

Study of the heat pump for a passenger electric vehicle based on refrigerant R744

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Abstract Energy management plays a crucial role in cabin comfort as well as enormously affects the driving range. In this paper energy balances contemplating the implementation of a heat pump and an expansion device in battery electric vehicles are elaborated, by comparing the performances of refrigerants R1234yf and R744, from -20°C to 20°C . This work calculates the coefficient of performance, energy requirements for ventilation (from 1 to 5 people in the cabin) and energy required with the implementation of a heat pump, with the employment of a code in Python with the aid of Cool-Prop library. The work ratio is also estimated if the work recovery device recuperates the work during the expansion. Comments on the feasibility of the implementation are as well explicated. The results of the analysis show that the implementation of an expansion device in an heat pump may cover the energy requirement of the compressor from 27% to more than 35% at 20°C in cycles operating with R744, and from 15% to more than 20% with refrigerant R1234yf, considering different compressor efficiencies. At -20°C , it would be possible to recuperate between around 30 and 24%. However, the risk of suction when operating with R1234yf at ambient temperatures below -10°C shows that the heat pump can only operate with R744. Thus, it is the only refrigerant that achieves the reduction of energy consumption at these temperatures.

Keywords: R744 (CO_2); Heat pump; Battery electric vehicle; Thermal comfort

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1 Introduction

During the last ten years, the sales of battery electric vehicles (BEV) have considerably increased [1]. The studies also predict that 30% of passenger cars (PXR) in 2032 will be EVs, Rietmann *et al.* [2]. Given the increasing popularity of BEVs, it is necessary to find the whole HVAC (heating ventilation air conditioning) system that satisfies not only the thermal requirements but also complies with the most actual standards.

Findings show that BEVs are more appropriate for city driving (i.e. short distances and optimal speeds) but not for long trips or high-speed journeys without recharging options, Greaves *et al.* [3]. Even though the analyses have proved that today's electric vehicles can meet all travel needs on almost 90% of days from a single overnight charge, Kempton [4], there are still some challenges to be faced in order to improve the driving range of BEVs,

Even if the image and interest towards electric vehicles is rather positive, according to Klamut [5], there are still perceived limitations: too high of a purchase price, lack of sufficient information about them and unsatisfactory technical parameters, mainly the long time needed to recharge the battery and the insufficiently long distance with one recharge. It is necessary in the short term, as attested by Varga *et al.* [6], to achieve improvements in the energy efficiency of HVAC systems, since this has a dominant influence not only on the BEVs range, but also on the perception of the consumers, and it can negatively affect the consumers' perception of BEVs in contrast with IC (internal combustion) vehicles.

2 Heating system in internal combustion cars vs. electric cars

In internal combustion vehicles, the heating of the cabin is reached by the heating energy released from the radiator, by the means of hot water. In opposition, as in electric vehicles, the radiator is not present thus the heat exhaust is not possible, the employed system relies on the transformation of electric energy from the traction battery into heat. This compromises the safety and durability of the battery, by subjecting it to thermal stress on account of its charge and discharge cycling, Lajunen and Suomela [7]. The studies of Garg *et al.* [8] have moreover identified six critical gaps in the design of an efficient battery management system:

- uncertainty in the battery estimation,
- mechanical design of robust battery pack,
- emerging battery technologies,
- sustainable and manufacturable battery pack,
- unified and conceptual model,
- safe location for easy installation and replacement of the battery pack.

Despite of the recent reduction of the costs and weight, and the increasing popularity of the lithium-ion batteries, investigation revealed that management of the charging and discharging processes, CO₂ and greenhouse gases emissions, health effects, and recycling and refurbishing processes research are not yet settled in a satisfactory manner, Hannan *et al.* [9].

3 Proposed model

The heat pump's (HP) system in electric vehicles differs from the traditional one, by the substitution of the mechanical compressor for an electric compressor. The electric compressor shows not only lower indirect and direct contributions to the TEWI (total equivalent warming impact), Petitjean *et al.* [10] but also benefits from low fuel consumption and low emissions purposes, Guyonvarch *et al.* [11].

3.1 Electric flux of the proposed model

Figure 1 shows that the cabin thermal and ventilation requirements can be achieved thanks to the transformation of electric energy into heating energy.

