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# Simulation of a scroll expander using R1233zd(E), R1234ze(Z) and their mixtures as drop-in replacements for R245fa

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## Abstract

This paper presents simulations of the performance of a 2 kW hermetic scroll expander, based on a model reported in literature, when replacing the original working fluid (R245fa) with fourth-generation refrigerants.

Calculations of micro organic Rankine cycles, equipped with the selected expander, show a slightly better performance when using R1234ze(Z) or R1233zd(E), as drop-in replacements of R245fa. Binary mixtures, characterized by a non-isothermal phase-change behavior, are considered as well. In particular, results of mixtures depend on the fluid temperature at the expander inlet. The most relevant result is that the mixture process for some hydrofluoroolefins causes a decrease of the maximum cycle temperature, after setting a fixed expander power output, and therefore the possibility of exploiting heat sources at lower temperatures.

## 1. Introduction

The organic Rankine cycle (ORC) is a technology for mechanical energy production with growing interest in the last few years due to its potential integration in distributed generation systems and its favorable characteristics to exploit low-temperature heat sources [1]. One of the main advantages is the possibility of matching the ORC operation to the heat source and heat sink characteristics by means of the selection of the working fluid among a considerable set of substances. ORC systems are successfully used in several geothermal and biomass-fired power

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plants, but there is also a great interest in ORC utilization to exploit waste heat and exhaust gases of combustion turbines and reciprocating engines as well as solar thermal energy.

As a core component of the ORC system, the expander has a vital role in the overall system performance. In general, expanders can be categorized into two types: the first is the dynamic type, such as axial turbine expanders; the second is the volumetric type, such as scroll expanders [2]. Currently, expanders with kW scales for organic working fluids are under development and demonstration. As a matter of fact, several types of commercial scroll machines can be modified into expanders and integrated into ORC systems for low grade heat recovery. In particular, numerous researchers [3] have investigated the performance of scroll expanders resulting from original hermetic refrigeration compressors, automotive air-conditioning compressors and open-drive scroll air compressors.

Paying attention to the specific experiments with scroll-type expanders, R123 and R245fa are the most tested working fluids, in spite of the non-zero ODP of R123 and the significantly high GWP of R245fa (around 1000). With reference to the latter, recent researches have proposed fourth-generation refrigerants as drop-in replacement. These relatively new fluids have zero ODP, a GWP value less than 6 [4] and an ALT of less than thirty days.

This paper aims at simulating the performance of a 2 kW hermetic scroll expander for use in a micro-scale Rankine cycle when replacing the original R245fa with fourth-generation refrigerants such as R1234ze(Z) [4,5] and R1233zd(E) [6] and even mixtures of hydrofluoroolefins.

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**Nomenclature**

ALT       atmospheric lifetime
AU        heat transfer coefficient, $W \cdot K^{-1}$
GWP       global warming potential
L         specific length, m
$\dot{m}$       mass flow rate, $kg \cdot s^{-1}$
Nu        Nusselt number
ODP       ozone depletion potential
ORC       organic Rankine cycle
Pr        Prandtl number
Re        Reynolds number
λ         thermal conductivity, $W \cdot m^{-1} \cdot K^{-1}$

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## 2. The expander model

The scroll expander simulated in the current paper is the one previously investigated by Lemort et al. [7].
As shown in Fig. 1, the evolution of the working fluid (R245fa) through the expander is decomposed into a number of consecutive steps: an adiabatic pressure drop (su → su,1) and an isobaric cooling down by contact with the metal
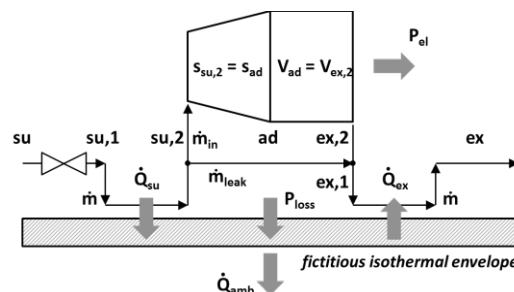


