be reduced.

Besides the GWP, the overall cycle efficiency depends on the choice of refrigerant [3]. Thus, selecting a proper working fluid is crucial regarding low emissions. The refrigerants, however, are subject to increasingly strict political regulations that lead to maximum allowed limits for the GWP, refrigerant charges, and include bans on specified characteristics of refrigerants [4]. In search for possible alternatives that satisfy the political restrictions, the current research focuses on natural refrigerants and hydrofluoroolefins (HFO) since both have near zero GWP values [5–8]. However, selecting the optimal refrigerant is complex and depends on many boundary conditions. Thus, evaluation criteria exist comparing and evaluating refrigerants. In addition

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to conventional energetic assessment metrics like seasonal coefficient of performance (*SCOP*), multiple evaluation methods estimate the environmental impact at different levels of complexity: The *Total Equivalent Warming Impact* (*TEWI*) [9], the *Life Cycle Climate Performance* (*LCCP*) [10] and the *Life Cycle Assessment* (LCA) [11]. However, to the authors' knowledge it is unknown how different ecologic evaluation methods influence the results regarding the refrigerant selection and whether the high complexity of the evaluation is necessary within the selection process. Thus, this work aims to analyze the influence of the evaluation method on the optimal refrigerant selection. In the evaluation, the *SCOP*, the *TEWI*, *LCCP*, and LCA are evaluated for ten refrigerants. The refrigerants are mainly low-GWP refrigerants, e.g. propane (R290). Additionally, conventional refrigerants such as R410A, R134a and R404A are included as well as R22, which has an ozone depletion potential (ODP) to include multiple environmental aspects and derive general conclusions.

The paper is structured as follows: Sections 2 describes and discusses the simulation model. We investigate three refrigerant cycle flowsheets since the flowsheet strongly influences the energetic performance of refrigerants. Additionally, the calculation methods of the assessment criteria are presented. Section 3 shows the results and highlights the differences of each evaluation method. Section 4 discusses the impact of the evaluation method on refrigerant selection and Section 5 draws the overall conclusions and give a suggestion for future work.

2. Method

This section describes the overall method and assessment criteria. Section 2.1 presents the heat pump modeling approach. Section 2.2 shows the evaluation of the energetic assessment criteria of the seasonal coefficient of performance. Sections 2.3 to 2.5 describe the evaluation of the ecologic criteria *TEWI*, *LCCP* and LCA. Finally, section 2.6 shows the selected parameter and the case study.

2.1. Heat pump modeling approach

In the present investigation, we evaluate three heat pump cycle configurations. For each cycle configuration a thermodynamically consistent modeling approach is used. A short description of the selected approach is presented. A detailed description is given in [12]. The modeling approach follows an optimization procedure using the *Python* scipy package [13]. Equation (1) shows its formulation.

$$\begin{aligned} &\max_{\vec{x}} COP(\vec{x}) \\ &s.t. \quad g(\vec{x},\vec{\theta}) \geq 0 \\ &\qquad \vec{x}_{\min} \leq \vec{x} \leq \vec{x}_{\max} \end{aligned} \tag{1}$$

In the optimization, the coefficient of performance (*COP*) is maximized by adjusting the process parameters $\vec{x}$. The process parameters depend on the individual cycle configuration and are presented below. For each process parameter, the optimization considers box-bounds. Additionally, the optimization is subject to inequality constraints $g(\vec{x},\vec{\theta})$. The inequality constraints depend on the process parameters $\vec{x}$ and on the temperatures of heat sink and source. The constraints ensure a physical and technical feasible operation and include (1) wet compressor prohibition, (2) subcritical operation and (3) minimal approach temperatures for all heat exchangers to satisfy the 2nd law of thermodynamics. The heat exchanger modeling uses a minimum approach temperature $\Delta T_{\min} = 2$ K. The expansion valves are assumed isenthalpic. Losses due to friction in the pipes, pressure losses, and heat losses to the surroundings are neglected.

For the compressor, a loss-based compressor model of a reciprocating compressor is used to evaluate refrigerant and operating point dependent isentropic and volumetric compressor efficiencies [14]. The model includes multiple loss mechanisms within a compressor and combines them to a single definition of the compressor efficiency. Thereby, losses due to friction of the piston, flow losses at the compressor valves, electrical losses of the inverter, and heat losses to the environment are included. Additionally, the model scales all effects for a predefined heat flow rate in the condenser. In this work, we consider a 10 kW heat pump for a residential building at the design point -10 °C ambient air temperature and a sink temperature of 55 °C. Thus, the size of the calculated heat pump does not vary between fluids, and a general comparison is possible. A fluid-dependent and operating point-dependent calculation is crucial since the compressor is the component with the highest irreversibilities in the cycle, and an inaccurate calculation can lead to significant differences between the fluids [15].

To account for the influence of the cycle configuration, the study includes three different flowsheets. All models are implemented in *Python* and use *REFPROP* version 10.0 [16] to calculate the fluid properties of all refrigerants. **Figure 1** shows the flowsheets.