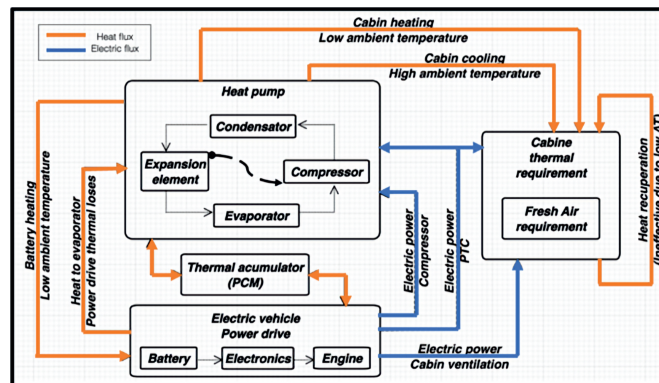


Figure 1: Energy flows within the proposed HP.

For fresh air requirements, the electric energy is simply transformed from the electric power drive of the BEV through the electric power ventilation.

3.2 Heat flux of the proposed model

Concerning the cabin thermal requirements of heating (when the ambient temperature is low) and cooling (when the ambient temperature is high), the electric energy from the battery can be transformed in two ways. The first way of transformation is directly through a PTC (positive thermal coefficient element) by Joule's first law. It means that all the energy will be directly taken from the battery. Another way for cabin conditioning is by the means of an HP, activated with an electric compressor. Only in cases when the heat pump is not operative, a PTC might be used. HP can provide heating and cooling to the cabin vehicle and decrease the electric requirements. The heat pump can also provide battery thermal conditioning to preserve the battery's life. The power drive thermal losses can also be redirected to the heat pump's evaporator to reuse this energy.

Another improvement can be reached by the implementation of a PCM (phase change material) that accumulates heat and protects the battery in a cost-effective way, Bashirpour-Bonab [12], Karimi and Li [13]. It was also reported that with the application of PCMs, the energy density of the battery pack would be increased, Kizilel *et al.* [14]. The studies of Agarwal and Sarviya [15], Ettouney *et al.* [16] placed the latent heat of the paraffin wax (a PCM widely utilized for automotive applications) for energy storage, between 176 and 210 kJ/kg (49–58 Wh/kg or 46–54 Wh/l). The energy density of a lithium-ion battery (LiB) is around 100–265 Wh/kg or 250–670 Wh/l. Those parameters are important at the moment of choosing one or another system, regarding the dimensions and size of it.

3.3 Heat pump operation, analysis, and improvements

The compression of the working fluid starts at the end of the evaporation, Fig. 2. The fluid leaves the evaporator in an overheated state, to avoid the injection of liquid into the compressor. The fluid is compressed from the pressure of the evaporator (P_{\min}) and enthalpy h_1 , until it reaches the pressure of the condenser (P_{\max}). During isentropic compression, the fluid at the end of the compression would reach a maximal temperature ($T_{\max}^{\text{isentropic}}$), yet in practice it is not possible given the irreversibility of the process. This means that the fluid will have the enthalpy h_2 and reach

a maximal temperature (T_{\max}) lower than $T_{\max}^{\text{isentropic}}$. Once the compression ends, the fluid enters the condenser until reaching the saturation curve in the liquid state. Then the fluid expands through a throttling valve, with an isenthalpic expansion after condensation, implying that the enthalpy at the end of the expansion (h_4) has the same value as it had at the beginning (h_3).

