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THERMOECONOMIC OPTIMIZATION OF KALINA CYCLE SYSTEMS FOR WASTE HEAT RECOVERY IN A DIESEL ENGINE

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Abstract. In this work, a thermoeconomic optimization of Kalina Cycle is carried out in order to recover waste heat from cooling water and exhaust gases in a diesel engine. For each heat source, it was evaluated two different structures of Kalina Cycle, regenerative and non-regenerative. The objective function for the thermoeconomic optimization problem is the profit from sale of Kalina Cycle additional power generation. The decision variables of the optimization problem are evaporation pressure, condensation pressure, waste heat recovery exchanger approach, pump isentropic efficiency, turbine isentropic efficiency, separator terminal temperature difference, regenerator effectiveness, superheater temperature increase, mass flow and ammonia concentration. The optimization problem, as well as the thermodynamic and economic modelling, were formulated and solved in EES (Engineering Equation Solver) software. The results of the thermoeconomic optimization problem allow to evaluate the total costs, thermal efficiency and net engine power output of the Kalina Cycle for the waste heat and others design parameters.

Keywords: Internal Combustion Engine, Kalina Cycle, Waste Heat Recovery, Optimization.

1. INTRODUCTION

Recently, due to the energy shortage, environmental pollutions, and climate change, the issues of energy saving have become more and more important. Waste heat recovery has great potential to increase energy efficiency and to reduce fuel consumption.

Despite the substantial improvements of diesel engine efficiency over the last few decades, a considerable amount of energy is still rejected to the environment (Teng et al., 2006). These losses, depending on engine operating conditions, are more than 50% of fuel energy (Teng et al., 2011), thus, a significant margin of improvement on the total system efficiency is still available. Over the last decade, different technologies have been proposed and evaluated by industry and academy (Saidur et al., 2012). A promising technology that seems to collect a lot of attentions, especially in the field of heavy duty engines, is the waste heat recovery with Kalina Cycle systems.

The aim of this paper is to present the procedures and results of a thermoeconomic optimization of Kalina Cycle systems to recover waste heat from cooling water and exhaust gases in a Wärtsilä W20V32 diesel engine of a power plant located in Espírito Santo, Brazil. The optimization results provide the profit from sale of Kalina Cycle additional power generation, costs of equipments and design parameters by means of the optimal decision variables: evaporation pressure (P_{evap}), condensation pressure (P_{cond}), waste heat recovery exchanger approach (APP), pump isentropic efficiency (η_p), turbine isentropic efficiency (η_T), separator terminal temperature difference ($\Delta T_{separator}$), regenerator effectiveness (ε_{reg}), superheater temperature increase ($\Delta T_{superheater}$), mass flow (\dot{m}_K) and ammonia concentration (x_{NH_3}), which finally reach the maximum objective function (F_{obj}). These results are discussed at the end of this work

2. ENGINE RECOVERABLE WASTE HEAT

The selected diesel engine is a turbocharged engine powered by intercooled four-stroke Diesel cycle with direct fuel injection. The main parameters of the recoverable waste heat (exhaust gases and cooling water) of the internal combustion engine (ICE) under design conditions are presented in Tab. 1. The exhaust gas composition is in Tab. 02.

