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Thermodynamic Optimization of heat recovery ORCs for heavy duty Internal Combustion Engine: pure fluids vs. zeotropic mixtures

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Abstract

This article focuses on the optimization of ORCs for heat recovery from heavy duty Internal Combustion Engines (ICEs), with particular attention to the optimal fluid selection. We considered two different ICEs featuring same power (10 MW) but different architectures: a two-stroke engine with exhaust temperature 250°C and a four-stroke engine with 350°C exhaust temperature. The analysis tackles the optimization of the heat integration between heat sources and ORC, the optimization of the cycle variables as well as the selection of the working fluid. In addition to conventional pure substances, such as hydrocarbons, refrigerants, and siloxanes, and recently synthesized refrigerants, (i.e., HFOs, HCFOs, and HFEs), also binary zeotropic mixtures have been considered. The optimization algorithm combines the evolutionary optimization algorithm PGS-COM with a systematic heat integration methodology which maximizes the heat recovered from the available heat sources. The methodology allows optimizing also the mixture composition. In total 36 pure fluids and 36 mixtures have been evaluated. HCFO-1233zde turns out to be the best or second best fluid for most cases. Cyclopentane is the best fluid for the engine with high exhaust temperature. Another promising fluid is Novec™ 649. The optimal cycles are supercritical with T-s diagrams resembling the ideal triangular cycle. The use of the mixtures leads to an increase of the exergy efficiency of around 2.5 percentage points (about 3.5 percentage point increase in net power output). Since the optimal cycle is supercritical, the temperature glide can be exploited only in condensation and, as a result, the advantage of mixtures compared to pure fluids is lower than the values reported in the literature.

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1. Introduction

In the last decades, the developed countries and recently the developing countries have shown an increasing interest in the possibility to reduce the primary energy consumption related to fossil fuel and reduce the emission of carbon dioxide. Considering the great diffusion of internal combustion engines both in industry (e.g., combined heat and power plants) and in transport, increasing the efficiency of such engines has a very important positive effect on the reduction of CO_2 emissions. A step change in terms of efficiency could be made by recovering the engine waste heat, available as hot flue gases, compressed air (intercoolers), cooling water and lube oil, and converting it into useful mechanical power with a Rankine cycle [1,2]. Indeed, a significant fraction of the thermal power introduced by the fuel, typically around 50-60%, is still available at medium-low temperature in the flue gasses and in the coolant. The technical and economic feasibility of recovering this heat increases with engine size and for engines running mainly at constant load [3,4], like engines for power production and large naval engines. As far as the heat recovery Rankine cycle is concerned, several papers report the advantages of Organic Rankine Cycles (ORCs) compared to steam cycles in terms of efficiency and costs [5–7]. However, to the best of our knowledge, a systematic study of the ORC considering the optimal working fluid selection, the optimization of the heat integration with all the possible heat sources (exhaust gases, cooling water, lube oil, intercoolers), and the optimization of the cycle variables (pressures and temperatures) is still lacking. Some works addressed the problem analyzing the selection of the working fluid among a limited number [6,8,9], others focused on the cycle optimization [7,10,11] and on the part-load analysis [12–14].

In this paper, we aim at performing a systematic thermodynamic optimization of heat recovery ORCs for large ICEs by devising an ad hoc optimization approach and screening a large number of promising fluids. Besides conventional and recently developed fluids (HFE, HCFO, HFO), we consider and optimize binary zeotropic mixtures. Economic and operational aspects of the analysis will be dealt with (for the best fluids identified) in a successive work using ad hoc methodologies capable of optimizing also the heat exchanger network [15,16].

Nomenclature

ALT	Atmospheric Lifetime
GWP	Global Warming Potential
HCFO	Hydro Chloro Fluoro Olefins
HFE	Hydro Fluoro Ether
HFO	Hydro Fluoro Olen
ICE	Internal Combustion Engine
ODP	Ozone Depletion Potential
ORC	Organic Rankine Cycle
PGS-COM	Particle Generating Set – Complex algorithm

2. Cycle optimization

In this paper, we tackle the following cycle optimization problem.

