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# Robust optimization of an Organic Rankine Cycle for heavy duty engine waste heat recovery

Elio Antonio Bufi<sup>a,\*</sup>, Sergio Mario Camporeale<sup>a</sup>, Paola Cinnella<sup>b</sup>

<sup>a</sup>Politecnico di Bari, Department of Mechanics Mathematics and Management, Via Re David, 200 - 70125 Bari, Italy

<sup>b</sup>Laboratoire DynFluid, Arts et Mtiers ParisTech, 151 Boulevard de l'Hopital, 75013 Paris, France

## Abstract

A robust parametric optimization of Organic Rankine Cycles (ORC) is carried out by taking into account uncertainties in the cycle input parameters. A typical engine driving duty cycle is considered and sampled in order to construct a suitable probability distribution describing the variability of the exhaust gases mass-flow and temperature. Besides, the environmental and condensing temperatures, specific heat ratio of the waste gases, turbine and pump efficiencies are also considered as uncertain. The parameter combination that maximizes the mean cycle efficiency and minimizes its variance is sought as optimal. Six organic fluids have been taken into account, namely R245fa, R245ca, R134a, R11, R113 and Novec649, with the best results provided by R11 and R113.

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*Keywords:* optimization; uncertainty quantification; heavy duty; heat recovery

## 1. Introduction

In recent years, the Organic Rankine Cycle (ORC) technology has received great interest from the scientific and technical community because of its capability to recover energy from low- grade heat sources. In some applications, as waste heat recovery (WHR) in the automotive field, ORC plants need to be as compact as possible because of geometrical and weight constraints. Effective solutions have been proposed by Honda [1] and BMW [2] for passenger cars and Cummins [3] for long-haul trucks. The performances of recently developed prototypes of ORC for automotive applications seem to be promising [4], with reduction of fuel consumption up to 12% and engine thermal efficiency improvements of 10%. However, currently no commercial ORC solutions in the automotive field are available. Indeed, the large range of operating conditions on typical duty driving cycles may lead to difficulties in the design of the ORC plant, resulting in hesitancy of the investors towards this applications and leading to a system performance improvement that is too low to justify the corresponding economic effort. In this work, a robust optimization approach is proposed in order to overcome these issues for a real-world application, namely the recovery of residual energy from the waste gases of a heavy duty diesel engine. The robust optimization approach has been applied in the past by Persky et al. [5] to the design of a power block and turbine of a supercritical  $CO_2$  solar Brayton cycle, in order to account for

\* Corresponding author contact:

E-mail address: [elioantonio.bufi@poliba.it](mailto:elioantonio.bufi@poliba.it)

the day-night cycle and seasonal variations, whereas Wang et al. [6] provided a deterministic parametric optimization by means of genetic algorithms of an ORC using a low grade heat source considering both thermodynamic and economic factors simultaneously. The effect of the key thermodynamic parameters on the net power output and the resulting surface of heat exchangers was examined. Here, a robust parametric optimization of the ORC is carried out by taking into account uncertainties in the cycle input parameters. The focus of the present work is to explore a way of accounting for the uncertainty about various input parameters and give a general approach for preliminary ORC component design. Robust optimization (RO) was initially introduced by Taguchi in the 1960s, with the introduction of a new paradigm for the design of an industrial product. By citing Marczyk [7], "optimization is actually just the opposite of robustness". This statement means that classical and robust optimizations lead to different solutions which are sensitive or insensitive to uncertain conditions, respectively. A typical engine driving duty cycle is considered and sampled in order to construct a suitable probability distribution describing the variability of the exhaust gases mass-flow and temperature. Besides, the ambient and condensing temperatures, the specific heat ratio of the waste gases, turbine and pump efficiencies are also considered as uncertain. An importance analysis based on the ANalysis Of VAriance (ANOVA) of the cycle performance is carried out in order to identify the most influential variables. Six working fluids of interest for WHR application have been analysed, namely: R245fa, R245ca, R11, R113, R134a and Novec649. The ORC parameters are optimized by means of a Non-dominated Sorted Genetic Algorithm (NSGA) [8] coupled with an uncertainty quantification method, based on a Monte-Carlo simulation of the thermodynamic cycle, with the objective to maximise the cycle thermal efficiency while minimising its variance. Constraints on the minimal efficiency are also explicitly accounted for. The outcomes of this process are the ORC parameters that ensure the best trade-off between high efficiency and a stable behaviour of the system, as well as confidence intervals on these parameters.

