Working fluid selection for Organic Rankine Cycle applied to heat recovery systems

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Abstract: The selection of suitable organic fluids for use in Organic Rankine Cycle (ORC) for waste energy recovery from many potential sources of low-medium temperature (up to 350 ºC) is a crucial step to achieve high thermal efficiency. In order to identify the most suitable organic fluids, several general criteria have to be taken into consideration, from the thermophysical properties of the fluids leading to the environmental impact and cost related issues. The aim of the study is to elaborate a tool for the comparison of the influence of different working fluids on performance of an ORC heat recovery power plant installation. A database of a number of organic fluids as well as a s oftware (code) which allows the user to select the proper organic fluid for particular application have been developed. Calculations have been conducted for the same heat source and installation component parameters. The elaborated tool should create a support by choosing an optimal working fluid for special applications and become a part of a bigger optimization procedure by different frame conditions.

Keywords: *Organic Rankine Cycle, Database, Heat Recovery*

Nomenclature

$\dot{Q}_{in}$ *heat flux input* ..... *.kW*
$\dot{m}$ *mass flow rate*.....*kg·s*$^{-1}$
π *pressure ratio*
h_i *specific enthalpy for process point i*...*kJ·kg*$^{-1}$
T_{high} *high system temperature*..... *°C*
T_{low} *low system temperature* ..... *°C*
p_{high} *high system pressure*.....*MPa*
p_{low} *low system pressure*.....*MPa*
$\eta_{turbine}$ *internal efficiency of the turbine*..... *%*
η_{pump} *internal efficiency of the pump*..... *%*
η_{system} *system efficiency* ..... *%*
P_{pump} *power used by the pump*..... *kW*
$P_{turbine}$ *output power of the turbine* ..... *kW*
$\dot{Q}_{out}$ *heat flux output in the condenser* ..... *.kW*

1. Introduction

Nowadays, with energy demand rising at an ever increasing rate, efficient use of energy has become a m ajor issue. One candidate suitable for improving efficiencies of existing applications and allowing the extraction of energy from previously unsuitable sources is the Organic Rankine Cycle. Applications based on t his cycle allow the use of low temperature energy sources such as waste heat from industrial applications, geothermal sources, biomass fired power plants and micro combined heat and power systems.

Waste heat represents the heat produced by machines, electrical equipment and industrial processes which has no practical use. Usually it's generated by fuel combustion or by chemical reaction. The difficulty of capturing, distribution or transformation into other forms of energy comes from the characteristics of the heat source and the high costs connected to the equipment needed to transform the heat into useful energy. Statistical investigations indicate that low-grade waste heat accounts for 50% or more of the total heat generated in industry [1]. There are several types of industrial waste heat sources, some of which are presented in Table 1.

Table 1. Waste heat sources and their quality. [2]

Waste heat source	Quality of waste heat and possible use
Heat in flue gases	The higher the temperature, the greater the potential value for heat recovery
Heat in vapor streams	As for heat in flue gases, but when condensed, latent heat is also recoverable
Convective and radiant heat loss from the exterior of equipment	Low grade – if collected, may be used for space heating or air preheating
Heat losses in cooling water	Low grade – useful gains if heat is exchanged with incoming fresh water
Heat losses in providing chilled water or in the disposal of chilled water	1. High grade if it can be utilized to reduce demand for refrigeration 2. Low grade if refrigeration unit used as a form of heat pump
Heat stored in products leaving the process	Quality depends upon temperature
Heat in gaseous and liquid effluents leaving process	Poor, if heavily contaminated & thus require alloy heat exchanger

Organic Rankine cycle is a Clausius – Rankine cycle which uses an organic fluid instead of water. The replacement of water with organic fluids brings a number of advantages over the classical steam process. Due to their thermophysical characteristics, such as low critical point, low boiling temperature and high molecular mass, the transformation of low temperature heat into useful electrical energy is possible and can be effective (higher efficiency than other possibilities).

Because of the low critical point relative to water and because the temperature level of the heat input is much lower than in the case of steam processes, the working pressures are lower and thus, they lead to a small-scale, low-cost installation which in most cases does not require permanent supervision [6].