Table 1. Design parameters of the recoverable waste heat of the ICE

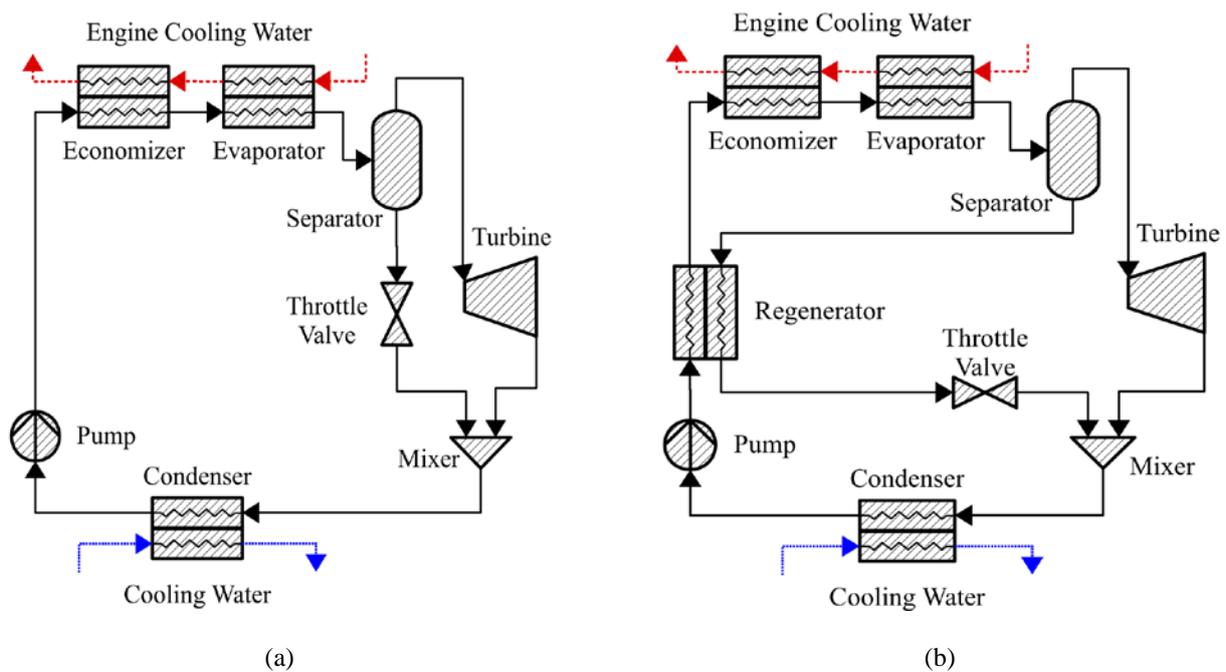
Parameter	Value
Cooling Water Mass flow Rate, m^3/h	100
Cooling Water Inlet Temperature, K	351.55
Cooling Water Outlet Limit Temperature, K	314.55
Exhaust Gas Mass Flow Rate, kg/s	16.7
Exhaust Gas Inlet Temperature, K	618.15
Exhaust Gas Outlet Limit Temperature, K	413.15

Table 2. Engine exhaust gas composition.

CO ₂ , %	H ₂ O, %	N ₂ , %	O ₂ , %	Air, %	SO ₂ , %
6.36	5.58	75.53	11.60	0.90	0.03

3. THERMODYNAMIC MODELLING

The physical structure of Kalina cycle systems to recovery waste heat from engine cooling water and engine exhaust gases are shown in Fig. 1.



