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Parametric Optimization of Organic Rankine cycles Using Zeotropic Mixtures in FPSO Units

César A R Sotomonte
Bruno S. Bunya
Grupo de Estudos em Tecnologias de Conversão de Energia, Federal University of Itajubá, Brazil
c_rodriguez32@unifei.edu.br
bruno.bunya@gmail.com

Thiago G. Correia Veloso
thiagogotelip@yahoo.com

Christian J. Rodríguez Coronado Rodriguez
christian@unifei.edu.br

Abstract. *An increase in the atmospheric concentrations of greenhouse gases as a result of excessive consumption of fossil fuels has been a major concern for several countries. However, the use of renewable energy sources is not yet economically feasible or are still in the conceptual stage. Therefore, increasing energy efficiency in industrial processes is the best short-term option for the reduction of greenhouse gas emissions. Currently, the Organic Rankine cycle (ORC) is a commercial option to increase energy efficiency in the industrial sector converting low-temperature waste heat into electric energy. The working fluid selection and optimization of the design parameters are the main approaches to improve the performance of these thermal systems. Recently, zeotropic mixtures are proving to be promising as a working fluid option in ORC cycles as a consequence of the better match temperature profile between the organic fluid, the heat source and cooling fluid during the vaporization and condensation processes. Thus, this article aims to find the optimal design of an ORC cycle for the generation of electricity in offshore oil and gas production processes. The thermodynamic model includes two configurations of the ORC cycle (with and without heat recovery) and the use of 12 possible mixtures as working fluid in which design parameters such as vaporization and condensation pressure, superheating, pinch point and effectiveness of the heat exchanger were optimized using as objective function the net power generated by the thermal system. Preliminary results indicate that heat recovery in the main gas compression unit is maximized by RE245CB2, i-Pentane and R236FA/C7H16 as the best options for working fluid, with a net power output close to 1.8 MW and providing up to a 18% increase in energy efficiency in the compression process.*

Keywords: *Optimization, Zeotropic Mixtures, Organic Rankine Cycle*

1. INTRODUCTION

In Brazil, the expansion of the oil and gas industry is directly linked to the recent discoveries of oil in the pre-salt layer. Floating Production Storage and Offloading (FPSO) units have become one of the commercially viable technological options for exploring deepwater oil deposits. Within these perspectives, offshore platforms have been used to expand the exploration and processing of oil and gas in various regions of the world.

From the point of view of atmospheric emissions, this industrial activity has a negative impact on the environment, mainly related to global warming and air contamination. For this reason, increasing the energy efficiency of its production process and reducing greenhouse gas emissions is one of the main objectives for the sustainable development of this industrial activity in different countries around the world.

Among the solutions proposed to meet energy requirements and reduce the impact generated by the consumption of fossil fuels, the organic Rankine cycle (ORC) shows itself as a promising technology, since it allows the use of low temperature thermal flows rejected during production processes, which can represent between 50 - 80% of the total primary energy source used.

The ORC cycle is similar to the conventional Rankine cycle, but uses a heavy molecular organic compound as a working fluid. The working fluids in an ORC cycle have a low boiling point and a latent heat of vaporization lower than water, allowing evaporation at lower temperatures, which provides better use of the heat provided by the heat source.

According to Schuster *et al.* (2010) the appropriate selection of the working fluid and operating parameters for ORC systems are crucial to maximize system performance; this decision being strongly dependent on the temperature level of the heat source.

Holistic approaches such as those developed in Pierobon *et al.* (2013) and Correa Veloso *et al.* (2018) that base the selection of the working fluid and operating parameters through an optimization that allows to evaluate different objectives independently taking into account several design criteria simultaneously present themselves as the best choice.

However, the aforementioned research rules out the possibility of using zeotropic mixtures as working fluids, which according to what was presented by Chys *et al.* (2012) and Liu *et al.* (2014) favor the thermodynamic performance of the ORC cycle.

