Simulation and optimization of an Organic Rankine Cycle

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Abstract: An Organic Rankine Cycle is an ideal model that describes power cycles processes that have a low temperature heat source such as biomass, solar energy or waste heat from conventional power plants. This kind of cycles can be modelled and simulated numerically using simple programming languages and specific libraries that contain essential information about phase transition and different properties for a great variety of substances. The aim of this project is to simulate numerically an ORC using Python 2.7 and the library Coolprop, find out how the power produced and the efficiency vary depending on different variables, and finally try to optimize it with some environmental conditions fixed.

I. INTRODUCTION

A Rankine Cycle (RC) is a thermodynamic cycle that is used to ideally model a thermal power plant and essentially the behaviour of its working fluid. This simplifies the study of the efficiency and the power production of this kind of plants. The simplest form of this thermodynamic cycle has 4 basic components: expander, condenser, pump and boiler.

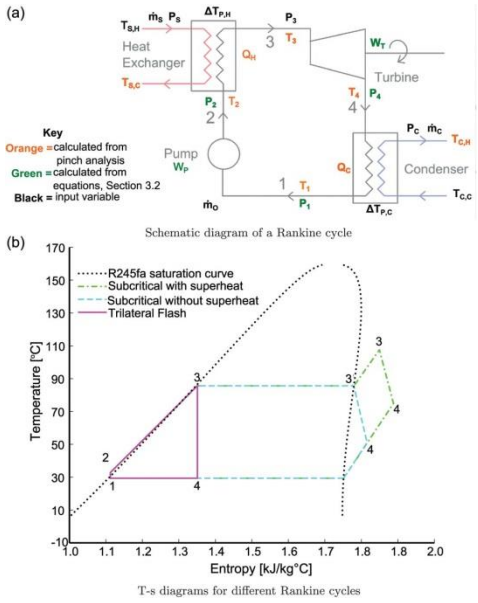

FIG 1: Schema of the main elements of a RC and example of a T-s diagram for R245fa fluid. Image from [1].

The working fluid goes through all these four elements, changing its state from liquid to saturated liquid-gas and from saturated to gas state if enough energy is provided in the boiler, this process is represented in Fig.(1). When the heat source is a low-temperature one, such as the one coming from power plants waste heat, biomass or solar energy or when the power plant is small, the fluid used is preferable to be an organic one, which main properties are a high molecular mass and a lower boiling temperature than water [2]. These types of RC are called Organic Rankine Cycles (ORC).

The first and main part of this work consists on doing a simulation of an ORC while taking into account not only the working fluid but also the hot fluid and the cold fluid of the heat exchangers (boiler and condenser) and also the coherence of the cycle, this means that the final state must coincide with the first one. It is impossible to know the last state before running the program at least one time, so some iteration is needed. Including the heat source and the cold source, we are taking into account the irreversibilities caused by the finite-time heat transfer between fluids [3].

The simulation programme is made with Python (version 2.7) programming language using CoolProp [4] library, which is a free-software tool similar to the NIST RefProp library.

The following section aim is to study the effects of different variables on the cycle thermal efficiency and work and to optimize our cycle providing the previous results. The variables studied are the ones that could be changed in a "real" plant once installed, such as the working fluid flow or the maximum and minimum pressures of the cycle, as well as the working fluid substance. The variables we consider fixed are the mass flow of the hot fluid and its initial temperature, and the geometric constants of the exchangers.

II. NUMERICAL SIMULATION

The program has been divided into 4 parts: the main program and 3 subprograms: boiler and condenser, expander and pump, and plotting. The most complex part out of the 4 mentioned is the boiler and condenser one. Coolprop library gives the different fluid state parameters given two of them and the fluid substance.

The main program. All the variables are defined, the subprograms are called and the efficiency and total power are calculated. As mentioned previously, there is iteration while the initial and the final working fluid temperature are not the same. This procedure is necessary as an initial temperature has to be defined in order to start the simulation, but this parameter depends on other variables and is not a definable start variable.

