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Systematic Nonlinear Sensitivity Analysis of Working Fluid Mixtures for Flexible Solar Rankine Cycles

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A systematic method is proposed for the selection of working fluid mixtures in a solar Organic Rankine Cycle (ORC) system in view of operating variability. The method is based on a sensitivity analysis procedure where several operating and design parameters that affect the cycle performance are assessed and investigated through an appropriate sensitivity index, which quantifies their impact on several important system performance indices. The proposed method is applied to 11 mixtures, which were previously identified to present increased energy and exergy performance in solar ORC systems. Among those mixture 70 % 1,1,1-trifluoro-propane / 30 % 1-Fluoromethoxy-propane is found to combine good performance in steady state conditions with reduced sensitivity to variability.

1. Introduction

ORC systems are an efficient technology for the generation of power through the utilization of solar radiation. Their operation is based on the absorption of heat through solar collectors which is subsequently transformed into useful power through the ORC. The selection of the appropriate working fluid for each application is important for the development of highly efficient ORC systems. The use of mixtures as working fluids involves significant advantages compared to pure components as they present increased exergetic efficiency due to their variable temperature profile during phase change. But the selection of the mixture that would result in optimum ORC system performance is a multi-dimensional problem. Most studies evaluate the efficiency of different mixtures for steady state operation (Mavrou et al., 2014) but an important limitation of this approach is that even a small change is an operating parameter might result in significant changes in the system performance. This is important as changes are common in system operation due to internal (e.g. malfunctions, fouling etc) or external (e.g. uncertainty in solar radiation) variance. Unless variance is accounted for during mixture selection or system design it will have detrimental effects on the system operability. To this end, an increasing number of recently published works are concerned with the study of off-design (i.e. other than nominal) (Quoilin et al. 2011) or dynamic (i.e. transient) (Wang et al. 2014) ORC performance. However, the consideration of different working fluids as a means to address variability has yet to be addressed.
In this work we propose a method for the simultaneous selection of optimum working fluid mixtures and ORC system characteristics under operating variability. The method is adapted from Seferlis and Grievink, (2001) where it was used as a post-optimality nonlinear programming analysis approach for chemical process systems, whereas recently Papadopoulos et al. (2013) used it to quantify and incorporate modeling uncertainties in the design of ORC working fluid mixtures under nominal operation. The adaptation proposed here employs a sensitivity analysis procedure which supports the identification of working fluid mixtures and ORC characteristics for flexible operation under variability considering successive steady states. The method determines the effects of variability resulting from the simultaneous consideration of multiple system design and operating parameters on a set of ORC performance

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indicators. It further supports the identification of parameters with high influence on the overall ORC-working fluid performance and the quantification of the overall system sensitivity with respect to these parameters. It is based on a formal and robust mathematical analysis framework that avoids assumptions regarding the effects of the selected design and operating parameters and subjective interpretations of the obtained results, while ensuring the validity of the resulting insights for a very wide design and operating ORC range.

2. Proposed approach

In order to develop flexible ORC systems it is required to simultaneously identify the working fluids and the system characteristics, which are able to tolerate external or internal variations while maintaining high operating efficiency. This is because potential unexpected changes in the system operation may result in significant deviations from the performance for which the system was initially designed. Some working fluids or system design and operating characteristics may be less sensitive to variability while others may result in significant deviations from their expected performance. As a result a systematic method is required to simultaneously classify working fluid candidates and operating/design ORC characteristics with respect to their ability to address variability. In this work a sensitivity analysis method is proposed which facilitates the identification of the parameters with the highest influence on the overall ORC-working fluid performance as well as the quantification of the overall system sensitivity with respect to these parameters. The steps of the proposed method are the following:

1) Let a vector $\mathbf{E}^{\mathbf{nom}}$ incorporating a total of N_ε nominal values for the design and operating parameters of an existing ORC system which will be subjected to variability, a set **D** of ORC working fluid candidates, a vector **X** of state variables of an ORC model and a vector **F** of totally N_F system performance indices.

