17th Brazilian Congress of Thermal Sciences and Engineering
November 25th-28th, 2018, Águas de Lindóia, SP, Brazil

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ENCIT-2018 - 0467
DEVELOPMENT OF A COMPUTATIONAL MODEL FOR SIMULATION OF ORGANIC RANKINE CYCLES (ORC)

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Abstract. *The need to reduce the environmental impacts generated by the consumption of fossil fuels has resulted in the intensification of the search for alternative sources of energy in the last decades. Among the most promising alternative technologies for electric power generation is the Organic Rankine cycle (ORC). ORC systems are applied to generate electricity in heliothermic and geothermal power plants, in ocean thermal energy conversion systems (OTEC), in biomass plants and waste heat recovery in industrial processes. This work aims to create a computational model that performs the ORC simulation for different fluids and applications and shows the best result for each case. For this, mathematical models were created for different architectures of the cycle. Then these models were implemented computationally through MATLAB software. The CoolProp library was used to obtain the thermodynamic properties of the working fluids. Finally, simulations were carried out with the purpose of verifying the model by comparing the data generated with those available in literature. The analysis shows that the computational model can simulate the Organic Rankine cycle and generate satisfactory results.*

Keywords: *Alternative energy, computational model, electricity generation, organic Rankine cycle, thermal simulation.*

1. INTRODUCTION

The demand for electric energy is growing continuously in the world. In Brazil, the Brazilian Energy Research Company (EPE) linked to the Ministry of Mines and Energy estimates that in 2050 electricity consumption will be of the order of 1600 TWh, about three times more than the 2015 consumption of 525 TWh, which means an average rate of increase of 3.2% per year (EPE, 2016).

Currently, the world energy matrix is highly dependent on fossil fuels (oil, coal and natural gas). In addition to generating negative environmental impacts (acid rain, air pollution, global warming, etc.), this type of fuel is finite.

The concepts of energy and development are directly linked, thus ensuring that the advancement of society needs a broad and economical energy supply. To reduce environmental impacts and to meet the demand for energy in the future, clean and renewable energy sources must be developed, and the efficiency of existing energy conversion processes must be increased. An effective way to achieve these objectives is through the use of organic Rankine cycles (ORC) in electric power generation.

ORC systems can be applied in the generation of energy in heliothermic, geothermal and biomass power plants (biogas, biodiesel, sugarcane bagasse, etc.), in ocean thermal energy conversion systems (OTEC) and in waste heat recovery in industrial processes (industries of cement, chemicals, food, etc.) (Tchanche et al. 2011).

Defining the cycle configuration and equipment types of an ORC depend on the working fluid that will be used based on the characteristics of the available heat source. Due to the large number of fluids that can be used, the dimensioning of an organic Rankine cycle must be done by means of simulation, that is, different configurations and fluids must be analyzed to determine the best scenario (Bao, Zhao, 2013).

In order to simulate an ORC cycle, it is necessary to determine the thermodynamic state of the working fluid at the inputs and outputs of the equipments. For this, state equations are used (thermodynamic functions that describe the state of a substance under certain physical conditions). Getting state equations for different fluids and implementing them into a computational tool is a laborious and time-consuming task. However, there are currently programs that have a library of state equations for dozens of fluids. One such software is CoolProp, developed by researchers at the University of Liège (Belgium) and the Technical University of Denmark. CoolProp is free and can be used in conjunction with other software and, furthermore, it is possible to simulate 122 different fluids (Bell et al., 2014).

An effective way to simulate a thermal cycle is through numerical analysis software. The purpose of this work was to use MATLAB and CoolProp to develop a computational tool for the simulation of organic Rankine cycles in basic and recuperative architectures. The main differential of this tool in comparison to those available in the market is that the user will define the scenario for an ORC application, different fluids and cycle configurations will be simulated and the tool will indicate the best fluid and the best operating conditions of the ORC for such scenario.

This model could be of great use for the development of energy efficiency projects of existing electricity generation systems and new generation ventures from renewable energy sources, which may contribute to the supply of electricity and reducing the environmental impacts.

2. ORGANIC RANKINE CYCLE

An ORC is basically composed of the same equipment as a conventional Rankine cycle. The main difference is that instead of using water as working fluid, an ORC system uses an organic fluid (Bao and Zhao 2013).

