Selection of working medium for low-temperature ORC based on thermodynamic, economic and environmental criteria

M Jankowski¹, A Borsukiewicz¹,*, P Klonowicz³

¹ West Pomeranian University of Technology, Chair of Heat Engineering, Piastów 19 avenue, Szczecin, 70-310, Poland
³ Institute of Fluid-Flow Machinery, Polish Academy of Science, Fiszera 14 st., Gdańsk, 80-231, Poland

E-mail: aborsukiewicz@zut.edu.pl

Abstract. This paper concerns multicriteria analysis of the selection of working medium for the low-temperature ORC microsystem. The criteria for the selection of the working medium are: thermodynamic efficiency (efficiency and power of the cycle), environmental impact and safety of the substance as well as the cost of installation on the basis of the heat exchanger surface analysis. The analysis was done for five organic fluids: R1234ze, R1234yf, R152a, R143a and propylene, and the source of the powering heat for the power plant is oil heated to the temperature of 85°C while cooling the screw compressor. Based on the results of calculations and analysis of the working substance properties it has been found that the fluid that best meets the criteria mentioned above is R1234yf. The minimal environmental impact and the smallest heat exchange surface of the vapour generator, with comparable turbine power and the ORC efficiency compared to other fluids, make it the best choice. The disadvantage of this liquid is the relatively high price (~ 140€/kg). A cheaper alternative may be R1234ze (~ 35€/kg). Its environmental impact is also negligible and the calculated heat exchange surfaces of the vapour generator are only slightly larger.

Keywords: ORC, working fluid, low-temperature power plant, waste thermal heat

1. Introduction and literature review

Vapour power plants working on a variety of working fluids are now commercially available and manufactured by many producers. They can be used to convert heat to electricity for very different thermal energy sources, and the match to the temperature of the power source is mainly based on the appropriate choice of the working medium. The purpose of this paper is to present the methodology for the working medium selection for the ORC microsystem fed with oil at the temperature of 85°C and this heat comes from the screw compressor cooling system. As the solution of the heat waste management from cooling the compressor is to be implemented by the manufacturer and the compressed air seller, the following criteria of working medium selection for the power plant were taken:
- thermodynamic criterion (maximizing the power and efficiency of the power plant),
- economic criterion (minimizing heat exchange surface of the vapour generator in the power plant, price of the fluid) and
- environmental criterion (relatively low potential for GWP greenhouse effect, zero ODP ratio, lack or low flammability and toxicity).

Selection of working fluids that can be used in ORC power plants is very large. Proper selection of the working medium for the ORC is a key issue affecting the whole success of the further work on the prototype preparation, research implementation and finally, implementation of the solution. The choice of the fluid affects the cost of the installation, its degree of complexity, efficiency, safety, operating costs and service life. A number of papers have been written on the principles of the organic fluids selection, the review of which has been made below. In [1] thermodynamic criteria for selection of an appropriate working fluid for subcritical and supercritical cycles were presented. The authors proposed equations based on the Jakob number, which allow the thermodynamic evaluation of the cycle and the selection of the working medium for the low-temperature ORC. Similarly, the criterion of thermodynamic evaluation of the usefulness of the working medium is presented in [2]. Yadong Zhu et al. [3] also refers to the thermodynamic aspects of the working medium selection in the ORC, but this includes aspects such as: concepts of entropy generation rate, revised entropy generation number, exergy destruction rate, entransy loss rate, entransy dissipation rate and entransy efficiency which are applied to the optimization of the Organic Rankine Cycle.

In [4] thermodynamic analysis of the cycle based on internal and external exergy efficiencies is presented, and on this basis the influence of working fluids on the organic cycle was analyzed. The optimization results presented in that paper show that the selection of working fluids depends greatly on optimal evaporation temperature. Guoquan Qiu presents the comparison and optimization of 8 mostly-applied working fluids nowadays: HFE7000, HFE7100, PF5050, R123, n-pentane, R245fa, R134a and isobutene and gives a preferable ranking by means of spinal point method [5].

New expressions for thermal efficiency of the subcritical and supercritical simple ORC are proposed in [6]. For the subcritical ORC without the superheating, thermal efficiency is expressed as a function of the Figure of Merit (FOM) while for the superheated subcritical ORC thermal efficiency is given in terms of the modified Jacob number. For the supercritical ORC, thermal efficiency is expressed as a function of dimensionless temperature.