In this order of ideas, the present work aims to evaluate the energy performance of an ORC for the use of low temperature heat sources in FPSO units for off-shore exploration. For this purpose, a multiobjective optimization based on genetic algorithms was developed using as selection criteria the net electrical power and the dimensions of the heat exchange equipment, in which, design parameters such as vaporization and condensation pressure, superheating at the turbine inlet and effectiveness of the heat recovery unit in the case of regenerative cycles were analyzed using 48 different working fluids and their respective mixtures.

2. METHODOLOGY

2.1 Mathematical model

The proposed ORC system (Fig. 1) is composed of the following equipment: pump, regenerator, evaporator, condenser and turbine.

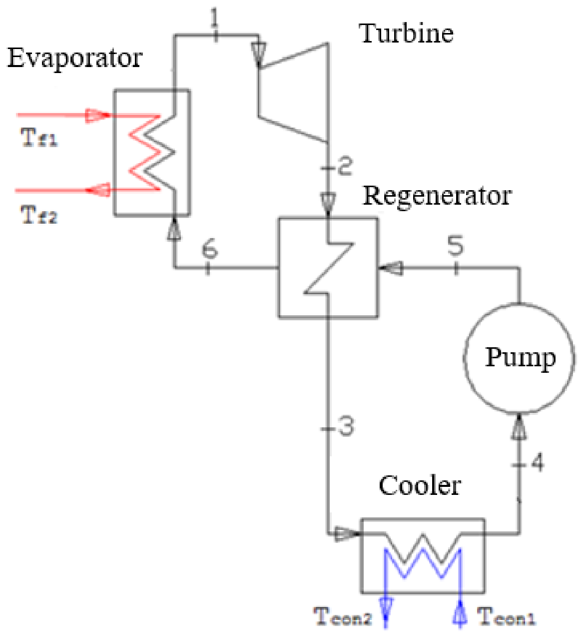

Figure 1. Organic Rankine Cycle

The minimum condensing pressure of the ORC cycle was set at 50 kPa, a pressure used by some commercial condensers. If required, the condensing pressure can be increased to raise the condensing temperature to 40 °C, the minimum established condensing temperature.

Studies like the one presented by Dai *et al.* (2016) show that the operation of the ORC cycle in supercritical conditions leads to a thermal decomposition of the working fluid. Thus, in order to disregard thermal stability analysis of the selected working fluids, the maximum vaporization pressure in the system cannot exceed 95% of the critical pressure and the inlet temperature in the turbine (T_1) cannot exceed the critical temperature of the working fluid.

The mathematical model was developed in order to compare and evaluate the performance of the organic Rankine cycle. Mass and energy balance equations that describe the performance of each component in the thermal system have been integrated into a computational model to provide the steady state operating point for a given target application (heat source) and environmental conditions (condensation temperature).

The mathematical model described allows to simulate two configurations of the ORC cycle, with and without heat recovery. The laws of conservation of mass and energy are the fundamental principles in the development of a thermodynamic system. These principles are defined for a control volume at steady state by Eq. (1) and Eq. (2), respectively:

$$\sum \dot{m}_e = \sum \dot{m}_s \tag{1}$$

$$\sum (\dot{m}h)_e - \sum (\dot{m}h)_s + \sum \left(\dot{Q}\right)_{cv} - \sum \left(\dot{W}\right)_{cv} = 0 \tag{2}$$

These principles are applied to the different components of the ORC system, assuming the following simplifications:

- The cycle operation occurs under permanent regime;
- There is no variation in the potential energy and kinetic energy of the working fluid throughout the cycle;
- There is no loss of heat to the environment in the pipes, turbine, pump and heat exchangers;
- Detailed calculations of pressure losses and heat transfer in the evaporator, recuperator and condenser, are ignored since they depend heavily on materials and design details of the heat exchangers;
- The isentropic efficiencies of the turbine and the pump are constant (η_b = η_t = 80%);
- The working fluid at the condenser outlet is saturated.