## 2. Thermodynamic cycle and parameters for WHR

### 2.1. Cycle configuration

In this work, the waste gases discharged from a four-stroke heavy-duty Diesel engine (338 kW) are used as the low-grade heat source of ORC. The residual energy is converted to supply the auxiliary electric devices of the vehicle. A sketch of the ORC layout is shown in Fig. 1a, along with a representation of the cycle in the temperature-entropy diagram for R245fa working fluid (Fig. 1b), for a baseline configuration with:  $p_{ev} = 0.545 p_{cr}$ ,  $\Delta T_{pp} = 8 \text{ K}$  and  $\Delta T_{TIT} = 5 \text{ K}$ , where  $p_{ev}$ ,  $\Delta T_{pp}$  and  $\Delta T_{TIT}$  are the evaporating pressure, pinch point temperature difference and turbine-inlet/evaporation temperature difference, respectively. The working fluid is compressed and pumped into the evaporator by the feed pump. After evaporation and a slight super-heating, the enthalpy drop is converted into electric energy by means of an expander coupled with a generator. In order to minimize the system size, no regenerations and thermal oil loops are considered. The pre-heating and evaporation energy is totally provided by the waste gases, and a turbo-expander provides the work output. Despite the wide-spread use of positive-displacement expanders for ORC applications, due to their low cost and manufacturing simplicity, their performance for small-scale applications as automotive WHR is rather poor, due to volumetric expander intrinsic problems as low adaptivity to volumetric ratios different from the nominal ones, resulting in losses for under- or over-expansions, internal leakages and lubricating issues [9]. On the other hand, turbo-expanders could provide higher performances in a wide range of operating conditions, but the high rotational velocities, high pressure ratios, complexity of the working fluids and the need for a compact geometry make the design of an efficient ORC turbine challenging. About this, some authors have proposed some design solutions in the past [10–13]. After the expansion, the fluid is cooled in the condenser in order to close the thermodynamic cycle. In this study, no sub-cooling is considered during the condensation and the heat exchanger between the source and the working fluid is modelled as perfect. The attention is focused on the main cycle outcomes which could be affected by the variability of the waste gases mass-flow ( $\dot{m}_w$ ) and temperature ( $T_{w,in}$ ), namely: the cycle thermal and exergy (2nd law) efficiencies ( $\eta_I = W_{net}/Q_{in}$ ,  $\eta_{II} = W_{net}/[Q_{in}(1 - \frac{T_0}{T_m})]$ , with  $W_{net}$  the net work of the cycle, given the energy input  $Q_{in}$ ,  $T_0$  and  $T_m$  the ambient and log mean temperature, respectively), representing the energy conversion efficiency and the maximum amount of extractable work, the volumetric expansion ratio ( $V_r$ ) and the turbine size parameter ( $S_T = \frac{\dot{V}_{t,out}^{0.5}}{\Delta H_t^{0.25}}$ , with  $\dot{V}_{t,out}$ ,  $\Delta H_t$  the turbine exit volumetric flow rate and enthalpy drop, respectively). Other variables of interest for the cycle analysis are: the condensing and ambient pressures ( $p_{cond}$ ,  $p_{amb}$ ), waste gas specific heat ( $c_w$ ), pump and turbine efficiencies ( $\eta_p$ ,  $\eta_T$ ).

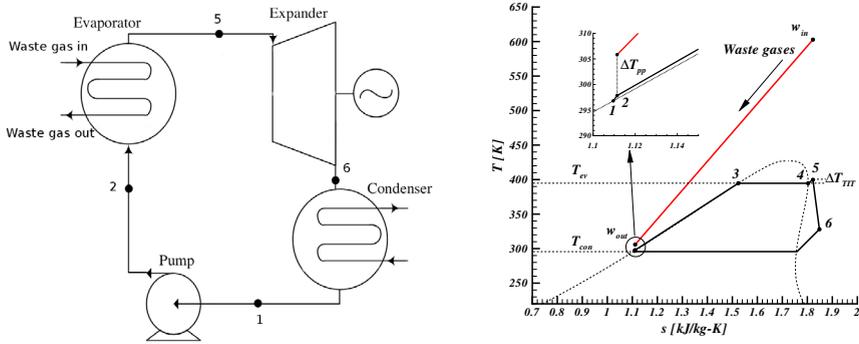


Fig. 1. (a) ORC layout (figure extracted from [14] and modified); (b) T-s diagram for R245fa fluid.