Given the set of hot streams made available by an internal combustion engine and the temperature of the available heat sink (cooling water or cooling air) determine:

- the working fluid selection (if a mixture, determine also the optimal composition)
- the heat integration between ORC and heat sources/sinks (including regenerator of the ORC)
- the mass flow rate of ORC
- the cycle variables (pressures, temperatures, etc)

which maximize the mechanical/electric power generated by the heat recovery ORC (this is equivalent to maximize the net efficiency of the overall system ICE + ORC) while guaranteeing the following techno-economic constraints:

- minimum vapor fraction in the expansion greater than 0.88%
- minimum temperature difference in each heat exchanger grater or equal to 5°C

It is a thermodynamic analysis aimed at finding the most promising working fluids and cycle configurations.

3. Methodology

First, a list of promising working fluids (pure fluids and binary mixtures) is determined on the basis of simple selection criteria (see Subsection 3.1). Then, for each selected fluid, the cycle configuration, cycle variables and heat integration are optimized with the algorithm described in Subsection 3.2. Fluids are ranked according to the achievable net electric efficiency of the integrated system (ICE + ORC). In addition to efficiency, a preliminary estimate of the minimum number of stages required for an axial turbine is performed on the basis of the maximum enthalpy drop of an impulse stage and the expansion volumetric ratio [12].

3.1. Fluid selection

Regarding the fluid selection, we considered the following selection criteria:

- good matching between the working fluid and the heat source and sink to reduce the heat transfer losses
- critical temperature close or slightly lower (<200°C or <320°C depending on the engine selected) than the flue gas inlet temperature (this allows to optimize the heat integration with the hot flue gas stream [17]
- condensation pressure at ambient temperature higher than 0.03 bar (current technological limit), preferably above atmospheric
- sufficient thermo-chemical stability, preferably up to the flue gas inlet temperature
- low environmental impact: low GWP, ODP and ALT
- non-flammable, non-toxic and non-corrosive
- fluid property data and validated correlations available in REFPROP v.9.1

We considered also flammable working fluids with the requirement of installing a thermal oil loop between the hot flue gases and the ORC. Due to the indirect heat transfer, the heat source temperature is decreased by 20°C, leading to an efficiency penalty for the ORC. For the group of novel fluid mixtures (namely mixtures of refrigerants, hydrocarbons, and siloxanes), validated correlations are not yet available in REFPROP, so the predictive method proposed by Lemmon and McLinden [18] was used.

3.2. Optimization Algorithm

We devised an ad hoc optimization algorithm capable of optimizing simultaneously the cycle variables, the heat integration between the ORC and the available heat sources/sinks and the composition of the working fluid (only for mixtures) and of accounting for the technical constraints listed in Section 2. The algorithm is shown in Figure 1(A).

The input data of the algorithm are the nature of working fluid (molecule or couple of molecules of the mixture), the heat sources and heat sink data, the upper and lower bounds for the pressures and temperatures of the cycle and the technical constraints reported in Section 2 (e.g., minimum vapor fraction in the expansion).

At the upper level, the evolutionary algorithm PGS-COM [19] optimizes the independent cycle variables (namely condenser pressure, turbine inlet pressure and superheat temperature) and the composition of the mixture (only for mixtures). PGS-COM is a derivative-free algorithm, coded in Matlab [20], specifically developed for non-smooth constrained black-box problems arising in the optimization of energy systems and power cycles [12,21]. For each combination of variables sampled by PGS-COM, we simulated the ORC in Matlab to determine the temperatures, pressures and enthalpies of all the streams. We used REFPROP [22,23] to evaluate the thermodynamic properties of the fluids and, for the sake of simplicity, we considered a single pressure level ORC with ideal turbine and no pressure drops across the components. Figure 1 (B) schematically represent the cycle process flow diagram. Nevertheless, more sophisticated models of the units can be easily included. The heat integration methodology automatically optimize the presence and size of the regenerator.

