Uncertainty Quantification of an ORC turbine blade under a low quantile constrain

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Abstract

Typical energy sources for ORC power systems, such as waste heat recovery or biomass, geothermal, and solar energy, typically feature variable heat load and turbine-inlet thermodynamic conditions. In this context, advanced uncertainty quantification and robust optimization methodologies are nowadays available and could be used during the ORC turbine design process in order to account for multiple uncertainties. This study presents a preliminary ANOVA and Uncertainty Quantification analysis, prior to apply robust shape optimization approach to ORC turbine blades, to overcome the limitation of a deterministic optimization that neglects the effect of uncertainties of operating conditions or design variables. The analysis is performed by applying a two-dimensional inviscid computational fluid dynamic model to a typical supersonic turbine cascade for ORC applications. The working fluid is siloxane MDM, which in the conditions of interest exhibits relevant non-ideal effects, here modeled by using of a Peng-Robinson-Stryjek-Vera equation of state.

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1. Introduction

Dense gases (DG) are defined as single phase vapors, characterized by complex molecules and moderate to large molecular weights. The use of dense gases as working media in turbomachinery is proposed for the development of widely distributed, small yield thermal energy conversion devices, referred to as Organic Rankine Cycle (ORC) turbines, where the proposed heat source (such as, for example, solar thermal collectors or waste heat from industrial processes) typically feature variable load and thermodynamic conditions. To improve the reliability of this technology, the resistance to variation in input conditions must be taken into account at an early stage of the development process. On the other hand, just a few highly uncertain thermodynamic data are available for many ORC working fluids, especially the heavier and more complex ones. This makes the development of high-fidelity equations of state describing the thermodynamic behavior of these fluids quite difficult (see [?] for a discussion). Furthermore the need
for a reduction in production costs of ORC systems is leading many constructors toward mass production techniques based on low-quality machining and assembling technologies, which might result in significant geometric tolerances on the final product.

Classic computational Fluid Dynamics (CFD) simulations are generally deterministic, where a set of constant input parameters result in a single solution. In order to evaluate the effects of input parameter variation in the CFD model, several stochastic approaches have been developed in recent years, which treat the problem solution as a vector of random variables depending, via the governing equations, on one or more stochastic input parameters. These may affect the solution via the equations themselves, via the initial and/or boundary conditions and via the geometry of the domain of definition. The results of these stochastic simulations is no longer a single deterministic solution, but rather the probability distribution function of the solution or at least its lower-order statistical moments, such as the expectancy and the variance. The interest of stochastic simulation is that the mean system performance can be evaluated along with its variability, and this information can be taken into account for system optimization. For instance, one can think of optimizing the mean system performance while minimizing some variability parameter to get a more robust design and avoid overfitting problems. The interested reader may refer, e.g., to Refs [?] and [?] for a discussion of robust optimization strategies and sample applications to isolated airfoils.

Recent research efforts have led to the development of several uncertainty quantification (UQ) methods, which may be classified as non-intrusive or statistical (e.g., the Monte Carlo method and the surface response method) or intrusive/non-statistical [e.g., polynomial chaos (PC) methods]. Among these methodologies, considerable interest has been received by PC methods because of their high accuracy and computational efficiency compared to other methods but they have the disadvantage to be intrusive approaches. Anyway, it is possible to develop non-intrusive formulations based on PC theory, such as chaos collocation methods (see e.g., [? ?]), which have demonstrated great capabilities: an undeniable advantage of these approaches is that they may be externally coupled with a black-box deterministic flow solver, without any need to modify it. As a consequence, non-intrusive methods are more versatile than intrusive ones, since they may be applied to different problems just by changing the black-box solver.

The present work investigates the accuracy and efficiency of a Sparse Polynomial Dimensional Decomposition for the analysis of dense gas turbine cascades in the presence of multiple sources of uncertainty, primarily related to the operating conditions. The more relevant uncertain parameters are identified in terms of their impact on the expected system performance, which allows to establish recommendations on the parameters that should be taken into account in the subsequent optimization phase and on possible choices of optimization criteria.

