This dissertation presents the development of a simulation model for the organic Rankine cycles. The purpose of the study is to model an organic Rankine cycle from the thermodynamic and heat transfer point of view, so as to determine the power output of the plant and to size the heat exchangers necessary for that duty. The model was considered for the recovery of low grade waste heat from both liquid and gaseous sources. The simulation also considered the use of different working fluids, some of which are considered new for heat recovery applications. Also, a study on the application of an organic Rankine cycle in a trigeneration system was conducted.

1.1. Organic Rankine cycles

The organic Rankine cycle comprises the same components as a conventional steam power plant (a boiler, a work-producing expansion device, a condenser and a pump). However, the working fluid is an organic component characterized by a boiling temperature lower than water at a given pressure, which allows for power generation from low heat source temperatures [1].

The layout of the organic Rankine cycle (ORC) is somewhat simpler than that of the steam Rankine cycle: there is no water-steam drum connected to the boiler, and one single heat exchanger can be used to perform the three energy supply phases: preheating, vaporization and superheating. Figure 1 shows a schematic representation of the essential components of an ORC plant.



Figure 1 Schematic diagram of an ORC plant.

The particularity of the organic Rankine cycle over the traditional steam cycle lays in the working fluid: an organic component is used instead of water. This organic compound is typically a refrigerant, a hydrocarbon (butane, pentane, hexane, etc.), a silicon oil or a perfluorocarbon. Its boiling point is lower than that of water at a given pressure, which allows for recovering thermal energy at a lower temperature than in the traditional steam Rankine cycle [1].

In recent years, there has been a great amount of waste heat energy being released into the environment, such as exhaust gases from turbines and engines and waste heat from industrial plants, which leads to serious environmental impacts. Not recovering this waste heat leads to higher fossil fuel consumption and emissions of CO, CO_2 , NO_x and other atmospheric pollutants. In addition, there are also abundant geothermal sources and solar energy available in the world, which are classified as low grade heat sources [2], thus requiring specific technology to be used.

It has been estimated that industrial low-grade waste heat accounts for more than 50 percent of the energy generated [3]. In general, heat is considered to be moderate-to-low grade if it is available at temperatures lower than 370 °C [3]. It should be mentioned that the correct denomination should be "waste thermal energy", although "waste heat" finds widespread use, in industry and the scientific literature

An organic Rankine cycle can make efficient use of low temperature waste heat such as geothermal energy to generate electricity. At these low temperatures a steam cycle would be inefficient, because of the enormous volume of low pressure steam, which would require very voluminous and costly piping, resulting in inefficient plants. Small-scale ORCs have been used, commercially or as pilot plants, in the last two decades. Several organic compounds have been used in ORCs to match the temperature of the available waste heat energy, which temperatures can be as low as 70-80°C. The efficiency of an ORC is estimated to be between 10% and 20%, depending on temperature levels [4].

1.2. Literature review

The most important concern in the study of an organic Rankine cycle is the improvement of the overall cycle efficiency, since the energy input temperature is lower than in a traditional Rankine cycle. The efficient operation of the cycle relies greatly on two factors: the working conditions of the cycle (namely, temperature and pressure levels) and the thermodynamic properties of the working fluids.

In the literature, experimental research on organic Rankine cycles has been widely explored, and authors have proposed different arrangements for the system, depending on design, heat sources and applications.

Larjola [5] constructed three ORC prototypes with high speed turbo generators, two for medium temperature waste heat, using R114 as the working fluid, and one for high temperature waste heat, using toluene as the working fluid. The study focused on the technical development of the prototypes that showed best performance and were economically viable for commercial production.

The ORC generating set proposed by Nguyen et al. [6] developed 1.5 kW using hot water as the heat transfer fluid and n-pentane as the working fluid. It was able to operate using low temperature heat at 81°C with a thermal efficiency of 4.3 %.

An experimental study as well as a numerical model of an organic Rankine cycle was presented by Quoilin et al. [7]. The prototype used refrigerant HCFC-123 as the working fluid and a hot air flow as the heat source. The performance of the prototype was used to validate the model, which was applied to investigate potential improvements on the prototype.

Srinivasan et al. [8] examined the exhaust waste heat recovery potential from a high-efficiency low-emission dual-fuel low-temperature combustion engine using an organic Rankine cycle. The fuel conversion efficiency improved by an average of 7% for all injection timings and loads while NO_x and CO_2 emissions recorded an 18% (average) decrease.