2.1.1 Heat source

Bearing in mind that in ORC technology the main constraint is the heat source, the first stage of the development of the thermodynamic model is focused on the characterization of this according to its chemical composition, temperature and molar flow.

Once the three parameters are defined, both the energy potential of the heat source and the operating restrictions of the thermal system can be established.

In this work, the main natural gas compression unit was considered as the heat source. The main characteristics of the heat source are summarized in Table 1.

Table 1. Operating conditions of the heat source

Temperature	431.15 K
Mass flow	61.8 kg/s
Pressure	8196 kPa
Chemical composition	%
H_2O	0.6
CO_2	3.0
CH_4	77.0
C_2H_6	9.2
C_3H_8	5.9
Others	4.3

The heat supplied by the heat source is calculated using the following expression:

$$\dot{Q}_{fon} = \dot{m}_{fon}(h_{f1} - h_{f2}) \tag{3}$$

2.1.2 Evaporator

The evaporator is modeled with a single countercurrent heat exchanger as can be seen in Figure 1. In this equipment all the heat is added to the cycle and the heat transfer process was divided into two stages, preheating and evaporation.

The evaporator performance is limited by the pinch temperature differential (pinch point - PP), which is defined as the smallest temperature difference that occurs in the heat exchanger between the working fluid and the heat source. In this model, the terminal and initial temperature differences in the minimum accepted heat exchanger (ΔT) are limited to 5 and 10 K respectively similar to the work presented in Correa Veloso *et al.* (2018); whereas, the minimum accepted pinch point is 5 K three degrees above the minimum value evaluated in Guo *et al.* (2011). Equation (4) represents the energy balance in this equipment and Eqs. (5-7) the system restrictions.

$$\dot{Q}_{evp} = \dot{m}(h_1 - h_{1v,sat}) + \dot{m}(h_{1v,sat} - h_6) \tag{4}$$

$$\Delta T_i = T_{f1} - T_1 \geq 10 \tag{5}$$

$$\Delta T_0 = T_{f2} - T_6 \geq 5 \tag{6}$$

$$PP \geq 5 \tag{7}$$

2.1.3 Turbine

The turbine performance is established according to the equipment's isentropic efficiency, which is defined mathematically for a turbine that does not have steam extractions such as:

$$\eta_{is,t} = \frac{\dot{W}_{real}}{\dot{W}_{is}} = \frac{h_1 - h_2}{h_1 - h_{2,is}} \tag{8}$$

Where $h_{2,s}$ is the enthalpy of the working fluid at the turbine outlet considering an isentropic expansion. The mechanical power of the turbine is calculated by Eq. (9):

$$\dot{W}_t = \dot{m}\,(h_1 - h_2) \tag{9}$$

2.1.4 Internal heat recovery

Part of the energy from the turbine exhaust flow can be recovered through an internal heat exchanger in order to do a preliminary warm-up of the working fluid before entering the evaporator.

Like the evaporator and the condenser, the terminal temperature differences in the heat exchanger (ΔT) and a pinch temperature differential are limited to 5 K. The performance of this equipment is limited by the effectiveness of the heat exchanger which in this specific case can be defined as:

$$T_3 = T_2 - \ \varepsilon\,(T_2 - T_5) \tag{10}$$

$$\Delta T_i = T_3 - T_{con1} \geq 10 \tag{11}$$

$$\Delta T_0 = T_4 - T_{con2} \geq 5 \tag{12}$$

$$PP_1 \geq 5 \tag{13}$$

The energy balance in this equipment is reduced to:

$$\dot{Q}_{reg} = \dot{m}\,(h_2 - h_3) = \dot{m}\,(h_6 - h_5) \tag{14}$$

2.1.5 Pump

Like the turbine, the thermodynamic model of the pump is established as a function of isentropic efficiency, which is a model input and can be defined mathematically as:

$$\eta_{is,p} = \frac{h_{5,s} - h_4}{h_5 - h_4} \tag{15}$$

Where $h_{5,s}$ is the enthalpy of the working fluid at the pump outlet considering an isentropic pressure rise. The electrical power consumed by the pump is calculated by Eq. (16):

$$\dot{W}_p = \dot{m}\,(h_5 - h_4) \tag{16}$$

Once the different energy flows of the thermodynamic system have been evaluated, both the net power output (W_n) and the thermodynamic efficiency of cycle (η) can be determined using the mathematical expressions given by Eqs. (17-18):

$$\dot{W}_n = \dot{W}_t \cdot \eta_g - \dot{W}_b \tag{17}$$

Where the efficiency of the electric generator (η_g) that was set to 98%.

