Robust Aerodynamic Shape Optimization of Supersonic Turbine Using Non-Intrusive Polynomial Chaos Expansion

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1. Abstract

A supersonic axial turbine stage has been optimized for aerodynamic efficiency under an influence of random variation in rotational speed. The turbine stage is based on the NASA M-1 rocket fuel turbopump, scaled to match the configuration of an LE-5-class liquid-hydrogen rocket engine. The required power output and expansion ratio as well as sizing constraints dictate that the turbine operate in supersonic flow regime, implying that a significant portion of loss generation is due to shock wave and its interaction with boundary layer. In addition to the mean efficiency, robust optimization deals with variance which must be evaluated. This is achieved by the use of Non-Intrusive Polynomial Chaos Expansion (PCE) so as not to resort to approaches such as Monte Carlo simulation which is computationally prohibitive. In order to reduce the simulation turn-around time, and thus the overall time requirement of optimization campaigns, flow simulation was carried out in quasi-3D RANS analysis. An in-house optimization environment, Dough, was used for the optimization, which employs a genetic algorithm assisted by the use of surrogate models. This approach offers the best of two worlds, the global optimization of GA without sacrificing efficiency. The surrogate models are built and enriched on-line, i.e., without the user intervention, and Radial Basis Function Network was used for this purpose. The optimized turbine geometry was shown to not only improve the mean efficiency but also ensured its robustness against rotational speed variability.

2. Keywords

Supersonic turbine, fluid dynamics, robust optimization.

3. Introduction

In the design of space launch systems, the performance of cryogenic rocket engine plays a significant role in the overall launch capability. As a large portion of launcher mass is reserved for fuel and oxidizer, the dry mass allowed for its engine system is extremely limited. Such stringent design requirement necessitates that each component be designed very tightly while ensuring sufficient robustness against system and environment variability.

For modern medium to heavy launchers utilizing liquid hydrogen and oxygen, expander-breed cycle is receiving attention due to its inherent robustness and its capability of achieving relatively high specific impulse. [1, 2] The cycle routes a tiny fraction of fuel around the combustion chamber wall to be heated and the resulting gas drives the turbine. Although simple in construction, the combination of required output, enthalpy drop, and sizing requirements necessitates the use of supersonic impulse turbine which is the focus of the present paper. Such turbines suffer from significant aerodynamic losses due to shock waves and their complex and unsteady interactions with boundary layer. As a result, current designs exhibit relatively low efficiency and a new design approach is strongly desired.

Further improvement of turbomachines exhibiting such complex flow physics is not straightforward and would be time-consuming if done manually. Therefore an efficient design exploration/optimization approach which combines an intelligent design space search and high-fidelity numerical simulation is
desired. One such type of approach, namely surrogate-assisted evolutionary algorithm, has been shown to be quite effective during the last decade [3, 4, 5]. At the same time, researches uncovered pitfalls of automatic optimization, among which the issue of over-optimization is well-known. [6]

Over-optimization happens because numerical optimization is quite adept at exploiting the weaknesses of underlying simulation codes, often undetected by human users. It is particularly evident when optimizing for a single operating condition. The simplest way to avoid this single-point over-optimization is to formulate the objective function by taking a weighted average of multiple operating points [4, 5]. Although it does not incur much extra computational burden, multiple-point approach is nothing more than an ad-hoc numerical workaround and still susceptible to over-optimization. [7]

Therefore, one really needs to resort to a non-deterministic approach that solidly takes into account variability of objective functions, by somehow modeling the mechanism by which uncertainties are propagated toward objective functions. If the computational requirement for the evaluation of a single design is not large, brute-force sampling, i.e. Monte Carlo simulation, can be readily employed, in fact should be used as it is the most reliable way of estimating variability. [8] Such an approach is impractical for optimization involving CFD simulations. One approach gaining some attention is uncertainty propagation modeling by the use of Polynomial Chaos Expansion (PCE) [9] which, if random variables are limited in number, requires only moderate number of samples per design. In this study, using a second-order variant of PCE, robust aerodynamic optimization of the first rotor of a supersonic impulse turbine was carried out. As will be explained later, the use of a second-order PCE results in three sample evaluations per design. This is equivalent to a multi-point formulation where an on-design and two off-design points are considered simultaneously. Thus in terms of computational load, these two formulations are the same. The difference is in the fact that the designer now has a practical indicator (mean and variance of the objective function) by which an optimization can be formulated.