An indicator, namely equivalent hot side temperature (TEHST) which is determined by the thermodynamic parameters at the liquid-vapor equilibrium state is proposed in [7] for the organic Rankine cycle optimization and fluid selection. The authors of the paper concluded that TEHST provides a more universal guideline on the ORC efficiency assessment as compared to some existing indicators such as boiling point temperature, critical temperature, Jacobs number and Figure of Merit.

Many guidelines for selecting the working medium for the ORC are presented in [8]. Some of them are cited below:
- working fluids with higher compressibility factors at the turbine inlet result in higher turbine isentropic work;
- fluids with higher values of ideal isobaric heat capacity are better suited to obtain high specific isentropic work;
- working fluids with higher molecular weights and compressibility factor are more suitable to obtain higher turbine efficiency;
- working fluids with low saturated liquid molar volume result in decreased ideal work in the pump.

In [9] the systematic design and selection of optimal working fluids for ORC based on computer aided molecular design and process optimization techniques are presented.

In [10] is made investigation of working fluids for the organic Rankine cycle (ORC) applications with a goal of identifying “ideal” working fluids for five renewable/alternative energy sources. The study suggests that a critical temperature of the working fluid and its critical ideal gas molar heat capacity have the largest impact on the cycle efficiency and volumetric work output.
Zahra Hajabdollahi et al. [11] propose Non dominated Sorting Genetic Algorithm (NSGA) for maximization the thermal efficiency and minimization the total annual cost (sum of investment cost, fuel cost and environmental cost) simultaneously. The optimization results show that the best working fluid is R123 from the thermodynamic viewpoint. Furthermore, R123 needs the highest investment cost while the environmental and fuel costs are the lowest.

Proper selection of heat exchangers in the ORC affects the cost of these devices, which represents the economic aspect of the installation, first the investment cost and then the operating costs of the power plant. The issue of selecting the type of heat exchangers: shell-and-tube or plate heat exchangers is presented in [12].

In this paper thermodynamic analysis of the low-temperature ORC using selected working fluids has been presented. However, the fluids were selected to meet the environmental criteria (low GWP greenhouse gas potential, zero ODP ratio). Then the influence of the type of fluid and the operating parameters of the power plant on the heat transfer surface was analyzed and other properties of working fluids were included. Based on this, a radar chart was prepared to evaluate the impact of each price criterion on the suitability of fluid as a working medium in the ORC.

2. Initial assumptions

2.1. Heat source

The energy source for the considered ORC system is the heat from the cooling of the screw compressor and the energy carrier is the LOTOS Corvus 46 oil. Basic parameters of the heat source, i.e. oil inlet and outlet temperatures and heat flux \( \dot{Q} \) are shown in Table 1, while Figure 1 presents the installation diagram.

| Oil temperature (inlet) | Oil temperature (outlet) | Heat flux \( \dot{Q} \) |
|-------------------------|--------------------------|-----------------------|
| \( t_{o1} \) [°C]       | \( t_{o2} \) [°C]        | 100 [kW]              |
| 85                      | 60                       |                       |

Table 1. Parameters of the heat source for the low-temperature system.

![Diagram of low-temperature ORC system.](image)

Figure 1. Diagram of low-temperature ORC system.
Thermophysical properties of the LOTOS Corvus 46 oil heat carrier (specific heat capacity and thermal conductivity) are summarized in Table 2.

Table 2. Thermophysical properties of the LOTOS Corvus 46 oil.

| Temperature of oil t [°C] | Specific heat $c_{po}$ [kJ/(kgK)] | Thermal conductivity $\lambda_o$ [W/(mK)] |
|---------------------------|-----------------------------------|------------------------------------------|
| 40                        | 1.954                             | 0.133                                    |
| 100                       | 2.173                             | 0.128                                    |

Density $\rho_o$ and kinematic viscosity $\nu_o$ of the oil were indicated using the equations below:

$$\rho_o = -0.682t + 884.83$$ (1)

$$\nu_o = 63772 \, t^{-1.986}$$ (2)

Specific heat $c_{po}$ and thermal conductivity $\lambda_{po}$ according to manufacturer's data are known for temperatures 40 and 100°C. For further calculations it is convenient to define these parameters as a function of temperature. After applying the linear approximation for the given values, the equations are:

$$c_{po} = 0.0037 \, t + 1.808$$ (3)

$$\lambda_o = -8 \cdot 10^{-5} \, t + 0.1363$$ (4)

2.2. Working media

Analysis of the low-temperature system was carried out for five organic fluids: R1234ze, R1234yf, R152a, R143a and propylene. Table 3 shows the short characteristics of selected working fluids, taking into account their environmental impact and flammability class while Table 4 shows the approximate market prices.