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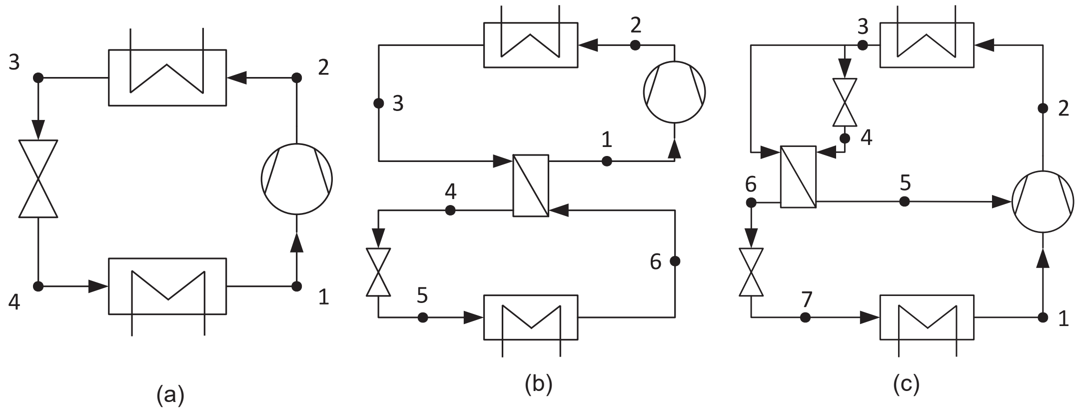

Figure 1: Selected heat pump cycle configurations for the case study.

The simple flowsheet (**Figure 1**a) consists of the four basic components. During the cycle calculation, the optimizer adjusts four optimization variables that specify the simple cycle. Equation (2) shows the optimization variables for the simple cycle.

$$\vec{x}_{\text{simple}} = \vec{x}_{\text{ihx}} = [p_{\text{eva}};\ p_{\text{con}};\ \Delta T_{\text{SH}};\ \Delta T_{\text{SC}}]^T \tag{2}$$

Thereby, the amount of superheating at the compressor inlet ΔT_{SH}, the amount of subcooling at the condenser outlet ΔT_{SC}, the evaporation pressure p_{eva} and the condensation pressure p_{con} are optimized. For each parameter set, the cycle efficiency *COP* is evaluated by equation (3).

$$COP_{\text{simple}} = \frac{\dot{Q}_{\text{con}}}{P_{\text{el}}} = \frac{h_2 - h_3}{h_2 - h_1} \tag{3}$$

The second flowsheet uses an internal heat exchanger (**Figure 1**b). The amount of superheating is shifted from the evaporator to the internal heat exchanger, recuperating heat from the high-pressure side. Thus, the evaporator outlet is saturated vapor. Within the used modeling approach, the internal heat exchanger provides heat for the necessary amount of superheating only and the calculation of the efficiency *COP* in the ihx-cycle is similar to the simple cycle stated in equation (3).

The third cycle uses vapor injection to increase the overall cycle performance (**Figure 1**c). For the vapor injection (vi), a two-stage compression model is used. After the first stage, a partial mass flow rate $\dot{m}_{\text{inj}}$ (state 5) is injected into the compressor. The injected mass flow rate arises from the expansion of a partial mass flow after the condenser to an intermediate pressure level and the heat transfer within the economizer (state 5). Due to the vapor injection, the cycle includes two additional degrees of freedom: (1) The intermediate pressure p_{int} of states 4 and 5 and (2) the injection ratio *y*, which is the ratio of injected vapor $\dot{m}_{\text{inj}}$, and total mass flow rate in the condenser $\dot{m}_{\text{con}}$.

$$y = \frac{\dot{m}_{\text{inj}}}{\dot{m}_{\text{con}}} \tag{4}$$

$$\vec{x}_{\text{vi}} = [p_{\text{eva}};\ p_{\text{con}};\ \Delta T_{\text{SH}};\ \Delta T_{\text{SC}};\ p_{\text{int}};\ y]^T \tag{5}$$

The injected mass flow rate at state 5 is assumed saturated vapor. Due to the two-step compression and vapor injection into the compression chamber, the cycle efficiency calculation is more complex than the simple heat pump cycle. Equation (6) shows the definition of the *COP* for the vi cycle.

$$COP_{\text{vi}} = \frac{h_2 - h_3}{(1 - y) \cdot \Delta h_{\text{com,step,1}} + \Delta h_{\text{com,step,2}}} \tag{6}$$

Thereby, $\Delta h_{\text{com,step}\,i}$ is the specific enthalpy difference due to the compression in step *i*. Since the mass flow within the evaporator and thus, the first compression step only includes a partial mass flow rate.

2.2. Seasonal coefficient of performance

To evaluate the annual energy consumption of a single-family house, we evaluate the seasonal coefficient of performance (*SCOP*). In this work, a weighting approach is used that divides a whole test reference year (TRY) into representative clusters. Here, we use the *k-medoids* clustering method [17] and a TRY of the city Aachen in Germany provided by the German Weather Service. A building energy model from the *AixLib* Modelica library calculates the heating demand of a defined operating point [18]. The building has a heating

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demand of 9.7 kW at nominal ambient air temperature. Equation (7) shows the resulting formula of the *SCOP*.

$$SCOP = \frac{\sum_i \dot{Q}_{\text{heating},i} \cdot \omega_i}{\sum_j \frac{\dot{Q}_{\text{heating},j}}{COP_j} \cdot \omega_j} \tag{7}$$

Here, the indices *i* and *j* indicate the selected cluster, ω_i is the weight of the cluster in hours, $\dot{Q}_{\text{heating},i}$ is heating demand of the building and thus, the condenser heat flow rate of the heat pump and *COP* is the evaluated *COP* for the defined flowsheet at the operating point of the cluster.