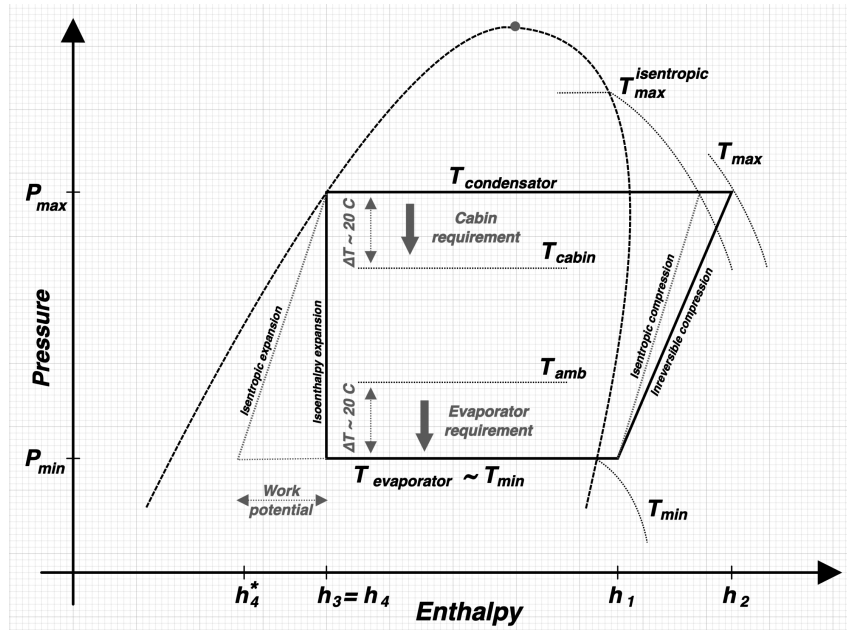


Figure 2: Diagram of an HP cycle.

The coefficient of performance (COP) of the heat pump (HP) is calculated by equation

$$\text{COP} = \frac{Q_{\text{cond}}}{W_c}, \quad (1)$$

considering the ambient temperatures (T_{amb}) of 10, 5, 0, -5, -10, -15, and -20°C. The atmospheric pressure (P_{atm}) of 1 atm is considered. The energy necessary for the evaporation is calculated by the means of the difference of enthalpy at the end (h_2^*) and at the beginning (h_3) of the condensation:

$$Q_{\text{cond}} = h_2^* - h_3. \quad (2)$$

The work of the compressor is obtained by the difference of enthalpy between the end of the compression (h_2) and the enthalpy at the beginning

of it (h_1),

$$W_c = h_2^* - h_1, \quad (3)$$

taking into account the real transformation (h_2^*)

$$h_2^* = \left(\frac{h_2 - h_1}{\eta_c} \right) + h_1. \quad (4)$$

The efficiency coefficient (η_c) of the electric compressor is considered in Eq. (4) between 0.75 and 1.0 and varies with a step of 0.05.

4 Choice of refrigerant

R134a (1,1,1,2-tetrafluoroethane) became popular as a substitution of R-12. With insignificant ozone depletion potential and a lower global warming potential (GWP), in comparison with the former standard automotive refrigerant R12, R134a presents similar thermodynamic characteristics.

However, the Kigali amendment report by the 28th Meeting of the Parties to the Montreal Protocol signed in 2016, Heath [17], reflects the global incumbency of the selection of the refrigerant, which visibly defines the intention of eradicating the employment of HFCs, among which R134a (GWP = 1430) is comprehended. Besides, an optimal replacement of R134a should not only have a lower GWP, but also a set of properties that fulfil the criteria of: a) enhancement of thermophysical compatibility, b) inflammability, c) low ozone depletion potential and d) cost-benefit.

4.1 R1234yf (2,3,3,3-tetrafluoropropene)

Refrigerant R134a is being phased out by R1234yf, given its similar thermophysical properties and its relatively lower 100-year direct global warming potential (GWP) of 4 and ozone depletion potential (ODP) of 0. It is also classified as a weakly flammable refrigerant (A2L) and low-toxic, according to the ASHRAE. If the safety conditions regarding the flammability of the R1234yf are met, this refrigerant can be charged into R134a systems and replace R134a, as it has adequate performance and good environmental properties, Lee and Jung [18], Ozgur *et al.* [19], Vaghela [20].

Despite the fact of the inconvenience of directly dropping R1234yf into an R134a system that will result in a notable change of pressure, Reasor *et al.* [21], researchers have found that a real enhancement of the cooling

capacity and COP can be reached with the introduction of an internal heat exchanger (IHX) Cho *et al.* [22], Direk *et al.* [23].

In addition to the implementation of the IHX, a system equipped with R1234yf requires a positive temperature coefficient (PTC) heater when the exterior temperature hits -10°C to compensate for the insufficient heat pump capacity. If a PTC heater is not employed, a bigger compressor is required, Feng and Hrnjak [24], Wu *et al.* [25].