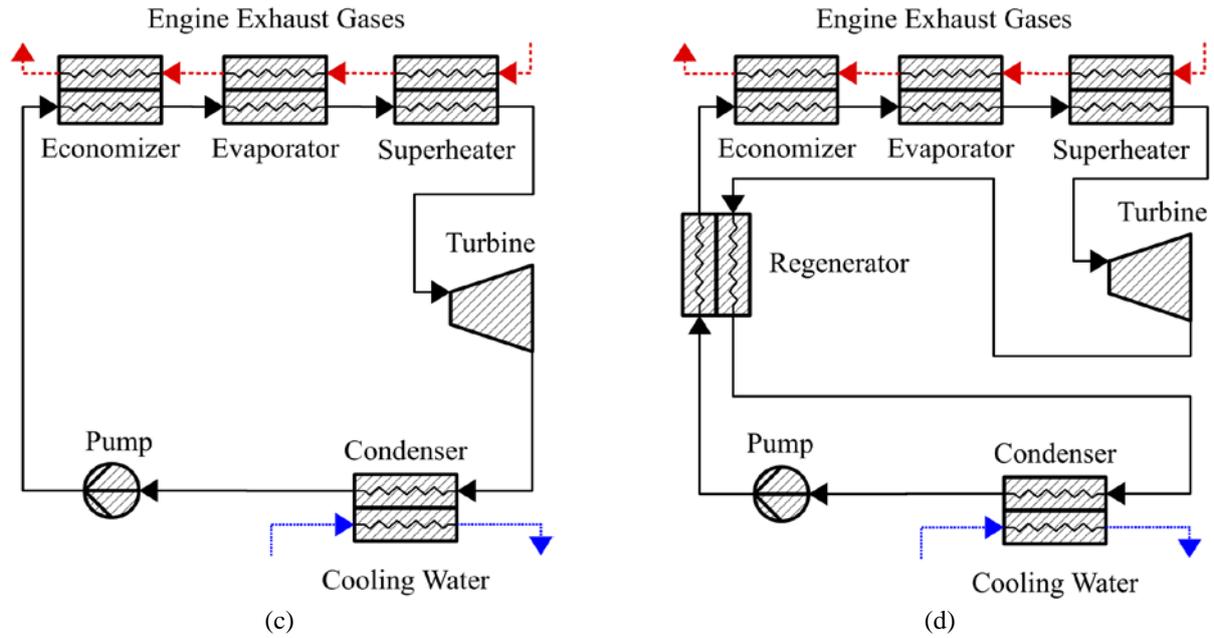


Figure 1. Schematic diagram: (a) non-regenerative Kalina cycle recovery system for engine cooling water, (b) regenerative Kalina cycle recovery system for engine cooling water, (c) non-regenerative Kalina cycle recovery system for exhaust gases, (d) regenerative Kalina recovery system for exhaust gases.

The following assumptions are made for mass and energy balance: each component is considered as a steady-state flow system and adiabatic, where kinetic and potential energy changes as well as heat and friction losses, are neglected.

The pump power (\dot{W}_p) is expressed in Eq. (1), where η_p is the pump isentropic efficiency, h_{in} is the working fluid specific enthalpy at the pump inlet, $h_{out,s}$ is the working fluid specific enthalpy at the pump outlet for an isentropic compression and \dot{m}_K is ammonia-water mass flow.

$$\dot{W}_p = \frac{\dot{m}_K (h_{out,s} - h_{in})}{\eta_p} \quad (1)$$

The heat addition process in the evaporator occurs at constant pressure and the heat transfer rate to the working fluid (\dot{Q}_{EVAP}) is given by Eq. (2), where h_{in} and h_{out} are the working fluid specific enthalpies at the evaporator inlet and outlet, respectively, and \dot{m}_K is the working fluid mass flow. This analogy can be applied for economizer and superheater.

$$\dot{Q}_{EVAP} = \dot{m}_K (h_{out} - h_{in}) \quad (2)$$

The heat transfer rate from the heat source flow (\dot{Q}_{HS}) can be determined by Eq. (3), where \dot{m}_{HS} is the heat source mass flow; $h_{HS,in}$ and $h_{HS,out}$ are the heat source specific enthalpies at the inlet and outlet of the evaporator, respectively.

$$\dot{Q}_{HS} = \dot{m}_{HS} (h_{HS,in} - h_{HS,out}) \quad (3)$$

The working fluid passes through the expander to generate the mechanical power. The expander power (W_E) is given by Eq. (4), where η_E is the expander isentropic efficiency, h_{in} is the working fluid specific enthalpy at the expander inlet and $h_{out,s}$ is the working fluid specific enthalpy at the expander outlet for an isentropic expansion.

$$\dot{W}_E = \dot{m}_K (h_{in} - h_{out,s}) \cdot \eta_E \quad (4)$$

The expander outlet working fluid is led to the condenser where it is condensed by transferring heat to water. This is a constant pressure process. The condenser heat rejection rate (\dot{Q}_{cond}) can be expressed as Eq. (5), where h_{in} and h_{out} are the working fluid specific enthalpies at the condenser inlet and outlet, respectively.

$$\dot{Q}_{cond} = \dot{m}_K (h_{in} - h_{out}) \quad (5)$$

The heat sink transfer rate (\dot{Q}_{HSK}) in the condenser of Kalina cycle is given by Eq. (6), where \dot{m}_{HSK} is the heat sink mass flow and $h_{HSK,out}$ and $h_{HSK,in}$ are the heat sink (cooling water) outlet and inlet specific enthalpies, respectively.

$$\dot{Q}_{HSK} = \dot{m}_{HSK} (h_{HSK,out} - h_{HSK,in}) \quad (6)$$

The regenerator energy balance can be evaluated by Eq. (7), where h_1 and h_2 are the working fluid inlet and outlet specific enthalpies at the regenerator after the pump, and h_3 and h_4 are the working fluid specific enthalpies at the regenerator inlet and outlet after the expander.

$$(h_2 - h_1) = (h_3 - h_4) \quad (7)$$

The Kalina cycle system net mechanical power output (\dot{W}_{net}) can be expressed as Eq. (8).

$$\dot{W}_{net} = \dot{W}_E - \dot{W}_p \quad (8)$$

The Kalina thermal efficiency (η_{cycle}) is the ratio between the net engine power output and the total heat input to the cycle. It can be expressed as Eq. (9):

$$\eta_{cycle} = \frac{\dot{W}_{net}}{\dot{Q}_{tot}} \quad (9)$$

Based on the heat transfer coefficient variation caused by different phase state, the evaporator and the condenser are divided into three sections.