There are different ORC architectures, but the two main ones are the basic (BORC) and the recuperative (RORC). A BORC consists of four main equipments: pump, evaporator, turbine and condenser. The RORC also has an additional heat exchanger (a recuperator). These two architectures are shown in Fig.1.

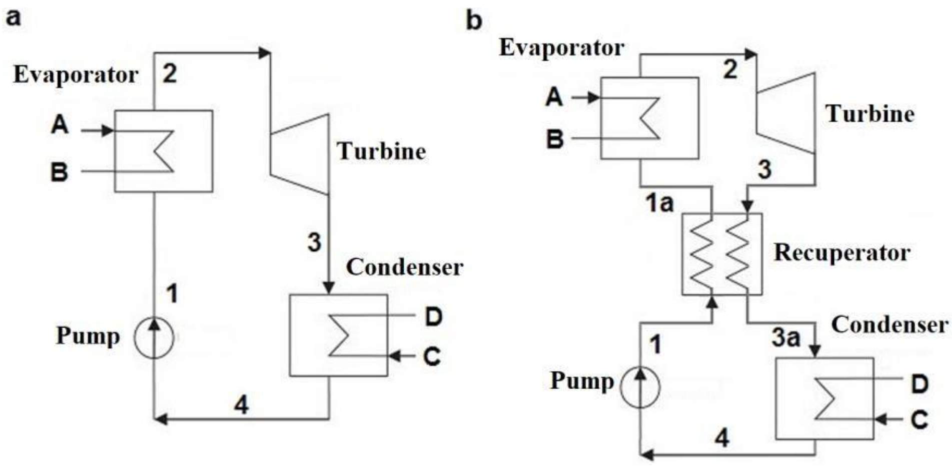

Figure 1. ORC architectures: (a) BORC and (b) RORC

The principle of BORC operation consists of four main processes: (1) a heat source is used to evaporate the working fluid in the evaporator; (2) vapour expands inside the turbine, which drives an electric generator; (3) the fluid leaving the turbine is cooled in a condenser, reaching the saturated liquid state; and (4) the fluid is then pumped back to the evaporator to receive more energy, completing the cycle (Tchanche, Pétrissans, and Papadakis 2014).

For each type of application, a different ORC system should be proposed, based on the characteristics of the available heat source. ORC dimensioning is a laborious process. It is necessary to select the best working fluid for the case and the appropriate architecture. Due to a large number of fluids available, the selection must be done through simulation, that is, different configurations and fluids must be analyzed in order to determine the best scenario.

The selection of the fluid becomes complex mainly for two reasons: (i) the working conditions of the cycle and the heat sources vary greatly from temperature of 80ºC to temperatures above 400ºC; (ii) hundreds of fluids can be used: simple hydrocarbons, aromatic hydrocarbons, perfluorocarbons, siloxanes, etc. (Bao, Zhao, 2013).

Several factors should be analyzed when selecting the most suitable fluid. The efficiency of the energy conversion and the cost of the electricity generated are the most important factors (Long et al., 2014). However, toxicity and flammability of the fluid, its thermal and chemical stability, its Global Warming Potential (GWP) and its ozone depletion potential (ODP) must be considered (Le et al., 2014).

Although several studies improve the selection of working fluid, none of them has obtained an optimal result, due to the variety of heat sources, as well as their working conditions and the wide range of possible fluids. Thus, there is a more suitable fluid for each case (Bao, Zhao, 2013), with its range of possible applications, related to its thermophysical properties (Hung et al., 2010).

Taking into account its thermophysical properties and saturated vapour curve types according to the variation of temperature and entropy (dT/ds) in the Temperature-entropy diagram, fluids can be classified in three categories: dry, wet and isentropic, as shown in Figure 2.

The type of fluid mainly influences the process of expansion in the ORC turbine (Quoilin, 2011):

- Dry fluids: the slope (dT/ds) is positive. So, the saturated vapour phase becomes superheated after isentropic expansion. The use of this type of organic fluid does not present a risk of corrosion in the turbine due to the superheated state at the outlet.
- Wet fluid: with a negative slope (dT/ds), expansion occurs in the saturated vapour zone, and it is necessary to superheat the fluid at the turbine inlet to avoid condensation and potential damage inside the equipment);
- Isentropic fluid: with an infinite slope (dT/ds), as the vapour expands along a vertical line in the T-s diagram, the saturated vapour at the turbine inlet remains saturated until it reaches the output of the turbine, not occurring condensation.