The performance of an ORC system using solar energy as the heat source and CO_2 in supercritical conditions, as the working fluid, was investigated by Zhang et al. [9]. The resulting power generation efficiency (ratio of power generation and solar radiation) ranged between 8.78-9.45%.

Manolakos et al. [10] also evaluated the performance of a solar ORC system, in this case, used specifically for desalinization with a reverse osmosis process. Using HFC-134a as the working fluid they proved that the developed plant achieved continuous operation under the intermittent availability of solar radiation. Nonetheless, the efficiency was lower than when tested at laboratory with a controlled thermal load.

Research has also been conducted for specific cases, like the use of organic Rankine cycles bottoming internal combustion engines, that is, the use of the exhaust gases from the engine as the heat source for the ORC.

Vaja and Gambarotta [11] employed a thermodynamic analysis to efficiently match an organic Rankine cycle with a stationary internal combustion engine. They considered three different working fluids, classified according to the shape of the vapor lines in the T–s diagram: overhanging, nearly isentropic and bell shaped. Also, three different cycle setups were considered and a second law analysis was performed. They demonstrated that a 12% increase in the overall efficiency could be achieved with respect to the engine with no bottoming.

The vast majority of prototypes reported in the literature were designed to generate electric power; with the exception of those used for reverse osmosis desalination [10] and to power vapor compression refrigeration cycles [3].

In terms of the heat source that was used in the experimental evaluation, some authors used hot air [7, 12] to simulate waste heat gases, while others used hot water [6, 13] and hot oil [3]. Some researchers started using a prototype in laboratory conditions, and then, tested it with real industrial waste heat, such as exhaust and combustion gases, from stationary engines [5, 8, 11, 14], and from automotive Diesel engines [15, 16]. Other heat sources include exhaust from solid biomass power plants [17], micro-gas turbines [18], and combined cycle power plants [19]. Solar panels have also been used to provide the thermal energy to the system [9, 10, 20, 21, 22].

Many researchers have conducted comparative studies of organic Rankine cycles on the selection of the proper working fluid to recover the same amount of wasted heat under the same conditions [23-25]. Analytical studies that seek a better performance of the cycle were carried out comparing different working fluids [16-22].

Organic fluids can be classified as dry, wet, and isentropic, depending on the slope of the saturation vapor line in the temperature-entropy diagram [26].

As presented on Fig. 2, at the end of the expansion process, the isentropic fluid (a) has an almost vertical vapor saturation line, the dry fluid (b) has a positive slope and thus expansion ends in the saturated vapor region, and the wet fluid (c) expansion ends in the two phase region.

In an ideal ORC, the working fluid expands isentropically through the turbine. The negative slope of the saturation vapor curve for wet fluids indicates the formation of condensate while expanding through the turbine. Since the impact of liquid droplets in the turbine blades is undesirable, only dry and isentropic fluids are recommended to be used in ORCs [27].



Figure 2. *T-s* process diagram comparison of working fluids: (a) isentropic, (b) dry, and (c) wet. [16]

Hung et al. [28] developed a parametric analysis and comparison of the efficiencies of organic Rankine cycles using benzene, ammonia, R11, R12, R134a and R113 as working fluids. Their study demonstrated that, for operation between two isobaric curves, the system efficiency increased for wet fluids and decreased for dry fluids. Isentropic fluids achieved an approximately constant value for high turbine inlet temperatures, and were most suitable for recovering low temperature waste heat.

Some years later, Hung [29] continued to study the efficiency of organic Rankine cycles using dry fluids such as benzene, toluene, p-xylene, R113 and R123. In his investigation p-xylene showed the highest efficiency and benzene the lowest. He also carried out an irreversibility analysis of the working fluids and found out that irreversibility depends on the type of heat source. As a result, pxylene had the lowest irreversibility in recovering high temperature waste heat, while R113 and R123 had a better performance recovering low temperature waste heat.

Roy et al. [30] investigated the parametric optimization and performance analysis of a waste heat recovery system by means of an organic Rankine cycle, using R-12, R-123 and R-134a as working fluids. The results showed that R-123 had the maximum work output and efficiencies among all the selected fluids.