4.2 R744 (Carbon dioxide)

Natural refrigerant R744, also known as CO_2 , started to generate interest already in 1834 when Evans and Perkins invented the vapour-compression cycle. Studies consider it the refrigerant of the future as well as a good option for applications with a big sink of temperature, Maina and Huan [26], Song *et al.* [27], Wu *et al.* [29], given its thermophysical properties, non-flammability according to ASHRAE, non-toxicity and considerably low GWP of 1 (when compared with R134a). However, Lorentzen [28] advocated that R744 is effective only when used in a transcritical cycle and encouraged its application in mobile air conditioning, where equipment space and weight is limited. Even if the thermodynamic properties of R744 are similar to these of R1234yf, R744 has a higher volumetric cooling capacity, which permits smaller components of the system, Großmann [29].

4.3 Transcritical cycle

R744 stands out thanks to its low critical temperature of 31.1°C . Above this critical temperature, the condenser will not effectively transfer heat. Moreover, since there is no condensation in the transcritical cycle, the condenser is respectively replaced by a gas cooler (GC). Since the CG is operating in the transcritical regime, it is of considerable relevance that the temperature is not constant during the cooling process. This means that GC not only suffers a temperature change but also an enthalpic difference at the end and beginning of the cooling, which difference is obtained by $h_2 - h_3$, in Fig. 3.

The advantages related to the high-pressure process include smaller equipment, which benefits the space-saving and good heating capacity at low temperatures, Wu *et al.* [24]. The transcritical process though is associated with high pressure. The pressure during a transcritical transformation is always higher than 73.7 bar. Hence, the components of the cycle are de-

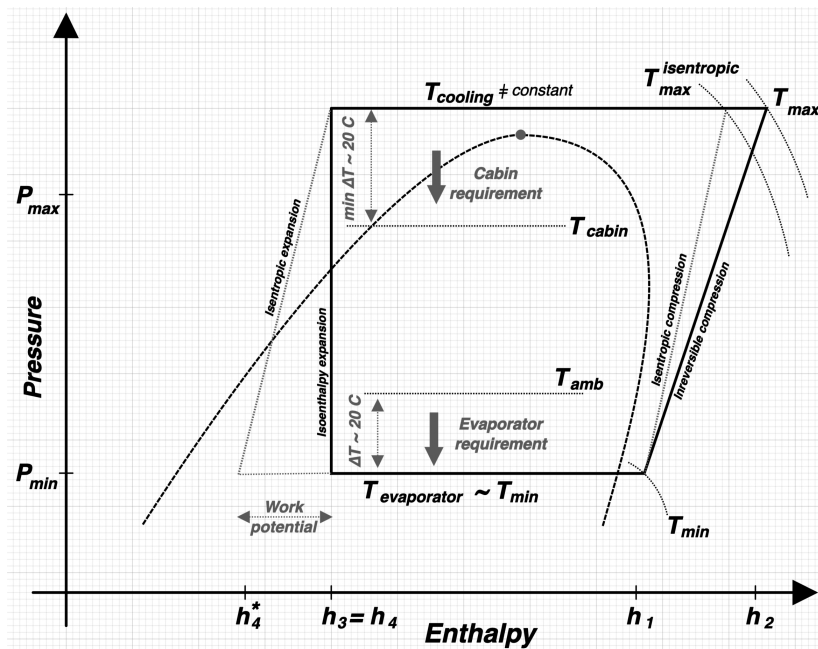


Figure 3: Scheme of classic behaviour of an HP operating in a transcritical cycle.

signed to work with this pressure. As a direct consequence, the components are costly, requiring attention to the safety.

4.4 Secondary loop

Modifications can improve the performance of the transcritical carbon dioxide up to the point to make it comparable with a conventional heat pump system, Ma *et al.* [30]. Among the adaptations, the most considered is the implementation of a dual loop that showed better performance in cold climates, Ma *et al.* [31], Menken *et al.* [32], Wang *et al.* [33, 34].

On the contrary, the dual loop does not exhibit good performance in warm climates and its addition to the system may cause worse regulation, giving the addition of extra elements to control. A summary of positive and negative characteristics of R134a, R1234yf and R744 is recapitulated in Table 1.

In this paper, the amount of heating energy in MJ per m^3 (v_e) for R1234yf and R744 will be estimated by equation

$$v_e = C_p \rho_2 T_m, \quad (5)$$

Table 1: Recapitulation of positive and negative aspects of R134a, R1234yf and R744.