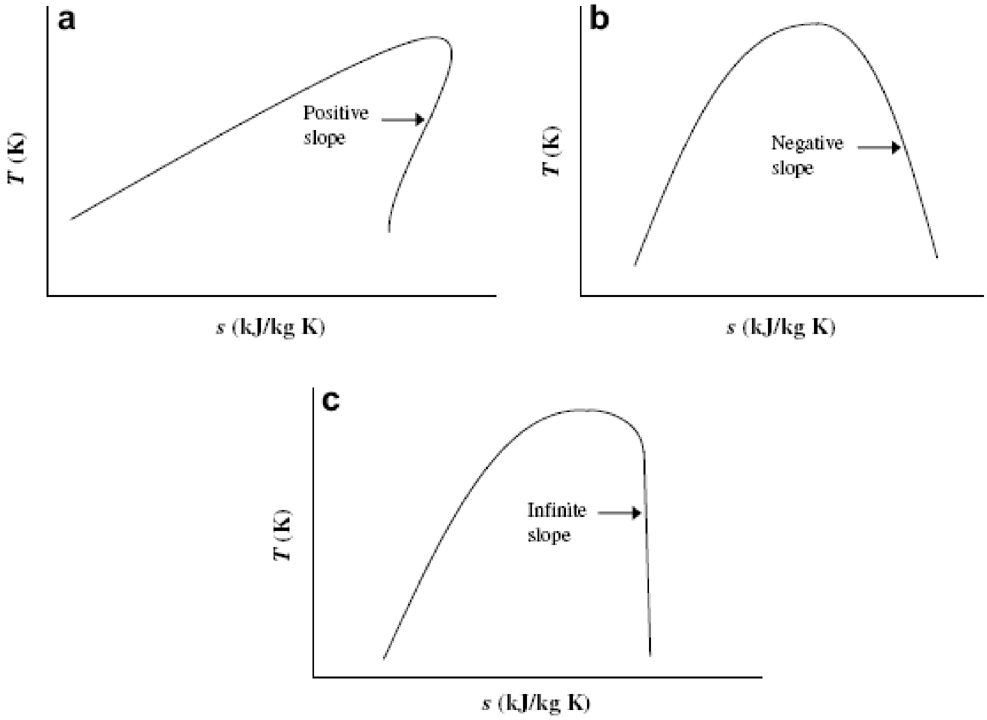

Figure 2. Typical saturation curves on T–s diagram for (a) dry fluid (b) wet fluid, and (c) isentropic fluid (Desai e Bandyopadhyay, 2009).

Using a dry fluid, the temperature of the working fluid at the turbine outlet is relatively high, and the fluid is in the superheated vapour state (Uusitalo et al. 2014). Thus, an internal heat exchanger (recuperator) can be adopted in the ORC to absorb heat from the fluid leaving the turbine and use it to preheat the fluid entering the evaporator (Feng et al. 2015). In this case, with the recuperator, the cycle efficiency is increased.

To achieve high thermal efficiency and provide good cycle operating conditions, some parameters can be adjusted (Quoilin, 2008), for example:

- Superheating degree: the difference between the turbine inlet temperature and the evaporation temperature of the fluid. Superheating can guarantee an increase in efficiency due to the increase in the heat addition temperature in the cycle. For wet fluids, it reduces the risk of condensation in the turbine. However, from the economic point of view it may increase the cost of the system.
- Subcooling: difference between the pump inlet temperature and the condensation temperature of the fluid. It is important to guarantee that only fluid in liquid state enters the pump.
- Pinch Point: is the minimum difference between the fluids in a point of the heat exchangers. It is an important parameter in ORC. A lower pinch point increases efficiency. However, this generates a larger area of heat exchange and therefore generates a significant increase in the costs of heat exchangers.

3. METHODOLOGY

This work was developed in three stages. Firstly, the mathematical modelling of two architectures of the organic Rankine cycle (basic and recuperative) was carried out. Then, the developed model was implemented computationally through MATLAB. To obtain the thermodynamic properties of the fluids, using CoolProp. Finally, simulations were performed for different working fluids with the purpose of testing and verifying the model through comparisons of the results generated with those available in the literature. These steps are described in more detail below.