4. Turbine Configuration

The turbine geometry chosen here is the first stage of the hydrogen (fuel) turbopump (FTP) turbine designed for M-1 rocket engine in the US in the 60s. The geometry of the nozzle and the rotor blades is given in Ref. [10]. The first stage (nozzle and the first rotor) was then scaled to match the fuel turbopump turbine of the LE-5 engine whose layout and design characteristics are given in Ref. [11]. The layout of the two-stage LE-5 FTP turbine is reproduced here in Fig. 1.

![Figure 1: LE-5 FTP turbine configuration, from Ref. [11].](image_url)

The airfoil shape of the first rotor is then parameterized with two B-spline curves for pressure and suction surfaces and circular arc sections are used for the leading and trailing edges. Each B-spline curve
consists of 6 control points with equally-spaced knots. The positions of the 4 interior control points are controlled through 5 distance parameters as shown in Fig. 2 while the two end points are positioned as a function of edge radius \(r\), blade metal angle \(\beta\), and wedge angle \(\delta\). The axial chord length and the blade stagger angle complete the parameterization resulting in 18 parameters. In the present study, the axial chord length is fixed.

Figure 2: Left: the original Rotor 1 airfoil definition from Ref. [10], right: parameterization by B-splines.

5. Flow Simulation

ANSYS CFX version 12 was used for the simulation of the first stage. The so-called frozen rotor approach was employed for the simulation of the first stage where no averaging was performed at the nozzle-rotor interface and the rotating domain was kept (frozen) in a fixed relative position. This permits minimal simulation time equivalent to steady simulation with mixing plane approximation used on the interface, although it does not fully capture unsteady phenomena. The governing equation solved is the Reynolds-averaged Navier-Stokes equations with Shear Stress Transport two-equation model [12] used as turbulence model. The flow simulation is simplified as a quasi-3D problem, with two layers of 2-d mesh representing the solution domain. The spanwise height of the flow passage expands linearly in the axial direction at a rate equivalent to the 3-d passage of the actual turbine. The computational mesh contains approximately 400,000 vertices including both the nozzle and rotor domains.

6. Optimization Algorithm

The optimization algorithm used in the current study is based on a combination of genetic algorithm and surrogate modeling, provided by an in-house optimization platform, Dough, developed at Iwate University. A similar approach was applied to various turbomachinery design optimization cases in the past. [13, 4] Genetic algorithms, or more broadly evolutionary algorithms, possess many favorable aspects for high-dimensional non-linear design space, but severely suffer from huge computational requirement. This disadvantage can be alleviated by interfacing the genetic algorithm and the target function evaluation, i.e. numerical simulation, by inserting an approximate model that can be evaluated at a fraction of the cost of the target function. The overall schematic of such surrogate-assisted evolutionary algorithm is shown in Fig. 3. The optimization algorithm used in the inner loop is a real-coded genetic algorithm with extended intermediate recombination and tournament selection operators. Radial Basis Function (RBF)
Network [14] is used as surrogate model. In initiating a surrogate-assisted optimization, a Design of Experiment (DoE) is carried out using Latin Hypercube Sampling (LHS) method to generate the initial sample set needed to construct the first surrogate model.

Robust design optimization is an approach which aims to optimize simultaneously for the mean and the variance of an objective function where variability may originate in several different types of random sources. This is contrasted against deterministic optimization approach where at best a predetermined set of conditions are considered discretely. The following section outlines how the propagation of uncertainties toward objective functions are modeled.