Fig. 1. Schematic representation of the expander simulation model

mass of the machine (su,1 → su,2) during the intake process; a first isentropic expansion down to the adapted pressure imposed by the built-in volume ratio of the machine (su,2 → ad) and a second adiabatic expansion at constant machine volume (ad → ex,2); an adiabatic mixing between the flow rates $\dot{m}_{in}$ and $\dot{m}_{leak}$ (ex,2 → ex,1) to account for leakages; an isobaric exhaust cooling down or heating up (ex,1 → ex). $P_{loss}$ in Fig. 1 takes into account both mechanical losses due to friction between moving elements (scrolls, journal bearings, Oldham coupling, thrust surface) and electromechanical losses in the asynchronous machine. $P_{el}$ is the electric power output. Reference to Lemort [8] is made here for a thorough description of the semi-empirical modelling approach. Although a more physically sound modelling can be proposed as regards mechanical and ambient heat losses [9,10], the model adopted by Lemort et al. [7] for the simulation of the 2 kW hermetic scroll expander is reliable with a maximum deviation between the prediction and the measurements of 2% for the mass flow rate, 6% for the power output, and 2 K for the exhaust temperature. In addition, the applicability of the model is sufficiently wide as regards the ranges of fluid pressure at the expander inlet (from 2 to 35 bar) and of pressure ratio (from 2 to 20) [7].

In order to simulate the performance of the expander in case of other working fluids, the procedure proposed and adopted in a former work [11] is here applied. In particular, based on the geometry of the expander, only heat transfer coefficients should be varied when changing the working fluid. Lemort et al. [7] proposed the following formula for calculating the heat transfer coefficient:

$$AU = 30 \cdot \left( \frac{\dot{m}}{0.1} \right)^{0.6}$$ (1)

where $\dot{m}$ and 0.1 (kg/s) are the mass flow rate and a reference value for normalization, respectively. Based on the consideration that orifices, flow passage areas and the general geometry of the scroll expander do not vary when changing the working fluid:

$$AU \propto \frac{Nu \cdot \lambda}{L} \propto Re^x \cdot Pr^y \cdot \lambda$$ (2)

where $Re^x \cdot Pr^y$ is introduced in place of the Nusselt number. According to Eq. (2) and considering the specific working fluid, the heat transfer coefficients can be reasonably revised by leaving intact the original structure modelling the expander, as adopted in a former work [11]. Further specific details on the overall modelling are reported in Refs. [7,8,11], here referred to for the sake of brevity. REFPROP 9.1 [12] has been used to include the thermodynamic and transport properties of the working fluid in the calculation environment implemented in the MATLAB® platform.

## 3. Results

This section presents the results of simulations of micro-ORC systems powered by the 2 kW scroll expander. As the main calculation assumptions, (i) the overall efficiency of the pump is set at 0.5, (ii) the pressure losses in both evaporator and condenser are neglected and (iii) the minimum fluid (condensation) temperature is set at 40°C without liquid subcooling. Thus, the calculation continues until the evaporation pressure corresponding to a determined power output from the expander is reached.

The model proposed by Lemort et al. [7] was validated for a certain degree of fluid superheating at the expander inlet. Thus, according to the above-mentioned assumptions, Fig. 2(a) reports the cycle efficiency for four levels of electric power output (1, 1.33, 1.67 and 2 kW) from the expander in case of two degrees of R245fa superheating (5 and 10 K) at the expander inlet. It is possible to appreciate that the figure of merit is shifted to the right by around 5 K in the case of higher superheating, but cycle efficiency variations are really negligible. Thus, the fluid superheating should be limited in order to use a heat source with a temperature as low as possible, e.g. a solar-based application [13]. According to this first result, the fluid superheating is set at 5 K in the following analysis.