The thermal efficiency of the cycle is defined as the ratio between the net electrical power and the heat supplied to the cycle, and represents the ability of the working fluid to convert heat into electrical energy:

$$\eta = \frac{\dot{W}_n}{\dot{Q}_{evp}} \tag{18}$$

Due to the complexity of the rigorous methods of dimensioning heat exchangers, an approximation of the dimensions of this equipment can be estimated using the logarithmic mean temperature (LMTD) and global heat transfer coefficients (U) as presented in Li *et al.* (2012); He *et al.* (2012); Lakew and Bolland (2010).

$$\dot{Q} = UA \cdot \left[\frac{(\Delta T_{hot} - \Delta T_{cold})}{\ln(\Delta T_{hot} \,/\, \Delta T_{cold})} \right] \tag{19}$$

The ORC cycle simulation is performed using a computer code written in MATLAB2014® and the calculation of thermodynamic properties using the REPROP 9.1® software. The numerical solution is validated with the ASPEN-HYSYS industrial process software, using the basic Rankine cycle and a water source at 413 K as a basis for comparison and different proportions of a mixture of n-pentane/n-butane as a working fluid. The validation of the results of the net electrical power showed that the relative error varies between 1 - 3% depending on the concentration of the working fluid evaluated.

2.1.6 Selection of working fluid

The selection of the working fluid is the design decision that most influences the technical and economic performance of the ORC cycle project. Although there are many options available for working fluids, there are also many restrictions in their selection, mainly related to the thermodynamic properties of fluids, safety and environmental impact.

The selection of the working fluid (pure substances) for a given application of the ORC cycle has been treated in numerous studies, most of them focused on low temperature sources, as can be analyzed in the works by Lakew and Bolland (2010); Tchanche *et al.* (2009); Kosmadakis *et al.* (2009); Mago *et al.* (2008); Saleh *et al.* (2007); among others.

When compared with zeotropic mixtures, the use of pure fluids leads to greater irreversibility in the heat transfer processes, a consequence of the constant temperature profile during the vaporization and condensation process. Thus, the use of zeotropic mixtures as a working fluid leads to a process of vaporization and condensation at variable temperature, increasing the temperature profile between the cold and hot fluid in the heat exchangers, reducing the irreversibilities in this equipment.

However, from the thermodynamic point of view, the use of zeotropic mixtures is an open question. Although several studies such as those presented in Chys *et al.* (2012); Liu *et al.* (2014); Dong *et al.* (2018); Bamorovat Abadi and Kim (2017) suggest that the use of mixtures of organic compounds as working fluids increase the thermodynamic efficiency of ORC cycles, other works such as those presented in Lecompte *et al.* (2014); Li *et al.* (2011, 2014); Wang and Zhao (2009) present results that indicate that the thermodynamic performance of the ORC cycle is lower when purchased with the use of pure fluids.

Thus, it can be concluded that the study of mixtures of viable organic compounds for working fluid must be carried out through an ORC system project, in which the parametric analysis of the thermal system must use more holistic methods that allow to evaluate the importance of different parameters such as vaporization pressure, condensation pressure, pinch temperature differential, overheating and system configuration under the thermodynamic performance of the cycle and equipment dimensions.

