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**Uncertainty quantification and sensitivity analysis of
the $k-\epsilon$ turbulence model closure coefficients for the
prediction of cavitating and non-cavitating flows around
the NACA66(MOD) hydrofoil and the PPTC propeller**

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To my mother.

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Abstract

The following Thesis presents the Uncertainty quantification and Sensitivity Analysis of the $k\varepsilon$ turbulence model applied to the numerical prediction of the cavitating and non-cavitating flows around the NACA66(MOD) hydrofoil and the PPTC (Potsdam Propeller Test Case) marine propeller. The turbulence model parameters are treated as epistemic uncertain variables, and the forward propagation of uncertainty is evaluated by using the Non-Intrusive Polynomial Chaos and the Polynomial Chaos-based Kriging approaches. The required simulations are performed by using a commercial CFD solver, namely the Simcenter Star CCM+. The Sobol indices are used to rank the relative contribution of closure coefficients to the total uncertainty in the output quantities. For the NACA66(MOD) hydrofoil, the ranking of the model parameters seems to be unaffected by the presence of the sheet cavity flow, while it varies with respect to the considered output quantity. Comparing the results of Polynomial Chaos and Polynomial Chaos Kriging, the Polynomial Chaos Kriging seems to be better performance than the Polynomial Chaos Expansion in terms of predictability when the DOE (Design OF Experiment) is composed by a set of few points. Instead, the both models have shown a similar predictability for a DOE of many points. For the PPTC propeller, the ranking of the model parameters seems to be affected by the presence of the sheet cavity flow. The ranking varies by varying the output of interest and comparing the results of Polynomial Chaos Expansion and Polynomial Chaos-based Kriging, as for the NACA66(MOD) hydrofoil, the Polynomial Chaos Kriging shows a lower prediction error than the Polynomial Chaos. In conclusion, a direct correlation between the ranking of coefficients of NACA66(MOD) and PPTC seems to not be present.

Introduction

The field of fluid dynamics is a branch of fluid mechanics aimed at predicting behaviours and evolutions of flows of fluids. Basically, fluid dynamics is based on the application of the Navier-Stokes equations in order to evaluate the velocity and pressure fields of fluids. As is well known, Navier-Stokes equations cannot be directly solved for all types of flow (such as transitional and turbulent flows) and for any body (such as complex geometries) but they must be modeled through other approaches. These approaches are: Direct Numerical Simulation (DNS) approaches, Large Eddy Simulation (LES) approaches and Reynolds-Averaged Navier-Stokes (RANS) approaches.

Generally, the Naval world often works by using RANS approaches in hydrodynamics simulations for the possibility of obtaining the mean flow field within reasonable time and computational costs. The implementation of RANS simulations must be coupled with turbulence model equations to close the RANS problem.

In this context, the $k - \varepsilon$ Turbulence model has been applied. It has been one of the first two-equations turbulence models developed to guarantee the closure of the RANS problem by introducing one transport equation for the turbulent kinetic energy k and one transport equation for the turbulent kinetic energy dissipation rate ε . These two equations are characterized by five calibration constants, i.e. $C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k$, which have been implemented in the model to balance the transport terms of the k and ε equations to correctly predict turbulent flows. These calibration coefficients were standardized to specific numerical values many years ago when the available computational tools were limited and their classical setting has now been questioned due to improvements in computer performance. This means that the five calibration parameters represent sources of uncertainty in the RANS approach because their universal numerical values are unknown.

The current research project has focused on the analysis of the uncertainties associated with the $k - \varepsilon$ Turbulence model constants for the prediction of cavitating and non cavitating turbulent flows around objects of naval interest.

Broadly speaking, uncertainties are associated with the lack of knowledge about one or more dimensions of quantities of interest and they propagate into the model making hard prediction of outputs. In accordance with their nature, they can be classified into six families: parameter uncertainties, parametric uncertainties, structural uncertainties, algorithmic uncertainties, experimental uncertainties, and interpolation uncertainties. The $k - \varepsilon$ model coefficients are related to the variability of input variables due to their estimation. Furthermore, those constants are also epistemic uncertainties whose uncertainty can theoretically be reduced by acquiring more knowledge.