2.2. Heat source characterisation

The hot source in automotive WHR applications is characterised by a variability in time, along with a level of uncertainty on the characterisation of the cycle performances. Here, the measured time histories of the waste gases mass-flow and temperature of a four stroke Diesel engine for heavy-duty railcar application have been used to model the source (see Fig. 2). The profiles represent a portion of a typical intercity train trip, characterized by frequent start and stop cycles that determine a very large variation of the mass-flow rate and temperature of the exhaust gas, while the gas temperature shows a variation within a range of 20 °C [15]. Although the behaviour is roughly periodic over cycle, it is perfectly repeatable. To account for its stochastic behaviour, a random sampling of  $\dot{m}_w$  and  $T_w$  has been carried out in order to fit two beta probability density functions (pdf) over the occurrence histograms. The shape (a, b), location (loc) and scale beta-pdf parameters are listed in Table 1 for the two variables.

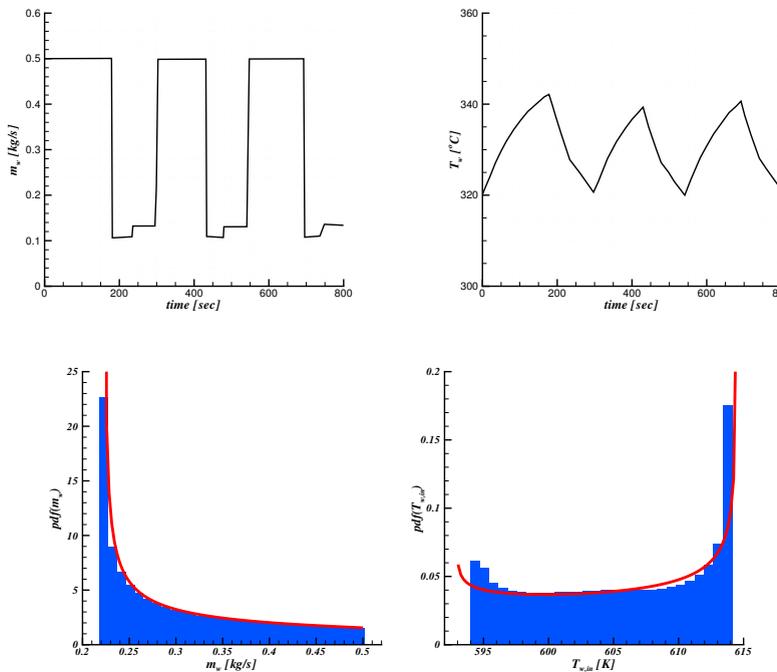


Fig. 2. Time evolution of the waste gases mass-flow rate (a) and temperature (b) (see. Peralez et al. [15]); histogram and beta pdf fitted for the exhaust gas mass-flow (c) and temperature (d).

Table 1. Beta-pdfs parameters for waste gases mass-flow ( $\dot{m}_w$ ) and temperature ( $T_w$ ).

Variable	a	b	loc	scale
$\dot{m}_w$	0.444	1.009	0.222 kg/s	0.284
$T_w$	0.847	0.666	592.9 K	21.58

### 2.3. Working fluids

Six organic fluids have been selected as candidates for the parametric optimization, and their main thermophysical properties are listed in Table 2. These are effective heat transfer fluids with a very low boiling point and are well known in ORC applications. The complex thermodynamic behaviour is described by multi-parameter equations of state (EOS) based on Helmholtz free-energy, as provided by the open-source library CoolProp [16].

Table 2. Properties of the working fluids of interest.

Fluid	Molecular weight (kg/kmol)	Critical pressure $p_c$ (MPa)	Critical temperature $T_c$ (K)	Equation of State (EOS)
R245fa	134.05	3.651	427.01	[17]
R245ca	134.05	3.941	447.57	[18]
Novvec649	316.04	1.869	441.81	[19]
R11	137.37	4.394	471.06	[20]
R134a	102.03	4.059	374.21	[21]
R113	187.38	3.392	487.21	[22]

### 3. Uncertainty Quantification and ORC sensitivity analysis

The ORC parameters listed in Section 2.1 and used for the computation of the cycle performances, are considered as exactly known and constant in common applications. We neglect the influence of fluid-property uncertainties on the cycle performance. These may be considered in future research. On the other hand, various cycle parameters have been modelled as independent random variables with pdf given in Table 3. These distributions have been propagated through the thermodynamic model and the mean, variance and pdf of the cycle outputs have been computed by means of Monte-Carlo simulations. Given the low computational cost of the model,  $N_{mc} = 10000$  samples are computed in each UQ case to extract the statistics. Additionally, a decomposition of the model outcome variance, by means of ANOVA, is carried out to identify the main contributors to the total variability.