2.2 Multiobjective optimization of ORC systems

A multiobjective optimization problem requires the simultaneous satisfaction of a number of different and generally conflicting objectives, making it impossible to find a solution that satisfies all objectives simultaneously. Therefore, it is necessary to find the set of optimal solutions. Thus, a multi-objective mathematical optimization problem has m decision variables to minimize or maximize n objectives subject to k restrictions.

$$\min F(X) = [f_1(X), f_2(X), ..., f_n(X)]^T \tag{20}$$

$$X = [x_1, x_2, ..., x_m]^T \tag{21}$$

Subject to:

$$g_i(X) \leq 0 \qquad i = 1, \ldots, k \tag{22}$$

$$h_i(X) = 0 \qquad i = 1, \ldots, k \tag{23}$$

$$x_{i,min} \leq x_i \leq x_{i,max} \qquad i = 1, \ldots, k \tag{24}$$

Genetic algorithms (GAs) apply an iterative and stochastic search strategy to find the ideal solution, simply imitating the principles of biological evolution. In this work, the NSGA-II method proposed by Deb *et al.* (2002) is employed, which is a multiobjective Genetic Algorithm that classifies the optimal solutions according to the Pareto dominance concept. In this way, using elements from the GAs such as the succession of generations and the population structure, at the end of the optimization process, a set of non-dominated solutions is obtained to be submitted to decision making by the analyst.

Two objective functions were considered in this optimization: minimization of global thermal conductance (UA_T) and maximization of net electrical power (W_n), these being the parameters that most influence the technical and economic feasibility of implementing heat recovery systems based on the ORC.

The following decision variables are selected for this research: working fluid, condensing temperature (T_4), vaporization pressure (P_1), overheating (SUP), heat recovery effectiveness (ϵ), pinch temperature differential in the evaporator and condenser (PP and PP_{con}) and the mass concentration (x) between the mixed working fluids. Although the decision variables are continuously changed within the optimization process, each one must be within a reasonable range of values. The variations in vaporization pressure, condensation temperature, superheating, effectiveness and pinch point are defined in the equations shown in Table 2.

Table 2. Main operating parameters of the ORC cycle

Working fluid	Discrete Variable
$0.2P_c \leq P_1 \leq 0.9P_c$	Discrete Variable
$20\ kPa \leq P_4$	Discrete Variable
$0^oC \leq SUP \leq 70^oC$	Discrete Variable
$0 \leq \epsilon \leq 0.9$	Discrete Variable
$5^oC \leq PP_{con}$	Discrete Variable
$0 \leq x \leq 1$	Discrete Variable
$\eta_{ORC} \geq 0.1$	Restriction

3. Results

The Genetic Algorithm is performed for 150 generations, evaluating different combinations of the design parameters. The distribution of results from the optimization process and the set of optimal solutions (Pareto frontier) are shown in Fig. (2) and Fig. (3), respectively.

