Efficient uncertainty quantification of turbulent flows

through supersonic ORC nozzle blades

E. A. Bufi[a,b]*, P. Cinnella[a]

[a]*Laboratoire DynFluid Arts et Métiers ParisTECH, 151 Boulevard de l'Hopital, 75013 Paris (France)*
[b]*Politecnico di Bari, Via Edoardo Orabona 4, 70126 Bari (Italy)*

Abstract

This work aims at assessing different Uncertainty Quantification (UQ) methodologies for the stochastic analysis and robust design of Organic Rankine Cycle (ORC) turbines under multiple uncertainties. Precisely, we investigate the capability of several state-of-the art UQ methods to efficiently and accurately compute the average and standard deviation of the aerodynamic performance of supersonic ORC turbine expanders, whose geometry is preliminarily designed by means of a generalized Method Of Characteristics (MOC). Stochastic solutions provided by the adaptive Simplex Stochastic Collocation method, a Kriging-based response surface method, and a second-order accurate Method of Moments are compared to a reference solution obtained by running a full-factorial Probabilistic Collocation Method (PCM). The computational cost required to estimate the average adiabatic efficiency, Mach number and pressure coefficient, as well as their standard deviations, to within a given tolerance level is compared, and conclusions are drawn about the more suitable method for the robust design of ORC turbines.

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* Corresponding author.
E-mail address: elioantonio.bufi@poliba.it

1. Introduction

The design under multiple uncertainties is a technique called Robust Optimization (RO), which allows achieving designs with stable performances under random variations of the design parameters. Here we consider an Organic Rankine Cycle (ORC) supersonic impulse expander working under stochastic operating and geometrical conditions. In order to carry out a robust design, which takes into account the non-deterministic nature of inputs, the sensitivity of the 2D turbulent flow through a geometry representative of a typical supersonic ORC turbine nozzle cascade is preliminarily investigated via different uncertainty quantification (UQ) algorithms coupled with an in-house finite-volume dense gas flow solver. The supersonic nozzle is designed by means of an in-house software based on the method of characteristics extended to dense gases [1], which are peculiar of ORC applications. Dense gases are molecularly complex gases with a strongly non-ideal thermodynamic behavior in a thermodynamic region above the liquid/vapor saturation curve, where the speed of sound exhibit a behavior opposite to that of standard gases when the fluid undergoes isentropic transformations. Unfortunately, experimental comparisons are not possible since for dense gas flows no experimental data of any kind are available in the literature up to now [2]. This is a well-known difficulty in the ORC community. Attempts to build experimental setups to provide data are currently underway at several universities. ORC systems are subject to multiple uncertainties, like fluctuating operating conditions, geometric tolerances and ill-known fluid properties, which should be taken into account at an early stage of the design process (see, e.g. [1]). Problems involving a high number of uncertain parameters suffer from the so-call "curse of dimensionality" problem [3,4], since the number of code runs required to approximate the statistical moments of the probability density functions associated to the output quantities of interest increases exponentially with the number of parameters. Besides, due to the complexity of the geometry and computational cost associated with the ORC geometries and working fluids, no advanced UQ method has been applied so far to these turbines and little work has been done on uncertainty quantification in turbomachinery in general [5]. A few applications of non-intrusive, sparse grid Generalized Polynomial Chaos methods to simple ORC turbine simulations exist [4,6]. For realistic applications such the ORC turbines considered in this paper, the overall computational cost of an UQ calculation becomes prohibitive. Computational cost is especially crucial when the aim is using robust design techniques in an industrial context. To overcome these limitations, the selection of efficient sampling techniques of the parameter space is of vital importance. Then, the aim of the paper is to assess and compare very different UQ techniques, in terms of accuracy and efficiency, for a realistic ORC nozzle configuration and to suggest useful guidelines to engineers and designers for selecting an efficient UQ method for this kind of problems.