Table 3. Cycle parameters distributions and variability ranges.

Parameter	Distribution	Range
$T_{amb}$ (K)	Uniform	[290-300]
$T_{con}$ (K)	Uniform	[293.15-303.15]
$c_w$ (J/kg-K)	Uniform	[1000-1200]
$\eta_P$	Uniform	[0.65-0.75]
$\eta_T$	Uniform	[0.75-0.85]
$T_{w,in}$ (K)	Beta	[592-615]
$\dot{m}_{w,in}$ (kg/s)	Beta	[0.1-0.5]

Three variables are considered for the parametric study of the cycle, namely: the evaporation pressure  $p_{ev} = p_2 = p_3 = p_4 = p_6$ , the pinch point temperature difference  $\Delta T_{pp}$  and the turbine inlet temperature  $T_{TIT} = T_6$ , expressed as  $T_{TIT} = T_{ev} + \Delta T_{TIT}$ . The remaining cycle parameters are treated as deterministic, namely:  $p_{ev} = 0.545 p_{cr}$ ,  $\Delta T_{pp} = 8 K$  and  $\Delta T_{TIT} = 5 K$ , for all of the working fluids of interest. In the following, such parameters are used as optimization variables, as shown in the next Section. The results of the analysis are shown in Table 4 in terms of mean  $\mu$  and coefficient of variation (defined as the standard deviation-to-mean percent ratio)  $CoV$  [%] of  $\eta_I$ ,  $\eta_{II}$ ,  $S_T$  and  $V_r$  for the six working fluids. The R11 and R113 provide the best thermal and exergetic performances with the lowest variability with respect to the other fluids. On the other hand, the R113 requires higher volumetric expansion ratio.

The decomposition of the cycle parameter variances by means of ANOVA provides the main contributions to the total variance of the cycle performances, expressed in terms of first order Sobol' indices. The results are shown in Fig. 3 for the R245fa case (similar results are observed for the other fluids). As expected, the turbine efficiency has the greatest influence on the cycle performances, with a contribution of 63% and 56.8% for  $\eta_I$  and  $\eta_{II}$ , respectively. A not negligible effect is also addressed to the condensation temperature. The size factor is mainly influenced by the exhaust gases mass-flow (87%), whereas the volumetric expansion ratio shows an almost total dependency on the condensation temperature (99.7%).

Table 4. Statistics (mean  $\mu$  and coefficient of variation  $CoV$  [%]) of the four outcomes of the thermodynamic model for the **baseline** configuration.

Fluid	$\mu_{\eta_I}, CoV_{\eta_I}$ (%)	$\mu_{\eta_{II}}, CoV_{\eta_{II}}$ (%)	$\mu_{S_T}$ (m), $CoV_{S_T}$ (%)	$\mu_{V_r}, CoV_{V_r}$ (%)
R245fa	0.145, 4.69	0.357, 4.99	0.0186, 14.2	15.8, 10.4
R245ca	0.161, 4.50	0.383, 4.76	0.0206, 14.38	25.4, 10.8
Novec649	0.122, 4.44	0.294, 4.73	0.0392, 14.5	33.3, 12.1
R11	0.187, 4.38	0.436, 4.65	0.0194, 14.12	23.7, 9.66
R134a	0.0878, 6.94	0.238, 7.20	0.0116, 13.80	3.66, 8.69
R113	0.188, 4.23	0.427, 4.47	0.0287, 14.4	47.8, 10.9