The total power produced and the thermal efficiency of the cycle are calculated with the following expressions.

$$\dot{W}_{TOTAL} = \dot{W}_T - \dot{W}_P \quad (1)$$

$$\eta = \frac{\dot{W}_T - \dot{W}_P}{\dot{Q}_{in}} \quad (2)$$

Where $\dot{W}_T$ is the power produced by the turbine or expander, $\dot{W}_P$ is the power given to the pump and $\dot{Q}_{in}$ is the heat transfer rate given to the working fluid in the boiler.

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The exchangers. The same function is used for both the boiler and the condenser, but in the first the cold fluid is the working fluid whereas in the second one is the hot one. The parameters and variables are shown in the following table:

	Parameters	Units	Description
Input	p_c	Pa	Cold fluid pressure
	p_h	Pa	Hot fluid pressure
	$\dot{m}_c$	kg/s	Cold fluid mass flow rate
	$\dot{m}_h$	kg/s	Hot fluid mass flow rate
	T_{h1}	K	Hot fluid start temperature
	T_{c1}	K	Cold fluid start temperature
	U	$W/K/m^2$	Heat transfer coefficient
	A	m^2	Exchanger area
	Fluids	-	Substances (hot and cold)
Output	$\dot{Q}_{in}$	W/s	Total heat exchanged
	T_{h2}	K	Hot fluid final temperature
	T_{c2}	K	Cold fluid final temperature
	h_{h2}	J/kg	Hot fluid final enthalpy
	h_{c2}	J/kg	Cold fluid final enthalpy

TABLE I: Parameters introduced as imput and output given by the subprogram exchangers.py.

The aim of this subprogram is to calculate the heat transferred from one fluid to the other, the final temperature and the final enthalpy of both fluids given the input parameters (Table I). The expressions used in the exchanger are:

$$\dot{Q}_{in} = UA \cdot \Delta T_{LMTD} \tag{3}$$

$$\dot{Q}_{in} = \dot{m}_h \cdot \Delta H_h = \dot{m}_c \cdot \Delta H_c \tag{4}$$

$$T_{LMTD} = ((T_{h1} - T_{c2}) - (T_{h2} - T_{c1}))/\ln\left(\frac{T_{h1}-T_{c2}}{T_{h2}-T_{c1}}\right) \tag{5}$$

Where ΔT_{LMTD} is the Log-mean temperature difference for the counter-current flow case and ΔH_i is the enthalpy difference between the first and the last state for both fluids [5].

The exchanger is divided into 3 parts depending on the state of the fluids: one part for the liquid state, another one for the saturated state and the final one for the vapour state. It is assumed that the changes of the fluids pressure are negligible and that the pressure is far below the critical pressure to avoid numerical issues.

The first part of this subprogram computes some essential initial parameters such as the initial enthalpy, the saturated liquid and gas state enthalpy, the maximum achievable enthalpy, the maximum heat exchangeable, and the minimum and maximum possible final temperatures for the hot fluid.

As the final hot fluid temperature is needed to calculate the heat exchanged, but only the physical and geometrical properties of the exchanger are known, a bisection method is implemented. The program that follows calculate the A (size of the exchanger, geometrical parameter) given T_{h2}. The first value of T_{h2} is the semi-sum of the maximum and minimum possible T_{h2}, and this value is varied depending on the resulting A until it is the same as the defined in the main program. In this way, when iteration ends all the parameters are known and the result are physically compatible with the geometry of the exchanger.

Expander and pump. It computes the working fluid state after the expander and pump given its previous state and the isentropic efficiency of the element. The input and output parameters of this subprogram are shown in Table II.