The temperatures of the source and sink, describing the operating point of the heat pump, are derived from the ambient air temperature given by cluster *i*. Additionally, a heat curve of a radiator system is coupled, using a nominal design temperature of 55/45 (supply temperature in °C / return temperature in °C), which is a common heating system in the German building stock. Thus, the heat pump operates at different working and load conditions.

The annual electricity demand $W_{\text{el,annual}}$ can be calculated using equation (8).

$$W_{\text{el,annual}} = \sum_j \frac{\dot{Q}_{\text{heating},j}}{COP_j} \cdot \omega_j \tag{8}$$

2.3. Total Equivalent Warming Impact

In addition to the energy evaluation, selected refrigerants and flowsheets are evaluated with regards to their environmental impact. Different approaches exist in the literature for this purpose. A comparatively simple estimation allows the calculation of the *Total Equivalent Warming Impact* (*TEWI*). The *GWP* evaluates refrigerants in terms of their direct emissions to the environment. This value indicates the global warming potential of the refrigerant, but does not take into account the actual amount of refrigerant released into the environment in case of leakage. In addition to the GHG emissions from refrigerant leakage, the *TEWI* also takes into account the GHG emissions from the electricity used to operate the heat pump. Thus, the *TEWI* considers direct and indirect emissions [9]:

$$TEWI = GWP \cdot m_{\text{ref}} \cdot (L_{\text{annual}} \cdot n + EOL) + (W_{\text{el,annual}} \cdot EM_{\text{GWP}} \cdot n) \tag{9}$$

Where L_{annual} is the annual refrigerant leakage, m_{ref} is the refrigerant mass, *n* is the system lifetime, *EOL* is the end of life refrigerant leakage, $W_{\text{el,annual}}$ is the annual electricity demand, and EM_{GWP} is the CO_2-emission factor of the electricity grid. The *TEWI* provides an approximation of the actual CO_2-emissions caused by a heat pump. However, this assessment method only covers the use phase and neglects further climate-relevant life cycle phases.

2.4. Life Cycle Climate Performance

To include further life cycle phase, an extension to the *TEWI* is the *Life Cycle Climate Performance* (*LCCP*). Compared to the *TEWI*, the *LCCP* includes further sources of equivalent GHG emissions. Like the *TEWI*, this is composed of direct (equation (11)) and indirect emissions (equation (12)) [19, 20].

$$LCCP = LCCP_{\text{DE}} + LCCP_{\text{IE}} \tag{10}$$

$$LCCP_{\text{DE}} = m_{\text{ref}} \cdot (n \cdot L_{\text{annual}} + EOL) \cdot (GWP + Adp.GWP) \tag{11}$$

$$\begin{aligned} LCCP_{\text{IE}} = {} & n \cdot W_{\text{el,annual}} \cdot EM_{\text{GWP}} + \sum_{i=1}^{n} \left(m_{\text{new},i} \cdot MM_i\right) + \sum_{j=1}^{m} \left(m_{\text{rec},j} \cdot RM_j\right) \\ & + m_{\text{ref}} \cdot (1 + n \cdot L_{\text{annual}}) \cdot RFM + m_{\text{ref}} \cdot (1 - EOL) \cdot RFD \end{aligned} \tag{12}$$

Here the additional variables stand for:

- *Adp.GWP*: *GWP* of the atmospheric decomposition products
- m_{new}: mass of the new material of the heat pump unit
- m_{rec}: mass of recycled material of the heat pump unit
- *MM*: emissions per kg of virgin material of the heat pump unit
- *RM*: emissions per kg of recycled material of the heat pump unit
- *RFM*: emissions from the production of the refrigerant
- *RFD*: Emissions from disposal of the refrigerant

The metric follows the so-called cradle-to-grave approach so that GHG emissions are captured regarding the entire life cycle. In addition to the GHG emissions captured by the *TEWI*, GHG emissions from energy contained in product materials and for refrigerant production, and disposal are also included. The additional parameters introduced in the *LCCP* supplement the *TEWI*, but account for only a small proportion in the overall analysis. However, *TEWI* and *LCCP* use equivalent GHG emissions and do not account for further assessment criteria that might be of importance to avoid misleading the fluid choice.

2.5. Life Cycle Assessment

The Life Cycle Assessment (LCA) includes all life cycle stages of a heat pump and introduces several assessment metrics. To utilize this method, first the overall goal of the assessment must be defined. In this case, the goal is the environmental evaluation of heat pumps and refrigerants in a single-family house in Germany. The LCA aims to investigate the influence of the refrigerant on environmental impact caused during the life cycle of a heat pump. Thereby, the environmental impact is divided into different environmental categories.

This work investigates the life cycle of an air-to-water heat pump (cf. section 2.1 and 2.6). The investigation focuses on the production of refrigerants and heat pump, the operation of the heat pump and the disposal (including a possible recycling). The function of the air-to-water heat pump is to provide space heating and domestic hot water over an observation period of 20 years, matching the heat pump's lifetime (cf. **Table 3**).

This study comprises four main environmental impact categories: global warming (GW), ozone depletion (OD), Photochemical Ozone Formation (POF) and Acidification (A). Overall, their normalized values (normalized by the maximum of each category) are weighted (cf. **Table 1**) and summed to one single LCA-value.

Table 1: Weighting factors for each environmental impact within the LCA.

Environmental impact	Weights in %
Global Warming (GW)	40
Ozone Depletion (OD)	30
Photochemical Ozone Formation (POF)	15
Acidification (A)	15

Since this work aims to compare multiple evaluation methods using the same overall technology, in this case the heat pump, these are the main environmental impact categories. In case different technologies should be compared, however, further impact categories are necessary to provide a full LCA and, thus, a proper ecologic comparison.