Fig. 2(b) reports the cycle efficiency as a function of fluid temperature at the inlet of the expander for four levels
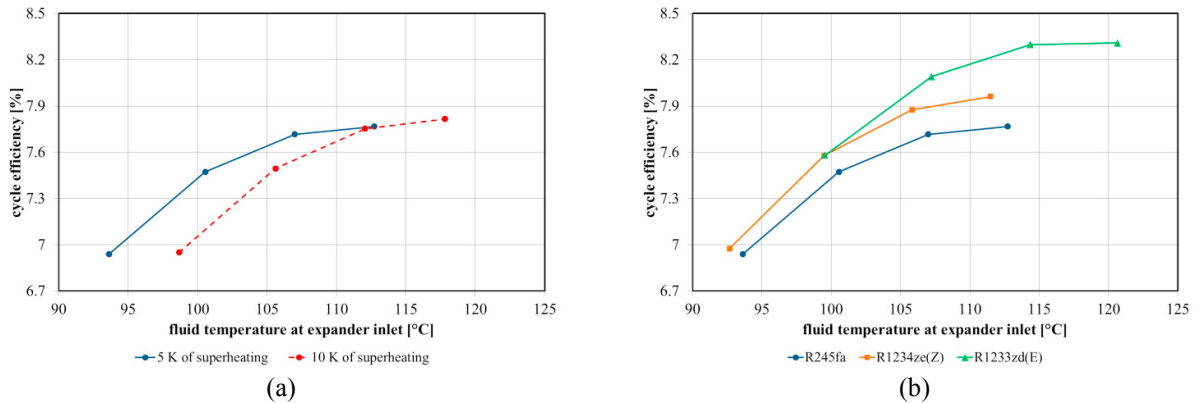
Fig. 2. (a) Cycle efficiency as a function of the fluid (R245fa) temperature at the expander inlet for four levels of electric power output from the expander (1, 1.33, 1.67 and 2 kW); (b) cycle efficiency as a function of the fluid temperature at the expander inlet (5 K of superheating) for four levels of electric power output from the expander (1, 1.33, 1.67 and 2 kW).

of expander power output (1, 1.33, 1.67 and 2 kW). Based on the calculations, R1234ze(Z) seems to perform even better than R245fa. As a matter of fact, a modest improvement of the cycle efficiency seems to be possible, even with a slight reduction of the fluid temperature. In case of operation with R1233zd(E), the cycle efficiency is greater but an increase of 6 to 8 K in the maximum cycle temperature is necessary for an electric power output from the expander ranging from 1 to 2 kW. These first simulations confirm that both R1234ze(Z) and R1233zd(E) are interesting drop-in replacement fluids for R245fa.

In order to extend the operation temperature range for the specific expander selected as the test case, other working fluids are taken into account. The REFPROP database include other two fourth-generation refrigerants, namely R1234yf and R1234ze(E). Thus, binary mixtures of R1234yf, R1234ze(E), R1234ze(Z) and R1233zd(E) are considered in the next analysis, even though no mixture data are available in the REFPROP database for such binary pairs and the mixing parameters have been estimated [12]. Thus, the next results should be considered as a preliminary assessment of performance trends.

Fig. 3 shows the results of the calculations of the cycle efficiency as a function of the fluid temperature at the expander inlet for four expander power outputs. Focusing on each curve, the two extreme points refer to the performance in case of pure fluids, whereas the other nine points consider nine mixtures (for each binary pair) with a 10 to 90 wt.% content of the first substance compared to the second in the pair (with a fixed step of 10 wt.%). Of course, the performance of each binary pair moves up and to the right in case of higher power output from the expander. Based on the results in Fig. 3, R1234yf and R1234ze(E) can be considered in case of reduced maximum cycle temperature, even though the lower the maximum cycle temperature, the lower the corresponding cycle efficiency. According to an increasing maximum cycle temperature, the calculations suggest the best binary pair as R1234yf-R1234ze(E), then R1234ze(E)-R1234ze(Z) and finally R1234ze(Z)-R1233zd(E).