	Parameters	Units	Description
Input	p_1	Pa	Working fluid initial pressure
	p_2	Pa	Working fluid final pressure
	T_1	K	Working fluid initial temperature
	$\dot{m}$	kg/s	Working fluid flow
	η	-	Turbine/Pump efficiency (0-1)
	Fluids	-	Working fluid substance
Output	$\dot{W}$	W/s	Power produced or given
	T_2	K	Working fluid final temperature
	h_2	J/kg	Working fluid final enthalpy

TABLE II: Parameters introduced as imput and output given by the subprogram turbine_pump.py.

The enthalpy is one of the parameters used to find the fluid state parameters needed, as it is unique for each state, also in the phase transition where pressure and temperature stay constant. The final enthalpy can be found with the following expressions for the isentropic efficiency:

$$\eta_{Pump} = \frac{h_1 - h_{2s}}{h_1 - h_2} \tag{6}$$

$$\eta_{Expander} = \frac{h_1 - h_2}{h_1 - h_{2s}} \tag{7}$$

Where η_i is the isentropic efficiency of each element, h_1 and h_2 are the start and final enthalpy of the fluid, and h_{s2} is the final enthalpy that would be if the process were isentropic, this means, with no changes of entropy during the process. Some examples from Cantera library website have been used and modified in this part [6].

Plotting. Finally, there is a last subprogram that contains the code needed to plot the results obtained (the power/efficiency depending on a variable) and a Rankine cycle. The input elements are arrays with the data x and y, and the main parameters of a RC, such as the maximum and minimum temperature and pressure.

III. RESULTS AND DISCUSSION

Once the program has been written and works properly, it is possible to analyse the behaviour of some parameters depending on the others. Two important parameters in power plants are the power produced and the efficiency of the process.

We want the cycle simulated to be organic, as it has been mentioned before as one of the principal aims. The first step is to choose the working fluid substance. It has to fulfil a series of conditions:

- The fluid state is recommendable to be entirely liquefied when going through the pump, as it works more efficiently [7]. As the cold fluid temperature in the condenser will be the ambient temperature and the fluid will be water, the boiling

temperature of the working fluid must be greater than the ambient temperature (298K) at the pressure defined in the condenser.

- In the same way, the turbine is more damaged if the fluid is a mixture of liquid and gas state. That is why the working fluid boiling temperature should be much lower than the hot fluid temperature.

- The critical pressure of the fluid has to be much greater than the pressure defined in the exchangers. The exchanger's simulation works properly providing the fluid pressure is not critical.

The initial state of the hot fluid is fixed and has the following parameters: $m_h = 31.94\ \frac{Kg}{s}$, $T_{h1} = 150\ ºC$, $P_s = 2.3\ bar$. This corresponds to a superheated steam and is similar to a realistic case of an industrial processing plant waste heat recovery [1].

The following table shows the boiling temperature at 3 different pressures and the critical pressure of different organic fluids:

Substances	T(ºC)			P_{crit} (atm)
	0.9 bar	1.013 bar	7 bar	
Novec649	46	49	119	18.4
R113	44	48	121	33.5
R141b	29	32	102	41.6
R365MFC	37	40	108	32.2
SES36	32	36	105	28.1

TABLE III: Substances that meet the requirements mentioned before, their boiling temperature at 3 different pressures and critical pressure.

These are some of the substances that meet the requirements. To decide which one will be the working fluid in the following simulations we can see which is the power produced and the efficiency of the cycle depending on the substance for a given RC. In this case, the maximum and minimum pressures chosen are the ones of the Table III.