2. Dense gas solver

In the numerical simulations presented in this work, the viscous governing equations are discretized using a cell-centered finite volume scheme for structured multi-block meshes of third-order accuracy, which allows the computation of fluids modelled by the Peng-Robinson-Stryjek-Vera cubic equation of state in order to take into account the real gas effects [7]. The closure of the RANS equations system is achieved by implementing the Spalart-Allmaras turbulence model. The scheme is obtained by correcting the dispersive error of the classical second-order accurate Jameson's scheme [8]. To preserve the high accuracy on non-Cartesian grids, the numerical fluxes are constructed by using weighted discretization formulas, which take into account the mesh deformations [9]. This ensures third-order accuracy on moderately distorted meshes and second-order accuracy at least on highly deformed mesh. The equations are then integrated in time using a four-stage Runge-Kutta scheme. Local time stepping, implicit residual smoothing and multi-grid acceleration are used in order to drive the solution to the steady state. The accuracy of the numerical solver has been already demonstrated in previous works [7-10].

3. Uncertainty quantification models

In this Section a short description of the UQ models used in this work is provided. Two non-intrusive models (Simplex Stochastic Collocation (SSC) and Bayesian-Kriging (BK) methods) and one deterministic model (Second Order Second Moment (SOSM) method) have been coupled with the dense gas solver in order to evaluate the response of the ORC injector to the stochastic variations of the inputs. As described in the next Section, the results are compared with those provided by a full-factorial analysis performed with a Probabilistic Collocation Method (PCM).

3.1. Probabilistic Collocation Method (PCM)

In the PCM [11] the multi-dimensional random space parameters is discretized in a full-factorial way by means of multiple one-dimensional tensor products. If we consider the generic partial differential equation system $L(\boldsymbol{x},\omega,u)=f(\boldsymbol{x},\omega)$ (where x are the spatial variables and $u=u(\boldsymbol{x},t,\omega)$ is the random solution depending on time, space and the random parameter ω), the solution is decoupled in a deterministic part $u(\boldsymbol{x},t)$ and in a stochastic part $h(\xi(\omega))$, where ξ is the input random variable. The random solution u is expanded by means of a Lagrange polynomial chaos according the equation (1):

$$u(\boldsymbol{x},t,\omega)=\sum_{i=1}^{N_p} u_i(\boldsymbol{x},t)h_i(\xi(\omega)) \tag{1}$$

The number of terms N_p for the expansion increases exponentially as function of the number of random variables n_ξ according to the relation $N_p=(P+1)^{n_\xi}$, where P is the degree polynomial. This feature is typical of the full-factorial sampling and introduces the "curse of dimensionality" problem, which has a dramatic impact on the computational costs. The statistics (mean and variance) are evaluated by means of a Galerkin projection of the solution on the polynomial basis, with the collocation points calculated as the nodes of the Gaussian quadrature integration performed by implementing the Golub-Welsch algorithm [12].

3.2. Simplex Stochastic Collocation with Extremum Diminishing (SSC-ED) method

To alleviate the high computational cost associated to a full-factorial sampling, a more efficient technique is proposed in [13]. The hypercubic space parameters is discretized in a unstructured way under the form of simplexes by means of an adaptive Delaunay triangulation. A random sampling is performed in order to avoid clustering of points and high order polynomial interpolation allows to reconstruct the random solution for each simplex. This method is suitable for dealing with discontinuities, such as shocks, thanks to the local smoother based on a Local Extremum Conserving criterion. A super-linear convergence is reached during the simplex refinement process. The statistics are evaluated using the definition of expectation by means of a Monte-Carlo integration on the polynomial interpolation. The refinement process for a generic simplex is carried out according to a local error, which depends exponentially from the local polynomial degree and the number of random variables. The adaptive random sampling of the space parameters is expected to improve the efficiency, leading to a lower overall number of deterministic calculations than the full-factorial sampling.