Table 3. Environmental characteristics of operating fluids for low-temperature ORC.

| Fluid          | Characteristics                                                                 |
|----------------|---------------------------------------------------------------------------------|
| R1234ze        | This fluid has a very low potential for greenhouse effect (GWP=7) and a zero ozone-depleting potential (ODP=0). The material safety data sheet is designated as non-combustible (safety group A2L). |
| R1234yf        | R1234yf, like its predecessor has a very low potential for greenhouse effect (GWP=4) and a zero ozone depletion potential (ODP=0). It is characterized by a moderate degree of flammability (safety group A2L). |
| R152a          | GWP ratio in the case of R152a equals: GWP=124 which makes it possible to qualify for a group of compounds with relatively low greenhouse effect potential. Moreover, ODP ratio equals zero, just as for previous fluids. It is flammable - it is classified as a safety group A2. |
| R143a          | R143a has a relatively high potential for generating a greenhouse effect – in its case the ratio equals: GWP=4470. ODP ratio of this factor is zero. In terms of flammability it was classified as a safety group A2. |
| propylene      | Propylene, also known as R1270, has a very low potential for creating a greenhouse effect (GWP=3) and zero ODP ratio. However, it is a combustible substance - belongs to the safety group A3. |
The impact of each of the studied environmental factors was also examined and their approximate market prices were checked (fluids prices are summarized in the table below).

Table 4. Approximate prices of analyzed working fluids for low-temperature system [13-14].

| Fluid | Price (€/kg) |
|-------|--------------|
| R1234ze | ~35          |
| R1234yf | ~140         |
| R152a propylen | ~16   |
| R143a | ~10          |
|       | no data      |

3. Mathematical model of a power plant

3.1. Determination of power and efficiency of ORC

ORC power output, assuming that the conversion of the factor expansion in the turbine and compression in the pump run without friction, was determined from the following dependence:

$$N_{ORC} = \dot{m}_{ORC} \left[ h_1 - h_{2s} - (h_{4s} - h_3) \right]$$  \hspace{1cm} (5)

Mass flow of the ORC fluid was determined from the equation of energy balance which, assuming the steady state and failure to take account of heat losses to the environment, leads to the equation:

$$\dot{m}_{ORC} = \frac{\dot{Q}}{h_1 - h_{4s}}$$  \hspace{1cm} (6)

The efficiency of ORC microsystem was determined from the dependence:

$$\eta = \frac{h_1 - h_{2s} - (h_{4s} - h_3)}{h_1 - h_{4s}}$$  \hspace{1cm} (7)

however, the heat flux $\dot{Q}$ in the formula (6) is the default value, whereas specific enthalpies appearing in formulas (5), (6) and (7) were determined using a database of Refprop 9.1 [15] based on the operating parameters (pressure, temperature and/or specific entropy) of the ORC.

3.2. Estimation of the heat exchange surface of the vapour generator in the ORC

The heat exchange surface of the vapour generator was estimated as two independent sections: the heating section and the evaporation and superheating section of the circulating medium. The surface of the heat exchange can be determined using the following dependence:

$$A = \frac{\dot{Q}}{k \Delta T}$$  \hspace{1cm} (8)

The formulas used to determine the particular quantities occurring in the above formula depend on the type of section under consideration.

Heating section

Heat flow at the heating section was determined from the dependence (9):

$$\dot{Q}_{heat} = \dot{m}_o c_{p \text{ir}} (t_{o1-2} - t_{o2})$$  \hspace{1cm} (9)

while the mass flow $\dot{m}_o$ was defined from the energy balance equation:
\[
\dot{m}_o = \frac{\dot{Q}}{c_{p\text{sr}}(t_{o1} - t_{o2})}
\]  

(10)

Mean specific heat in the relations (9) and (10) was determined from the equation:

\[
c_{p\text{sr}} = \frac{\int_{t_{o1}}^{t_{o2}} c_{po}(t)dt}{t_{o1} - t_{o2}}
\]

(11)

where \(c_{po}(t)\) is designated by (3) while the oil temperature leaving the evaporation section \(t_{o1-2}\) was determined from the equation of energy balance, which after appropriate transformations leads to dependence:

\[
t_{o1-2} = t_{o1} + \frac{\dot{m}_{ORC}(h_5 - h_{4s})}{\dot{m}_o c_{p\text{sr}}}
\]

(12)

Value of specific heat capacity \(c_{p\text{sr}}\) in the above formula was calculated using the equation (11) however, the appropriate temperature range for the heat carrier (oil) was considered. Due to the fact that the temperature \(t_{o1-2}\) is unknown, it was necessary to adopt an initial value \(t_{o1-2}\), and then performing a series of iterations to calculate the proper value of \(c_{p\text{sr}}\).