2) For every working fluid in **D**, external or internal variability is emulated by imposing a vector of infinitesimal variations **dE** on each element of vector $\mathbf{E}^{\mathbf{nom}}$ hence resulting in vector $\mathbf{E} = \mathbf{E}^{\mathbf{nom}} + \mathbf{dE}$ which represents the perturbed system conditions. The variations of the performance indices in **F** are then calculated by simulating the ORC model for each element of **E**.

3) For every working fluid in **D,** the effects of the design and operating parameters to the performance indices in **F** are identified by generating a local sensitivity matrix **P** around $\mathbf{E}^{\mathbf{nom}}$. Note that the elements in **P** represent the scaled derivatives of the performance index values in **F** with respect to the system parameters that change under the influence of variability represented by **E**.

4) For every working fluid in **D,** the major directions of variability are derived by calculating the eigenstructure of matrix $\mathbf{P}^T\mathbf{P}$ followed by the rank-ordering of the resulting eigenvectors $\{\mathbf{\Theta}_i\}_{i=1}^{N_\varepsilon}$ based on the magnitude of the corresponding eigenvalues.

5) For every working fluid in **D**, the dominant direction of the system variability is identified as the eigenvector $\mathbf{\Theta}_1$ directions associated with the largest in magnitude eigenvalue of $\mathbf{P}^T\mathbf{P}$. The dominant direction of variability represents the combinations of the design and operating parameters in **E** that cause the largest change in the performance indices in **F** in a least squares sense.

6) For every working fluid in **D**, a dimensionless sensitivity metric $\Omega(\zeta, d)$ is then calculated accounting for the aggregate performance indices variability within a wide variation range explored through a dimensionless parameter variation magnitude coordinate ζ along the dominant direction $\mathbf{\Theta}_1$ as follows:

$$
\begin{aligned}
&\underset{\forall d\in\mathbf{D},\zeta}{Calculate} \quad \Omega(\zeta,d) = w^{\Omega}(\zeta)\sum\left|\left(F_j(\mathbf{X},d,\mathbf{E}(\zeta)) - F_j(\mathbf{X},d,\mathbf{E}^{\mathbf{nom}})\right)/F_j(\mathbf{X},d,\mathbf{E}^{\mathbf{nom}})\right| \\
&\text{s.t.} \quad \mathbf{h}(\mathbf{X},d,\mathbf{E}(\zeta)) = 0 \quad and \quad \mathbf{g}(\mathbf{X},d,\mathbf{E}(\zeta)) \le 0 \\
&\quad\quad \left(\left(\varepsilon_i(\zeta) - \varepsilon_i^{nom}\right)/\varepsilon_i^{nom}\right) - \theta_{1,i}\cdot\zeta = 0 \quad \forall i \in \{1,\ldots,N_\varepsilon\} \\
&\quad\quad \mathbf{X}^L \le \mathbf{X} \le \mathbf{X}^U, \quad \zeta \in [-\zeta_{\lim}, \zeta_{\lim}]
\end{aligned} \tag{1}
$$

Term $w^{\Omega}(\zeta)$ is a weighting factor accounting for the significance of each variation segment within the parametric sensitivity space and matrices **h** and **g** represent the model equality and inequality constraints.

7) For every working fluid in **D**, an $\Omega(\zeta', d)$ is calculated at a desired point ζ' and an augmented vector **aF** is developed which contains both the performance indices and $\Omega(\zeta', d)$ .The elements of **aF** are used in a multi-objective optimization problem formulation considering the working fluids in **D** as the decision parameters in order to select the ones that simultaneously minimize all performance indices in **F** as well as the sensitivity index (or indices) in Ω by generating a Pareto front (Papadopoulos et al., 2013). The Pareto

optimality conditions represent a minimization problem but maximization or combinations may be defined and solved in a similar manner by changing the direction of the inequality signs appropriately.