2. Methodology

2.1. CFD

This study makes use of high-fidelity numerical simulations, applying an inviscid real-gas CFD model based on the Open Source code SU2 [? ] [? ]. Here, blade-to-blade effects are of interest, considering a straight stream-tube around midspan. The real-gas thermodynamic behavior of the working fluid is treated by means of the well-known cubic Peng-Robinson equation of state. Total Pressure $P_{in}^t$, total Temperature $T_{in}^t$, and axial flow direction are assigned at the inlet, while static pressure $P_{out}^s$ is given at the outlet. The nominal operating point is given Table 1. The onset of spurious pressure wave reflections from the downstream boundary is avoided by placing the outflow boundary three axial chords away from the trailing edge. In the context of the robust blade optimization, the objective function that will be used is the same as the one considered for the sensitivity analysis. It is defined as the standard deviation of the azimuthal pressure distribution evaluated half axial chord downstream the blade trailing edge [? ], denoted as $\Delta P$ in the following. Indeed, the minimization of this quantity in a supersonic cascade is expected to reduce the strength of the shock generated in the rear suction side of the blade, with beneficial effects on both the cascade efficiency and the aerodynamic forcing acting on the following rotor. Computations are run on a coarse mesh of 7k cells, in order to dramatically decrease the computation time. The Mach number and Pressure field on the blade-to-blade surface are reported for the nominal case, for the baseline configuration in Figure 1. Results are on good agreement with previous CFD analyses of the same cascade configuration [? ].
Table 1. Nominal Operating Conditions.

<table>
<thead>
<tr>
<th>$P_{in}^t$</th>
<th>$T_{in}^t$</th>
<th>$P_{out}^t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 bars</td>
<td>545.15 K</td>
<td>1.072 bars</td>
</tr>
</tbody>
</table>

Figure 1. Euler Computation using SU2 on a coarse mesh (7k cells) at nominal point: Mach (left) and Pressure (right) contours.

2.2. ANOVA Analysis

In this subsection, we recall some definitions about the ANOVA analysis, especially the sensitivity Sobol indices. The objective consists here to perform an efficient Uncertainty Quantification in order to quantify the influence of each uncertain parameter on the quantity of interest $Y$. $\mathbf{X} = (X_1, X_2, ..., X_N)$ denotes a list of input random variables (random vector), and $Y$ a scalar random output. We assume the $N$ input random variables $\mathbf{X}$ are independent. Let us suppose that the response of the output can be represented by a $N$-dimensional function $y = f(\mathbf{x})$. We consider our model output in its functional expansion form as follows

$$y = f_0 + \sum_{1 \leq i \leq N} f_i(x_i) + \sum_{1 \leq i < j \leq N} f_{i,j}(x_i, x_j) + \ldots + f_{1,2,...,N}(x_1, x_2, ..., x_N)$$  \hspace{1cm} (1)

The terms in the ANOVA can then be expressed as unconditional and conditional expectation of $f(\mathbf{x})$

$$E[Y] = f_0$$ \hspace{1cm} (2)
$$E[Y|x_i] = f_0 + f_i(x_i)$$ \hspace{1cm} (3)
$$E[Y|x_i, x_j] = f_0 + f_i(x_i) + f_j(x_j) + f_{i,j}(x_i, x_j),$$ \hspace{1cm} (4)

and so on. The total variance $\text{Var}[Y]$ of the output $Y$ is found to be the summation of all partial variances, namely

$$\text{Var}[Y] = \sum_{1 \leq i \leq N} \sum_{i_1 < \ldots < i_T} \text{Var}[f_{i_1,\ldots,i_T}]$$ \hspace{1cm} (5)

We define the global sensitivity indices

$$S_{i_1,\ldots,i_T} = \frac{\text{Var}[f_{i_1,\ldots,i_T}]}{\text{Var}[Y]}$$ \hspace{1cm} (6)

and the first-order sensitivity indices

$$S_i = \frac{\text{Var}_{X_i}[E[Y|X_i]]}{\text{Var}[Y]}$$ \hspace{1cm} (7)
We outline that the first-order sensitivity indices are positive, and their sum equals unity.

$$\sum_{i=1}^{N} S_i = 1$$  \hspace{1cm} (8)