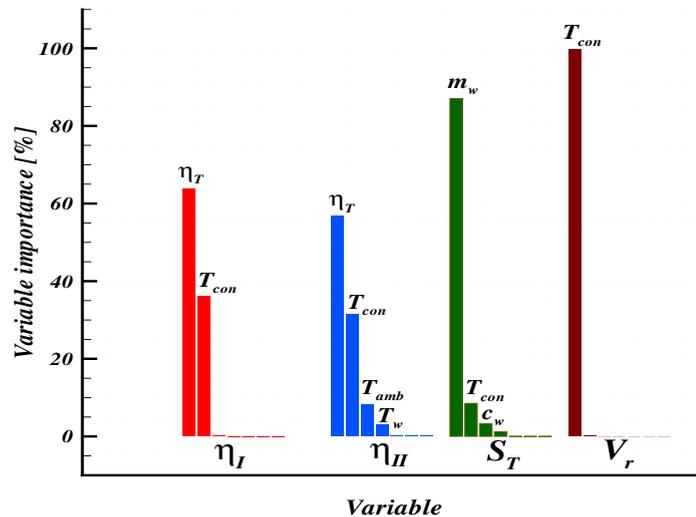


Fig. 3. Variance decomposition by means of ANOVA and evaluation of the uncertain cycle parameters contribution to the total variance for the thermodynamic model outcomes with R245fa.

## 4. Cycle optimization

### 4.1. Deterministic optimization

A preliminary analysis on the search for the best cycle parameters that maximise the thermal efficiency has been carried out by means of a single-objective Genetic Algorithm (GA). The optimization variables are  $[p_{ev}, \Delta T_{pp}, \Delta T_{TIT}]$ , whereas the objective is the maximisation of  $\eta_I$ . The main cycle parameters are considered constant and equal to values included in the ranges of the distributions used for the UQ analysis (see Table 3), such that:  $T_{amb} = 295\text{ K}$ ,  $\dot{m}_w = 0.4\text{ kg/s}$ ,  $T_{w,in} = 610\text{ K}$ ,  $T_{con} = 303\text{ K}$ ,  $c_w = 1100\text{ J/kg-K}$ ,  $\eta_p = 0.7$  and  $\eta_T = 0.8$ . The infeasible individuals of the population at each generation are penalised in order to discard them in the successive iteration, whereas the search domain is limited, such that:  $0.4p_{cr} \leq p_{ev} \leq 0.8p_{cr}$ ,  $0.1\text{ K} \leq \Delta T_{TIT} \leq 10\text{ K}$ ,  $7\text{ K} \leq \Delta T_{pp} \leq 10\text{ K}$ . The population size at each generation is set with  $N_p = 40$  individuals and, among them,  $N_{elite} = 20$  are chosen as "elite". The average fitness of the population, as well as the best fitness, is calculated at each generation. If the difference between those values is less than a specified tolerance ( $\epsilon = 1E - 10$ ), the convergence is reached. In this application, the latter is

attained after 11 generations for all of the fluids.

The best variable sets, along with the best solution, are shown in Table 5. It can be noticed an average improvement of 1% for  $\eta_I$  with the highest effect on the R11 case. Afterwards, the optimum variable sets have been used to carry out an UQ analysis in order to compare the statistics of the cycle performances with respect to the baseline configuration (see Table 4), for the same uncertain parameters (see Table 3). The results are provided in Table 6 and show a decrease of the variability of  $\eta_I$  of 0.2%, and a general improvement of  $\eta_{II}$  with a 17% increase for R11 and R113. On the other hand, there is an increase of the mean size factor and expansion ratio across the expander and a still high variability, which implies an higher complexity of the turbine.

Table 5. Optimum variable sets for the six working fluids after the **deterministic optimization**.

Fluid	$p_{ev}$ (MPa)	$\Delta T_{TIT}$ (K)	$\Delta T_{pp}$ (K)	$\eta_I$
R245fa	2.918	9.9	7.5	0.151
R245ca	3.149	9.4	8.9	0.171
Novec649	1.492	0.5	8.8	0.124
R11	3.509	9.8	7.1	0.208
R134a	3.237	9.9	7.7	0.100
R113	2.703	9.8	8.5	0.192

Table 6. Statistics (mean  $\mu$  and coefficient of variation  $CoV$  [%]) of the four outcomes of the thermodynamic model for the **deterministic optimized** configuration.