Fluid selection for any type of ORC application is a very important step in designing an efficient working system. There are many important aspects that need to be taken into consideration before choosing an organic fluid. In this context a special fluid database with an implemented selection algorithm has been created with the possibility of continuous development.

2. Database

The database has been assembled in MS Excel due to the wide spread of the program and the fact that it facilitates the structuring and organization of data sets in an easy and intuitive way. Another major advantage of MS Excel is the relative ease with which one can import data either from other databases or from experimental data. The characteristics of the fluids have been sorted in two major groups, each containing multiple parameters: thermophysical characteristics and environmental characteristics.

2.1. Themophysical characteristics

One of the thermophysical characteristics of the organic fluids is the slope of the saturation curve in the temperature-entropy diagram. It can be negative, isentropic or positive, as shown in Fig. 1.

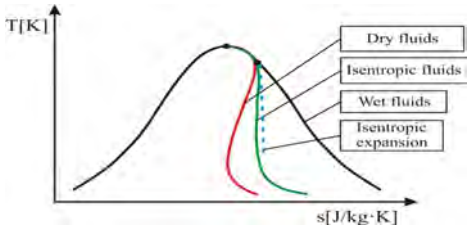

Fig. 1. Typical T-s diagram for dry, isentropic and wet fluids

In the case of dry and isentropic fluids there is no need for overheating. Because of the theoretical isentropic expansion in the turbine, in the case of wet fluids, overheating must be applied in order to avoid the creation of liquid droplets during the expansion in the turbine which would damage the turbine blades. Due to this characteristic the database contains information about the type of saturation curve for each contained fluid.

For practical reasons the low pressure value has been set to just above the atmospheric pressure (0.15 MPa). This limit must be imposed in order to avoid infiltration of air in the installation which would lead to the damaging of components. Also, for the moment, the low temperature value has been set to the value of normal ambient temperature (20 °C). Of course the real frame conditions of a real process, especially the temperature of the cooling medium, determine these values, which can be varied.

Another important characteristic is the boiling temperature at the low pressure value of the fluid. If it's lower than the ambient temperature then the minimal pressure value at which the fluid is in a liquid state at room temperature must be identified and set as the new low pressure value. This has to be done in order to maintain the highest possible value for the pressure ratio π of the expander, as a higher pressure drop yields a higher efficiency and it has been done for each fluid in the database.

There are other thermophysical parameters that must be taken into consideration when choosing a working fluid. Some of these are:
- low freezing point, so that the fluid will not solidify when it's in the low-temperature area of the process;
- the critical pressure and temperature should be above the highest values of these parameters in the process;
- the vaporization heat and the density of the fluid should be high, as a fluid with these characteristics will absorb more energy from the source in the evaporator and thus reduce the required flow rate, the size of the facility, and the pump consumption.

2.2. Environmental characteristics

Although high system efficiency is the main goal when designing heat recovery systems, one has to take into account the environmental characteristics for safety and practical considerations. For example, as the HCFCs still contain chlorine and have an associated Ozone Depletion Potential, they will be phased out in the EU Community from the 1st of January 2010 [3]. So, the availability of HCFCs for equipment servicing following the phase-out may not allow for predictable economical use.

Two main environmental characteristics are the ODP (Ozone Depletion Potential) and the GWP (Global Warming Potential). ODP represents the relative amount of degradation that a fluid can cause to the ozone layer. The standard of reference has been set for trichlorofluoromethane (R11). It has the value of 1 and the maximum potential of ozone depletion among chlorocarbons because of the three chlorine atoms in its composition. [4]

GWP represents a parameter that quantifies the contribution of a given mass of greenhouse gas to global warming. The standard of reference in this case is set for carbon dioxide with a given value of 1. Another important characteristic is the safety classification. After a careful analysis the ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) classification has been chosen because of the high number of organic fluids covered and the relative simplicity of the annotations of the safety classes. These are as follows in Table 2:

Table 2. ASHRAE safety classification. [5]

Flammability	Low toxicity	High toxicity
High	A3	B3
Low	A2	B2
Non-flammable	A1	B1

2.2.1. Toxicity classification [5]

Refrigerants are divided into two groups according to toxicity:
• Class A signifies refrigerants for which toxicity has not been identified at concentrations less than or equal to 400 ppm;
• Class B signifies refrigerants for which there is evidence of toxicity at concentrations below 400 ppm.