Substance	Efficiency(%)	Power (kW)
Novec649	9.75	133.28
R113	13.92	203.46
R141b	14.86	317.14
R365MFC	12.84	257.84
SES36	11.81	222.06

TABLE IV: Substances, efficiency of an ORC and power produced, given some specific conditions: T_{1hot} = 423 K, T_{1cold} = 298 K, $\dot{m}_{hot}$ = 31.94 kg/s, $\dot{m}_{working}$ = 7 kg/s, $\dot{m}_{cold}$ = 40 kg/s, $p_{condenser}$ = 0.9 bar, p_{boiler} = 7 bar, ΣUA_{boiler} = 67.5 kW/K, $\Sigma UA_{condenser}$ = 40.5 kW/K, η_{pump} = 0.6, $\eta_{turbine}$ = 0.9

We can see that both Efficiency and Power have the same order of magnitude for every substance, but they differ significantly. We can see that in the case of the RC parameters chosen, the substances R113 and R141b are the ones with the best efficiency, and R141b and R365MFC are the ones with better Power production. It is clear, then, that more thermal efficiency does not mean more power produced.

If we study how Power and Efficiency varies depending on different parameters for each fluid, it will be easier to determine the best working fluid substance in our simulation.

A. Variables effect on total power and efficiency

There are some parameters than can be modified in a "real" cycle. Some of them are the working fluid flow and the cold fluid flow, and the pressures at the boiler and the condenser. The following figures show the Power and Efficiency depending on these four parameters for each substance of tables III and IV.

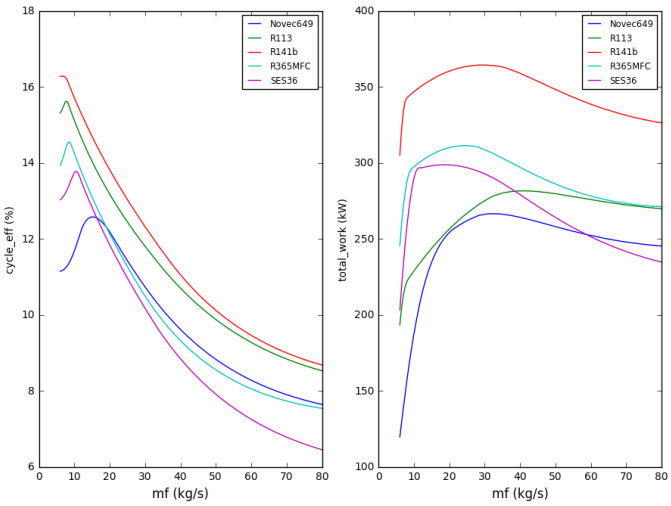

FIG 2: Efficiency and total Power depending on the working fluid flow and substance.

The efficiency and the total power have approximately the same behavior for each substance. On one hand, the efficiency has a very pronounced peak for low m_f, whereas on the other hand the total work has a smoother peak located around 30 kg/s. It is also easy to observe that the first part of the work curve has a pronounced slope for all the substances, which corresponds to the "complete" ORC, where the working fluid reaches the gas state.

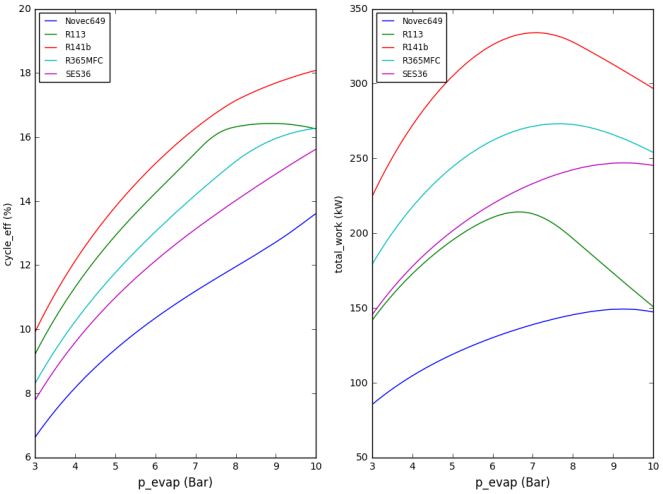

FIG 3: Efficiency and total Power depending on the maximum pressure of the cycle (pressure at the boiler) and the working fluid substance.