3.1 Mathematical Modeling

The computational model was based on the mathematical models developed in the works of Quoilin et al. (2011), Meinel, Wieland, and Spliethoff (2014) and Imran et al. (2014). Figure 3 shows ORC architecture adapted for simulation and Table 1 describes each step according to the Figure. Numbers identified the cycle points, and letters, on their turn, the external sources.

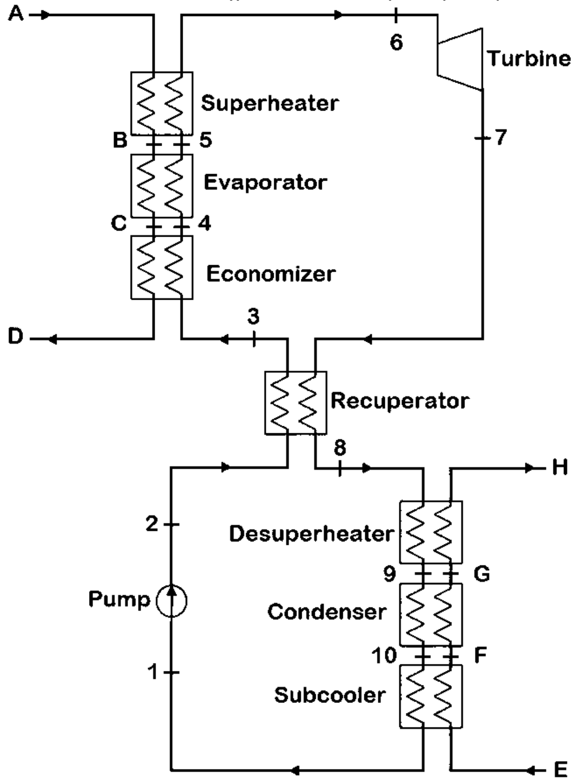

Figure 3. ORC architectures adapted for simulation.

For the simulation, evaporator and condenser were divided into three parts to facilitate the modelling, with each part of the exchanger having a different heat transfer process. In the economizer, the working fluid, in liquid state, is heated to saturation. In the evaporator, there is a change of liquid phase to vapor and, in the superheater, the saturated steam is superheated to ensure better efficiency and to prevent the condensate formation at the outlet of the turbine. In the superheater the superheated steam leaving the turbine is cooled to the state of saturation. In the condenser there is a phase change from vapor to liquid and in the subcooler, the saturated liquid is subcooled to ensure that there is no vapor in the pump.

Table 1. Description of flows in the main points of the ORC

Point	Flow description	Fluid
1	Subcooler outlet / Pump inlet	Organic fluid (liquid)
2	Pump outlet / Economizer inlet (BORC) or Recuperator outlet (RORC)	Organic fluid (liquid)
3	Recuperator outlet / Economizer inlet	Organic fluid (liquid)
4	Economizer outlet / Evaporator inlet	Organic fluid (liquid)
5	Evaporator outlet / Superheater inlet	Organic fluid (vapor)
6	Superheater outlet / Turbine inlet	Organic fluid (vapor)
7	Turbine outlet / Recuperator inlet (RORC) or Desuperheater inlet (BORC)	Organic fluid (vapor)
8	Turbine outlet (BORC) or Recuperator outlet (RORC) / Desuperheater inlet	Organic fluid (vapor)
9	Condensator outlet / Subcooler inlet	Organic fluid (liquid)
10	Subcooler outlet / Pump inlet	Organic fluid (liquid)
A	Superheater inlet	Heating fluid
B	Superheater outlet/Evaporator inlet	Heating fluid
C	Evaporator outlet/ Economizer inlet	Heating fluid
D	Economizer outlet	Heating fluid
E	Subcooler inlet	Cooling fluid
F	Subcooler outlet/ Condensator inlet	Coolinf fluid
G	Condensator outlet/ Desuperheater inlet	Cooling fluid
H	Desuperheater outlet	Cooling fluid

The first step to simulate the ORC is to define the heating and cooling fluids and their states conditions from points A to H. The second step is to choose the working fluids through a pre-selection. Then it is necessary to simulate the fluids pre-selected according with the heating and cooling fluids temperatures.