3.3. Bayesian Kriging (B-K)

The third approach we compare is a Kriging-like surrogate model of the random output, derived by using a Bayesian framework [14]. We are interested in the value of a quantity of interest (QoI) as function of certain random variables at n locations ξ_i contained in the hypercube space parameters. At m of these locations the QoI is observed and known (by running a deterministic calculation) while at the remaining m-n points it needs to be estimated. Following a Bayesian inference approach, the probability distribution of the QoI can be calculated as the posterior distribution resulting from the combination of a multivariate normal prior distribution and likelihood function. In the latter, the covariance matrix takes into account the spatial correlation among the random variables by means of a geometrical correlation range. Then, for each location ξ_i, the solution is approximated by a Gaussian distribution with a certain mean and variance. The error of the surrogate model respect to the observation is provided at the random locations *i* by the standard deviation, as $\sqrt{\hat{\Sigma}_{ii}}$, where $\hat{\Sigma}$ is the covariance matrix.

3.4. Mean Value Second Order Second Moment method (MVSOSM)

The Mean Value Second Order Second Moment method (MVSOSM or simply SOSM) is a so-called deterministic UQ model which computes the statistics of the random QoI by means of a Taylor expansion around the mean value. In this work the mean and variance are obtained with a second and a first order truncated expansion respectively, according to equations (2)-(3):

$$\mu_{QoI} = QoI(\mu_{\boldsymbol{x}}) + \frac{1}{2}\sum_i \frac{\delta^2 QoI}{\delta x_i^2}(\mu_{\boldsymbol{x}_i})\sigma_{x_i}^2 \tag{2}$$

$$\sigma_{QoI}^2 = \sum_i (\frac{\delta QoI}{\delta x_i}(\mu_{\boldsymbol{x}_i})\sigma_{x_i})^2 \tag{3}$$

The cross derivatives are neglected in the Taylor expansion, i.e. the interaction among the random parameters are not considered here. If a centered scheme is used for all the derivatives, the number of deterministic calculations N_p varies linearly with the number of random variables n_ξ, as $N_p = 2n_\xi + 1$. The method requires a relatively low number of samples and is expected to be cheap in terms of computational costs. An additional deterministic calculation is required in order to evaluate the QoI at the mean value of the random inputs.

4. Results

The objective of this work is to assess which is the more suitable UQ model for performing a sensitivity analysis of the ORC injector designed with the MOC under stochastic input parameters. After discussing the deterministic numerical results at nominal conditions, we analyse the stochastic solutions provided by the different UQ methods under investigation.

4.1. Nominal operating conditions results

First of all, the performances at nominal operating conditions have been evaluated by means of the dense gas solver. A deterministic run requires about 10 hours of CPU time on a single processor machine. The Reynolds-Averaged-Navier-Stokes (RANS) equations where solved numerically on a structured C-shaped mesh with $384 * 128$ cells. The inlet total thermodynamic conditions, periodicity in peripheral direction and a supersonic outlet are imposed as boundary conditions. The working fluid is penta-fluoro-propane R245fa, largely used in ORC applications, and the operating conditions are chosen close the saturation curves in the supercritical region, characterized by significant dense gas effects. The injector geometry has been preliminarily designed by using the MOC, with the inlet total reduced pressure and temperature (p_r^0, T_r^0), the target massflow G and the Mach number Me at exit section (see table 1) as input conditions.

p_r^0	T_r^0	G [kg/(s*m)]	M_e
1.28	1.15	20	2

Table 1. Design parameters of the ORC expander and nominal thermodynamic conditions

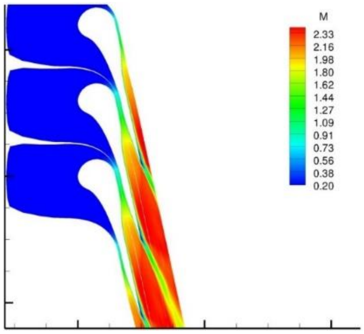

Fig. 1. Mach number distribution for a viscous deterministic calculation at nominal operating conditions