The logarithmic temperature difference method is used in this present study, given by Eq. (10), where $DTML$ is the logarithmic mean temperature difference, ΔT_1 and ΔT_2 are the maximum and minimum temperature differences at the heat exchangers ends, respectively.

$$DTML = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} \quad (10)$$

The heat transfer (\dot{Q}_i) in each section can be calculated by Eq. (11), where, U_i and A_i are the overall heat transfer coefficient and the heat transfer area of each section, in that order. The values of U_i are obtained by Larsen et al., 2014.

$$\dot{Q}_i = U_i \cdot A_i \cdot DTML \quad (11)$$

The exhaust gases are considered as mixtures of ideal gases, composed of six elements, see Tab. 2. Their specific heat varies with temperature for each element (n), as showed in Eq. (12):

$$c_{ps,g} = \frac{1}{\sum y_{n,i} \cdot M_n} \cdot \sum y_{n,i} \int_{T_0}^{T_i} \bar{c}_{p_n} dT \quad (12)$$

4. ECONOMIC MODELLING

When evaluating the costs of a plant, it is necessary to consider the annual cost associated with the purchase and operation of each plant component. The expressions for obtaining the purchase equipment costs (PEC) are presented in Tab. 3.

For all heat exchangers, the purchase equipment costs are a function of the heat transfer surface area, the construction material and the temperature difference. For the evaporator and the condenser in this present study, the PEC is given by Turton et al., 2012.

For the pump and the expander, the purchase equipment costs are a function of isentropic efficiency, pressure ratio and temperatures. In these equipments the PEC was calculated using a Frangopoulos Cost Equations from Uche, 2001. However, purchase equipment costs calculated using these equations have been parameterized according to Turton et al., 2012.

This procedure was necessary for optimization, since the objective function needs to be direct function of decision variables.

The expressions for obtaining the purchase equipment costs (PEC) are presented in Tab. 3.

Table 3. Equipment cost functions.

Equipment	Cost Equation
	$PEC = A \cdot e^{B \cdot \ln C \cdot FBI \cdot (D \cdot F2T + E \cdot F2P)} \cdot FBN \cdot FBT$ $FBI = \eta_T \cdot \dot{m}_k$ $F2T = T_{in} - T_{out} - T_{out} \cdot \ln \frac{T_{in}}{T_{out}}$ $F2P = T_{out} \cdot \ln \frac{P_{in}}{P_{out}}$ $FBN = 1 + \left(\frac{1 - 0,9}{1 - \eta_T} \right)^3$ $FBT = 1 + 5 \cdot e^{\left(\frac{T_{in} - 1100}{18,75} \right)}$
Expander	
Heat Exchangers	$PEC = 10000 + 324 \cdot (A^{0,91})$
Pump	$PEC = A \cdot e^{(B \cdot \ln(C \cdot \dot{m}_k \cdot D \cdot (P_{in} - P_{out})))} \cdot FDN$ $FDN = 1 + \left(\frac{1 - 0,8}{1 - \eta_b} \right)^3$

The value of the cost equation constants (A, B, C, D, E) in Tab. 3 are showed in Tab. 4, 5, 6 and 7, which are calculated for each ammonia concentration.

Table 4. High Pressure Pump Constants Costs.

Ammonia Concentration	$x < 65$	$65 < x \leq 75$	$75 < x \leq 85$	$x > 85$
A	4,951	8,115	297.8	1,092
B	0.6876	0.6907	0.7003	0.7102
C	0.00128	0.03074	0.07344	0.021
D	5.476	0.1157	5.733	3.215

Table 5. Low Pressure Pump Constants Costs.

Ammonia Concentration	$x < 65$	$65 < x \leq 75$	$75 < x \leq 85$	$x > 85$
A	3,157	2,389	1,641	5,177
B	0.3977	0.4306	0.4305	0.4307
C	0.1519	0.07358	0.09725	0.00533
D	1.851	0.7032	1.329	1.889

Table 6. High Pressure Expander Constants Costs.

Ammonia Concentration	$x < 75$	$75 < x \leq 85$	$85 < x \leq 95$	$x > 95$
A	42,037	43,279	43,161	40,701
B	0.3557	0.37	0.3743	0.36
C	0.00524	0.00293	0.00342	0.00395
D	0,01	0.01	0.01	0.012
E	5.683	7.82	6.024	6.186

Table 7. Low Pressure Expander Constants Costs.