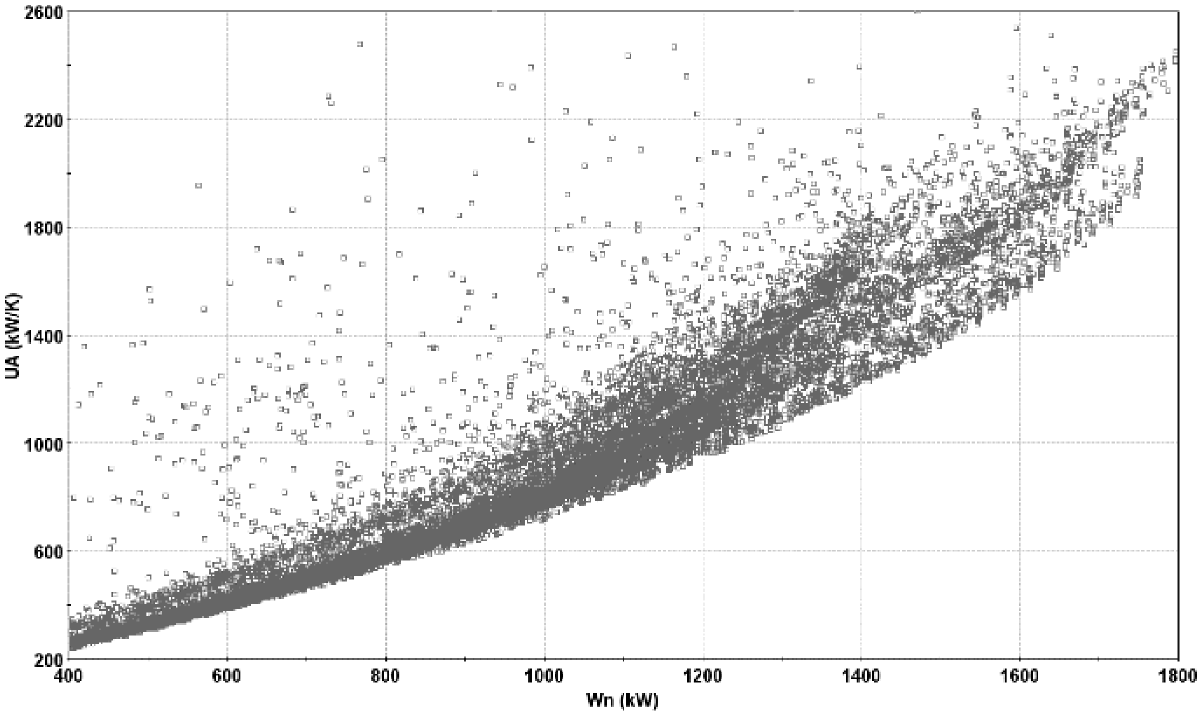

Figure 2. Distribution of genetic algorithm results

In Figure. (3), it can be seen that the optimal solutions are presented by power generation ranges, in which the choice of the optimal solution is strictly related to the working fluid used, with the configuration of the cycle and with the design parameters, since, only the correct combination of these variables allows to achieve the best technical-economic performance of the thermal system.

The results of the Pareto frontier shows that the RE245CB2 presents the best working fluid option from the point of view of electricity generation, generating between 1750 - 1800 kW. However, under these design conditions, the largest area required by the thermal system is achieved with an overall thermal conductance ranging from 2200 - 2450 kW/K.

N-Butane (C_4H_{10}) is the fluid that presents itself as the best option from the point of view of the total heat exchange area required by the thermal system with an overall thermal conductance varying between 200 - 450 kW/K with a capacity to generate electricity between 400 - 650 kW. On the other hand, a mixture of R235FA/C7H16 at 98% presented as the best working fluid option for thermal systems designed to operate between 650 - 1750 kW.

From the mathematical modeling developed in section 2 it is evident that the thermodynamic performance and dimensioning of the equipment is directly proportional to the molar flow of the working fluid, variation of the enthalpy in the turbine, heat added to the thermodynamic cycle and heat rejected to the environment through the condenser.

From the analysis of the conventional Rankine cycle, it is known that the increase in the pressure of the working fluid