Once all the stream temperatures of the ORC are determined, the heat integration between ORC streams and heat sources/heat sinks is optimized with the methodology proposed by Maréchal and Kalitventzeff [24]. Given the available hot and cold streams (including the superheated vapor discharged from the ORC turbine which could be used within a regenerator), the heat integration methodology determines the maximum mass flow rate of the working fluid which can be generated (the so called “maximum heat recovery target”). The heat integration methodology uses a reformulation of the Pinch Analysis “heat cascade” [25] as a linear program [26] where the ORC flows and the mass flow rate of cooling water/air are optimization variables. In our implementation, the linear program is solved with the Matlab “linprog” algorithm. Once the mass flow rate of the ORC is computed, the mechanical power recovered by the ORC and the efficiency of the integrated ICE + ORC system can be easily determined. Such performance value is returned to PGS-COM as output of the optimized black-box function (which comprises the cycle model and the heat integration methodology). It is worth noting that the routines for the calculation of the fluid properties and the heat integration optimization method generate non-smooth points in the black-box function. For this reason, we selected the algorithm PGS-COM. One optimization run takes about 30 minutes. Each run has been repeated 5 times to minimize the risk of finding local optimal.

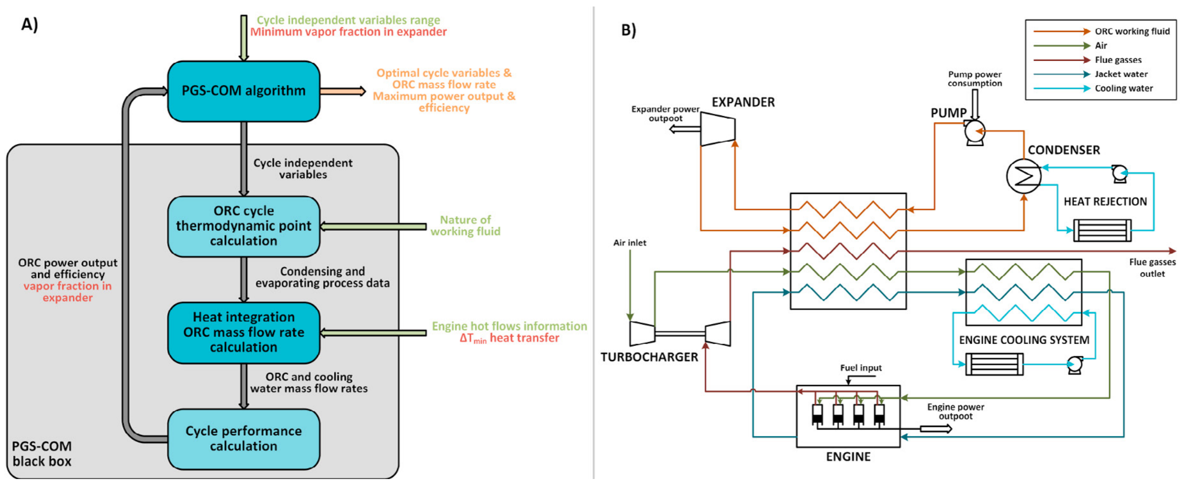

Figure 1. (A) Block diagram of the optimization algorithm. (B) Process flow diagram of the integrated system ICE + heat recovery ORC cycle.

4. Results

We considered two possible heat recovery applications represented by two large Diesel engines of the same size (10 MW of mechanical power output) but with opposite features (see Table 1):

- Man S60-MC6: two-stroke and 10.2 MW of power output
- Wärtsilä 46DF: four-stroke and 10.3 MW of power output.

Considering two engines with considerably different exhaust temperatures allows assessing the effects of this parameter on the optimal fluid selection, cycle configuration and ORC efficiency.

We fully optimized the heat recovery ORC for each of the two engines. First, we selected 36 pure fluids (HCFO, HFC, HFO, inorganic fluids, hydrocarbons, ethers, alcohols, siloxanes, and ketones) and 36 mixtures (HFC, HFE, HFO, inorganic fluids, hydrocarbons, ethers, alcohols, siloxanes, and ketones) for the two engines on the basis of the criteria described in Section 3.1. Then, for each of the engine and each of the selected fluids, we optimized the cycle with the algorithm described in Section 3.2.

Table 1: selected internal combustion engines characteristics (sources [27,28]).