The variable $X_i$ total effect on the quantity of interest, denoted as the total sensitivity index is estimated by

$$S_{T_i} = 1 - \frac{\text{Var}_{X_i}[\mathbb{E}[Y|X_{-i}]]}{\text{Var}[Y]}$$  \hspace{1cm} (9)

where $X_{-i} = (X_1, ..., X_{i-1}, X_{i+1}, ..., X_N)$. It is indeed the sum of all sensitivity indices containing $X_i$. Here, the total sensitivity indices are positive and lower than 1, and their sum might superior to 1:

$$\sum_{i=1}^{N} S_{T_i} \geq 1, \quad 0 \leq S_{T_i} \leq 1.$$  \hspace{1cm} (10)

The sensitivity indices presented above are computed using Variance-based adaptive strategies aiming to build a cheap metamodel by employing the sparsePDD approach with its coefficients computed by regression. The stepwise regression approach is selected, in order to retain only the most influential polynomials in the Polynomial Dimensional Decomposition (PDD) expansion. It results in a much smaller number of calls to the deterministic model to compute the final PDD coefficients.

2.3. Uncertain Variables

As suggested in [7,8], we study the variability of the output considering uniform uncertainties on the operating conditions, namely $P_{in}^t$, $T_{in}^t$ and $P_{out}^o$, while the inlet flow angle is considered constant and equal to zero (axial inlet flow). The inlet conditions are strongly linked to the ORC heat source, and thus subjected to variations due to "operating" constraints (as found in Waste Heat Recovery systems, Solar Concentrators, Boilers, etc...). The static pressure imposed at the turbine outlet, $P_{out}^o$, is instead dependent of the cold source temperature (water cooling, air coolers, cooling tower...) and the pressure loss due to pipeline connection to the condenser. Its variability is of a very different nature. In this study, we analyse three different scenarios, summarized in Table 2.

In the case of air coolers, the temperature variability during the day might be within a range of 25K, involving a high variability on the outlet static pressure modeled as the case 1 (Table 2). In the case of a water lake, the temperature is considered much more steady in the day scale, modeled as the case 2. We also investigate the case of cold source "hot and steady", or suggested to high pressure losses due to the pipeline connection from the turbine outlet to the condenser inlet.

<table>
<thead>
<tr>
<th>Case</th>
<th>$P_{in}^t$</th>
<th>$T_{in}^t$</th>
<th>$P_{out}^o$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\mathcal{U}[7.6, 8.4]$ bars</td>
<td>$\mathcal{U}[541.15, 549.15]$ K</td>
<td>$\mathcal{U}[1, 2]$ bars</td>
</tr>
<tr>
<td>2</td>
<td>$\mathcal{U}[7.6, 8.4]$ bars</td>
<td>$\mathcal{U}[541.15, 549.15]$ K</td>
<td>$\mathcal{U}[1, 1.2]$ bars</td>
</tr>
<tr>
<td>3</td>
<td>$\mathcal{U}[7.6, 8.4]$ bars</td>
<td>$\mathcal{U}[541.15, 549.15]$ K</td>
<td>$\mathcal{U}[1.8, 2]$ bars</td>
</tr>
</tbody>
</table>

Table 2. Variability of the uncertain inputs for the ANOVA analysis.

3. Results

In this section, we present the results of the ANOVA analysis applied to $\Delta P$, subject to the variability of operating conditions, for three different cases detailed in Table 2. The mesh is constructed with GMSH, in the mesh format SU2. SU2 Input and output of interest are interfaced with a sparsePDD in-house code. A Latin Hypercube Sampling of size 100 is performed for each of the three cases, in which the quantity of interest $\Delta P$ is evaluated running SU2. The total and first order Sobol indices are evaluated (Figure 3).
Statistics of $\Delta P$ are computed (Table 3). The Probability Density Function (pdf) is plotted in each case, illustrating the variability of the output of interest (Figure 2).

**Case 1: Outlet Pressure highly Variable.** In this case, the influence of $P_{out}^n$ is totally dominant, with a total Sobol Index (SI) of 99.5%. The inlet condition influence is very low: a total SI of 1.04% for the inlet pressure, and a negligible one for the inlet temperature.

For this set of uncertain input, it is clearly advised to consider the inlet conditions as deterministic, and only taking into account the variability of the static outlet pressure.