The field that analyses and studies sources of uncertainty is named Uncertainty Quantification theory. Uncertainty Quantification theory can be divided in two sections. The first is named Forward Propagation of uncertainties or Forward Approaches and the second one is called Backward Propagation of uncertainties, also known as Backward Approaches. The calibration constants of the $k - \varepsilon$ Turbulence model has been investigated by a Forward Approach; briefly, they have been considered as initial variables whose uncertainties propagate through model calculations by influencing output evaluations. The main scope of a Forward Propagation of uncertainties approach is to calculate the lower statistical moments (i.e. mean value and standard deviation).

Forward Approaches are classified into Probabilistic Strategies and Non-probabilistic Strategies but Probabilistic Strategies, which have been employed in this work, are more robust than Non-probabilistic Strategies and are mainly used in Uncertainty Quantification problems. Probabilistic Strategies are characterized by Sampling methods, Local Expansion-based methods, Most Probable Point-based methods, Numerical Integration-based methods, Functional Expansion-based methods and General Surrogate-based methods. In this work, we have taken into account the Polynomial Chaos Expansion as Functional Expansion-based method and Polynomial Chaos-based Kriging as General Surrogate method to investigate the sources of uncertainty of the applied turbulence model.

In few words, Functional Expansion-based methods generate metamodels by involving orthogonal or orthonormal univariate or multivariate polynomials as basis functions while General Surrogate-basis methods use other types of basis functions. In fact, the five calibration constants have been considered as initial random variables where each turbulence coefficient has been associated with a sensitivity interval/random domain.

Subsequently, the Sensitivity Analysis of the $k - \varepsilon$ Turbulence model constants has been conducted to investigate the most important parameters affecting the output calculations.

Sensitivity Analysis is classified into Local Sensitivity Analysis and Global Sensitivity Analysis. Local Sensitivity Analysis investigates the weight of each single variable on the response determination by varying one variable per time and keeping the others fixed while Global Sensitivity Analysis investigates the entire parameter space by modifying all constants simultaneously.

In this project, a Global Analysis has been applied. The main Global Sensitivity methods are respectively ANOVA methods, Screening-based methods, Regression-based methods, Correlation-based methods, McDiarmid diameters, Moment-Independent Importance Measures methods and Metamodel-based methods and in this study, the Sobol decomposition which is an ANOVA method has been applied. The method is based on the decomposition of the total variance of outputs into partial variances. Partial variances describe the importance of individual variables and their interactions.

The Uncertainty Quantification study has been applied for two objects of naval interest. In particular, one two-dimensional and one three-dimensional cases have been investigated. The first part of study has treated the propagation of uncertainty and the sensitivity analysis of the $k - \varepsilon$ turbulence coefficients for the prediction of a cavitating and non-cavitating flow regime around the NACA66(MOD) hydrofoil.

The NACA66(MOD) hydrofoil has been analyzed from a global point of view, where outputs of interest have been lift and drag coefficients and from a local point of view where outputs of interest have been pressure and friction coefficients.

Considering the global analysis of the hydrofoil, Polynomials Chaos Expansions from a second order expansion to a fifth order expansion have been applied. For each polynomial expansion, a Design Of Experiment has been generated by sampling the numerical values of the five calibration constants in accordance with their sensitivity intervals. Each set of sampled calibration constants has represented a collocation point. For each collocation point, the hydrodynamic simulation have been directly conducted by using the commercial solver Simcenter Stat CCM+. Furthermore, cavitation has been simulated by using the Schnerr-Sauer cavitation model. For each Polynomial Chaos Expansion, Leave-One-Out Cross-Validation error, statistical moments, Posterior Probability Distributions and Sobol indices have been calculated.

After, a comparison between the Polynomial Chaos Expansion and Polynomial Chaos Kriging has been carried out to evaluate (if possible) the best-adapted metamodel. Specifically, two Design Of Experiment, named "set of few points" and "set of many points" have been employed. For each of them, Polynomial Chaos and Polynomial Chaos Kriging have been generated from a second to

a tenth polynomial degree and the different polynomial expansions have been involved to evaluate the trends of Leave-One-Out Cross-Validation error and Sobol indices.