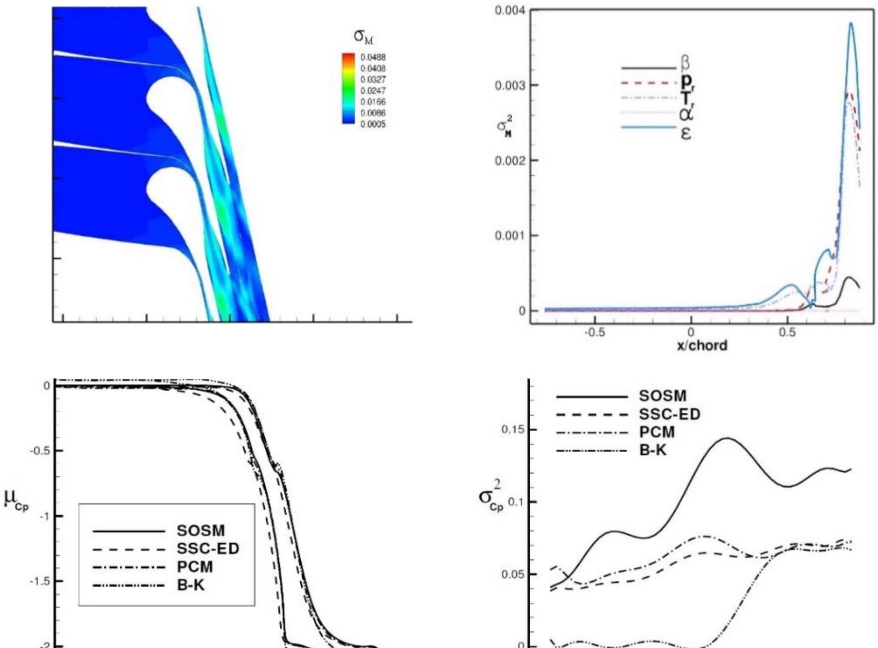

Fig. 2. From top-left to right: (a) Standard deviation contours of the Mach number; (b) ANOVA analysis of the Mach number; (c) Mean pressure coefficient along the blade wall; (d) Variance of the pressure coefficient along the nozzle axis

Figure 1 shows the results at nominal operating conditions in terms of Mach number distribution. The flow expands up to a Mach number of 2 in the exit cross section area, as expected from the MOC design. Afterwards it continues to accelerate guided by the suction side wall and then is decelerated by a weak oblique shock departing from the trailing edge. A viscous wake is visible at the exit and an interaction between the oblique shock and the boundary layer can be noticed close to the suction side wall. These phenomena are expected to be cause of high variability in the flow and, then, a UQ analysis is carried out.

4.2. Full-factorial sensitivity analysis with PCM

Five uncertain parameters are considered in this analysis: inlet total reduced pressure and temperature (p_r, T_r), with a variability of 5% around the nominal point, and inlet flow incidence angle β, blade thickness ε, stagger angle θ, with a variation of 1% around the design values. First of all, a full-factorial analysis via PCM has been carried out. By considering a second order polynomial chaos expansion and the five uncertain parameters, the number of deterministic calculations is $N_p = 243$, requiring 3000 hours of total calculation time. Second-order polynomial chaos was found to provide a good compromise between accuracy and computational cost [6]. In figure 2a the distribution of the Mach number variance shows the presence of regions with high uncertainty close to the wall of the divergent part and to the trailing edge, which can be addressed to the viscous effects. In a second step the random space parameters cardinality has been lowered in order to take into account only the most influential random parameters by means of an analysis of variance (ANOVA) [15]. This allows reducing the number of the deterministic calculations and, then, saving computation time. Figure 2b compares the contributions of the five uncertain parameters to the global variance of the Mach number and shows a great influence of the blade thickness, the inlet total pressure and temperature, while the incidence and stagger angles have a negligible effect. As consequence, the uncertain parameter space is reduced to these three uncertain variables and the four UQ models are applied to the reduced space in order to compare their performances in terms of accuracy and calculation time requirements.