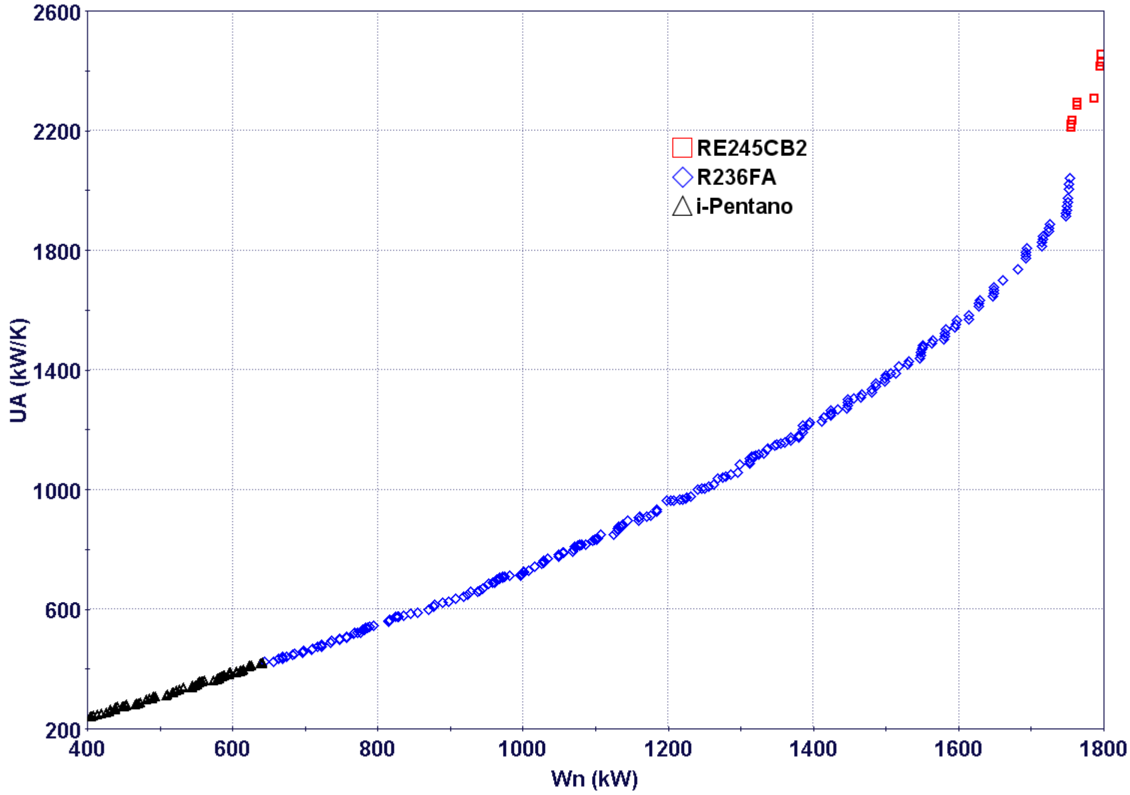

Figure 3. Pareto frontier of objective functions

during the addition of heat to the cycle increases the efficiency of the thermal system. The results obtained in this work are observed, being that the configuration of the ORC cycle and working fluid used, or the maximum performance of the thermodynamic system, a variable vaporization pressure occurs, or can be observed for a mixture R235FA/C7H16 in the Fig. (4).

For all fluids and corresponding mixtures evaluated, it is observed that the generation of electricity increases with the decrease of the pinch point, since this parameter is inversely proportional to the heat flow supplied to the thermal system, thus increasing the mass flow of the working fluid at the evaporator outlet favoring the generation of electrical power in the cycle.

The overheating and effectiveness of the internal heat recovery unit, when compared to the pinch point and vaporization pressure, have little influence on the generation of electricity in the thermal system. Regardless of the working fluid used, a slight degree of overheating of the working fluid before its expansion in the turbine generates an increase in the generation of energy from the thermal system by increasing the variation of enthalpy in the turbine, where the maximum value of overheating is limited by the difference between the temperature of the heat source and the temperature of entry into the turbine.

The preheating of the working fluid (regenerative cycle) before entering the evaporator has no direct influence on the ability of the ORC cycle to generate electricity, since the variation in the effectiveness of the internal heat exchanger does not modify the molar flow of the working fluid. and / or the variation of enthalpy in the turbine. However, the use of this equipment allows lower pinch point values to be established in the evaporator without violating the restrictions established in the mathematical model indirectly favoring the generation of electricity in the cycle.

4. Conclusions

In this research work, a thermodynamic model and multiobjective optimization were performed for a low temperature heat recovery system using an ORC cycle. The optimization model was developed for two configurations of the ORC cycle (with and without heat regenerator) operating with eighteen working fluids and their respective azeotropic mixtures.

The application of genetic algorithms to optimize the energy performance of heat recovery projects proved to be a powerful and effective tool to determine the "trade-off" for the different objectives established. The results show that the optimization of small-scale ORC systems should not be evaluated independently, since there is more than one optimal solution that must be considered in the decision-making process.