3. Implementation

3.1 Solar ORC system configuration

The system employed in this work is presented in Figure 1, consisting of three subsystems: the solar collector, the storage tank and the ORC. The solar collector heats water, which is stored in the tank. If the temperature at the collector outlet $T_{FPC,out}$ is greater than the temperature inside the tank T_s then the three-way valve allows the water to flow to the tank. Otherwise it is directed back to the collector for further heating. The temperature inside the tank is monitored and at all times must be lower than a predefined $T_{s,max}$ in order to avoid phase change. If the temperature inside the tank becomes greater than a predefined $T_{min,ORC}$ then the ORC is activated. Circulators are added to the system in order to impose the desired mass flow rates.

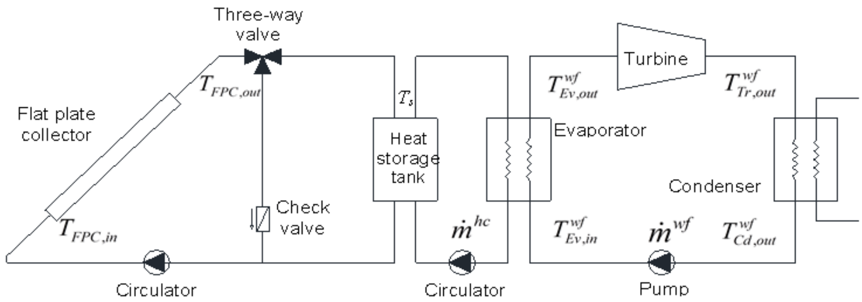

Figure 1: Layout of the investigated solar ORC system

3.2 Investigated mixtures

To illustrate the proposed methodology, four mixtures (Table 1) are investigated in several concentrations, as they were previously shown (Mavrou et al., 2015) to present favorable trade-offs between power generation and overall system operating performance under nominal operation. These mixtures were synthesized in (Papadopoulos et al., 2013) for optimality using a CAMD approach. Note that the different mixture concentrations are investigated with a 10 % interval of increment. The term “mixture concentration” used in the elaboration of the results represents the amount of the first component in the binary mixture.

Table 1: Investigated working fluid mixtures of vector ***D***

ID	Investigated concentrations	Component 1	Component 2
M1	30-40 & 60-70 %	1,1,1-Trifluoro-propane	2-Fluoromethoxy-propane
M2	30-40 & 60-70 %	1,1,1-trifluoro-propane	1-Fluoromethoxy-propane
M4	60 %	Neopentane	1,1,1-Trifluoro-2-trifluoro-methyl-butane
M5	60-70 %	Neopentane	2-Fluoromethoxy-2-methylpropane