For each fluid, it is possible to obtain the enthalpies and entropies at the evaporator and condenser inlets and outlets and then determine states 4, 5, 9 and 10. With the values of superheating and subcooling degrees it is possible to determine the states 6 and 1. The enthalpy values at the turbine outlet and pump output are also obtained assuming isentropic processes. Then, applying the 1st and 2nd Law of Thermodynamics to a control volume that includes the working fluid in the turbine, it is possible to determine the enthalpy at turbine outlet as a function of the turbine isentropic efficiency. Similarly, for a control volume that includes the working fluid in the pump, it is possible to determine the enthalpy at the pump outlet. With known values of enthalpy and pressure, states 7 and 2 has been defined. If temperature in state 7 is higher than in state 2, it is possible to use a recuperator. Thus, in this case, with the value of the pinch point, the states 3 and 8 are defined too.

It should be noted that for the basic cycle, since there is no recuperator, state 3 is equivalent to 2, so it is for state 8 which is equivalent to 7. For wet fluids, there is usually a two-phase fluid at the turbine outlet, in this case there is no superheater and thus state 9 is equal to state 8.

From Eqs. 1 to 8, were calculated the heat transfer rate in the evaporator ($\dot{Q}_{evap}$) and in the condenser ($\dot{Q}_{cond}$) for the BORC and RORC, the heat recovery rate in the recuperator ($\dot{Q}_{recup}$), the mechanical power generated in the turbine ($\dot{W}_{turb}$), the electric power in the generator ($\dot{W}_{ger}$), the system net power ($\dot{W}_{liq}$), the back work ratio (BWR), and the thermal efficiency of the cycle (η_{cycle}). For these calculations, the 1st Law was applied again to the control volumes including the working fluid in each of the equipment of the cycle.

$$\dot{Q}_{evap} = \dot{m}_w(h_6 - h_3) \tag{1}$$

$$\dot{Q}_{cond} = \dot{m}_w(h_8 - h_1) \tag{2}$$

$$\dot{W}_{pump} = \dot{m}_w(h_2 - h_1) \tag{3}$$

$$\dot{W}_{turb} = \dot{m}_w(h_6 - h_7) \tag{4}$$

$$\dot{W}_{gen} = \eta_{gen}\dot{W}_{turb} \tag{5}$$

$$\dot{W}_{net} = \dot{W}_{gen} - \dot{W}_{pump} \tag{6}$$

$$BWR = \frac{\dot{W}_{pump}}{\dot{W}_{turb}} \tag{7}$$

$$\eta_{cycle} = \frac{\dot{W}_{net}}{\dot{Q}_h} = \frac{\dot{W}_{net}}{\dot{m}_h(h_A - h_D)} \tag{8}$$

3.2 Computation Implementation

After the development of the mathematical model, the computational implementation was carried out to create the simulation model for the ORC. The program was written in Matlab. The thermophysical library CoolProp was used to obtain the thermodynamic parameters of the heating and cooling fluids and the working fluid (temperature, pressure, enthalpy, entropy, etc.).

The computational model analyses the data of a heat source for the thermal cycle and determines the most suitable fluid for the system, the properties of the fluid at certain points of the cycle, equipment dimensioning, estimates of the generated electric power and thermal efficiency.

Figure 4 illustrates the flowchart describing the computational simulation made in Matlab. In the simulation, firstly, the user must enter with the parameters of the heating and cooling system sources. Subsequently, the process of pre-selection of the working fluid begins. In this step, the user can choose between one or more types of fluids, (wet, dry and isentropic) to carry out the simulation. Also in the pre-selection stage, the user must determine the maximum desired index of ODP (Ozone Depletion Potential) and GWP (Global Warming Potential) for the fluid.

After completing the pre-selection process, the user can also define parameters such as equipment efficiency, and choose the configuration of the desired cycle. Finally, the cycle is simulated for all pre-selected fluids, and then the results obtained are presented (net power, thermal efficiency, etc.) for the fluid that presents the best performance among the simulated ones.