From the results, it is evident that it is not possible to define a comprehensive guideline to determine the optimum

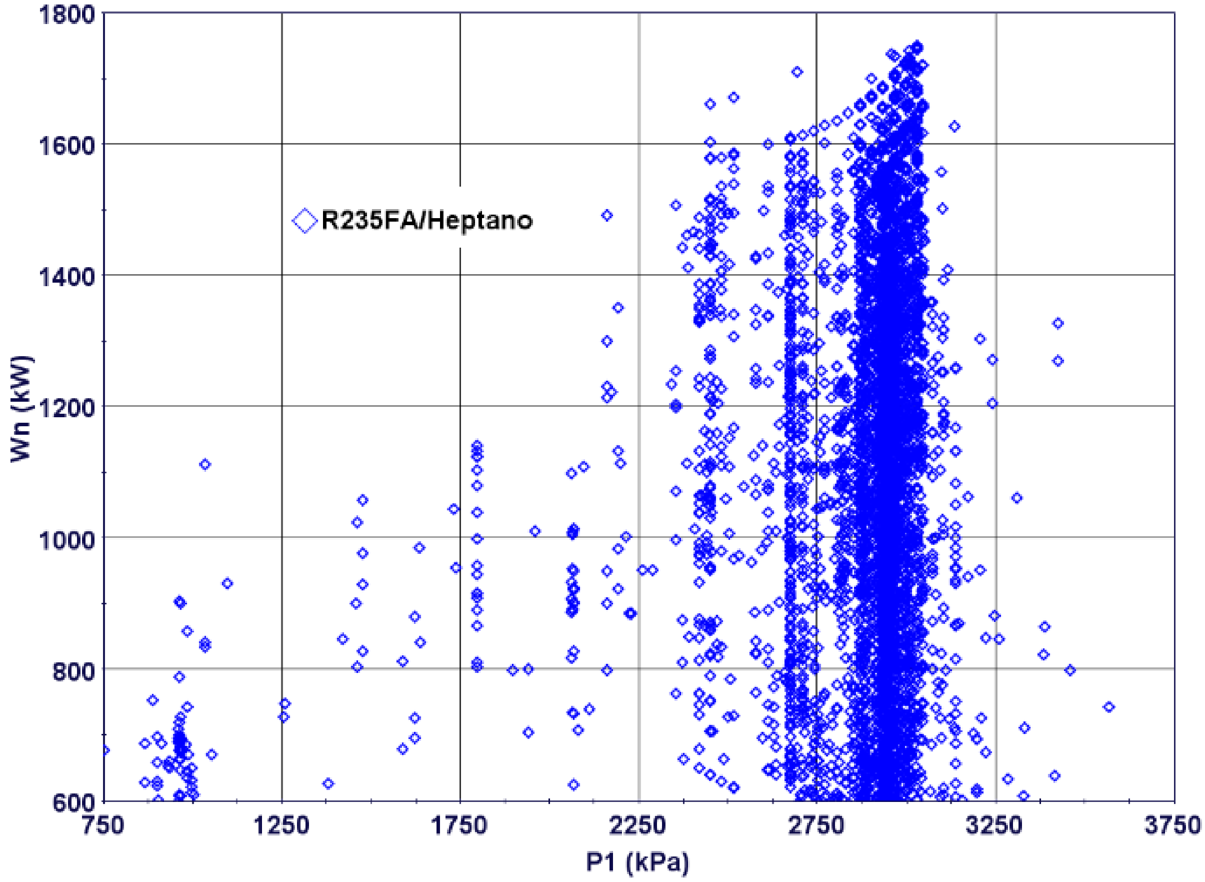

Figure 4. Variation of the electrical power of the cycle as a function of vaporization pressure

design of the cogeneration system, since for each working fluid considered in the optimization, the design variables influence the evaluated objectives differently and magnitude. Thus, a good engineering judgment in conjunction with sophisticated analysis tools is required for each application of the thermal system, since the set of optimal solutions is modified according to different technical and thermodynamic considerations.

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