2.6 Case study

Within the present case study, we consider ten refrigerants of different fluid groups (hydrocarbons, hydrofluoroolefins, hydrofluorocarbons and chlorofluorocarbons) to account for several effects when evaluating the ecologic parameters. **Table 2** presents the selected refrigerants and their fluid properties.

Table 2: Properties of the investigated refrigerants [16, 21].

Refrigerants	Safety	GWP	Adp. GWP	ODP	T_{crit} in °C	ΔT_g in K
R436A	A3	3	0	0	115.89	7.2
R32	A2L	675	0	0	78.11	0
R1270	A3	2	0	0	91.06	0
R290	A3	3	0	0	96.74	0
R22	A1	1760	0	0.055	96.15	0
R410A	A1	1920	0	0	71.34	0.1
R454C	A2L	146	0	0	85.67	7.5
R134a	A1	1300	1.6	0	101.06	0
R404A	A1	3940	0	0	72.12	0.4
R1234yf	A2L	4	3.3	0	94.70	0

In addition to the refrigerant properties, further parameters for the ecologic assessment are necessary. Thus, **Table 3** provides an overview of the constant parameters.

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Table 3: Parameters for ecologic assessment. [2]

Parameter	Value
Temperature difference of source	5 K
Lifetime of heat pump (*n*)	20 a
Annual leakage rate (L_{annual})	2 %
Refrigerant mass (m_{ref})	2.5 kg
End of life leakage (*EOL*)	20 %
Heat pump mass (simple cycle)	150 kg

Due to missing data within the literature, the emissions due to the disposal of the refrigerants (*RFD*) are neglected, which is a similar approach to Wan et al. [20] and Yang et al. [2]. For the emissions due to refrigerant production (*RFM*), values of Hwang et al. [10] are used.

The heat pump itself has an assumed constant mass of 150 kg for all refrigerants. However, additional mass is added for the ihx and the vi cycle due to additional piping and further components (e.g. internal heat exchanger). The mass of the basic configuration (simple cycle) of the heat pump is split into four main materials: steel, aluminum, copper, and plastic. **Table 4** shows their share of the total heat pump mass in the basic configuration, their recycling material percentage, and their emissions during production. The additional mass for the more complex cycle configurations consists of copper (piping) and steel (heat exchanger) only.

Table 4: Share of materials with in the heat pump and their individual emissions during production [2, 10].

Material	Share of heat pump in %	Recycling percentage in %	Emissions virgin materials in $kg_{CO2\text{-}eq}/kg$	Emissions recycled materials in $kg_{CO2\text{-}eq}/kg$
Steel	46	29	1.8	0.54
Aluminum	12	67	12.6	0.63
Copper	16	40	3.0	2.46
Plastic	23	7	2.8	0.12

Lastly, equation (13) defines the specific grid emissions for the main investigation. The curve was derived by using the specific emissions of the German grid of the last ten years and predict the general trend for the next 20 years.

$$EM_{\mathrm{grid}} = 405 \cdot 0.9542^{year} \text{ in } g_{CO2}/kWh_{el} \quad (13)$$

In the equation, *year* represents the current lifetime of the heat pump starting with one. Besides equation (13), two constant values are used for section 3.5 to analyze the sensitivity of the results in section 3.2 to 3.4. Here, zero emissions and 50 g/kWh are selected to account for a grid that has no emissions at all and a grid that uses only solar generated power.

3. Results

The following section presents the results of the conducted case study (cf. section 2.6). Section 3.1 shows the results of the energetic assessment for all three investigated flowsheets. Afterwards, sections 3.2 to 3.4 show the results for the ecologic assessments using the energetic assessment of the ihx flowsheet. Finally, a sensitivity analysis is conducted to evaluate the influence of specific parameters on the ecologic assessment results.

3.1. *SCOP*

Figure 2 shows the results of the energetic assessment using the seasonal coefficient of performance (*SCOP*) of all three mentioned flowsheets using the boundary conditions stated in section 2.6.

For the simple cycle (grey bars), the pure fluid R32 shows the highest efficiencies with 3.82, whereas R1234yf shows the lowest efficiencies with 3.29. Besides R1234yf, the pure refrigerants show significantly higher efficiencies than the investigated mixtures. For the flowsheet with vapor injection (vi – blue bars) the absolute values for the efficiencies increase. Overall, the efficiencies increase by a mean value of approximately 6 %. The improvements mainly result from reduced throttling losses since only a partial mass flow rate must overcome the whole pressure difference. Additionally, the mean temperature in the condenser is reduced, leading to reduced losses due to heat transfer in the condenser.

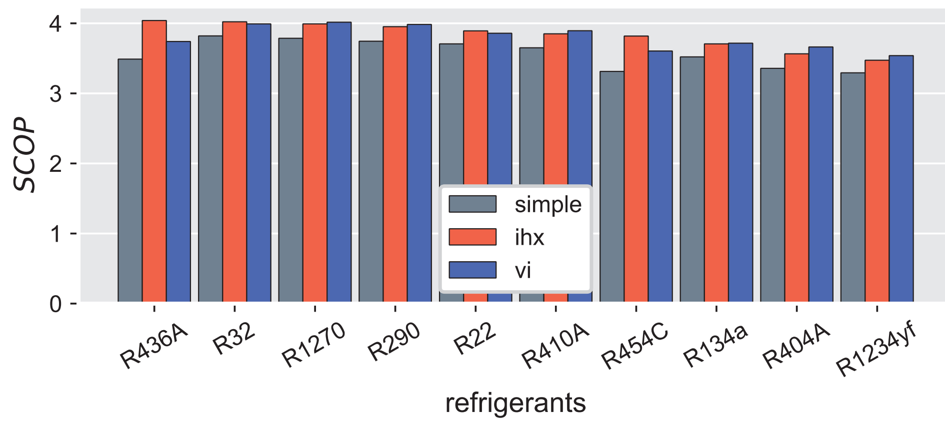

Figure 2: *SCOP* evaluation for the selected refrigerants within all three investigated cycle configurations. The refrigerants are sorted by their highest value in the ihx cycle.