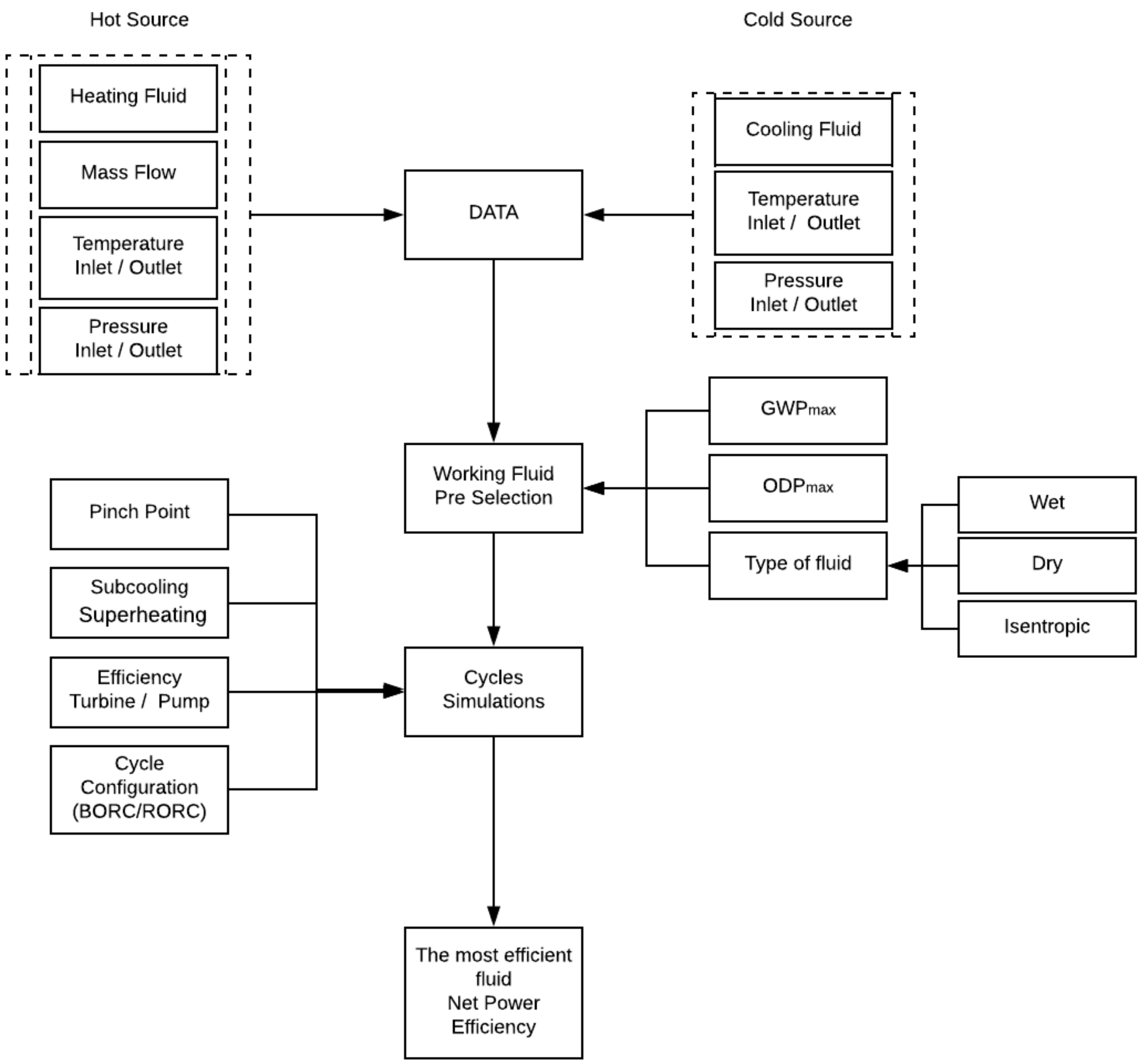

Figure 4. ORC simulation flowchart.

3.2 Verification

After the computational implementation of a mathematical model, it is important to perform the test and the model verification. In this work, this is being done by means of comparison with the literature data, that is, certain simulations are performed with the same parameters available in the works of other authors. Finally, the results (cycle efficiency, net power, etc.) should be compared. If necessary, adjustments should be made in the model in order to improve the reliability of the simulation results, to maximise the tool applicability and to minimise the data processing time.

4. RESULTS AND DISCUSSION

For the simulation, a main code was developed to simulate the BORC or RORC cycle. Besides this code, two other auxiliary codes were elaborated for the fluid pre-selection and another one for plot T-s diagram (Temperature versus Specific Entropy) of the working fluids.