2.2.2. Flammability classification [5]

Refrigerants are divided into three groups according to flammability:
• Class 1 indicates refrigerants that do not show flame propagation when tested in air at 21°C and 101 kPa;
• Class 2 indicates refrigerants having a lower flammability limit of more than 0.10 kg/m^3 at 21°C and 101 kPa and a heat of combustion of less than 19 kJ/kg;
• Class 3 indicates refrigerants that are highly flammable as defined by a lower flammability limit of less than or equal to 0.10 kg/m^3 at 21°C and 101 kPa or a heat of combustion greater than or equal to 19 kJ/kg.
The database interface allows the user to select the type of installation for which the fluid data will be analyzed. Momentarily the installation layouts that are available are:

- Undercritical single stage;
- Undercritical single stage with recovery;
- Undercritical two-stage;
- Supercritical single stage.

The major fluid parameters are introduced for each existing fluid in the database, with the possibility of adding either other fluids and/or other parameters of interest. The general layout of the existing list with some of the parameters present in the developed program can be seen in Fig. 2:

		Critical point					
Working fluid	Boiling point at p=0.1 MPa [°C]	Temperature [K]	Pressure [MPa]	Molar mass [g/mol]	Slope	Toxicity group	ODP
R11 (Trichlorofluoromethane)	23,77	471	4,41	137,37	Isentropic	A1	1
R113 (Trichlorotrifluoroethane)	47,6	487,26	3,39	187,37	Positive	A1	0,9
R114 (Dichlorotetrafluoroethane)	3,5	419,1	3,25	170,9	Positive	A1	0,85
R115 (Chloropentafluoroethane)	-39,1	353,1	3,15	154,5	.	A1	0,4
R116 (Chloropentafluoroethane)	-78,2	293,1	3,04	138	.	A1	0
R12 (Dichlorodifluoromethane)	-29,8	385	4,41	120,91	Negative	A1	0,82
R123 (Dichlorotrifluoroethane)	27,8	456,9	3,7	152,93	Positive	B1	0,02
R124 (Chlorotetrafluoroethane)	-11	395,5	3,62	136,5	Isentropic	A1	0,022
R125 (Pentafluoroethane)	-48,5	339,4	3,63	120	Isentropic	A1	0
R13 (Chlorotrifluoromethane)	-81,3	302	3,97	104,5	Negative	A1	1
R1381 (Bromotrifluoromethane)	-57,75	340,08	3,95	148,91	.	A1	13
R134a (Tetrafluoroethane)	-26,1	374,2	4,06	102	Isentropic	A1	0
R14 (Tetrafluoromethane)	-127,8	227,5	3,75	88	Negative	A1	0
R141b (dichlorofluoroethane)	32,05	477,6	4,25	117	.	.	0,1
R142b (chlorodifluoroethane)	-9,8	410,4	4,12	100,5	.	A2	0,07
R143a (Trifluoroethane)	-47,6	346,1	3,78	84	.	A2	0
R152a (Difluoroethane)	-25	386,5	4,52	66,1	Negative	A2	0
R21 (Dichlorofluoromethane)	8,92	451,7	5,71	102,9	Negative	.	0,04
R218 (Octafluoropropane)	-36,7	345,1	2,68	188	.	A1	0
R22 (Chlorodifluoromethane)	-40,8	363,3	4,99	86,5	Negative	A1	0,05

Fig. 2. Fluid list with selected available fluids and parameters

Each fluid has a series of static parameters, such as ODP, GWP, molar mass, boiling point at atmospheric pressure and others, which are introduced when the fluid is added to the database and which never change. The dynamic parameters such as the cycle efficiency, the mass flow rate and the pressure ratio are calculated and are modified with the alteration of the input parameters which will be described in the following section.