In the vi cycle, the mixtures (e.g., R454C) show higher improvements (approx. 8 %) compared to the pure fluids (4 %). Nevertheless, the overall refrigerant ranking does not vary. Thus, R32 still shows the highest efficiency in the vapor injection cycle.

The ihx cycle (red bars) lead to the overall highest *SCOP* value. Additionally, the ranking of the refrigerants changes. Compared to the simple and vi flowsheet, R436A shows the highest efficiency of 4.04. Overall, the improvements range from approx. 16 % (R436A) to 5 % (R22) with much higher values for the zeotropic mixtures (e.g., R454C and R436A). Main reason for the higher improvements of zeotropic mixtures is the temperature glide (cf. **Table 2**) in combination with an internal heat exchanger. In the simple and vi flowsheet, the pinch point in the evaporator is located at the refrigerant outlet due to the amount of super heating necessary for a safe heat pump operation. Thus, the temperature glide of the zeotropic mixtures leads to a decrease in the mean temperature during heat transfer, increasing heat transfer losses and thus, lowering the efficiency. In the ihx flowsheet, however, the amount of superheating is shifted into the internal heat exchanger. Thus, the pinch point shifts to the evaporator inlet resulting in higher evaporation pressures and overall, higher efficiencies. For zeotropic mixtures, the increase in pressure can exceed the improvements of pure refrigerants due to the temperature glide, especially if the temperature glide matches the temperature difference of the heat source. Therefore, the observed improvements are higher for zeotropic mixtures following findings within the literature [12].

Since the highest differences occur when using the ihx cycle due to the utilization of the temperature glide of zeotropic mixtures, *SCOP* values of the ihx cycle are used in the following ecologic assessments to exploit the full potential of fluid choice. Additionally, the refrigerants will be sorted by their energetic ranking in the ihx cycle, starting with R436A with the highest *SCOP* and ending with R1234yf with the lowest.

3.2. *TEWI*

Figure 3 shows the results for the *TEWI* evaluation of the mentioned refrigerants separated by their cause. For the operational evaluation, the results of the *SCOP* using the ihx cycle are selected.

Similar to the energetic evaluation, R436A shows the best performance and leads to the lowest emissions with overall 18.950 kg_{CO2eq} emissions during the heat pump's lifetime. Additionally, the main contributor to the *TEWI* are the emissions related to the energy demand and thus, are proportional to the *SCOP* (cf. section 3.1). For the low-GWP (<150) refrigerants, the share of the emissions due to energy demand is 99 % and higher, proving that the direct emissions are negligible. For refrigerant with high GWP (e.g. R404A with a GWP of 3.940), the share is 75 %. Due to the high influence of the emissions due to the energy demand and thus, the influence of the indirect emissions due to the power generation in Germany, the additional categories do not lead to changes in the refrigerant ranking regarding the optimal refrigerant choice. Considering the ban on high-GWP refrigerants, the *TEWI* evaluation shows similar results compared to the assessment of the energetic efficiency *SCOP*. Thus, the *SCOP* is sufficient when selecting a refrigerant compared to the *TEWI* evaluation in case low-GWP refrigerants are studied that satisfy current regulations.

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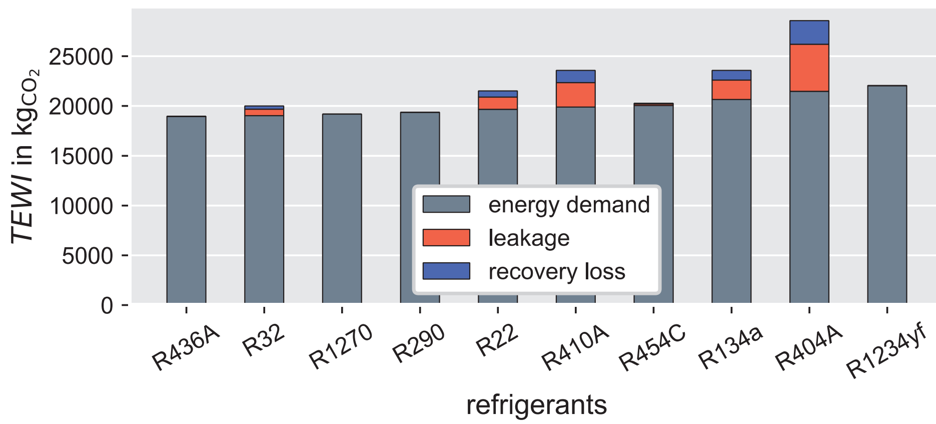

Figure 3: *TEWI* values for the investigated refrigerants. The value is split into each share regarding the emissions related to energy demand, leakage and recovery losses. The refrigerants are sorted by their *SCOP* value within the ihx cycle.