In conclusion, a local analysis of NACA66(MOD) hydrofoil has been applied by using a second-order Polynomial Chaos . There have been studied the evolutions of Leave-One-Out Cross-Validation error, statistical moments and Sobol indices of pressure and friction coefficients along the longitudinal development of the hydrofoil. The study has been conducted for a fully wetted flow.

As mentioned, the second study has been applied for a three dimensional geometry, i.e. Potsdam Propeller test Case. The flow analysis has been studied for both a cavitating and non-cavitating flow regimes by applying two advance ratio of $J = 1.019$ and $J = 1.408$. For these two operating points, a Polynomial Chaos Expansion of the second order has been employed to calculate Leave-One-Out Cross-Validation error, statistical moments, Posterior Probability Distributions and Sobol indices of thrust and torque responses.

A further analysis of the difference between the Polynomial Chaos Expansion and the Polynomial Chaos Kriging has been applied in order to investigate the trends of Leave-One-Out Cross-validation error and Sobol indices. The analysis has been applied for a polynomial series ranking from second to tenth degree expansions.

The thesis has been organized as follows:

- The first chapter, named "Uncertainty Quantification theory" is a review of the types of sources of uncertainty and the existing methods employed for studying the Uncertainty Quantification.
- The second chapter, called "Sensitivity Analysis" is a review of the typologies of Sensitivity Analysis and the existing methods employed for treating the Sensitivity Analysis.
- The third chapter is a presentation of the problem of interest and its state of the art.
- The fourth chapter is a detailed description of the Polynomial Chaos Expansion, the first method used for the Uncertainty Quantification analysis, in terms of its theoretical foundations and numerical applications.
- The fifth chapter explains the theory of the Polynomial Chaos-based kriging, the second surrogate model applied for the Uncertainty Quantification analysis.
- The sixth chapter treats the Sobol decomposition which has been the methodology employed for the analysis of the Sensitivity Analysis. Theoretical background and computation of Sobol indices have been shown.
- The seventh chapter is an introduction to Navier-Stokes equations and a review of the most common turbulence models developed in RANS approaches. Furthermore, the $k - \varepsilon$ turbulence model, which is the applied turbulence model in this study, is described in detail.
- The eighth chapter is an introduction to the phenomenon of cavitation. A review of the cavitation models involved in numerical simulations is presented and the Schnerr-Sauer cavitation model, which is the cavitation model used in this work, is explained in detail.
- In the ninth chapter, simulation setup and the geometry characteristics of the NACA66(MOD) hydrofoil, the first geometry analyzed, are described.
- In the tenth chapter, simulation setup and the geometry characteristic of the PPTC propeller, the second geometry analyzed, are described.
- The eleventh chapter concerns the results of NACA66(MOD) hydrofoil.
- The twelves chapter concerns the results of PPTC propeller.
- the thirteenth chapter summarizes the conclusions about the results associated with the both geometries of interest.

Chapter 1

Uncertainty Quantification theory

1.1 Introduction: Uncertainty Quantification, what and why

Since ancient times, guided by curiosity and desire, humans have always looked at the world around them in order to understand how the mechanisms behind physical phenomena work.

Initially, the understanding of nature was primarily driven by practical applications where knowledges were acquired through experience and when human observation failed to reach a concrete conclusion, superstitions and myths emerged. Over time, mathematical models have been developed to describe and study phenomena. Briefly, models are based on the idea of predicting quantities of interest (keeping a certain level of precision) by starting from known initial quantities and by applying a mathematical law which is a good approximation of the true phenomenon. Unfortunately, discrepancies between the reality and the model arise, leading to uncertainty. In other words, no phenomenon can be perfectly reproduced; therefore, divergences between what the reality is and what we know constitutes uncertainties. Given a phenomenon of reference, uncertainties are directly associated with the lack of knowledge about one or more dimensions of that phenomenon and their presence make hard the predictability of events.

Uncertainty Quantification aims to identify and reduce (if possible) the sources of uncertainty to improve the tools of studying phenomena. Uncertainty Quantification problems treat certifications, predictions, verifications, validations, estimations, data assimilations and much more. In next sections, a classification of uncertainties has been presented and a hierarchy of methodologies about the Uncertainty Quantification theory has been proposed as current state of the art of this wide field of study. Specifically, the sources of uncertainty have been described, as well as the types of uncertainty and the approaches used to analyzing uncertainties for both forward and backward approaches in probabilistic and non-probabilistic contexts.