Refrigerants' overview			
	R134a	R1234yf	R744
PROS	TDP similar to R12 ODP = 0 GWP _{R134a} < WP _{R12} (1400 _{R134a} < 10700 _{R12})	TDP similar to R134a ODP = 4 GWP = 4 Very low flammability = A2L Low toxicity Does not require total re-design of the system	Big sink of T ODP = 0 GWP = 1 Non-flammable Non-toxic Smaller components, given higher volumetric cooling capacity
CONS	HFC	PTC needed at low temperature ^o	Only efficient when operating at trans-critical cycle, requires redesign of the system

TDP – thermodynamic properties

where C_p is the latent heat at constant pressure of the refrigerant in consideration (in J/kgK), ρ_2 is the density at the end of the compression in kg/m³, and T_m is the logarithmic mean temperature difference. In order to compare how HPs with different refrigerants need to be replenished with additional heating when all the heat requirements are not covered. The radius ratio of the pipeline (R) is consequently calculated by

$$R = \sqrt{\frac{v_e^{\text{R1234yf}} + v_e^{\text{R744}}}{2}} \quad (6)$$

and the logarithmic mean temperature difference T_m at a counterflow process is found from equation

$$T_m = \frac{T3 - T_{\text{amb}} - T2 + T_{\text{cab}}}{\ln\left(\frac{T3 - T_{\text{amb}}}{T2 - T_{\text{cab}}}\right)}, \quad (7)$$

where $T3$, $T4$, T_{amb} , and T_{cab} are the temperatures at the end of condensation, at the end of expansion, ambient and cabin, respectively in K.

5 Work recovery expanders

It is possible to obtain work potential from the difference of enthalpy ($h_3 - h_4^*$) at the end of isentropic expansion when performed through an ideal device that makes possible the work recovery.

Throttling valves are traditionally used to expand the fluid, in order to lower the pressure at the end of condensation. However, exergy analysis made by Bruno *et al.* [35] showed that the expansion process during the transcritical operation is the process that contributes to the largest exergy destruction in the CO₂ cycle.

Studies of Baek *et al.* [36], Ferrara *et al.* [37], Kohsokabe *et al.* [38], Ma *et al.* [30] reported that the implementation of an expander unit, in replacement of the valve, leads to an improvement in COP of a CO₂ cycle under transcritical operation, in some cases similar to traditional heat pumps.

The work potential of the expander, defined by relation

$$W_e = h_4^* - h_4, \quad (8)$$

is the enthalpic difference between h_4 and the result of the isentropic transformation h_4^* . This work potential is compared with the energy necessary for the compression

$$\text{Work ratio} = \frac{W_e}{W_c}. \quad (9)$$

6 Ventilation and energy requirements

The ventilation requirements are calculated according to the Czech regulation 20/2012 of January the 9th, 2012 concerning the technical requirements on constructions. This regulation establishes the minimal air exchange rate with external air at 20 cubic meters per hour per passenger. The air exchange rate assumed in this paper will be 30 m³ per hour per occupant of the vehicle cabin.

Thus, the ventilation work will be given by

$$\dot{Q}_{\text{air.exchange}} = N \rho_{\text{air}} \text{rate}_{\text{air}} C_{p\text{air}} \Delta T_{\text{ex}}, \quad (10)$$

where $\dot{Q}_{\text{air.exchange}}$ is the energy, necessary for the air exchange in function of the number of people in kW; N is the number of people; ρ_{air} is the density of the air equal to 1.225 kg/m³; rate_{air} is the recommended air exchange rate of 30 m³ per hour per occupant of the vehicle cabin; $C_{p\text{air}}$ is the specific heat capacity at constant pressure of air of 1.00 kJ/(kgK) [39]; ΔT_{ex} is the difference in temperature between the cabin and exterior in K.

The optimal temperature difference is established at 20°C, given that bigger differences might affect the constructive materials and parameters.

The pressure at the evaporator is calculated given that under certain conditions of temperature, the risk of suction might appear when the pressure in the evaporator is lower than the atmospheric pressure.

The result obtained by Eq. (10) is divided by COP of the heat pump in the worst condition. This means that the compressor works at an efficiency of $\eta_c = 0.75$. Then, to this result, a minimal ventilation requirement of 0.1 kW is added to make the air flow through the system, as expressed by

$$P_{HP} = \frac{\dot{Q}_{\text{air.exchange}}}{\text{COP}_{(0.75)}} + 0.1. \quad (11)$$

Studies of Abas *et al.* [40] reported that following the international tendencies and agreements to preserve the environment, natural refrigerants (CO_2 , NH_3 , HCs) and a few synthetic media (R-152a, R-1234yf) are optimal options for modern refrigeration, air conditioning and heat pumping systems. For the transcritical cycle, the compressor works up to 100 atm. Ammonia, hydrocarbons and R-152a are not analyzed in this paper, given that they do not meet all the safety criteria (flammability and toxicity, among others).