3.3. *LCCP*

Figure 4 shows the results of the *LCCP* evaluation. The results are divided into their individual categories and compared to the *TEWI* (cf. section 3.2).

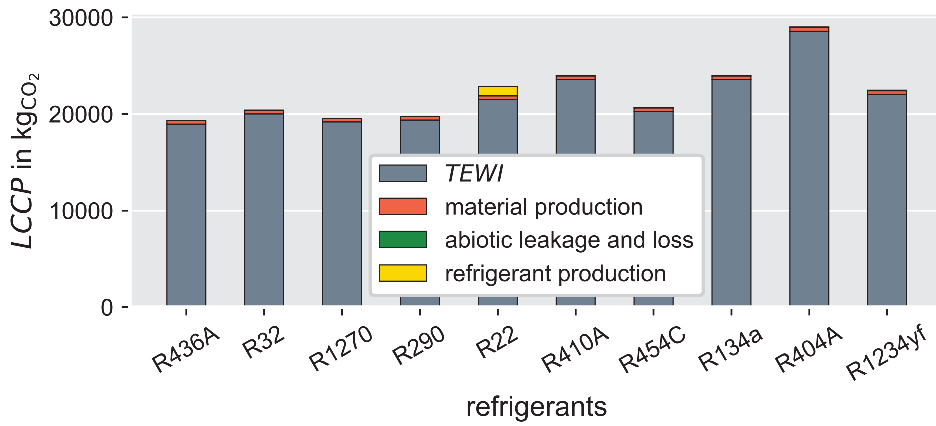

Figure 4: *LCCP* values for the investigated refrigerants. The bars show the share of the *TEWI* and the additional factors within the *LCCP* analysis. The refrigerants are sorted by their *SCOP* value within the ihx cycle.

Compared to the *TEWI*, the *LCCP* accounts for the CO_2-equivalent emissions of the lifecycle *cradle to grave*. However, the main differences between the *TEWI* assessment (grey bars) and the *LCCP* occurs for R22 since the production of R22 and the chemical reactions required have a high energy consumption as well as byproducts with high GWP values. The production of the materials of the heat pump shows only a minor influence on the *LCCP* of a heat pump with a defined refrigerant. Additionally, the composition and weight of a heat pump do not vary between the refrigerants in the current modeling approach leading to identical values. However, the differences in materials due to a refrigerant change and possible bigger components (e.g., larger heat transfer area) is negligible since the influence of the materials of a 150 kg heat pump is already below 1 % of the total emissions. Therefore, a significant influence regarding the CO_2-emissions is unlikely.

Overall, the *LCCP* results are similar to the *TEWI* and *SCOP* results especially for the low-GWP refrigerants. Thus, the more complex evaluation method is not required during a low-GWP refrigerant comparison. Additionally, the figure shows the results for the ihx cycle only. However, the total ecologic assessment conducted for this paper included the evaluation of all three flowsheets. The comparison of the selected flowsheets leads to the conclusion that the emissions due to additional components within the heat pump are negligible, if improvements in the energy efficiency occur. Thus, more complex flowsheet are always beneficial from a CO_2-emission related point of view as long as the *SCOP* improves.

Besides the CO_2-emissions, the construction and operation of a heat pump influences further environmental impact categories. Thus, the following section presents the results of the LCA, which accounts for multiple environmental impacts.

3.4. LCA

Figure 5 shows the results of the LCA analysis. The LCA value of a refrigerant is the sum of all normalized values in the individual environmental impact category multiplied with the weights in **Table 1**.

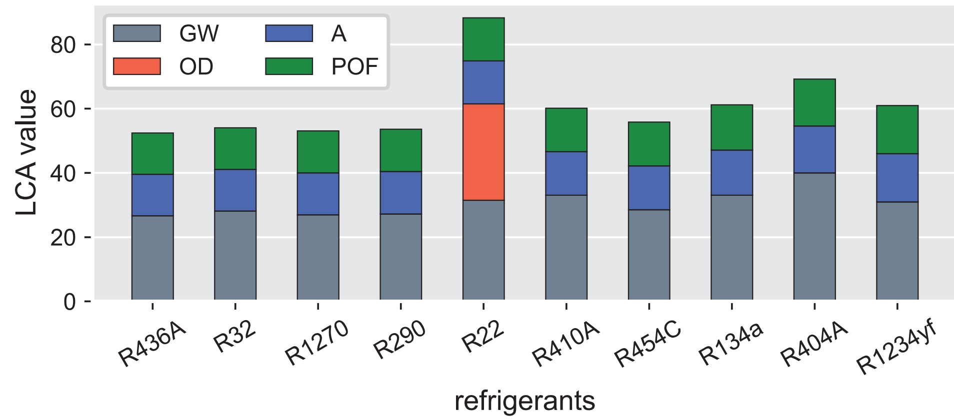

Figure 5: LCA values for the investigated refrigerants. GW: global warming, A: acidification, OD: ozone depletion, POF: photochemical ozone formation.

The most apparent difference compared to the previous results is the huge discrepancy between R22 and the other refrigerants due to the ozone depletion bar (OD – red). Since all other refrigerants have an ODP of zero the differences are to be expected and within the current regulation. Regarding the other impacts, no huge differences occur between the refrigerants. R436A still shows the lowest overall environmental impact and thus, is still favorable. The photochemical ozone formation (POF) and the acidification (A) of the refrigerants are mainly related to the power generation. Thus, the influence of the *SCOP* increases further.