3.3 Performance indices, design/operating ORC parameters and multicriteria assessment

The parameters used in vector **F** as system performance indices include the ORC thermal efficiency (η_{ORC}), the net generated power ($\dot{W}^{net}$), the volume ratio across the turbine (V^{Tr}), the mass flow rate of the working fluid ($\dot{m}^{wf}$), the evaporator temperature glide (ΔT_{gl}^{Ev}), calculated as the difference between the temperature at evaporator outlet and the corresponding bubble point temperature, the ORC total operating duration (t_{op}), and an irreversibility metric (Ir), calculated as the difference between the maximum power that can be extracted from a heat source at T_s and the net generated power. Note that apart from t_{op} all parameters are considered as averaged values over the total ORC operating duration. Among these parameters η_{ORC}, $\dot{W}^{net}$ and t_{op} are required to be maximized while all the rest are required to be minimized. The parameters in vector **E** that were varied in the solar ORC system are the following: the mass flow rate for the collectors installed in series ($\dot{m}_{FPC}$), the total mass flow rate of the solar collector subsystem ($\dot{m}_{FPC,sub}$), the minimum temperature in the storage tank that would result in ORC activation/deactivation ($T_{min,ORC}$), the heat carrier mass flow rate in the evaporator ($\dot{m}_{hc}$), the total collector area connected in line (A_{coll}) and the volume of the heat storage tank (V). These parameters are considered because their change may significantly affect the ORC performance. Parameter $\dot{m}_{FPC}$ influences temperature at the collector outlet ($T_{FPC,out}$) with lower $\dot{m}_{FPC}$ resulting in higher $T_{FPC,out}$. Parameter $\dot{m}_{FPC,sub}$ represents the number of installed collector loops. As it increases, the heat transferred to the storage tank increases accordingly. Parameters $T_{min,ORC}$ and $\dot{m}_{hc}$ impact directly on power generation. All these parameters refer to the solar ORC system operation. Additional important parameters refer to the capacity (i.e. size) of some solar ORC components hence they are considered as design parameters. Parameters such as A_{coll} and V may also change during operation. For example, a malfunction in part of the collector will reduce the nominal capacity of the system, whereas a leak in the tank may also reduce the amount of stored water. As a result, the influence of this type of variability in the ORC performance is also worth investigating. In particular, A_{coll} impacts on $T_{FPC,out}$. Finally, V is considered due to the fact that it represents the ORC heat source capacity. The above elaboration highlights the nonlinear associations among the system components and thus the importance of the employed nonlinear sensitivity analysis.

3.4 Technical details

The proposed investigation considers solar radiation, wind velocity as well as ambient temperature using actual hourly averaged data for an entire year for a typical location in northern Greece. At nominal point (i.e. in vector $\mathbf{E}^{nom}$) the mass flow rate per collector area connected in line is $\dot{m}_{FPC}$= 0.44 kg/s. The minimum temperature in the tank that would lead to ORC activation/deactivation is $T_{min,ORC}$ =80 ^oC. The mass flow rate of the solar collector subsystem is set equal to $\dot{m}_{FPC,sub}$= 2.64 kg/s. The heat carrier mass flow rate in the evaporator is $\dot{m}_{hc}$= 0.264 kg/s. The total collector area connected in line at nominal point is A_{coll} = 22 m^2 and the volume of the storage tank is V = 3690 L. Finally, the maximum allowed temperature inside the tank $T_{s,max}$ is assumed 95 ^oC in order to avoid phase change.

4. Results

4.1 Evaluation of the sensitivity index

This section illustrates the implementation of steps 1 through 6 of the proposed methodology. Based on step 5, the combined consideration of design and operating parameter changes along the $\mathbf{\Theta}_1$ eigenvector direction causes the largest change in the performance indices of vector **F** compared to other directions. However, not all parameters have the same impact in defining the $\mathbf{\Theta}_1$ direction. Parameter $\dot{m}_{hc}$ is of particular influence in the dominant direction of variability for most of the investigated mixtures (9 out of 11). This is reasonable as it directly affects the generated power. Figure 2 illustrates the sensitivity index Ω(ζ) which represents the combined effect of all parameters of vector **E** (i.e. the change of all parameters of $\mathbf{E}^{nom}$) on the change of all investigated performance criteria of vector **F** for magnitudes defined by coordinate ζ. The use of coordinate ζ assists in setting a common basis for the comparison of all the mixtures with respect to Ω(ζ). Mixtures with a steep profile especially close to ζ=0 (i.e. the nominal ORC operating point) prove sensitive to variability as they present significantly different performance for operation at other than the nominal point. These mixtures should be avoided as they might have detrimental effects in the ORC performance. On the other hand, mixtures with a flatter profile can efficiently absorb the effects of variability and should be preferred. The mixtures that according to Figure 2 should be further considered as they present a flatter profile close to ζ=0 are 60 % M2 and 60 % M1.There are some additional important observations that can be derived considering Figure 2 and expression (1):

1) The ORC performance of some mixtures deteriorates in different directions. For example 60 % M2 exhibits a flatter profile in the negative direction than 70 % M2, while both mixtures perform similarly in the positive direction.