Logarithmic mean temperature difference \(\Delta T\) in the equation (8) is given by the formula:

\[
\Delta T = \frac{\Delta T' - \Delta T''}{\ln \frac{\Delta T'}{\Delta T''}}
\]

(13)

while the individual temperature differences are:

\[
\Delta T' = t_{o1-2} - t_5
\]

(14)

\[
\Delta T'' = t_2 - t_{4s}
\]

(15)

where: \(t_5\) – evaporation temperature of the medium, \(t_{4s}\) – condensate temperature at the outlet of the pump. Value of heat transfer coefficient \(k\) was estimated using the program SSP G7 SWEP [16].

Evaporation and superheating section
The heat flux for the evaporation and superheating section is determined by the dependence:

\[
\dot{Q}_{ev-sup} = \dot{m}_o c_{p\text{sr}}(t_{o1} - t_{o1-2})
\]

(16)

Logarithmic mean temperature difference \(\Delta T\) is given by the formula (13), whereas the differences in temperature are determined by equations:

\[
\Delta T' = t_{o1} - t_1
\]

(17)

\[
\Delta T'' = t_{o1-2} - t_5
\]

(18)

The coefficient \(k\) is determined the same way as for the heating section.
4. Results and discussion

Analysis of the low-temperature system was carried out for five organic fluids: R1234ze, R1234yf, R152a, R143a and propylene. The results of the thermodynamic analysis are presented in the form of power Nu and efficiency $\eta_{ORC}$ characteristics of the ORC system, depending on the superheating temperature $t_f$ of the organic medium. Characteristics were made by applying curves on their area, reflecting the state of the working medium for different degrees of superheating $\Delta t_p$ and evaporation temperatures $t_{evp}$. The range of variability of both parameters was dependent on the type of fluid used.

In addition, the curves of the estimated evaporator heat exchange surface were drawn on the chart. The curves: $A=f(t)$ – heat. and $A=f(t)$ – ev.-sup., correspond to the sections of medium heating and evaporation and superheating, while the curve $A=f(t)$ – tot. represents the total heat exchange surface of the vapour generator.

Figure 2 shows the power output values of the cycle as a function of the live vapour temperature for different degrees of vapour superheating: vapour without superheating, vapour superheated by 2,5 5 7,5 10 and 12,5 K. Trend lines illustrating the tendencies of change in heat transfer surface are also presented and additionally, for the total surface area the points corresponding to the values on the basis of which the trend line has been drawn have been added. In the remaining figures (Figures 3-6) only trend lines were applied, while points for specific values were omitted for better graph readability.

Since the energy flow fed to the $Q_d$ is a constant value for all considered calculation variants, the variability process of the cycle efficiency, for individual operating factors, is identical with the power diagrams of the cycle, that is why these charts were not included in this study.

![Figure 2. Dependence of power and heat transfer surface for ORC with R1234ze in function of vapour temperature at turbine inlet.](image-url)
Figure 3. Dependence of power and heat transfer surface for ORC with R1234yf in function of vapour temperature at turbine inlet.

Figure 4. Dependence of power and heat transfer surface for ORC with R152a in function of vapour temperature at turbine inlet.
Figure 5. Dependence of power and heat transfer surface for ORC with R143a in function of vapour temperature at turbine inlet.

Figure 6. Dependence of power and heat transfer surface for ORC with propylene in function of vapour temperature at turbine inlet.
In order to compare the power plant rating for different working fluids, Figure 7 shows the values of these power levels as a function of the vapour temperature at the turbine inlet for the two extreme variants: when the vapour is not superheated ($\Delta T=0$) and for the vapour superheated by $\Delta T=12.5$ K.

Figure 7. Comparison of the ORC power as a function of vapour temperature at the turbine inlet for the variants without vapour superheating ($\Delta T=0$K) and for superheated vapour ($\Delta T=12.5$ K).

As can be seen from the calculation results in Figure 7, a significant impact on the plant rating (and efficiency) has evaporation temperature of the working medium, while the degree of superheating does not significantly affect these parameters, for example for R1234ze evaporated at 65°C the theoretical power of 9.00 kW was obtained, whereas for this fluid, when it was assumed that it would be evaporated at 65°C and superheated by 12.5 K (that is the vapour temperature at the inlet to the turbine will be 77.5°C), the plant rating is 9.04 kW. It should also be noted that the vapour superheating has a very negative impact on the total heat exchange surface of the vapour generator – the heat exchange surface of the vapour generator (dry saturated vapour) is approx. 26.5 m², whereas for the vapour superheated by 12.5 K it increases to almost 49.3 m².