To demonstrate the overall influence of the *SCOP* and the dependency of the environmental assessment criteria, **Figure 6** shows the normalized environmental functions (*TEWI*, *LCCP*, LCA) and the *SCOP*. Additionally, linear functions are included within the figure to show the overall trend.

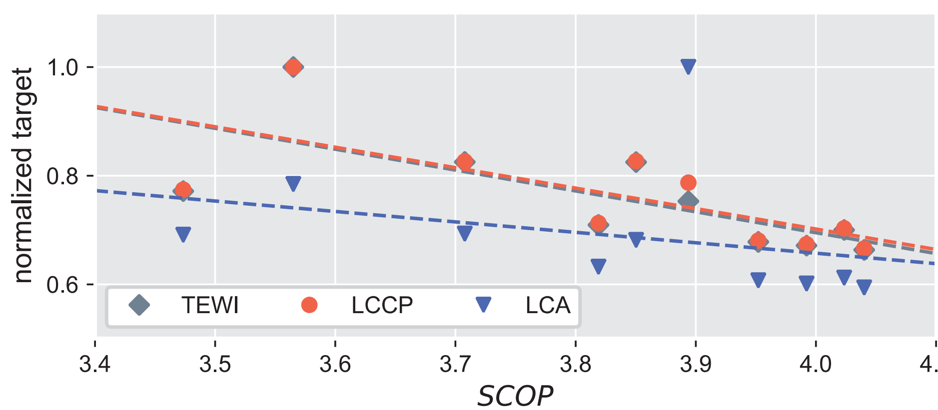

Figure 6: Correlation between the *SCOP* and the ecologic assessment parameters *TEWI*, *LCCP* and LCA. The ecologic parameters are normalized using the maximum value of the present investigation.

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The figure shows that the ecologic assessment criteria strongly depend on the *SCOP* and follow a linear curve. The highest differences occur for R22 in the LCA assessment since R22 has an ODP, which is not assessed within the *SCOP* and the energy demand related emissions. Nevertheless, all three linear regression curves offer a good fit for low-GWP and zero ODP refrigerants. Hence, using the *SCOP* offers an accurate assessment criterion when selecting a refrigerant under current regulations (ODP = 0 and GWP < 150).

Table 5 summarizes the results of a refrigerant selection in dependency of the investigated targets. The best performing refrigerant does not vary when the target function is adjusted. However, the ranking of the other refrigerants is offset.

Table 5: Overview of the refrigerant ranking in dependency of the target function.

	SCOP		***TEWI***		***LCCP***		**LCA**	
Ranking	Ref.	$\Delta SCOP$	Ref.	$\Delta TEWI$	Ref.	$\Delta LCCP$	Ref.	ΔLCA
1	R436A	0 %	R436A	0 %	R436A	0 %	R436A	0 %
2	R32	-0,4 %	R1270	1,2 %	R1270	1,2 %	R1270	1,2 %
3	R1270	-1,2 %	R290	2,2 %	R290	2,2 %	R290	2,2 %
4	R290	-2,2 %	R32	5,5 %	R32	5,6 %	R32	3,0 %
5	R22	-3,6 %	R454C	6,9 %	R454C	7,0 %	R454C	6,4 %
6	R410A	-4,7 %	R22	13,5 %	R1234yf	16,3 %	R410A	14,7 %
7	R454C	-5,5 %	R1234yf	16,3 %	R22	18,2 %	R1234yf	16,3 %
8	R134a	-8,2 %	R410A	24,4 %	R410A	24,1 %	R134a	16,6 %
9	R404A	-11,8 %	R134a	24,4 %	R134a	24,1 %	R404A	32,0 %
10	R1234yf	-14,0 %	R404A	50,7 %	R404A	50,1 %	R22	68,3 %

Since the energy demand related emissions strongly depend on the emissions during the power generation, the influence of the emissions factor is evaluated in the following section.

3.5. Influence of the power related emissions

The results of the ecologic assessment show that the environmental impact of a heat pump is mainly influenced by the energy demand. Thus, in the following the influence of the specific emissions related to the power generation is evaluated. Since the energy demand dominates the emissions due to the production and disposal of the heat pump for the German grid emissions (with average values of approx. 290 g/kWh – cf. equation (13)), **Figure 7** shows the influence of lower specific emissions on the *LCCP*.

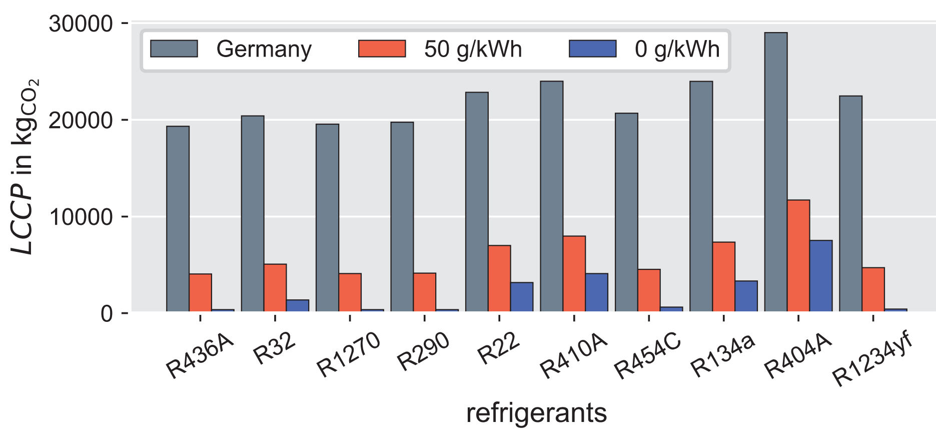

Figure 7: *LCCP* values for all investigated refrigerants using different specific grid emissions. The refrigerants are sorted by their *SCOP* value within the ihx cycle.