Again, all the curves have a similar behavior for each substance. The efficiency curve is ascendant for all the pressures except for the R113 substance, which presents a maximum efficiency for 7.5 bar approximately. Although efficiency grows with the boiler pressure, the work does not. In the case of the power produced, there is a maximum at one boiler pressure.

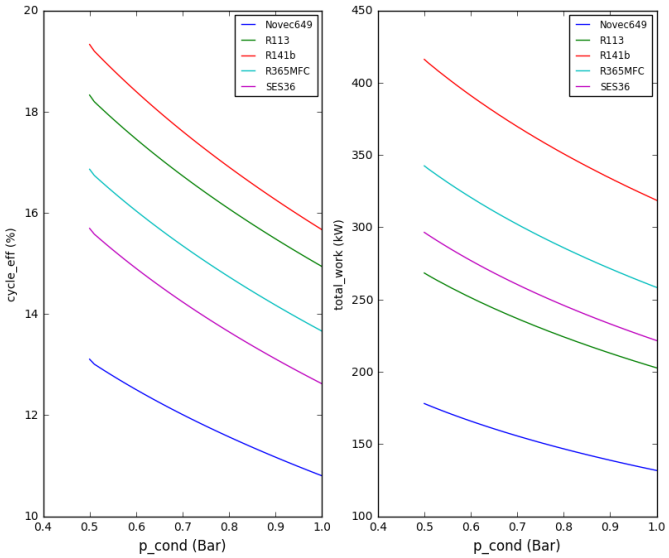

FIG 4: Efficiency and total Power depending on the minimum pressure of the cycle (pressure at the condenser) and the working fluid substance.

In this case both plots are very similar and the efficiency and the total work decrease with the pressure at the condenser. Although it seems that the lower the pressure, the better the ORC will be, it has to be taken in account that a liquid state after the condenser is desired. As it is known, the boiling temperature decreases with pressure, and we need the working fluid boiling temperature to be greater than the cooling fluid temperature.

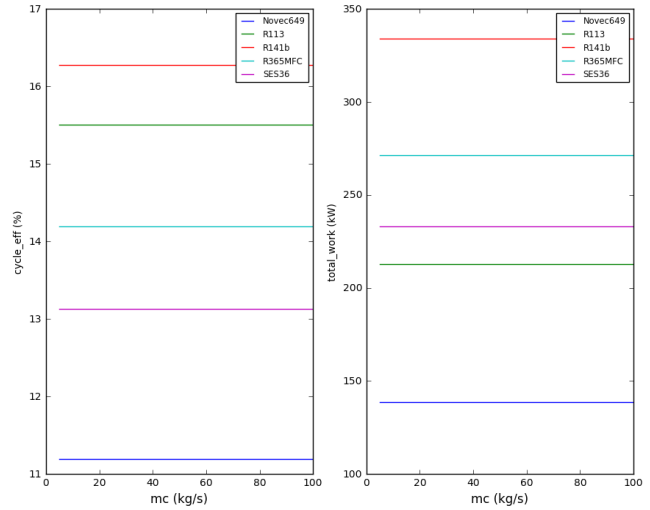

FIG 5: Efficiency and total Power depending on the cold fluid flow and the working fluid substance.

Finally, we can observe that for this simulation the cold fluid flow has no impact either on the efficiency or the power produced. This means that the flux is always great enough to provide enough cooling to the working fluid.

It is important to notice that more efficiency (given by equation (2) does not mean more power produced, as it can be seen in Fig (3), where the maximum of power happens at a different pressure than the maximum efficiency. In the following section the parameter optimized will be the power.

Looking at the figures is clear that the fluid with a major efficiency and power production in the cycle is the R141b fluid. From now on, it will be the one used in all the simulations.

B. Optimization of the cycle.

In this section, an optimization of an ORC is done using the dependences found in the previous section.

First of all, the pressure at the condenser has been set at the minimum one for which the fluid reaches de liquid state.