Ammonia Concentration	$x < 75$	$75 < x \leq 85$	$85 < x \leq 95$	$x > 95$
A	34,896	33,164	45,948	20,634
B	0.49	0.5052	0.5225	0.5228
C	0.00365	0.00305	0.00948	0.00401
D	9.991	0.02122	0,0132	0,01
E	4.21	5.208	0.818	8.85

The Frangopoulos Equations were originally applied to steam turbine and water pump. So, it was necessary an adjustment for the cost equation constants in equipment cost for each pump or expander and ammonia concentration. To calculate the cost constants for each equipment, it was minimized the error between the PEC calculated using Turton et al., 2012 and Uche, 2001, for the same power and design parameters, as shown in Eq. (14).

$$\text{Minimize} = \sum_{i=1}^n (PEC_{Frangopoulos} - PEC_{Turton})^2 \quad (14)$$

Based on these costs, the general equation for the cost rate (\dot{Z}_i , in \$/s), associated with the capital investment and the maintenance costs for each component, is obtained using Eq. (15), where the purchase equipment costs (PEC_i) are shown in Tab. 3, maintenance factor (φ) is 1.06, the hours of plant operation per year (N) are 7446 hours, and the annual capital recovery factor (CRF) is shown in Eq. (16), where $j = 0.1$ is the rate and n are 20 years.

$$\dot{Z}_i = \frac{PEC_i \cdot CRF \cdot \varphi}{N \cdot 3600} \quad (15)$$

$$CRF = \frac{j \cdot (1 + j)^n}{(1 + j)^{n+1} - 1} \quad (16)$$

The general equation for total cost is given by Eq. (17), where i is the number of equipments.

$$\dot{Z}_{tot} = \sum \dot{Z}_i \quad (17)$$

5. THERMOECONOMIC OPTIMIZATION PROBLEM

The thermoeconomic optimization problem has eight degrees of freedom for non-regenerative Kalina Cycle and nine degrees of freedom for regenerative Kalina Cycle, represented by their decision variables and consists of maximizing the objective function defined by the profit from sale of Kalina Cycle energy, expressed in Eq. (18), where P is the energy sale price and equal to 155 US\$/MWh in this work.

$$F_{obj} = (\dot{W}_{net} \cdot P) - \dot{Z}_{tot} \quad (18)$$

The constraints are imposed by the physical, thermodynamic and cost models of the installation. For each heat source, their lower and upper bounds were determined (Tab. 8 and 9).

All thermodynamic, thermoeconomic modelling and optimization problem were developed in EES Software ("Engineering Equation Solver - EES," 2017). To solve the thermoeconomic optimization problem, it was used a stochastic method, genetic algorithm, available in EES Optimization Tool. According to Whitley, 2001, Biegler and Grossmann, 2004, this method differs from traditional search procedures mainly because they don't work with just one point, but with a set of them, using only the objective function, without needs for derivatives or other auxiliary calculation, and present simple programming and good results even when dealing with multimodal functions. Furthermore, there is a large interest in science community for the use of this optimization programming technique (Cordeiro et al., 2011; Koch et al., 2007; Pires et al., 2013). The genetic algorithm parameters chosen in EES Optimization Tool were 32 individuals, 256 generations and 0.058 mutation rate (De Jong, 1975).

Table 8. Decision variables and their lower and upper boundaries for cooling water as heat source.

Decision Variable	Guess	Lower Bound	Upper Bound
Evaporation pressure, <i>bar</i>	20	15	50
Condensation pressure, <i>bar</i>	12	5	15
Waste heat recovery approach, <i>K</i>	5	0	10
Pump isentropic efficiency	0.75	0.4	0.99
Turbine isentropic efficiency	0.80	0.5	0.99
Separator terminal temperature difference, <i>K</i>	5	0	20
Regenerator effectiveness	0.30	0	1
Mass flow, <i>kg/s</i>	1.0	0	10
Ammonia concentration	0.80	0.4	0.99

Table 9. Decision variables and their lower and upper boundaries for exhaust gas as heat source.