2) The equality and inequality constraints of expression (1) are forced to be satisfied for every value of ζ. In case that violation does not allow the system to operate in a feasible way, this indicates the limit of the feasible region. Note that it is generally preferred to select mixtures with a wide feasibility region.

3) Several mixtures present a sharp change in the slope of their Ω(ζ) curve after a specific value of ζ, different for each working fluid. Beyond this ζ the profile of the Ω(ζ) curves becomes flatter which means

any change in the investigated parameters beyond this ζ would not result in a significant change in the system performance.

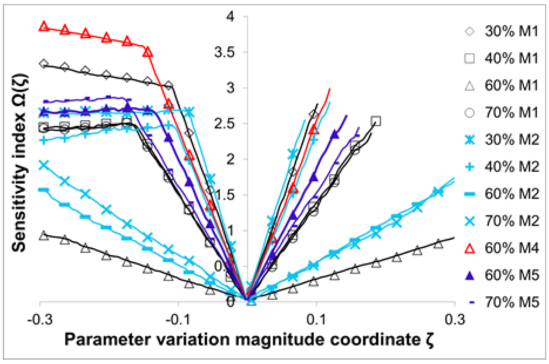

Figure 2: Sensitivity index Ω(ζ) with respect to parameter variation magnitude coordinate ζ.

4.2 Mixture selection for flexible ORC operation under variability

This section elaborates on the implementation of step 7 of the proposed methodology. The idea of step 7 is to consider the sensitivity index of each mixture as an additional indicator simultaneously with the performance indices at nominal operating settings in vector **F** and then select mixtures with optimum nominal ORC performance and minimum sensitivity to variability. System nonlinearity requires that a wide range of values for ζ' need to be investigated in order to ensure appropriate mixture selection. To this end the investigated values of ζ' are 0.03 and 0.06 in both the positive and negative directions. Note that the upper and lower limits are set at ζ'= ±0.06 to allow the investigation of the sensitivity characteristics of all mixtures. This is because the sensitivity of several mixtures may not be evaluated for values of ζ' greater than 0.06 or lower than -0.06 as their Ω(ζ) profiles (Figure 2) are discontinued due to constraint violations. The subsequent Figures illustrate the resulting Pareto fronts with dashes representing mixtures of suboptimal performance

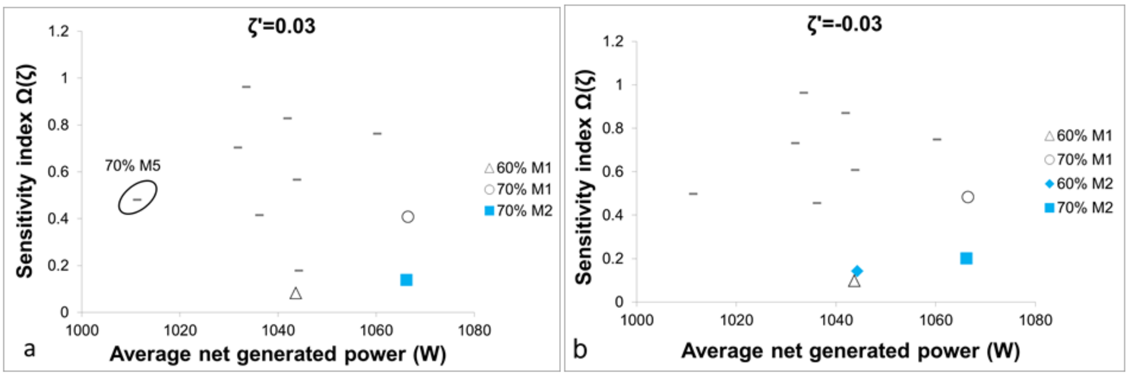

Figure 3:a) Pareto front of sensitivity index against average net generated power at ζ'=0.03, b) Pareto front of sensitivity index against average net generated power at ζ'=-0.03