1.2 Sources of uncertainty

As introduced, sources of uncertainty are associated with the limited knowledge of a problem. They are responsible for predictive inaccuracies and model failures. They can be related to physical or non-physical variables and can also arise to model structures, aleatoric fluctuations and other factors. Globally, taking into account Figure 1.1, we can classify the uncertainties in six main families: **parameter uncertainties**, **parametric uncertainties**, **structural uncertainties**, **algorithmic uncertainties**, **experimental uncertainties** and **Interpolation Uncertainties**. They are following explained and represent the core of the Uncertainty Quantification theory [1, 2, 3, 4].

1.2.1 Parameter uncertainties

Parameter uncertainties are associated with the measurement errors, sampling errors, variability of the model and use of surrogate data. These uncertainties are input variables represented by unknown parameters of the model. They specify features of a particular application context or they are more global input parameters.

1.2.2 Parametric uncertainties

Parametric uncertainties are related to the variability of input variables or they are associated with the lack of knowledge of a specific dimension of an input variable. They arise from the estimation of the model parameters under a given model specification.

1.2.3 Structural uncertainties

Structural uncertainties arise from the discrepancy between the true phenomenon and the mathematical model involved to describe it. They are strictly connected to the accuracy of the model and they are also named **model inequality**, **model bias** or **model discrepancy**.

1.2.4 Algorithmic uncertainties

Algorithmic uncertainties come from numerical errors and numerical approximations. Repeating the same calculations, the results may vary by the presence of Algorithmic uncertainties. These uncertainties include aspects such as data quality, hyperparameter settings and sensitivity to input changes. They are also called **numerical uncertainties**, **discrete uncertainties** or **residual uncertainties**.

1.2.5 Experimental uncertainties

Experimental Uncertainties arise from the variability of experimental measurements. They are also named as **observation errors**.

1.2.6 Interpolation uncertainties

Interpolation Uncertainties are due to the lack of available data collected from simulations and experimental data. They are also named **code uncertainties**.

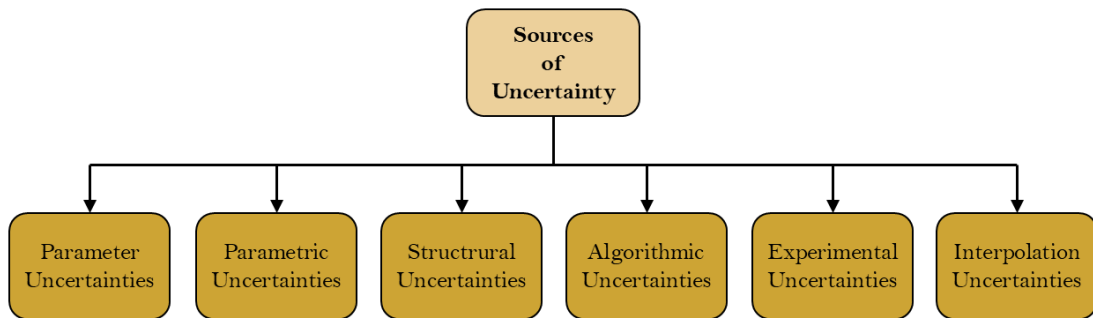


Figure 1.1: Sources of Uncertainty.

1.3 Types of uncertainty

In the previous section, a classification of sources of uncertainty has been applied in reference of dimensions where uncertainties arise. Each source can be sub-classified by considering its "be-

haviour” inside the problem of interest as represented in figure 1.2. In detail, sources of uncertainty can be **epistemic uncertainties** or **aleatoric uncertainties** [5, 6, 7, 8].

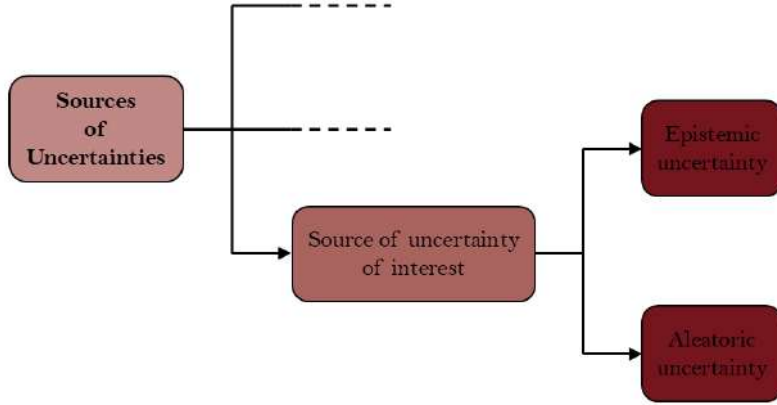


Figure 1.2: Types of Uncertainty.