Decision Variable	Guess	Lower Bound	Upper Bound
Evaporation pressure, <i>bar</i>	90	25	200
Condensation pressure, <i>bar</i>	14	8	25
Waste heat recovery approach, <i>K</i>	10	0	20
Pump isentropic efficiency	0.75	0.4	0.99
Turbine isentropic efficiency	0.80	0.5	0.99
Separator terminal temperature difference, <i>K</i>	100	0	200
Regenerator effectiveness	0.50	0	1
Mass flow, <i>kg/s</i>	1.0	0	10
Ammonia concentration	0.80	0,4	0,99

6. RESULTS AND DISCUSSIONS

Figure 2 shows objective function evolutions with function calls for engine cooling water and exhaust gases heat recovery. Fig. 2a refers to cooling water as heat source and Fig. 2b refers to exhaust gases as heat source.

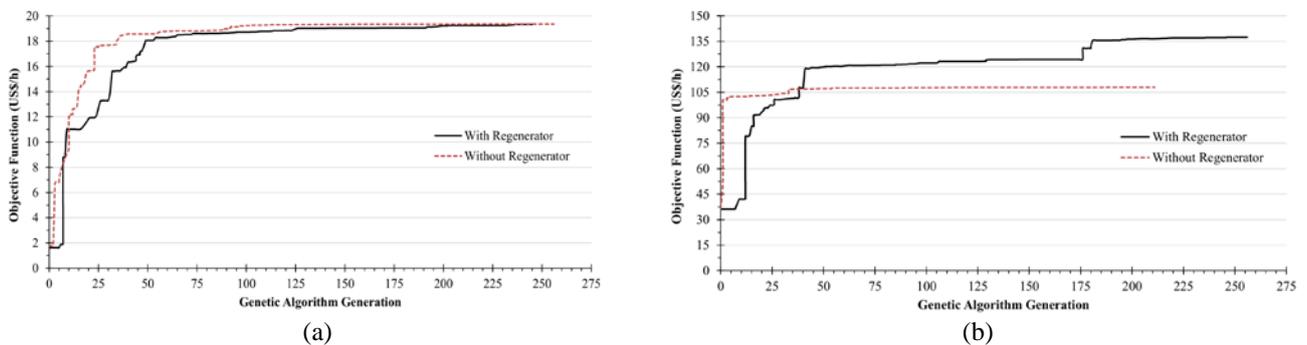


Figure 2: Objective function versus genetic algorithm generation for; (a) cooling water as heat source; (b) exhaust gases as heat source.

The optimization values for the decision variables are shown in Tab. 10 and 12 for cooling water and exhaust gases as heat source respectively. The optimization results are shown in Tab. 11 and 13 for cooling water and exhaust gases as heat source, respectively. All the results are divided into cycles with and without regenerator.

Table 10. Optimal decision variables in Kalina Cycle recovering engine cooling water heat.

Cycle	x_{NH3} (-)	P_{evap} (bar)	P_{cond} (bar)	APP (K)	$\Delta T_{separator}$ (K)	ϵ_{reg} (-)	η_p (%)	η_T (%)	\dot{m}_K (kg/s)
Without regenerator	0.953	23.17	12.47	9.9	6.19	-	80.92	90.99	3.21
With regenerator	0.841	19.29	11.08	9.9	9.27	0.353	81.05	91.01	5.17

Table 11. Optimal parameters values in Kalina Cycle recovering engine cooling water heat.

Cycle	W_{net} (kW)	η_{cycle} (%)	$T_{HS,out}$ (K)	\dot{m}_{HSK} (kg/s)	PEC _{tot} (US\$)	F_{obj} (US\$/h)
Without regenerator	197.0	5.77	321.35	154.0	463,282	19.37
With regenerator	187.6	5.16	319.35	165.1	403,899	19.34

Table 12. Optimal decision variables in Kalina Cycle recovering engine exhaust gases heat.

Cycle	x_{NH3} (-)	P_{evap} (bar)	P_{cond} (bar)	APP (K)	$\Delta T_{separator}$ (K)	ϵ_{reg} (-)	η_p (%)	η_T (%)	\dot{m}_K (kg/s)
Without regenerator	0.922	199.9	13.1	20.0	115.4	-	77.24	88.78	2.11
With regenerator	0.944	132.7	12.51	19.9	152.2	0.960	76.50	88.55	2.51

Table 13. Optimal parameters values in Kalina Cycle recovering engine exhaust gases heat.