The first observation in Figure 3 is that despite their high operating performance some mixtures exhibit high sensitivity in the presence of variability which implies less confidence on the achievable performance.The mixtures that exhibit high sensitivtiy are likely to require a more elaborate and difficult to implement operating strategy in order to maintain high ORC operating efficiency under variability.For example, from the mixtures of Figure 3a 70 % M2 is the most desirable option for the considered ζ'= 0.03. This is an interesting observation considering that Mavrou et al. (2015) (who investigated mixture selection without considering variability) found 70 % M5 (highlighted in Figure 3a) as the optimum mixture, which is suboptimal in this Pareto front. However, it is necessary to investigate other ζ' values and performance indices prior to reaching a final conclusion. We therefore investigate the Pareto fronts for ζ'= -0.03, observing several differences. While mixtures 60-70 % M1 and 70 % M2 appear in both Pareto fronts in Figures 3a and 3b, 60 % M2 is in the Pareto front only of Figure 3b.This is a verification of the need to consider both positive and negative directions in ζ. Considering that variability may appear in any potential direction, it is desirable to select a mixture that appears in both directions (i.e. in the Pareto fronts of both Figures). Mixture 70 % M2 has one of the lowest values in terms of sensitivity hence it is selected. In a similar fashion the Pareto fronts of all system performance criteria against the sensitivity index were investigated. The results are summarized in Table 2.

Table 2: Mixtures presenting optimum trade-off between performance and sensitivity for ζ'=±0.03

	$\dot{W}^{net}_{avg}$ (W)	$\dot{m}^{wf}_{avg}$ (kg/s)	t_{op} (h)	$\eta_{ORC,avg}$ (%)	Ir_{avg} (W)	$\Delta T^{Ev}_{gl,avg}$ (K)	V^{Tr}_{avg}
			ζ'=0.03				
Selected mixture	70 % M2	70 % M2	70 % M2	70 % M2	60 % M1	70 % M2	60 % M1
Additional mixtures in Pareto fronts	60 – 70 % M1	40 & 60 % M1 70 % M5	60 % M1 70 % M5	60 % M1 70 % M5	-	60 % M1 70 % M5	-
			ζ'=-0.03				
Additional mixture in Pareto fronts	60 – 70 % M1 60 % M2	40 & 60 % M1 60 % M2 70 % M5	60 % M1 70 % M5	60 % M1 60 % M2 70 % M5	-	60 % M1 60 % M2 70 % M5	-

As mentioned earlier, some profiles appear to have different slopes between adjacent values of ζ indicating different sensitivity and it is therefore required to investigate additional points at ζ'= ±0.06. Due to space restrictions these Pareto fronts are not reported, but differences are observed only in the negative direction. However, the mixtures in these Pareto fronts indicate a lower performance in the considered indices compared to the mixtures in the Pareto fronts at ζ'= ±0.03 hence the mixtures selected in Table 2 do not change. As a result, the mixture with the optimum trade-off between low sensitivity index and high overall performance is 70 % M2, considering that it appears with the highest frequency in Table 2.

5. Conclusions

In this work a systematic methodology is presented for the selection of ORC working fluid mixtures under the influence of variability. This is done by imposing changes of small magnitude in the steady state system behavior in view of different mixtures. The method is implemented in seven steps each based on a formal and robust mathematical procedure resulting in useful insights. The dominant direction of variability is investigated as it represents the worst-case variability scenario thus reducing the analysis effort while targeting the sensitivity investigation effectively. Furthermore the proposed sensitivity index provides valuable insights regarding the sensitivity of each mixture to variability for a wide range of the investigated parameters. Steep sensitivity index profiles indicate mixtures highly influenced by variability compared to mixtures with a flatter profile, so their use should be avoided. Finally, the proposed multi-criteria assessment approach unveils important trade-offs between the desired good performance at nominal point and minimum sensitivity to variability.

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