7. Uncertainty Propagation by Polynomial Chaos Expansion

A stochastic variable, $f^*$, which is a function of a deterministic vector, $\mathbf{x}$, and a random variable, $\xi$, can be approximated through a modal decomposition using Polynomial Chaos Expansion [15, 9, 16] as follows.

$$f^*(\mathbf{x}, \xi) = \sum_{i=0}^{P} f_i(\mathbf{x})\Psi_i(\xi)$$

where $f_i$ are the deterministic coefficients and $\Psi_i$ the stochastic basis functions. There are $P + 1$ terms present in Eq. 1 and $P$ is a function of the number of random variables, $m$, and the order of the expansion, $p$, as follows.

$$P + 1 = \frac{(m + n)!}{m!n!}$$

(2)

If we assume a normal distribution for the random variable, $\xi$, the basis functions are Hermite polynomials. Though it is not a requirement for $\xi$ to be normally distributed, we only treat such a source of randomness in the discussion that follows. The most important feature of PCE is that the basis functions are orthogonal with measure $p_N(\xi)$ (probability density function of $\xi$),

$$\langle \Psi_i(\xi), \Psi_j(\xi) \rangle = \int_{-\infty}^{\infty} \Psi_i(\xi)\Psi_j(\xi)p_N(\xi)d\xi = \delta_{ij}$$

(3)

where we denote the inner product above with $\langle \cdot, \cdot \rangle$ and $\delta_{ij}$ is the Kronecker delta. For reference, Hermite polynomials of a scalar random variable $\xi$ are given as follows.

$$\Psi_0(\xi) = 1, \quad \Psi_1(\xi) = \xi, \quad \Psi_2(\xi) = 1 - \xi^2, \quad \Psi_3(\xi) = \xi^3 - 3\xi, \ldots$$

(4)

The corresponding inner products, $\langle \Psi_i^j(\xi) \rangle$, are

$$\langle \Psi_0^0(\xi) \rangle = 1, \quad \langle \Psi_1^1(\xi) \rangle = 1, \quad \langle \Psi_2^2(\xi) \rangle = 2, \quad \langle \Psi_3^3(\xi) \rangle = 6, \ldots$$

(5)
Suppose that we somehow know the values of the deterministic coefficients, \( f_i \), for a given vector, \( \mathbf{x} \). The statistics of the stochastic variable, \( f^*(\mathbf{x}, \xi) \), such as mean and variance can be evaluated as follows.

\[
\bar{f}^* = E(f^*(\xi)) = \int_{-\infty}^{\infty} f^*(\xi)p_N(\xi)\,d\xi
\]

\[
= \int_{-\infty}^{\infty} \sum_{i=0}^{P} f_i \Psi_i(\xi)p_N(\xi)\,d\xi
\]

\[
= \int_{-\infty}^{\infty} f_0 \Psi_0(\xi)p_N(\xi)\,d\xi
\]

\[
= f_0 \int_{-\infty}^{\infty} (1)p_N(\xi)\,d\xi
\]

\[
= f_0
\]

\[
\text{Var}(f^*(\xi)) = E\left(\left[f^*(\xi) - \bar{f}^*\right]^2\right) = \int_{-\infty}^{\infty} \left[f^*(\xi) - \bar{f}^*\right]^2 p_N(\xi)\,d\xi
\]

\[
= \int_{-\infty}^{\infty} \left[\sum_{i=0}^{P} f_i \Psi_i(\xi) - f_0\right]^2 p_N(\xi)\,d\xi
\]

\[
= \int_{-\infty}^{\infty} \left[\sum_{i=1}^{P} f_i \Psi_i(\xi)\right]^2 p_N(\xi)\,d\xi
\]

\[
= \int_{-\infty}^{\infty} \sum_{i=1}^{P} f_i^2 \Psi_i^2(\xi)p_N(\xi)\,d\xi
\]

\[
= \sum_{i=1}^{P} f_i^2 \int_{-\infty}^{\infty} \Psi_i^2(\xi)p_N(\xi)\,d\xi
\]

\[
= \sum_{i=1}^{P} f_i^2 \langle \Psi_i^2(\xi) \rangle
\]

where we used the orthogonality of \( \Psi_i \) and the fact that \( E(\Psi_i) = 0, \ i > 0 \). Since the inner product terms, \( \langle \Psi_i^2(\xi) \rangle \), are known a priori from Eq. 5, the mean and the variance can be expressed as functions of deterministic coefficients \( f_i \), where the leading coefficient \( f_0 \) represents the mean and those of the higher-order terms contributing to the variance.