Flow	Feature	Units of measurement	Man S60-MC6	Wärtsilä 46DF
	Cycle type	-	Two-stroke	Four-stroke
	Power output	kW	10 200	10 305
	Efficiency (full load)	%	49.59	45.33
Exhaust gas	Mass flow rate	kg/s	26.53	19.00
	Thermal power	kW	3 607	4 892
	Temperature range	°C	245 - 120	354 - 120
Scavenge air	Mass flow rate	kg/s	26.00	18.40
	Thermal power	kW	3 970	3 789
	Temperature range	°C	198 - 48	253 - 50
Jacket water	Mass flow rate	kg/s	21.06	23.16
	Thermal power	kW	1 490	1 653
	Temperature range	°C	80 – 63	91 - 74

4.1. Pure fluids

The best three pure fluids for the two-stroke engine are HCFO-1233zde, HFE-245fa2, and HFO-1336mzz. These are non-flammable, and thus they can be directly coupled with the flue gasses. Figure 2 (A), (B), and (C), respectively show the composite curves, exergy composite curves (the area between the hot and cold curves is equal to the exergy loss of the heat transfer process) and T-entropy diagram of the best pure fluid HCFO-1233zde. As shown in Figure 2 (C), it has an isentropic expansion, because the saturation curve of the vapor phase in the T-s diagram is almost vertical. The second and third best choices are dry fluids featuring a large regenerator. For all the three working fluids, the optimal cycle has a trans-critical configuration. The optimal cycle variables are reported in Table 2. The difference in ORC power output between the three fluids is limited to 12 kW, corresponding to 0.14% of overall efficiency. On the other hand, the cycle pressures are different, as shown in Table 2. In all the cases, while the expansion enthalpy drop is limited, two axial stages are necessary due to the high volumetric expansion ratio (in the range 26-39). The mass flow rate of the working fluid is always in the range 27-31 kg/s. From an environmental point of view, HCFO-1233zde and HFO-1336mzz are preferable because of their lower GWP (respectively equal to 1 and 2) compared to HFE-245fa2 (GWP equal to 812). The ODP is equal to 0 in any case.

Table 2: Best pure fluids and mixtures cycle performances and parameters for both engines.

		Fluid (Weight fraction wt%)		W_{out} ORC kW	η_{exe} %	Turbine inlet temperature °C	Turbine inlet pressure bar	N° of expander stages -
Man S60-MC6	Pure fluids	HCFO-1233zde		1 802.5	75.71	196.31	38.61	2
		HFE-245fa2		1 795.9	75.44	197.86	36.17	2
		HFO-1336mzz		1 790.1	75.19	195.38	30.52	2
	Mixtures	HCFO-1233zde (90)	HFC-134a (10)	1 867.8	78.45	206.85	42.17	2
		HFO-1336mzz (97)	HFC-134a (3)	1 827.5	76.76	195.07	31.55	2
		Isobutane (56)	Pentane (44)	1 694.7	71.18	170.02	38.60	2
Wärtsilä 46DF	Pure fluids	Cyclopentane		2 456.5	73.82	235.54	42.70	2
		Ammonia		2 443.1	73.42	325.00	166.93	4
		HCFO-1233zde		2 420.2	72.73	256.34	43.56	2
	Mixtures	Cyclopentane (82)	Cis-Butene (18)	2 540.4	76.35	233.78	47.04	2
		Cyclopentane (78)	Heptane (22)	2 528.9	76.00	235.26	36.44	2
		Ammonia (98)	Water (2)	2 523.2	75.83	324.86	165.34	4

Cyclopentane, ammonia, and HCFO-1233zde are the best pure fluids for the four–stroke engine. The first two are flammable and toxic, thus less attractive from a safety point of view. While cyclopentane is an isentropic fluid, ammonia has a wet expansion, and then the vapor fraction at the turbine outlet can be an issue. In these cases, ammonia and HCFO-1233zde have a trans-critical cycle, while the optimal configuration for cyclopentane are slightly sub-critical. The difference in ORC power output between the three fluids is only 37 kW, corresponding to 1.09% of ORC power output, but negligible for the overall system (ICE+ORC). The higher ORC power output compared to the Man engine is a direct consequence of the lower efficiency of the ICE which makes available a greater amount of waste heat. The higher temperature of the heat sources justifies the higher first law efficiency of the optimized ORCs, whereas the second law efficiency is lower because the matching between the hot sources profile and the ORC features larger temperature differences. In this case, the three optimized cycles differ in many aspects, as shown in Table 2. Cyclopentane has a an evaporating pressure close to the critical one, HCFO-1233zde features a fully trans-critical while ammonia has a trans-critical cycle with an evaporating pressure 54 bar higher than the critical one. The high value of evaporating pressure of the ammonia working fluid can lead to operational and safety problems, while the low condensing pressure of cyclopentane can cause air leakages. Another disadvantage of ammonia is that it requires four axial turbine stages to handle the high isentropic enthalpy difference (512 kJ/kg). On the other hand, the other two fluids have a high volumetric ratio, equal to 26 for HCFO-1233zde and 107 for cyclopentane, which require at least two axial stages. The mass flow rate of the working fluid is 29 for HCFO-1233zde, 15 kg/s for cyclopentane and only 5 kg/s for ammonia. From the environmental point of view, the only relevant issue is that cyclopentane has a GWP of 11.