Fluid	$\mu_{\eta_I}, CoV_{\eta_I}$ (%)	$\mu_{\eta_{II}}, CoV_{\eta_{II}}$ (%)	$\mu_{S_T}$ (m), $CoV_{S_T}$ (%)	$\mu_{V_r}, CoV_{V_r}$ (%)
R245fa	0.158, 4.57	0.441, 5.61	0.0244, 14.3	25.0, 10.4
R245ca	0.171, 4.40	0.524, 5.42	0.0288, 14.4	40.8, 10.8
Novec649	0.129, 4.37	0.393, 5.38	0.0610, 14.6	61.8, 12.1
R11	0.201, 4.27	0.609, 5.24	0.0287, 14.1	37.4, 9.60
R134a	0.108, 5.83	0.328, 6.88	0.0131, 13.8	5.70, 8.59
R113	0.198, 4.16	0.601, 5.12	0.0445, 14.4	76.6, 10.9

#### 4.2. Robust optimization

The RO allows to take into account the variability of the cycle parameters, reduce the sensitivity of the performances and evaluate the optimal trade-off of the optimization variables for a stable behaviour of the ORC system. The optimization is carried out by means of a multi-objective genetic algorithm (NSGA) with the aim to maximise the mean thermal efficiency while minimise its variance. The evaluation of the two statistics is carried out by coupling the Monte-Carlo method, already used for the UQ analysis, with the NSGA. The uncertain parameters are chosen and set as shown in Table 3 and, for each generation, the population size is  $N_p = 40$  and the convergence is checked, below a prescribed tolerance ( $\epsilon = 1E - 10$ ), on the Euclidean distance between the centroids of two successive optimal Pareto fronts. The results are shown in Fig. 4 for the six working fluids, in terms of optimal Pareto fronts compared with the baseline and deterministic optimized configuration computed with the UQ, and in Table 7, where the statistics of the thermodynamic outcomes are listed for the individuals selected on the Pareto fronts. For all of the solutions, it can be noticed that the deterministic optimization lies on the high variance branch of the Pareto front, thus providing good performance but also high variability. A further analysis has been carried out by changing the operating point and performing two deterministic optimizations with the cycle parameters fixed at the lower (det. opt. low) and upper (det. opt. high) bound of the variability range (see Fig. 4). It can be noticed that the results are independent on the operating conditions and the variance of the deterministic individuals is always high. An improvement of the stability is observed for the robust individuals, which have been selected on the vertical branch of the Pareto front in order to consider high performance with lower variance with respect to the deterministic optimization. The individual #R245fa (see Fig. 4a) shows a relative decrease of the coefficient of variation by 7.7% with a high mean performance  $\eta_I = 0.157$ . A lower performance variability is observed also for #R245ca (-3.18%, see Fig. 4b), #Novec649 (-6.17%, see Fig. 4c), #R11 (-4.68%, see Fig. 4d), #R134a (-5.15%, see Fig. 4e), #R113 (-5.05%, see Fig. 4f). By comparing the baseline/deterministic configurations with respect to the individual with the lowest variance and the individual #R245fa (similar results for the other fluids, see Fig. 5) in terms of pdf( $\eta_I$ ) (evaluated by fitting beta pdfs over the occurrence histograms), an overlapping is visible in the region of the high performances. Then, the deterministic individual could be considered also as a good candidate thanks to its high mean performance  $\mu_{\eta_I}$ .