1.3.1 Epistemic uncertainties

Epistemic uncertainties are generated by a the lack of knowledge of a specific dimension of a problem of interest; they can be reduced by acquiring more knowledge (by gathering more data) or refining the models in theory but it is not possible in practice. They are also named **systematic uncertainties**.

1.3.2 Aleatoric uncertainties

They describe the natural variability of a quantity of interest. They cannot be reduced and depend on the nature of the system. They are also called **stochastic uncertainties**

1.4 Approaches for studying uncertainties

In this section, the methods developed to investigate the sources of uncertainty are discussed. Broadly speaking, Uncertainty Quantification is basically analyzed by involving two main methodologies, i.e. **forward approaches** and **backward approaches** [7, 9, 10, 11]. The type of the applied approach depends on the aims of the problem and the desired outcomes.

1.4.1 Forward approaches

A forward approach at analyzing to analyze how the propagation of uncertainties of input variables influences the output evaluations. It focuses on the influence on the outputs from the parametric variability listed in the sources of input uncertainty where the probability distributions are known at priori. In other words, pre-specified probability distributions are propagated to investigate the uncertainty distributions of solutions. The main aims of this approach are:

- Evaluation of the probabistic moments, i.e. mean value and standard deviation.
- Evaluation of the reliability of outputs
- Complete assessment of output probability distributions.

1.4.2 Backward approaches

In backward approaches, the posterior distributions are available and the goal is to calculate the most suitable input variables that ensure the target statistical properties for the output of interest. In other words, the available data is assimilated to infer the initial distributions or model errors. The backward propagation of uncertainties is a generalization of parameter estimation error analysis. Three typical scenarios can be identified in backward propagation:

- **Bias Correction scenario** aims to quantify the model inequality (i.e. the discrepancy between the experimental data and the mathematical model).
- **Parameter Calibration scenario** aims to quantify unknown parameters of the model.
- **Bias Correction and Parameter Calibration scenario.**

In the two approaches, the relationships between input and output values in Forward and Backward Approaches can be summarized as illustrated in Figure 1.3.

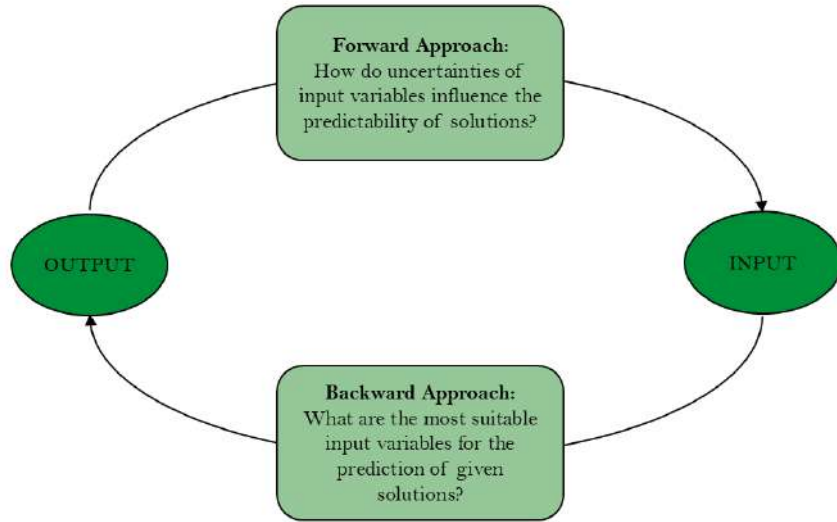


Figure 1.3: Uncertainty approaches.