5. Conclusions
The purpose of this study is a multicriteria evaluation of chemical substances for use as working fluids in the low-temperature ORC power plant powered by waste heat with an initial temperature of 85°C and a final temperature of 60°C. A summary of the obtained calculation results and analysis of the thermophysical properties of the substances, to ensure optimum selection of the ORC microsystem, is the radar chart shown in Figure 8. It classifies the fluids tested for each of the criteria, while the top of the pentagon represent the best result for the given criterion.
Figure 8. Radar chart of adopted assessment criteria for selected for analysis working fluids for low-temperature system.

The fluid that best meets the specified criteria is R1234yf. The minimal impact on the environment and the smallest heat exchange surface of the evaporator, with comparable turbine power and efficiency of the ORC system in relation to the other fluids, make it the best choice. The disadvantage of this fluid is relatively high price (~140€/kg). A cheaper alternative may be R1234ze (~35€/kg). Its environmental impact is also negligible and the calculated heat exchange surfaces of the vapour generator are only slightly larger.

Acknowledgements
This work has been founded by The National Centre for Research and Development from The Smart Growth Operational Programme (European funds) within the project No. POIR.01.01.01-00-0512/16 carried out jointly with the Marani Sp. z o.o. company.

References
[1] Mikielewicz D, Mikielewicz J A thermodynamic criterion for selection of working fluid for subcritical and supercritical domestic micro CHP, (2010) Applied Thermal Engineering, 30 (16), pp. 2357-2362.
[2] Mikielewicz D, Mikielewicz J Criteria For Selection Of Working Fluid In Low-Temperature ORC, Chemical and Process Engineering 2016, 37 (3), 429-440
[3] Yadong Zhu, Zhe Hu, Yaodong Zhou, Liang Jiang, Lijun Yu, Applicability of entropy, entransy and energy analyses to the optimization of the Organic Rankine Cycle, Energy Conversion and Management 88 (2014) 267–276.
[4] Long R, Bao Y J, Huang X M, Liu W Energy analysis and working fluid selection of organic Rankine cycle for low grade waste heat recovery Energy 73 (2014) 475-483
[5] Qiu G, Selection of working fluids for micro-CHP systems with ORC, Renewable Energy 48 (2012) 565-570
[6] Javanshir A , Sarunac N, Thermodynamic analysis of a simple Organic Rankine Cycle, Energy 118 (2017) 85-96
[7] Li J , Alvi J Z , Pei G , Su Y , Pengcheng L , Guangtao G , Jie J Modelling of organic Rankine cycle efficiency with respect to the equivalent hot side temperature , Energy 115 (2016) 668-683
[8] Mirko Z, Stijepovic , Linke P , Papadopoulos A I , Grujic A S , On the role of working fluid properties in Organic Rankine Cycle performance, Applied Thermal Engineering 36 (2012) 406-413
[9] Papadopoulos A I , Stijepovic M , Linke P,  On the systematic design and selection of optimal working fluids for Organic Rankine Cycles, Applied Thermal Engineering 30 (2010) 760–769
[10] Brown J S, Brignoli R, Quine T,  Parametric investigation of working fluids for organic Rankine cycle applications, Applied Thermal Engineering 90 (2015) 64-74
[11] Hajabdollahi Z, Hajabdollahi F, Tehrani M, Hajabdollahi H, Thermo-economic environmental optimization of Organic Rankine Cycle for diesel waste heat recovery, Energy 63 (2013) 142-151.
[12] Walraven D, Laenen B, D’haeseleer W, Comparison of shell-and-tube with plate heat exchangers for the use in low-temperature organic. Rankine cycles, Energy Conversion and Management 87 (2014) 227–237.
[13] Czynniki chłodnicze – Refrigerants, raport of Bitzer, version 18, online acces [19.09.2017r.]
[14] Czynniki chłodnicze, środki spieniające, rozpuszczalniki, oleje chłodnicze i chłodziwa (Refrigerants, foaming agents, solvents, cooling oils and coolants )– price list of Morsmarket, online acces [21.09.2017r.].
[15] NIST. Refprop 9.1, Standard Reference Database 23, Version 9.1, Reference Fluid Thermodynamic and Transport Properties. National Institute of Standards and Technology, Gaithersburg, MD, USA, 2013.
[16] http://swep.net/support/ssp-calculation-software.