It worth noting that for both engines, beside HCFO-1233zde, Novec^{TM} 649 appears as an interesting choice since the achievable power production (1688 kW for Man S60-MC6 and 2244 kW for Wärtsilä 46DF) are close to the optimal values. Moreover, it has the smallest isentropic enthalpy difference across the expander compared to all the fluid analyzed, and considering the volumetric ratio, it remains one of the best solution. The cycle is in both cases a trans-critical configuration with an evaporating pressure lower than 20 bar, and the condensing pressure around 0.5 bar.

4.2. Binary mixtures

The best three binary mixtures for the Man S60-MC6 engine are HCFO-1233zde/HFC-134a (0.9/0.1), HFO-1336mzz/HFC-134a (0.97/0.03), and isobutane/pentane (0.56/0.44). Figure 2 (D), (E), and (F), respectively show the composite curve, the exergy composite curves the T-s diagram of the best mixture. The cycle configuration is trans-critical in all the cases. As reported in Table 2, the cycle power output of 1868 kW for the best fluid and it drops to 1699 kW for the last mixture because it is flammable and requires the thermal oil loop. Differently from the pure fluids, the optimal turbine inlet temperatures vary considerably from one mixture to another. The turbine inlet pressure is lower than 43 bar for all the mixtures, so we do not envisage any technological problem. In these cases, the volumetric ratio imposes the need of at least two expansion stages for all mixtures. The mass flow rate of the non-flammable mixtures (i.e., 27 and 30 respectively for the first and second best mixture) is almost double compared to the mixture of hydrocarbons (16 kg/s). From the environmental point of view, since HFC-134a has a GWP of 1430, likely it will be banned, even if the mass fraction in the optimized mixtures is low. However, also the hydrocarbons have a high GWP (= 20).

For Wärtsilä engine, the best mixtures are all flammable: cyclopentane/cis-butene (0.82/0.18), cyclopentane/heptane (0.78/0.22), and ammonia/water (0.98/0.02). The maximum power output is around 2530 kW, which corresponds to an overall ICE+ORC efficiency of 56.46%. The optimal cycle configuration is trans-critical for cyclopentane/cis-butene and ammonia/water and slightly sub-critical for cyclopentane/heptane.

It has to be noticed that for the best refrigerant mixtures for the Man engine and the hydrocarbon mixtures for the Wärtsilä engine, the mixing parameters available in REFPROP were not experimentally calibrated but estimated with the predictive methodology [18]. Thus, the results for these mixtures are affected by a higher uncertainty.

5. Conclusions and future work

In this work, we proposed a methodology and an algorithm for the systematic thermodynamic optimization of heat recovery Organic Rankine Cycles. The methodology is capable of optimizing not only the cycle but also the heat integration with the available heat sources/sinks. Due to the limited computational time, it can be used to perform a systematic screening of the working fluids. We applied the methodology to assess the most promising cycles and fluids for the heat recovery from two heavy duty internal combustion engines: a two-stroke Diesel engine featuring a relatively low exhaust temperature (245°C) and four-stroke engine featuring a higher exhaust temperature (354°C).