1.5 Methodologies for investigating the forward propagation of uncertainties

Forward approaches involve probabilistic or non-probabilistic strategies that can be non-intrusive or intrusive. Non-intrusive applications are the most used strategies because they do not need the variation of any governing equation of the system while intrusive methods require the alteration of one, some or all governing equations of the system. Generally, Intrusive models are more expensive than non-intrusive models [12].

1.5.1 Probabilistic strategies

Probabilistic strategies are named so because the initial variables of a problem are random variables with own probabilistic distributions. They are more rigorous approaches than non-probabilistic methods are therefore the most commonly strategies involved in the Uncertainty Quantification theory. Probabilistic strategies can be classified into six macro-families of methods to study the Forward Propagation of Uncertainties: **sampling methods**, **functional expansion – based methods**, **local expansion – based methods**, **most probable point –based methods**, **numerical integration – based methods** and **general surrogate – based methods**.

Sampling methods

Sampling methods or also named **simulation – based methods** involve the creation of artificial models to mimic real-world phenomena. These methods leverage repeated random sampling to approximate complex systems or processes. The sampling distribution is created by using the many artificial generated datasets. Inferences are then based on this sampling distribution. Simulation-based methods are non-intrusive and among others we have: **Monte Carlo methods**, **quasi Monte Carlo** and **pseudo Monte Carlo methods** [8, 13, 14, 15, 16, 17, 18, 19, 20].

Functional expansion-based methods

Functional expansion-based methods are used to represent data specified on a desired domain as an expansion of basis set in a continuous manner. Basis functions of functional expansion-based methods are univariate or multivariate orthogonal or orthonormal polynomials. They are also named as **spectral methods** [21]. Among others we have **Polynomial Chaos Expansion**, **Wavelet Expansion**, **Karhunen – Loeve Expansion** and **Neumann Expansion** [8, 22, 23].

Local expansion-based methods

These methods take advantages (and are mainly used) for relatively small input variability and outputs that do not express high non-linearity. Among others there are **Taylor series expansion** and **perturbation method** [24].

Most probable point-based methods

Most probable point-based methods consist in predicting specific performances which often represent some failure in structural reliability applications. These methods determine the most probable point by involving approximation strategies applied to performance functions. Among others we have **First – order Reliability methods** and **Second – order Reliability methods**.

Numerical Integration-based methods

Numerical Integration methods are based the application of numerical integration techniques to determine the probabilistic moments, among others there are **Full Factorial Numerical Integration method** and **Dimension Reduction method** [25].

General Surrogate-based methods

General surrogate-based models represent the response surface of output values by involving other approaches than basis functions. Among others, there exist **Kriging** and **Polynomial Chaos – based Kriging** [26, 27, 28, 29, 30, 31, 32].

1.5.2 Non-probabilistic strategies

Non-probabilistic approaches are less used than probabilistic approaches to study the Uncertainty Quantification for their lower robustness. They are based on specific defined laws and the most used methods in the current category are **Interval analysis**, **Fuzzy theory**, **Possibility theory** and **Evidence interval**.

Interval analysis

The main objective of interval analysis is to provide a simple way of calculating upper and lower bounds of a function's range in one or more variables in order to reduce rounding and measurement errors. These endpoints are not necessarily the true supremum or infimum of a range since the precise calculation of those values can be difficult or impossible; the bounds only need to contain the function's range as a subset. The scope is to substitute single uncertain variables with arithmetic intervals which describe ranges of possibilities [33].

Fuzzy theory

The Fuzzy theory is based on manifold. In this context, uncertainties are represented and quantified by using Fuzzi numbers and Fuzzi logic. Probabilistic strategies are suitable for dealing with well-defined random variables while Fuzzy theory is employed for imprecise, vague, or subjective information, which makes it a valuable tool in Uncertainty Quantification [34].

Possibility theory

Possibility theory is an uncertainty theory for handling incomplete information which is based on set functions. Possibility theory uses pairs of dual set functions which are the possibility and necessary measures. Possibility theory can be sub-classified into **Quantitative Possibility theory** and **Qualitative Possibility theory** [35].

Evidence theory

The theory of evidence was developed by Glenn Shafer in 1976 as a new way to represent uncertainty. The non-probabilistic approach of this theory is based on belief functions which need to be defined by introducing some condition [36].