The equations of state and parameters that are used for the purpose of this paper are limited to those of R744 and R1234yf. As listed in the documentation of CoolProp library by Bell *et al.* [41], the calculations are based on the results obtained by Richter *et al.* [41], Span and Wagner [42], for R1234yf and R744 respectively.

7 Results and discussion

7.1 Coefficient of performance

Results of COP estimations are summarized in Fig. 4 for R1234yf and R744, correspondingly. Each line represents the operation of the compressor affected by its performance. As expected from various studies, Fukuda *et al.* [43], Großmann [29], Shin and Cho [44], COP of both refrigerants is comparable at moderate temperatures, with COP of R1234yf becoming better at higher temperatures, in comparison with R744.

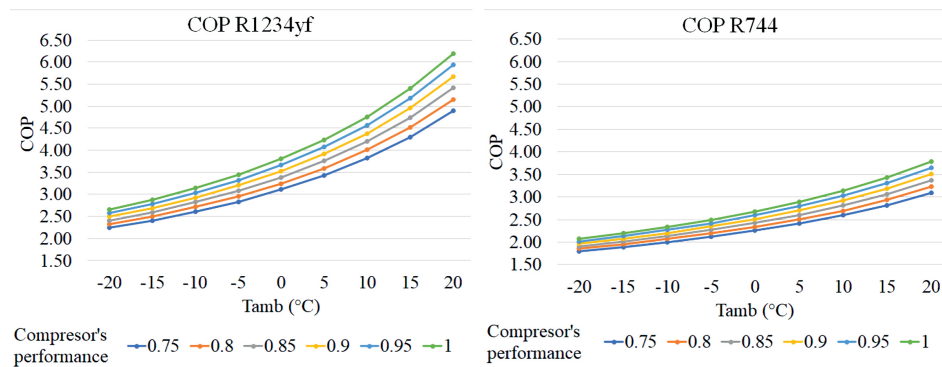


Figure 4: Comparison of COP of HP operating with R1234yf and R744 refrigerants at different temperatures and compressor performances of 0.75, 0.8, 0.85, 0.9, 0.95, and 1.00.

7.2 Energy density comparison for R1234yf and R744 in MJ per cubic meter

From the estimation of the energy density, it is also possible to detect that R744 has greater values of energy density than R1234yf. Figure 5 shows the energy density of both refrigerants in a range of temperatures between -20°C and 20°C , with steps of 5°C . It is notorious from this exposition that R744 maintains a greater energy density than R1234yf in the whole range of study of this paper.

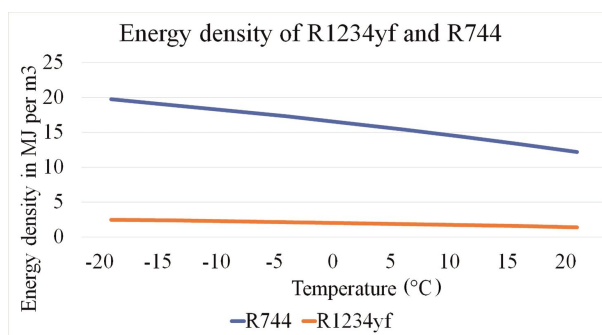


Figure 5: Energy density in function of the temperature of R1234yf and R744.

As for the radius ratio of the pipes, the results shown in Fig. 6 reveal that the mean radius ratio is about 3 times smaller in systems operating with R744 than in those operating with R1234yf.

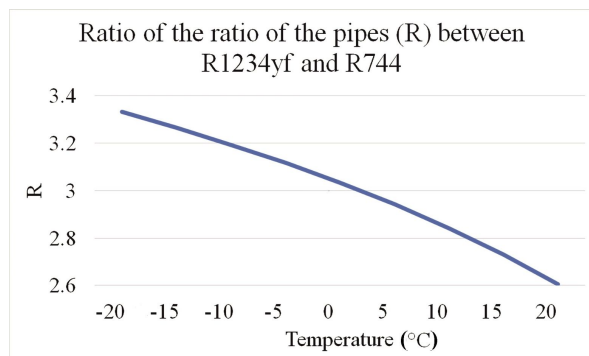


Figure 6: Pipe radius ratio for R1234yf and R744.