The study of a larger selection process was made by Maizza and Maizza [31], who examined the thermodynamic and physical properties of twenty nonconventional working fluids to be used in organic Rankine cycles. Of the fluids analyzed R123 and R124 showed best system performance and wide operative ranges.

The thermodynamic screening of 31 pure component working fluids for organic Rankine cycles was carried out by Saleh et al. [32] using the BACKONE equation of state. The fluids were alkenes, fluorinated alkenes, ethers and fluorinated ethers. They showed that the definition of an optimum working fluid would depend on its properties and the type of cycle used.

Other authors have concentrated their investigations on the optimization of the performance of the organic Rankine cycle with different working fluids under different working parameters [2, 17, 23, 33-35].

Wei et al. [36] carried out a performance analysis and optimization of an organic Rankine cycle using HFC-245fa as the working fluid. Their main findings were that maximizing the usage of exhaust heat is a good way to improve system output net power and efficiency. They also found that, when ambient temperature increases, the system output net power and efficiency deteriorates with the departure from nominal state by possibly exceeding 30%.

The effects of the thermodynamic parameters on the performance of an organic Rankine cycle were examined by Dai et al. [2], and these parameters were optimized for each working fluid with the exergy efficiency as an objective function by means of a genetic algorithm. Their results showed that the cycles with organic working fluids were more efficient than the cycle with water in converting low grade waste heat to useful work. The cycle using R236EA had the highest exergy efficiency, and the addition of an internal heat exchanger into the ORC system would not improve the performance under the given waste heat conditions.

Nguyen et al. [27] studied parametrically the advantages and disadvantages of several alternative working fluids and recommended the use of dry organic fluids. They also realized that, as expected, all performance indicators were low at low heat source temperatures, and improved as this temperature raised. They also discussed the influence of various external and internal operating parameters, such as heat source and heat sink temperatures, turbine and pump isentropic efficiencies and the addition of an internal heat exchanger, on the overall performance of the energy recovery and conversion system.

For the operation of such cycles, studies have also been carried out in the development of dynamic simulation models which can help predicting the behavior of the system under the variation of operational parameters.

Wei et al. [37] proposed two approaches to design a dynamic model for an organic Rankine cycle, based on moving boundary and discretization model techniques. Both models were validated against experimental data. The moving boundary model was less complex than the discretized version and, as a result, it was more acceptable for control design applications.

As it has been previously established, many researchers have conducted studies on the selection of the proper working fluid, that is, the one that showed best performance under prescribed operating conditions [3, 11, 16, 18-22, 24, 32]. Other authors have concentrated their investigations in optimizing the performance of the cycle with different working fluids [2, 17, 23, 33-35]. However, even when the cycle performance was evaluated, the operating parameters, such as the heat source mass flow and temperature, were maintained constant during these simulations.

To the author's knowledge, there has been little or no analysis on the cycle performance while varying the operating conditions, namely, the input data for the available heat source. The author wishes to explore the output and efficiency of the cycle under varying inlet conditions. Also, there has been little or no investigation on the two new working fluids addressed: R1234yf and R1234ze, for ORC applications. Only two studies utilizing R1234yf were found [38, 39].

Nonetheless, it is important to evaluate the performance of the cycle while varying the operating parameters in order to obtain the optimum power output under different working conditions.

1.3. Research Objectives

The present work focuses on the simulation of the organic Rankine cycle under steady state operation. There are three key areas which the dissertation addresses:

- Thermodynamic simulation of the system
 - Determining the power output and thermal efficiency of the organic Rankine cycle under various mass flow rates and inlet thermodynamic states of both liquid or gaseous waste heat source using three different dry working fluids.
- Heat exchanger simulation
 - Sizing of the heat exchangers used to recover and reject the waste heat in the ORC processes.
- Thermodynamic study of an ORC based trigeneration system
 - Thermodynamic analysis and validation of a trigeneration system using an ORC to recover the waste heat.

1.4. Dissertation Organization

- Chapter 2 describes the development and results of a thermodynamic model for the ORC system, based on a first law analysis.
- Chapter 3 details the heat exchanger models used for their sizing, considering the most suitable type of exchanger for each ORC application.
- Chapter 4 illustrates the association of an ORC system to a trigeneration system using the information gathered in the simulation.
- Chapter 5 presents the dissertation main conclusions and suggestions for future work.