Afterwards, an iteration method has been implemented to find the maximum work while changing the boiling pressure and the working fluid flow. The maximum in the power vs boiler pressure, Fig.(3), moves towards left when the mass flow increases, and the maximum in the power vs mass flow, Fig.(2), moves towards right when the boiler pressure decreases. This phenomenon happens until a certain point where the maximum work is reached. In this point the mass curve flattens in the zone of the maximum.

The ORC obtained is the one in the Fig (6).

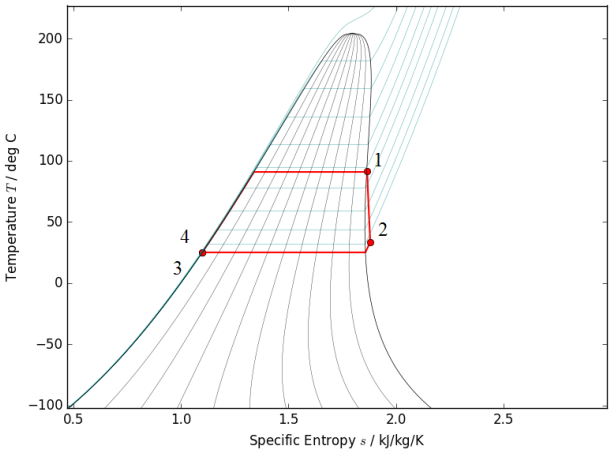

FIG 6: Optimized Rankine cycle in the T-s diagram. 1: Fluid state after the boiler and before the turbine; 2: Fluid state after the turbine; 3: Fluid state after the condenser and before the pump; 4: Fluid state after the pump.

The value of the different variables and parameters are shown in the following table.

	Parameters	Value
Input	UA_{boiler}	67.5 kW/K
	$UA_{condenser}$	40.5 kW/K
	P_{boiler}	5.4 bar
	$P_{condenser}$	0.79 bar
	P_{hot_fluid}	2.3 bar
	T_{h1}	423.15 K
	T_{c1}	298 K
	$\dot{m}_h$	31.94 kg/s

	$\dot{m}_c$	400 kg/s
	$\dot{m}_f$	9.23 kg/s
	Working fluid	R141b
	Hot fluid	Water
	Cold fluid	Water
	η_{pump}	60%
	$\eta_{turbine}$	90%
Calculated parameters and ouptut	T_{h2}	385.94K
	T_1	364.40K
	T_2	306.80K
	T_3	298.13K
	T_4	298.67K
	$\dot{Q}_{in}$	2486.4kW
	$\dot{W}_{turbine}$	350.6kW
	$\dot{W}_{pump}$	-5.2kW
	Efficiency	13.88%
	Total Work	345.4kW

TABLE V: Parameters of the optimized simulation.

IV. CONCLUSIONS

The principal aims of this project were to simulate numerically an ORC, determine how the power produced and the efficiency of the cycle depend on the different variables and try to optimize the cycle afterwards.

Although the simulation works and the power and efficiency found have realistic values, the program could be more complex either including more elements to the cycle (regeneration, re-heat) or taking into account singularities and changes of pressure in the exchangers. Nevertheless, the behaviour of the studied parameters (power produced and efficiency) is similar to the one it would be if these corrections were applied.

It has been shown the impact of some variables on the efficiency and the total power produced in our ORC. In this part we can conclude that the working fluid mass flow rate and the maximum pressure present a value for which the power has a maximum, this can be seen in Fig (2) and Fig. (3) respectively. Work and efficiency decrease with the minimum pressure of the cycle (pressure at the condenser), Fig.(4), and the cooling fluid mass flow rate has no impact in our simulation, as it can be seen in Fig.(5).

Finally, an optimization of an ORC has been done providing the previous results. All the input data and the results obtained are in Table V. The chosen working fluid has been R141b, and the cycle obtained would generate 345.4 kW approximately.

Acknowledgments

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