7.3 Ventilation energy requirements

In Fig. 7, it is possible to appreciate that, when the ambient temperature drops to -10°C , the pressure at the HP operating with R1234yf descends below the atmospheric pressure. This behaviour represents the technological risk of suction and is not appreciated in an HP operating with R744.

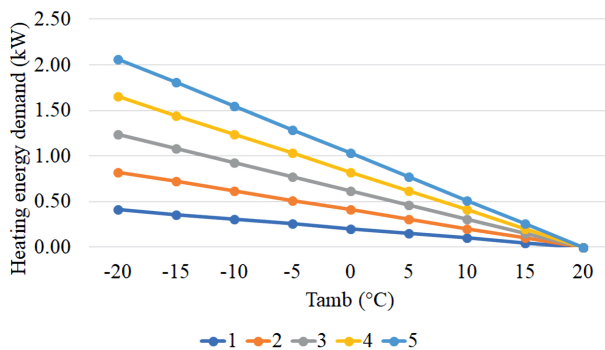


Figure 7: Heating energy requirements without implementation of HP.
The energy is entirely provided by the battery.

7.4 Implementation of an HP and electric energy demand

The effects of implementation of a heat pump, as per Eq. (11), are shown in Fig. 8 for R1234yf and R744. Given the technical supposition that a cycle operating with R1234yf will require the evaporation pressure to attain a value below the atmospheric pressure when outside temperatures drop below the -10°C , the COP will be considered 1 at this temperature. From

the obtained results, it is noticeable that the energy requirement is bigger when functioning at temperatures below -10°C with R1234yf because is not possible to operate, given the risk of suction.

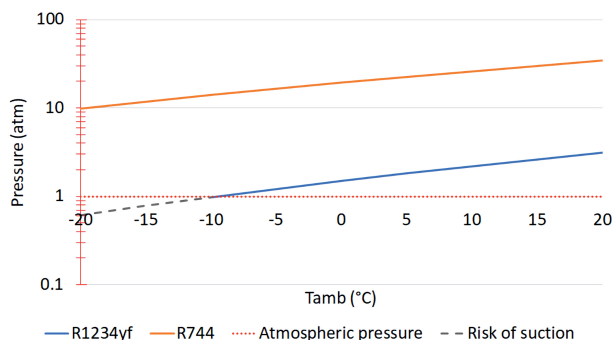


Figure 8: Pressure variation in function of the ambient temperature. When the cycle operates below -10°C with R1234yf, the risk of suction is shown for pressures below the atmospheric pressure.

7.5 Work potential

The difference of enthalpy, with the addition of an expansion device, imposes a work potential. The energy ratio between W_e and W_c for R1234yf and R744 is shown in Fig. 9, considering T_{amb} and working with different compressor performances. In these results the positive increment of the work potential ratio with the temperature is noticeable when operating with R744, but not with R1234yf. The latter one shows a decrement in work potential, while the temperature increases.

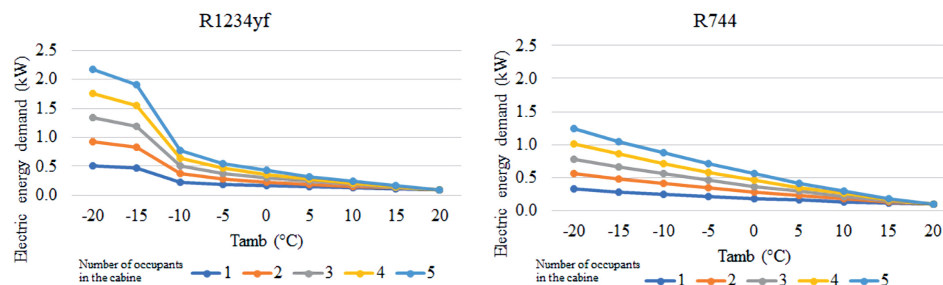


Figure 9: Electric energy requirement with the implementation of HP operating with R1234yf and R744.