The grey bars show the results mentioned in section 3.3. When using a lower power with a lower specific emission ratio which results from the usage of only solar power (red bars – 50 g/kWh), the lifecycle related emissions decrease significantly due to the high influence of the energy related emissions. For most refrigerants, the decrease is similar to the reduction in grid related emissions (approx. 80 %). However, the best performing refrigerant does not change since R436A has a single digit GWP value (3) and the emissions related to material productions are similar for all refrigerants. Thus, the ranking does not change and, the *SCOP* has significant influence on the ranking due to the low GWP of most refrigerants.

Reducing the emissions to a net zero (blue) bars, the dependency on the *SCOP* is lost since no emissions occur due to the energy demand. Thus, the GWP is the main influencing parameter. However, current regulations demand low-GWP refrigerants leading to quite low emission rates. Due to the low energy related emissions, the impact on the environmental impact category of climate change is close to zero whereby other environmental impact categories become more dominant – e.g., material and water usage. Thus, for a zero-emission grid, ecologic assessment criteria based on CO_2 emissions only are insufficient. Nevertheless, there is no country currently with a net zero power grid. Therefore, the authors suggest that the *SCOP* is a sufficient evaluation category when selecting low-GWP refrigerants for a heat pump application.

4. Discussion

The investigations in section 3 show that a correlation between the environmental impact of a heat pump and its individual *SCOP* exists. Thus, the authors conclude that the *SCOP* is a sufficient evaluation criterion when comparing different refrigerants and heat pump systems for residential applications using current regulations regarding a low-GWP (<150) and a zero ODP. Since most electric grids over the globe have emissions higher than 100 g_{CO2}/kWh, which also will not change significantly within the upcoming decade, the described trend will be similar soon. Additionally, the effect increases for electric grids that have higher significantly emission rates than the mentioned 100 g_{CO2}/kWh, reducing the influence of leakages and production even further. Even for lower values (cf. section 3.5), the energy related emissions are more significant still compared to production and leakage related emissions. On top of that, a zero-emission electric grid does not imply that the systems efficiency (*SCOP*) can be neglected since lower efficiencies lead to higher power demand and thus, bigger infrastructure, which once again leads to emissions and the usage of other resources.

Besides the impact on global warming, there are further environmental impact categories of a heat pump, e.g., the mention resource usage. Within the conducted LCA, four out of 16 commonly used environmental categories were used and weighted individually. The results strongly depend on the selected weighting factors and thus, should be investigated further. Additionally, future studies should include further categories to assess the whole impact on the environment. Nevertheless, the selected categories show the strong impact of the *SCOP*.

In this regard, future investigations should include the analysis of more complex flowsheets that improve the cycle efficiency. The present study shows that the impact of the additionally components due to the more complex flowsheet is negligible as long as the cycle efficiency increases. However, additional target functions such as costs must be included in future analysis to assess the energy efficiency, environmental impact, and the economic aspects for a feasible transition towards a net-zero building sector.

Overall, the refrigerant R436A, which is a zeotropic mixture of propane (R290) and isobutane (R600a) shows the best ecologic performance when using a flowsheet with an internal heat exchanger. Additionally, the hydrocarbons R290 and R1270 lead to high efficiencies and thus, low environmental impacts. Furthermore, hydrofluoroolefins (HFO) show lower efficiencies than the hydrocarbons leading to a bigger environmental impact. Additionally, most HFOs lead to the formation of trifluoroacetic acid (TFA) when leaked into the atmosphere. The impact of TFA on the overall lifecycle performance was neglected within the study due to insufficient data. Thus, the actual ecologic performance of HFO will decrease when TFA formation is included in the lifecycle. Thus, the authors conclude that hydrocarbons pave the way towards long-term environmentally friendly solutions in residential heat pumps. Due to their high flammability (A3), however, additional safety measures must be implemented that might worsen the overall ecologic performance. The influence of the additional factors should be investigated in future studies.

5. Conclusions

In the present paper, the influence of the evaluation method with focus on ecologic assessment criteria on the selection of a refrigerant for heat pump systems is investigated. We apply four evaluation methods (*SCOP*, *TEWI*, *LCCP* and LCA) and study ten refrigerants, ranging from high to low-GWP refrigerants. The investigation shows that the main influence on the ecologic performance of a heat pump in a residential building in Germany is the energy demand and the related emissions. Thus, the *SCOP* is the key metric that is sufficient for the ecologic assessment. The key findings of the investigations are:

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1. Since *TEWI* and *LCCP* assess CO_2-equivalent emissions only, they strongly depend on the energy demand related emissions and thus, the *SCOP*.
2. When using low-GWP and zero ODP refrigerants, the *SCOP* is a sufficient assessment criterion when selection a refrigerant for a heat pump application.
3. Adjustments in the cycle configuration or the selected flowsheet that improve the *SCOP* are recommended since the overall emissions of the heat pump can be reduced. This effect is valid for specific power grid emissions of 50 g_{CO2}/kWh and higher.
4. The hydrocarbon zeotropic mixture R436A shows the overall best performance in combination with an internal heat exchanger flowsheet.
5. Further research regarding the influence of TFA and a more detailed LCA are necessary to validate all findings of the present work and over a proper comparison to other technologies, e.g., hydrogen related systems.

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