As a result of the simulations, the cycle efficiency in Fig. 3 is not always a strictly monotonic function of the maximum cycle temperature. This is justified by focusing on possible mixtures of R1234yf and R1233zd(E), as an example. Fig. 4 presents some cases corresponding to 1 kW of electric power output from the expander in T-s diagrams. It is possible to appreciate that increasing the percentage of R1233zd(E) in the binary mixture results in larger cycle area, as well as in higher cycle efficiency, as shown in Fig. 3(a). The phenomenon of the temperature glide is evident during the evaporation and the condensation processes of the mixtures and the cycle efficiency initially increases with the temperature at the expander inlet in case of higher content of R1233zd(E) in the mixture. The case of pure R1233zd(E) presents the larger cycle area, but is characterized by a slightly lower maximum cycle temperature than the other case in Fig. 4(b). On the other hand, the case in Fig. 4(b) referring to the mixture presents an average evaporation temperature slightly lower than the case with pure R1233zd(E) and an average condensation temperature higher than 40°C.
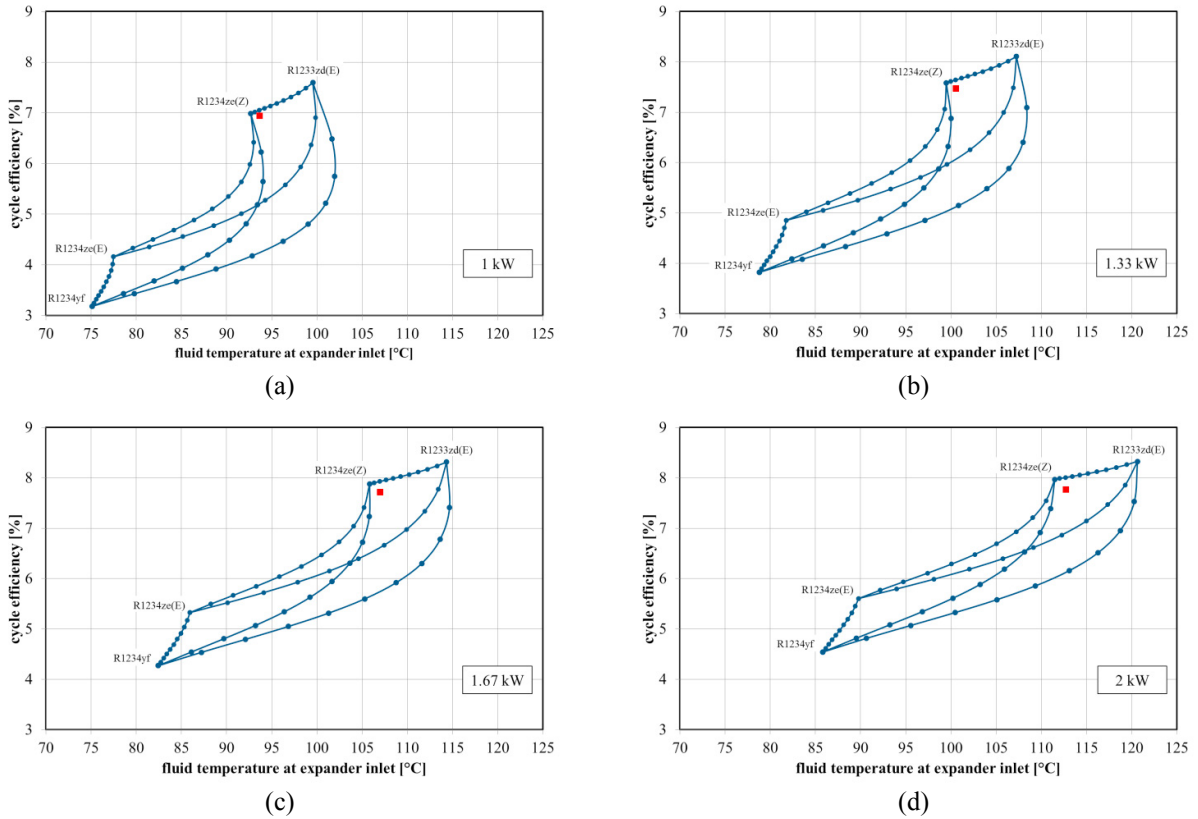
Fig. 3. Cycle efficiency as a function of the fluid temperature at the expander inlet for four electric power output from the expander (1, 1.33, 1.67 and 2 kW). The square refers to the result obtained with R245fa as the working fluid.
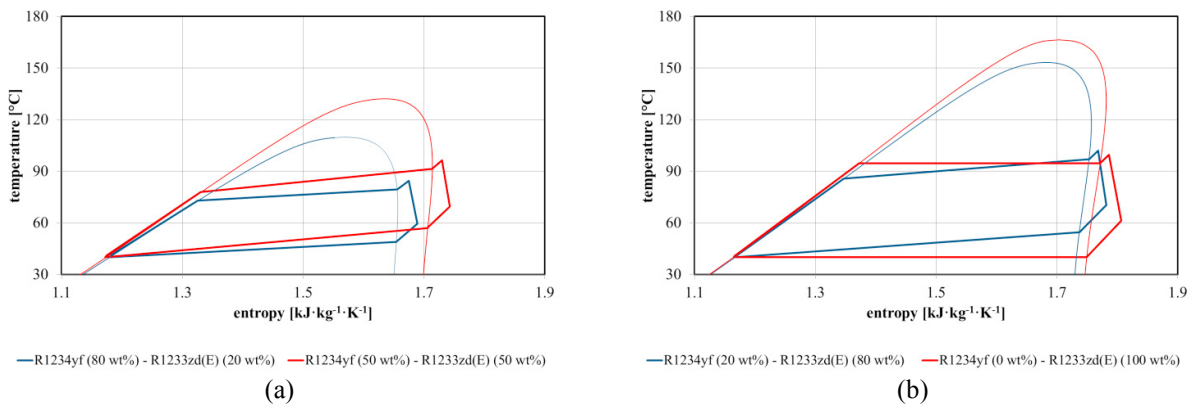