Cycle	W_{net} (kW)	η_{cycle} (%)	$T_{HS,out}$ (K)	\dot{m}_{HSK} (kg/s)	PEC _{tot} (US\$)	F_{obj} (US\$/h)
Without regenerator	864	23.4	413.25	135.2	1,073,213	108.2
With regenerator	1075	29.2	413.55	124.8	1,215,073	137.4

7. CONCLUSIONS

This work had as objective to carry out thermoeconomic optimizations of Kalina Cycles systems recovering the waste heat of both engine exhaust gases and cooling water and to compare regenerative and non-regenerative cycles. The optimizations for all the four cases converge within the generation's number adopted as was showed in Fig. 2.

The results for the cooling water heat recovery showed that the non-regenerative cycle produces the highest profit for this case studied, 19.37 US\$/h. Even though the regenerative cycle presented a lower total purchase equipment cost, the non-regenerative cycle produces the highest net power (197 kW) and has the highest thermodynamic efficiency (5.77 %). It's important to point out that neither cycles recover all the energy potential of the cooling water, as the heat source outlet temperature of both cycles didn't reach its limit value of 314.5 K.

The results for the exhaust gases heat recovery showed that the regenerative cycle produces the highest profit for this case studied, 137.4 US\$/h. Although the regenerative cycle presented a higher total purchase equipment cost, the regenerative cycle also produces a higher net power (1075 kW) and has the highest thermodynamic efficiency (29.2 %). In this case both cycles recover all the energy potential of the exhaust gases, as the heat source outlet temperature of both cycles reach its limit value of 413 K.

This work optimized two Kalina Cycle configurations as alternatives for diesel engine waste energy recovery. The recovery of both exhaust gases and cooling water can produce up to 1,272 kW which represents a profit of 156.8 US\$/h for the case studied. Once that the internal combustion engine analyzed produces 9,000 kW of mechanical net power, this additional power by means of heat recovery (1,272 kW) means 14.13% of repowering of the power plant.

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9. REFERENCES

- Biegler, L.T., Grossmann, I.E., 2004. Retrospective on optimization. *Comput. Chem. Eng.* 28, 1169–1192.
- Cordeiro, A.S., Vieira, L.S., Cruz, M.E., 2011. Exergoeconomic optimization and improvement of a cogeneration system modeled in a process simulator using direct search and evolutionary methods. *Int. J. Energy Environ.* 2, 463–476.
- De Jong, K.A., 1975. Analysis of the behavior of a class of genetic adaptive systems. *University of Michigan*.
- Engineering Equation Solver - EES, 2017.
- Koch, C., Cziesla, F., Tsatsaronis, G., 2007. Optimization of combined cycle power plants using evolutionary algorithms. *Chem. Eng. Process. Process Intensif.* 46, 1151–1159.
- Larsen, U., Nguyen, T.-V., Knudsen, T., Haglind, F., 2014. System analysis and optimisation of a Kalina split-cycle for waste heat recovery on large marine diesel engines. *Energy* 64, 484–494.
- Pires, T.S., Cruz, M.E., Colaço, M.J., 2013. Response surface method applied to the thermoeconomic optimization of a complex cogeneration system modeled in a process simulator. *Energy* 52, 44–54.
- Saidur, R., Rezaei, M., Muzammil, W.K., Hassan, M.H., Paria, S., Hasanuzzaman, M., 2012. Technologies to recover exhaust heat from internal combustion engines. *Renew. Sustain. Energy Rev.* 16, 5649–5659.
- Teng, H., Klaver, J., Park, T., Hunter, G.L., van der Velde, B., 2011. A Rankine Cycle System for Recovering Waste Heat from HD Diesel Engines - WHR System Development. *SAE Tech. Pap.* 2–4.
- Teng, H., Regner, G., Cowland, C., 2006. Achieving High Engine Efficiency for Heavy-Duty Diesel Engines by Waste Heat Recovery Using Supercritical Organic-Fluid Rankine Cycle. *SAE Tech. Pap.* 1–3.
- Turton, R.A., Bailie, R.C., Whiting, W.B., Shaeiwitz, J.A., Bhattacharyya, D., 2012. Analysis, Synthesis and Design of Chemical Processes, Prentice Hall International Series in the Physical and Chemical Engineering Sciences. *Pearson Education*.
- Uche, J., 2001. Thermoeconomic Analysis and Simulation of a Combined Power and Desalination Plant [thesis]. *Universidad de Zaragoza, Zaragoza*.
- Whitley, D., 2001. An overview of evolutionary algorithms: practical issues and common pitfalls. *Inf. Softw. Technol.* 43, 817–831.

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