For Eqs. 6 and 7 to be used for the evaluation of mean and variance, the deterministic coefficients must be known. This is where various methods based on Polynomial Chaos Expansion differ. In the present study, we chose the simplest approach first proposed by Walters, et al. [17]

To determine the deterministic coefficients, \( P + 1 \) samples are first chosen for \( \xi = \{\xi_0, \xi_1, \ldots, \xi_p\} \) and numerical simulation is carried out for each sample of \( \xi \). This results in the following system of linear equations.

\[
\begin{bmatrix}
\Psi_0(\xi_0) & \Psi_1(\xi_0) & \cdots & \Psi_P(\xi_0) \\
\Psi_0(\xi_1) & \Psi_1(\xi_1) & \cdots & \Psi_P(\xi_1) \\
\vdots & \vdots & \ddots & \vdots \\
\Psi_0(\xi_p) & \Psi_1(\xi_p) & \cdots & \Psi_P(\xi_p)
\end{bmatrix}
\begin{bmatrix}
f_0 \\
f_1 \\
\vdots \\
f_p
\end{bmatrix}
= \begin{bmatrix}
f^*(\xi_0) \\
f^*(\xi_1) \\
\vdots \\
f^*(\xi_p)
\end{bmatrix}
\]

where the right hand side vector represents the results of numerical simulation corresponding to each realization of random samples. The deterministic coefficients, \( f_i \), are obtained by solving Eq. 8.

8. Results

8.1. Reference Turbine

The flow field obtained from a frozen-rotor simulation of the reference geometry is first discussed. Figure 4 shows density gradient of the reference turbine. Around the trailing edge of the nozzle pressure side, an expansion fan is observed, followed by a relatively strong shock wave which impinges upon the nozzle
suction side upstream of the adjacent blade. The reflected shock wave then pierces the detached bow shock generated by the blunt leading edge of the rotor. From the suction side of the nozzle, similar expansion/shock pattern is visible around the trailing edge. The shock wave from this side also impinges on the detached shock of the rotor leading edge, albeit at a slightly different location.

8.2. Optimization Problem

The first stage of the scaled M-1 turbine is optimized for total-to-static adiabatic efficiency, evaluated by the following formula.

\[
\eta_{TS} = 1 - \frac{T_{0,\text{out}}}{T_{0,\text{in}}} \frac{T_{0,\text{in}}}{T_{0,\text{out}}} \gamma - 1
\]

where \(T_{0}, p, \) and \(p_{0}\) denote total temperature, static pressure, and total pressure, respectively, and the subscripts in and out the nozzle inlet and Rotor 1 outlet. The rotational speed, nominally set to 10080 RPM, is taken to be a random variable with 2.5% standard deviation while in operation. With this in mind, the objective of the optimization was chosen such that the optimal design maximize the mean efficiency while ensuring a lower bound on the mean minus 3 times the standard deviation. If the efficiency exhibits a normal distribution (though it is not strictly the case), the latter criterion ensures that 99.7% of efficiency variation falls above this value. The statistical information is estimated using second-order Polynomial Chaos expansion, which requires at least 3 samples of the random variable. Thus for each design candidate explored by the optimizer, three rotational speeds are numerically simulated. The three speeds are 9828 RPM, 10080 RPM, and 10332 RPM, respectively corresponding to \(\xi = -1.0, \xi_1 = 0.0, \) and \(\xi = 1.0.\) Let \(\eta_i\) be the efficiency evaluated for each sample \(\xi_i,\)

\[
\eta_i = f^*(\xi_i), \ i = 0, 1, 2.
\]

then from Eq. 8 we have

\[
\begin{bmatrix}
\Psi_0(\xi_0) & \Psi_1(\xi_0) & \Psi_2(\xi_0) \\
\Psi_0(\xi_1) & \Psi_1(\xi_1) & \Psi_2(\xi_1) \\
\Psi_0(\xi_2) & \Psi_1(\xi_2) & \Psi_2(\xi_2)
\end{bmatrix}
\begin{bmatrix}
f_0 \\
f_1 \\
f_2
\end{bmatrix}
= \begin{bmatrix}
f_0^*(\xi_0) \\
f_1^*(\xi_1) \\
f_2^*(\xi_2)
\end{bmatrix}
= \begin{bmatrix}
\eta_0 \\
\eta_1 \\
\eta_2
\end{bmatrix}
\]

which can be solved for the deterministic coefficients, \(f_i\). Finally, using Eqs. 6 and 7 the mean and the variance are obtained.