Fig. 4. T-s diagrams for four cases of mixtures of R1234yf and R1233zd(E), corresponding to 1 kW of electric power output from the expander.

Ultimately, further simulation results are reported in Fig. 5, with reference to the expander efficiency, for a better characterization of the behavior of the expander. The values of the expander efficiency in Fig. 5, as well as the shape, for the cases simulated and shown in Fig. 3 are consistent with experimental data on scroll-type expanders [14]. Apart from the strong dependence on the pressure ratio, as expected [14], slight variations are calculated despite the binary pair.
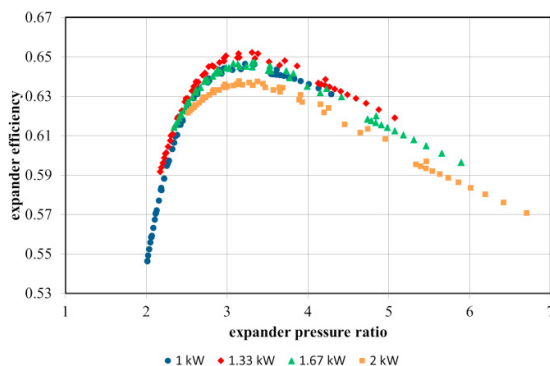
Fig. 5. Expander efficiency vs. pressure ratio for the cases reported in Fig. 3.

## 4. Conclusions

A model reported in literature [7] for simulating the performance of a 2 kW hermetic scroll expander has been revised and used to study the behavior of the machine in case of replacement of the original working fluid (R245fa) with fourth-generation refrigerants and even their mixtures.

Calculations of micro-ORC systems with the selected expander have resulted in a slightly better performance when using R-1234ze(Z) or R1233zd(E) as drop-in replacements of R245fa. Binary mixtures, characterized by a non-isothermal phase-change behavior, have been also considered. In particular, mixtures of selected hydrofluoroolefins show results depending on the fluid temperature at the expander inlet. The most relevant result is that the mixture process for some fluids causes a decrease of the maximum cycle temperature, after setting a fixed expander power output, and therefore the possibility of exploiting heat sources at lower temperatures.

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