Because the program is developed in MS Excel the interface and the fluid data are stored in the same document on different worksheets. Fig. 3 presents captions from both the interface and the database and the flow of data through them:

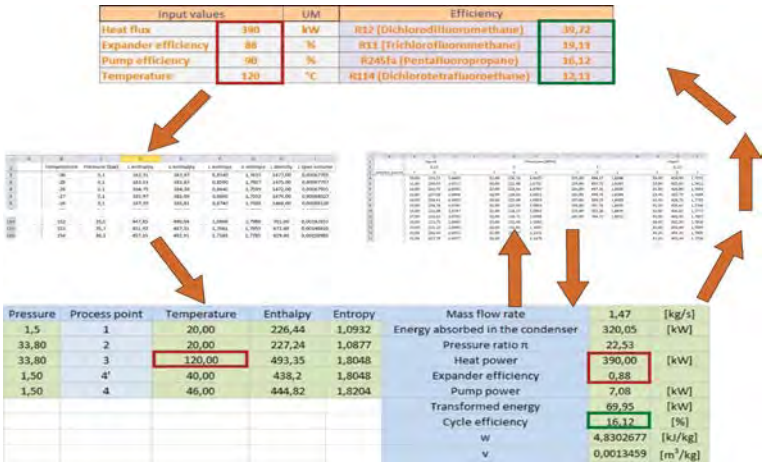

Fig. 3. Flow of data through the program

For each fluid from the database there are three worksheets. One contains the liquid and vapor enthalpy and entropy and other parameter values for the fluid along the saturation curve, one contains temperature, enthalpy and entropy values for the different process points and the third worksheet contains the calculation interface for the fluid and all the functions needed to implement the calculation procedure in the program.The user introduces the values for the input parameters, marked by the red rectangles, and the program returns the output parameters, marked with the green rectangles. For example, the program reads the temperature value introduced by the user and, by using the ”MATCH” function from Excel, it extracts the values for the enthalpy, entropy and pressure from the first data worksheet (saturation property curve) for each fluid. With these values, the program calculates and extracts values for the parameters for each process point and, finally, it returns the cycle efficiency. This value is introduced in the fluid list and it is updated whenever the input parameters are modified. From here the program returns a list of the fluids which yield the highest efficiencies (the top 4 in example from Fig. 3) for this set of input parameters.

3. Calculation procedure

As mentioned above, beside the general and environmental properties, the program returns the cycle efficiency for each fluid. This is done by employing a set of functions embedded in Excel which interrogate, search, match and return the desired data.

For the moment, the program executes calculations for a standard single stage cycle without recovery. The general layout of the installation, the process points and the T-s diagram (in this case for R114) can be seen in Fig. 4.

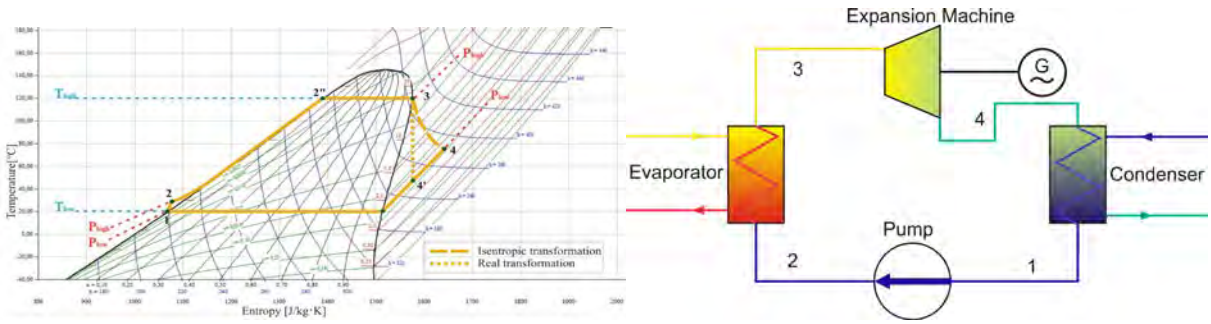

Fig. 4. T-s diagram and installation layout for a simple one-stage process

At the current state, the major input parameters for the program are the heat flux transferred to the system and the temperature at the inlet of the turbine (process point 3 in this case). The program calculates the efficiency of the cycle without overheating. So after introducing the heat flux and the turbine inlet temperature, the program chooses the corresponding pressure from the saturation curve for each fluid. The low pressure value is set to just above the atmospheric pressure (at 0.15 MPa) and the low temperature is set to the standard ambient temperature (20 °C).