Analysing now the output of interest, it comes $\mathbb{E}[\Delta P] = 11.5 \text{kPa}$, with a large standard deviation $\text{Var}^\uparrow[\Delta P] = 3.21 \text{kPa}$. The 95% quantile, 17.3 kPa is very high. The pdf shape is characterized by a long tail. The high variability of $\Delta P$ and its pdf shape definitively justifies the interest of the robust optimization approach, focused on tail: minimizing $\Delta P$ 95% quantile and its mean.

**Case 2: Low Outlet Pressure - Low Variability.** In this case, the influence of $P_{out}^n$ is still largely dominant, with a total Sobol Index (SI) of 92.1%. The inlet temperature influence is again negligible, its total SI being equal to 0.16%. For the inlet pressure, the total SI is 8.24%.

For this set of uncertain input, it is advised to consider the inlet temperature as deterministic, and taking into account for the variability of $P_{in}^n$ and $P_{out}^n$.

Analysing now the output of interest, it comes $\mathbb{E}[\Delta P] = 7.94 \text{kPa}$, with a low standard deviation $\text{Var}^\uparrow[\Delta P] = 0.30 \text{kPa}$. The 95% quantile, 8.42 kPa is quite close to the mean. The pdf shape is unimodal. The low variability of $\Delta P$ in this case indicates that the framework of deterministic optimization approach might be largely sufficient. This case exhibits lower $\Delta P$ values, so less losses with respect to the other cases.

**Case 3: Large Outlet Pressure - Low Variability.** In this case, the influence of $P_{out}^n$ is still dominant, with a lower total SI of 75.3%. The inlet temperature influence is again negligible. For the inlet pressure, the total SI is 24.7%, showing that in this case, the variability of the inlet and outlet pressure must be taken into account. Analysing now the output of interest, it comes $\mathbb{E}[\Delta P] = 16.6 \text{kPa}$, with a standard deviation of $\text{Var}^\uparrow[\Delta P] = 1.29 \text{kPa}$. The 95% quantile is 18.7 kPa. The pdf shape is unimodal. The variability of $\Delta P$ demonstrates the interest of the robust optimization approach in this case. This case exhibits higher $\Delta P$ values, so more losses with respect to the other cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\mathbb{E}[\Delta P]$</th>
<th>$\text{Var}^\uparrow[\Delta P]$</th>
<th>5% Quantile</th>
<th>95% Quantile</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11.5</td>
<td>3.21</td>
<td>7.69</td>
<td>17.3</td>
</tr>
<tr>
<td>2</td>
<td>7.94</td>
<td>0.30</td>
<td>7.42</td>
<td>8.42</td>
</tr>
<tr>
<td>3</td>
<td>16.7</td>
<td>1.29</td>
<td>14.7</td>
<td>18.7</td>
</tr>
</tbody>
</table>

Table 3. Statistics of $\Delta P$, for the three different cases: mean, standard deviation, 5% and 95% quantiles (in kPa).

4. Conclusion

In the framework of robust optimization of an ORC turbine cascade, a preliminary analysis of the impact of the uncertain input has been investigated. Three different scenarios on the static outlet pressure are considered: a large variability (case 1), a low variability associated with a low value (case 2) and a low variability associated with a large value (case 3). An ANOVA analysis is performed, and statistics of the output of interest $\Delta P$ are evaluated, with the sparsePDD method. It has been shown that the three approaches exhibit different behaviours. In all cases, the inlet temperature has a negligible impact and the outlet static pressure has dominant influence on $\Delta P$. More specifically, in the first case, the inlet pressure influence can be disregarded; due to the high variability of $\Delta P$, the robust optimization is expected to have a large impact on the geometry, with respect to the deterministic optimized one; this is also valid for the third case. Instead, for the second case, due to the low variability of the quantity of interest, deterministic optimization should give a similar result.
Figure 2. $\Delta P$ pdf for the three cases: (a) Case 1, (b) Case 2, (c) Case 3.
Figure 3. $\Delta P$ Sobol Indexes for the three cases: (a) First Order Indexes, (b) Total Order Indexes. Case 1, 2 and 3, respectively in red, green and blue.