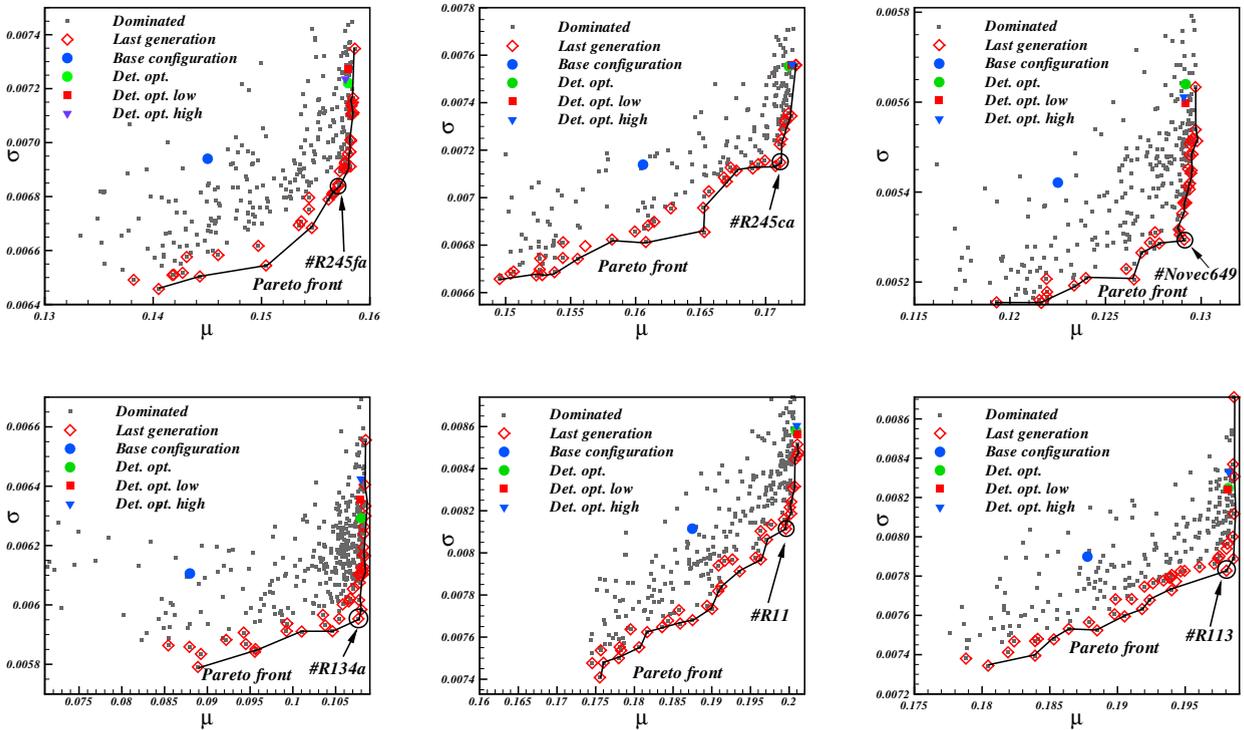


Fig. 4. Pareto fronts and dominated individuals of the robust optimization for the six fluids, along with the baseline and deterministic optimized configurations. From top-left to right: (a) R245fa; (b) R245ca; (c) Novec649; (d) R134a; (e) R11; (f) R113.

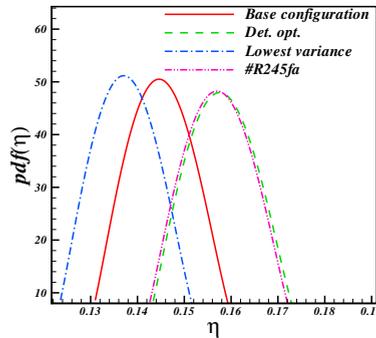


Fig. 5. Probability distributions of the thermal efficiency for the R245fa case and comparison of the baseline/deterministic configurations with the lowest efficient individual and #R245fa.

**5. Conclusions**

An UQ analysis has been carried out on a ORC system for WHR heavy duty applications. The variability of the heat source has been taken into account by considering a real engine duty cycle and the probability density functions of exhaust gas mass-flow and temperature have been evaluated. The expander efficiency and the condensing temperature have resulted the most influential parameters on the thermal and exergy efficiencies. The fluids R11 and R113 have shown the best results for this application and this behaviour has been observed also after the deterministic optimization, with an improvement in terms of mean values and decrease of variability. The robust optimization has provided a global reduction of the performance variability, however, by considering the high mean values of the deterministic individuals, the deterministic solution can be considered as a good compromise.

Table 7. Comparison of statistics (mean  $\mu$  and coefficient of variation  $CoV$  [%]) of the four outcomes of the thermodynamic model for the **robust** configurations.

Case	$\mu_{\eta_I}, CoV_{\eta_I}$ (%)	$\mu_{\eta_{III}}, CoV_{\eta_{III}}$ (%)	$\mu_{S_T}$ (m), $CoV_{S_T}$ (%)	$\mu_{V_r}, CoV_{V_r}$ (%)
RO (#R245fa)	0.157, 4.21	0.375, 4.57	0.0190, 14.01	24.1, 10.3
RO (#R245ca)	0.171, 4.26	0.397, 4.49	0.0216, 14.2	40.7, 10.8
RO (#Novoc649)	0.129, 4.10	0.301, 4.30	0.0458, 13.8	61.4, 11.9
RO (#R11)	0.200, 4.07	0.45, 4.25	0.0196, 14.6	35.03, 9.54
RO (#R134a)	0.108, 5.53	0.281, 5.92	0.0118, 14.2	5.76, 8.46
RO (#R113)	0.198, 3.95	0.436, 4.18	0.0294, 14.5	78.4, 11.01

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