With the value of the heat flux, the program calculates the mass flow rate:

$$\dot{m} = \frac{\dot{Q}_{in}}{h_3 - h_2} \tag{1}$$

where h_2 *and* h_3 represent the enthalpy values for process points 2 and 3.
By obtaining the high pressure value from the saturation curve, the program calculates the pressure ratio which is a good indicator for the system efficiency.

$$\pi = \frac{p_{high}}{p_{low}} \tag{2}$$

The internal efficiencies of the turbine and the pump are also input values. They can be selected from a drop-down list within the range of 0% to 100%, leading to a number of four input parameters. The expansion in the turbine is theoretically isentropic. The values for the irreversible process are obtained from the internal efficiency of the turbine.

$$\eta_{turbine} = \frac{h_3 - h_4}{h_3 - h_4'} \tag{3}$$

where the enthalpy values are obtained from the database for each fluid by matching the temperature and entropy values. By obtaining the value for the enthalpy in process point 4 the other parameters are extracted from the database. The power required for the pump is calculated with the following formula:

$$P_{pump} = \frac{v \cdot (p_{high} - p_{low})}{\eta_{pump}} \cdot \dot{m} \tag{4}$$

The output power of the turbine is calculated with the help of the internal efficiency of the turbine and by extracting the enthalpy values for process points 3 and 4 from the database:

$$P_{turbine} = \dot{m} \cdot \eta_{turbine} \cdot (h_3 - h_4) \tag{5}$$

The heat flux extracted in the condenser is calculated with the following formula:

$$\dot{Q}_{out} = \dot{m} \cdot (h_4 - h_1) \qquad (6)$$

After obtaining the values for each of these parameters, the program calculates the system efficiency as follows:

$$\eta_{system} = \frac{P_{turbine} - P_{pump}}{\dot{Q}_{in}} \cdot 100 \ [\%] \qquad (7)$$

The program returns the value for the system efficiency for each fluid in the database. If the input parameters lead to data that is outside the set conditions it will return "N/A" which signifies that the fluid is not suitable for the given input parameters.

In the current version the program returns a list of fluids which allow the highest system efficiencies for the input data set. In the following months more data and calculation procedures will be introduced so the program can calculate efficiencies of other types of installations, as shown in Figures 5, 6 and 7.

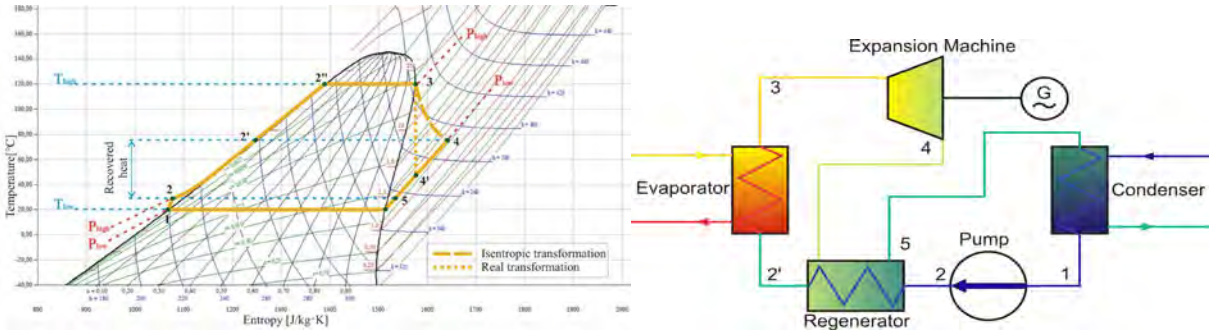

Fig. 5. T-s diagram and installation layout for a one-stage with recovery process