Also, a graphical interface (Guide) was developed, a tool available in Matlab and presented in Figure 5, which allows greater ease of interaction between the user and the proposed computational model. The interface created is elaborated according to the flow chart of Figure 4, where the user must enter the parameters in order to have the result presented through the interface. To facilitate the use of the interface, an instruction panel has been made available. The information also makes value suggestions to fill in the parameters.

Figure 5. Graphical interface (Guide)

To initiate the verification process of the computation tool, simulations of the ORC were performed using the first code created. The results were compared with the literature. The results of one of these simulations are presented in Tab. 2. In this specific case toluene was considered at an evaporation temperature of 300°C and a condensation temperature of 35ºC. The efficiencies of pump and turbine were considered 80% and it was considered the basic cycle. For comparison, the SmoWeb tool was used, which is an online platform for simulating thermal cycles (SmoWeb, 2018).

Table 2. Some results of the tool in the first verification for an ORC with toluene

Parameters	Developed Tool	*SmoWeb*
Thermal efficiency	21.73 %	21.73 %
Net power output	1841.48 kW	1840.15 kW
Pump power	62.84 kW	62.80 kW
Turbine power	1904.33 kW	1902.95 kW
Heat transfer rate in evaporator	8474.55 kW	8468.45 kW
Heat transfer rate in condenser	6633.07 kW	6628.29 kW

It is observed that, in general, the results were very close to the simulated condition. The cycle efficiency calculated by the developed tool was the same as calculated by the SwoWeb tool. Considering other fluids and other working conditions, the results were also satisfactory.

When the computational model was finished, other tests were performed to evaluate if the fluids indicated as more efficient by the tool for certain scenarios were the same ones pointed in the literature and also, to check if the values of net power and thermal efficiency were similar. The results of one of these simulations are presented in Tab. 3.

Table 3. Some results of the tool in the final verification for an ORC with benzene

Parameters	Developed Tool	Song et al. (2015*)*
Fluid with highest efficiency	Benzene	Benzene
Evaporation Temperature	211ºC (484 K)	207ºC (480 K)
Mass flow rate	0,63 kg/s	0,68 kg/s
Net Power Output	90,8 kW	86,44 kW
Thermal Efficiency	21,3%	21,8 %

The parameters used in Song et al. (2015) were used for this comparison. Five fluids were analyzed for the heat recovery of exhaust gases in a diesel engine for the basic cycle: benzene, toluene, cyclohexane, nonane and decane. The temperature of the gas was considered 300ºC at the inlet and 105ºC at the outlet. The efficiencies of pump and turbine were considered 80%. The higher efficiency was achieved by benzene in the simulation with the developed tool, as well as in the reference used. It is observed that the results were similar. The difference between the calculated efficiency and the reference was only 2.3%. For other parameters the difference was slightly higher, which can be explained by the differences between the input values in the simulation. In the calculation performed using the developed tool the heating fluid was considered as air. In addition, some input values, such as the cooling fluid conditions in the condenser for example, were unavailable and were estimated. Thus, it can be considered that, on the basis of the available data, the results were satisfactory.

5. CONCLUSIONS

For an ORC system, simulation is important because there are many options of fluids and possible configurations for the cycle and only through a computational tool can it safely determine the best scenario for each electric power generation system.

In this work, it was developed a mathematical model for an ORC simulation. This model was implemented in Matlab and an interface was created to facilitate interactivity with the user. The differential of this tool is the ability to analyze different fluids based on the parameters defined by the user and then present the fluid, cycle configuration and operating conditions that offer the highest net power and higher efficiency.

Based on the analysis and comparison with the literature, the model that was developed presented satisfactory results. In all the simulations performed for comparison, the results were similar. Considering that some parameters were estimated and considering the differences generated by the use of CoolProp instead of other tools to obtain the thermodynamic properties, it is considered that the model developed meets the objective of the work and can be used for ORC simulation for solar energy, ocean energy, geothermal energy, biomass, residual heat recovery and other applications.

6. ACKNOWLEDGEMENTS

The authors would like to thank the Federal Institute of Minas Gerais (IFMG) – Formiga campus, for their financial support and Prof. Thaís Lopes Reis for proofreading.

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8. RESPONSIBILITY NOTICE

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