4.3. UQ models comparison

The reduced parameter space has been sampled by using the UQ models described in the previous Section. The results are shown in figures 2c-2d under the form of pressure coefficient mean (along the blade wall) and variance (on the nozzle blade axis). The mean distributions provided by the four models show similar results, with variations below 2% respect to the PCM, while the analysis of the variance diagram reveals that SOSM results are not very accurate, due to the first order approximation of variance and neglecting cross interaction. The B-K model, trained with a set of 20 observations, under-estimates the variance in the leading edge region respect to SSC-ED and PCM which, instead, show very close results. However, the three models all agree about the higher variance on the trailing edge, where the viscous effects are important.

UQ model	N_p	Polynomial order	Calculation time [hours]
PCM	27	2	264
SSC-ED	25	83%→3; 17%→2	270 (+2.1% for LEC criterion)
B-K	20	-	193
SOSM	7	-	73

Table 2. Performance analysis of the UQ models

The analysis of the UQ models performances (see table 2) in terms of calculation time provides that the SSC-ED model is the more expensive, with a computational cost higher and a number of deterministic calculations required Np slightly lower than PCM, but with higher accuracy. Indeed, a third order polynomial reconstruction is obtained on 83% of the total simplexes after refinement, against the 2th global order of PCM. In order to compare these two UQ models based on a polynomial expansion with the B-K surrogate model, a B-K error based criterion has been used. The nodes of the PCM full-factorial and SSC-ED multi-dimensional grids of the parameter space have been used as training set for the B-K model and the cell center values as prediction set. In this way, a criterion to compare the efficiency of the discretization of the space parameters is provided. The maximum error value of the B-K predictions with the PCM and SSC-ED grids is compared with that provided by the B-K for 20 randomly distributed observations (see figure 3). The SSC-ED provides the lower error, with a value slightly below the B-K one. This analysis shows that the random adaptive unstructured SSC-ED grid refinement criterion is very accurate for this application, but its computational cost remains relatively high. Finally, the SOSM method is the cheapest one, with only 7 deterministic calculations required, however its low accuracy for calculating second moments makes it suitable only for fast preliminary analyses.

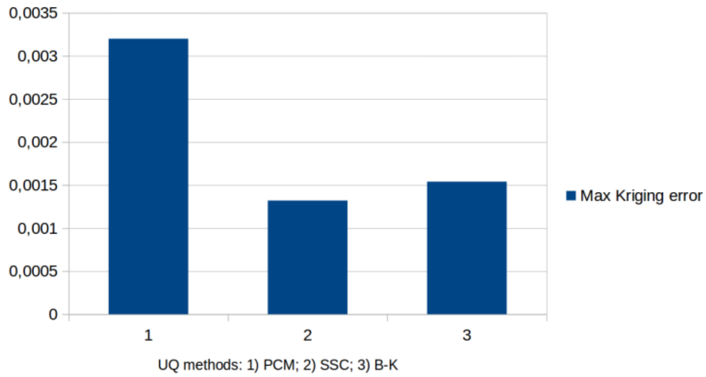

Fig. 3. Comparison of the maximum Kriging error among the PCM, SSC-ED and B-K grids

5. Conclusions

In this work a comparison of different UQ methods, coupled with a numerical solver suitable for dense gas calculation for ORC applications, has been carried out in order to choose the more efficient and accurate one. The PCM, SSC-ED and B-K provide similar quantitative results. PCM and SSC-ED use approximately the same number of samples and then lead to a similar computational cost, however the SSC-ED is more accurate thanks to the higher order polynomial approximation and better distribution of points in the space parameters grid. Also PCM and B-K lead to almost the same results, but B-K is 70% faster for a slightly higher error. Then, for the present application, the B-K results to be a good compromise between low computational cost requirement and accuracy. The SOSM, with cross-derivatives neglected and first order expansion of the variance, shows low accuracy but gives useful information for engineering design purposes with a very low computational cost.

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Biography

Elio A. Bufi is a mechanical engineer and PhD student of the DynFluid Laboratory ENSAM ParisTECH in joint agreement with Polytechnic of Bari. His domain of interest covers the uncertainty quantification and the robust design of supersonic ORC expanders.