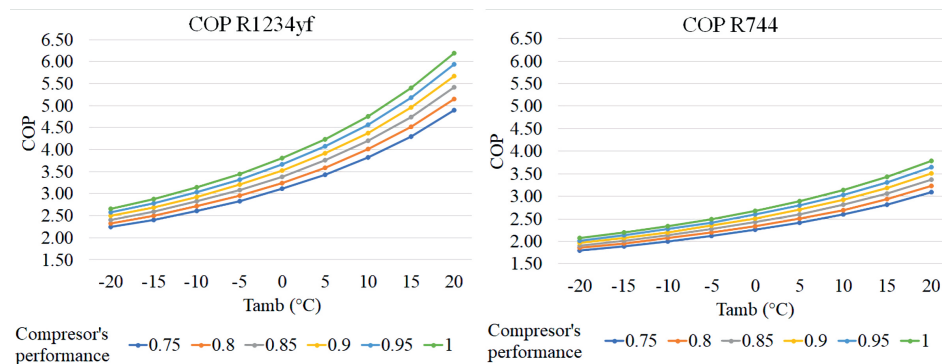


Figure 10: Work potential estimation of HP with R1234yf.

8 Conclusions

The rapid increase of sales of electric vehicles during the last years proves the interest on the market. However, the Achille's heel of the technology is still the electric energy consumption for cabin heating, ventilation, air conditioning and drive range, especially in low ambient temperature conditions.

The present paper analyzed and calculated systems and materials that serve to reduce the electrical consumption in electric vehicles for passenger use. The paper focused on the heat pump operating with CO_2 in comparison with cycles operating with R1234yf. The considered range of ambient temperature extends between -20°C and 20°C . Within this range, the properties were obtained with the aid of Python library CoolProp and then applied to the equations. Regarding the comparison between the refrigerants, coefficient of performance was calculated. Also, energy density, pipeline radius ratio and other ventilation energy requirements with the implementation of an HP were estimated.

The implementation of a work recovery element was correspondingly calculated and discussed. In parallel, phase change materials were contemplated for their application in electric vehicles. The compensation of factors such as the ambient temperature, number of passengers and driving cycle (urban, country, highway) increases the vehicle power consumption up to 5–20%, if achieved with the sole implementation of a positive thermal coefficient.

The alternative strategy is to use a heat pump and air conditioning for heating and cooling the cabin, respectively. The current research focuses on cycle optimization and using alternative refrigerants. Refrigerant R1234yf

is currently used and is suitable from a thermodynamic point of view until the ambient temperature reaches -10°C . For heating below -10°C the evaporator suffers a negative pressure, which is not achievable from a technological point of view, due to the risk of ambient air suction.

This limitation does not reach R744. The low-pressure loop is over-pressured at an extremely low ambient temperature. Moreover, the use of R744 as refrigerant means a 4 times smaller pipeline cross-section due to its higher density. Heat pumps based on R744 can be constructed as very compact devices. The small size and high efficiency at the extremely low temperature is an advantage of R744, in contrast with the disadvantage of high pressure and temperature requirement. This problem can be significantly amended by using an indirect cycle. The first loop tolerates high pressures and temperatures, based on R744. The second loop comprises the low-pressure cycle and is based on water with glycol as a running fluid.

The study presents the basic energy balance. We note that the dominant heat requirement is for the heating of fresh air. This part of heat requirement depends on the number of passengers, and it is typically 60–70% of the overall heating requirement. The second part of the heating requirement (40–30%) depends on the quality of cabin thermal isolation and not on the number of passengers.

Several studies focus on heat pump cycle optimization. One of the discussed modifications is using an expander, instead of an expansion valve. This paper presents the theoretical potential of expander work as a ratio between the work gained with the expansion device and the compressor demand, which can be used as recovery energy for the electric compressor of the cycle. Nevertheless, it is necessary to be aware of the fact that removing the work from the cycle is translated into an increase in heat demand for the evaporator. In the situation when there is not enough heat for the evaporator, there is no reason for expansion through a power recovery expander.

The work is also focused on phase change material (PCM) applications. This strategy starts to be reasonable from the moment that PCM allows for a higher energy density, in comparison with the BEV battery, which is currently about 100–265 Wh/kg. Another aspect of using PCM can be its volumetric density. The typical value of Li-Ion battery is in the range of 250–670 Wh/cm³. PCM seems to be far from such parameters and its deployment should be assessed from a point of view other than the weight and volume of its installation. An alternative can be thermal storage based on the chemical reaction, but this technology is not mature yet.

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