8.3. Design of Experiment

Before starting a surrogate-assisted optimization, a set of 50 points in design space were sampled by Latin Hypercube sampling. Out of the 50 samples evaluated numerically by the CFD code, 42 samples

Figure 4: Reference turbine, left: density gradient, right: entropy.
met the convergence criteria. This sample set provided the initial database upon which an RBF Network surrogate model was constructed. The mean value of total-to-static efficiency of the reference turbine given by Eq. 9 is 55.77% with standard deviation of 1.026%. Figure 5 shows the distribution of mean efficiency and standard variation of each sample in the DoE. A general trend is that an improvement in mean efficiency is accompanied by an increase in standard deviation, i.e. at the expense of robustness. The task of robust optimization is then to find a blade shape with an improved mean efficiency that does not degrade away from the nominal rotational speed, although such a solution is yet to be exposed in the DoE.

![Figure 5: Mean efficiency and its standard deviation of DoE samples.](image)

### 8.4. Optimization

Three optimization campaigns were carried out successively. After 164 outer optimization iterations (thus after 214 CFD runs including the DoE), the best design achieved mean efficiency of 55.98% with standard deviation of 1.180% (in efficiency). The optimized blade shape is compared with that of the reference blade in Fig. 6. A respectable improvement of mean efficiency was thus obtained without sacrificing the robustness of the reference design. Figure 7 shows a comparison of density gradient between the reference and the optimized designs. An interesting feature can be observed in the density contours that in the optimized blade the detached leading edge shock undergoes more complex reflection pattern on the rotor suction side. It should also be noted that downstream of the detached bow shock and the subsequent expansion fan, there exists another weaker shock on each side, which is a result of slight inflection present shortly after the leading edge radius. The shock on the pressure side coalesces into the detached shock further downstream just before the latter hits the suction side of the adjacent blade. The resulting interaction of these two shocks and the developing boundary layer from the suction side creates a markedly different pattern when compared to that of the reference blade. The entropy contours indicate that the peak in entropy production near the wall is reduced in the optimized blade. On the other hand, entropy production immediately after the detached shock reflection is more prominent than the reference blade. Around the trailing edge of the rotor, the pair of trailing edge shock waves are visibly weaker as shown in the density gradient contours.

Monte Carlo simulations with 100000 normally distributed samples of $\xi$ were then ran by using PCEs obtained for the reference and the optimized blade. Figure 8 shows the resulting histogram of the efficiency distribution for each case. Note that this is not strictly the distribution pattern of efficiency as obtained through the simulation code, as doing so would be impractical, but it nicely depicts the outcome of the robust optimization. The mean shift is obvious while the band of $\pm \sigma$ has not been compromised as a result of optimization which is not guaranteed should a multi-point optimization be the case.
9. Concluding Remarks

Optimization of a supersonic impulse turbine was carried out while taking into account the propagation of uncertainty in rotational speed to the efficiency. Variability in the efficiency was estimated by the use of second-order Polynomial Chaos expansion which required three collocated samples per design. The computational load is therefore unchanged if compared to three-point optimization approaches often employed in aerodynamic shape optimization of turbomachinery blades. By basing optimization criteria more formally on stochastic theory, the constraints on variability could be defined more clearly rather than an ambiguous weighted average done in multi-point optimization. The optimized rotor blade achieved an respectable improvement in mean efficiency while maintain the same level of robustness as the reference design, in a relatively small number of iterations. The technique proposed in the study can be very easily implemented on existing optimization platforms. The study posed the robust optimization problem as mono-objective, which was acceptable if seen as a design refinement. However as the next step, it should also be cast as a multi-objective optimization and other exploratory techniques should be employed to reveal trade-offs between the mean efficiency shift and its variability.
Figure 8: Histogram of efficiency distribution, top: reference, bottom: optimized. Red line: mean, blue lines: mean ± standard deviation.

10. Acknowledgements

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References