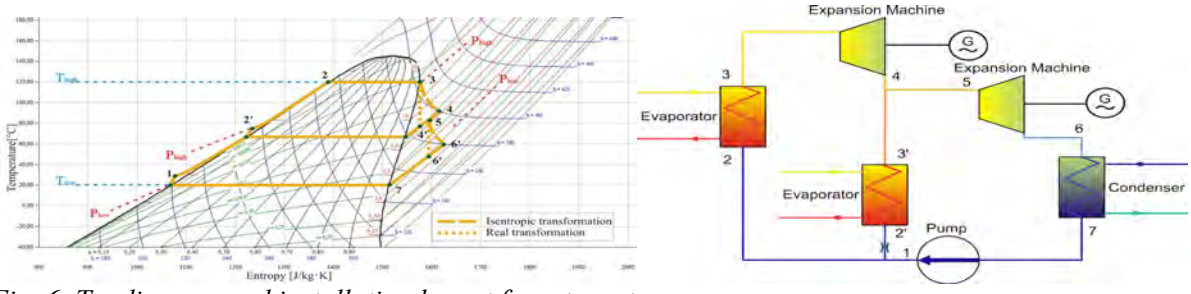

Fig. 6. T-s diagram and installation layout for a two-stage process

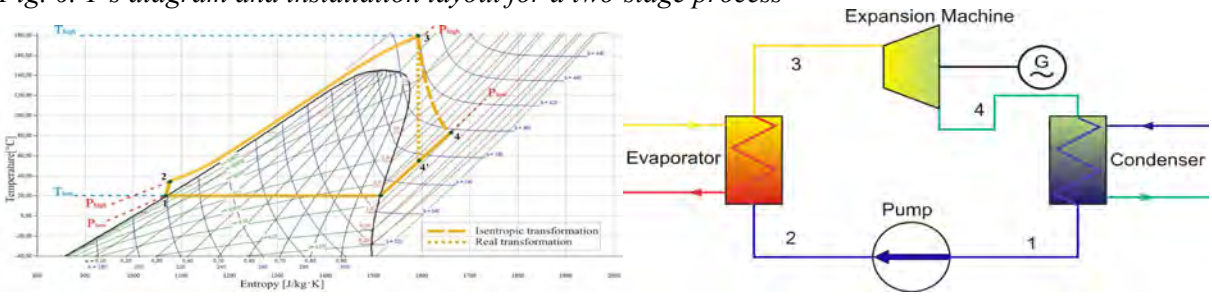

Fig. 7. T-s diagram and installation layout for a supercritical one-stage process

Further steps will consist of introducing the possibility of overheating and thus moving away from the saturation curve, the possibility of modifying the set values for the low pressure and

temperature as well as different sorting criteria such as cost, environmental aspects, availability and others.

4. Conclusions

Fluid selection is a major step in designing heat recovery systems based on the organic Rankine cycle. Although at this moment the sorting criterion for the fluids is the system efficiency, further development of the proposed program will create the possibility for different sorting criteria.

Developing this application has revealed that a program dedicated to fluid selection for heat recovery systems has a high degree of complexity. Although this application can give an idea to the user about the performance of different fluids applied to the same type of installation, one has to remember that the data still has to be compared to experimental data.

While the program is a good indicator for the influence on the system performance of different organic fluids, returning other fluid parameters in the process, the final decision of selection of an organic fluid for a given set of frame conditions remains to be made by the engineer designing the system. Costs related to fluid purchase, lifetime costs, taxes and availability may lead the designer to choose a lower efficiency yielding fluid.

To increases the level of complexity of the program and to bring the results, from theoretical, closer to real, measurable values, the interface from the heat source and the system will be investigated.

Another task that needs to be considered within the next steps is the investigation of energy and exergy losses in the expansion machine and exergy losses in the heat exchangers.

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