The best cycle configuration turns out to be the trans-critical one for both case studies and essentially all the best fluids. This result is not surprising since supercritical cycles can reach a better thermodynamic matching with the linear temperature profile of the hot flue gases (the T-s diagrams resemble the ideal Lorentz cycle). HCFO-1233zde appears to be a promising fluid both the engines analyzed, in particular with the low-temperature exhaust gasses. It has a relatively low critical temperature, which allows obtaining a trans-critical cycle configuration, and a high molar mass, which limits the enthalpy drop and the number of expander stages. Furthermore, the condensing pressure is higher than the atmospheric one. Another promising pure fluid is NovecTM 649 because it achieves close to maximum efficiency, it needs two expansion stage, it is not flammable, and it has a low environmental impact (GWP = 1 and ODP=0). The use of optimized mixtures leads to an increase of the exergy efficiency of around 2.5 percentage points (about 3.5 percentage point increase in ORC power output). Since the optimal cycle is supercritical, the temperature glide can be exploited only in condensation and, as a result, the advantage of mixtures compared to pure fluids is lower than the values reported in the literature. This little efficiency advantage is likely not sufficient to compensate the reduction of heat transfer coefficient which affects mixtures.

The techno-economic optimization of the cycles will be performed in a future study with the methodology proposed in [16].

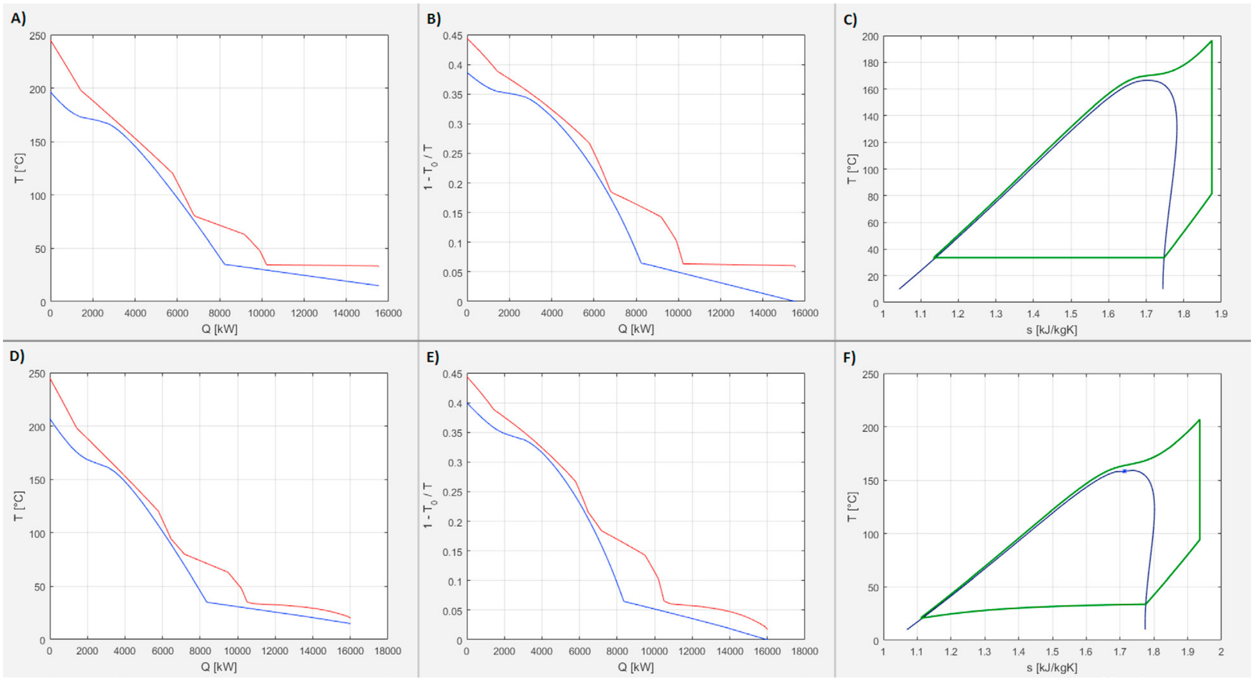

Figure 2: (A) T-Q diagram, (B) exergy loss diagram, (C) T-s diagram of HCFO-1233zde as best pure fluid for Man S60-MC6 engine. (D) T-Q diagram, (E) exergy loss diagram, (F) T-s diagram of HCFO-1233zde/HFC-134a (mass fraction 0.9/0.1) as best mixtures for Man S60-MC6 engine.

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