1.6 Methodologies for investigating the Backward Approaches of Uncertainties

In Backward approaches, the posterior distributions are available and the goal is to calculate the most suitable input variables that ensure the target statistic properties for the output of interest. The main tool used in backward analysis is the **Bayesian inference** which is based on the Bayes' theorem [37].

In conclusion a graphical representation of the Uncertainty Quantification theory is given in Figures 1.4, 1.5 and 1.6.

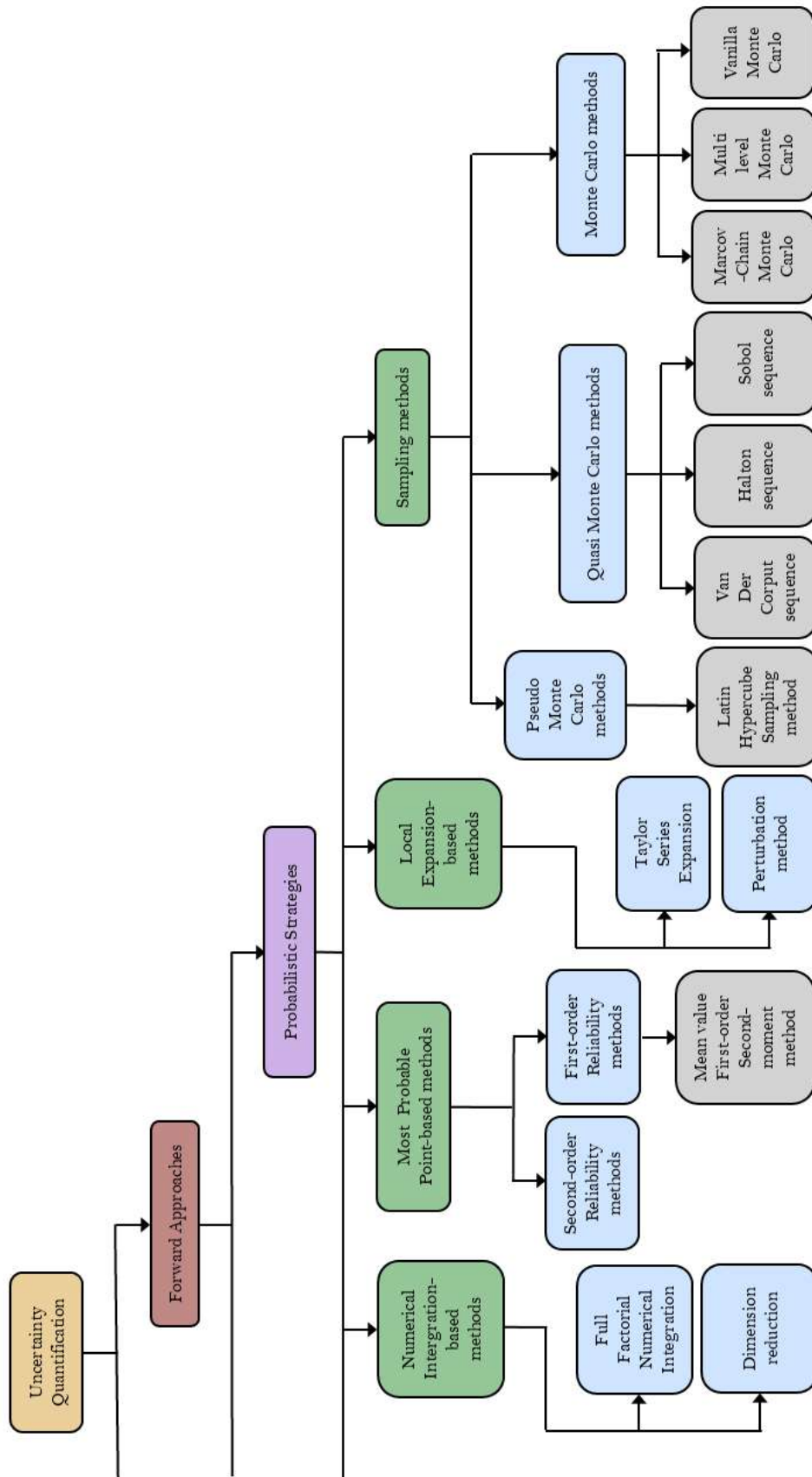


Figure 1.4: Uncertainty Quantification - part 1

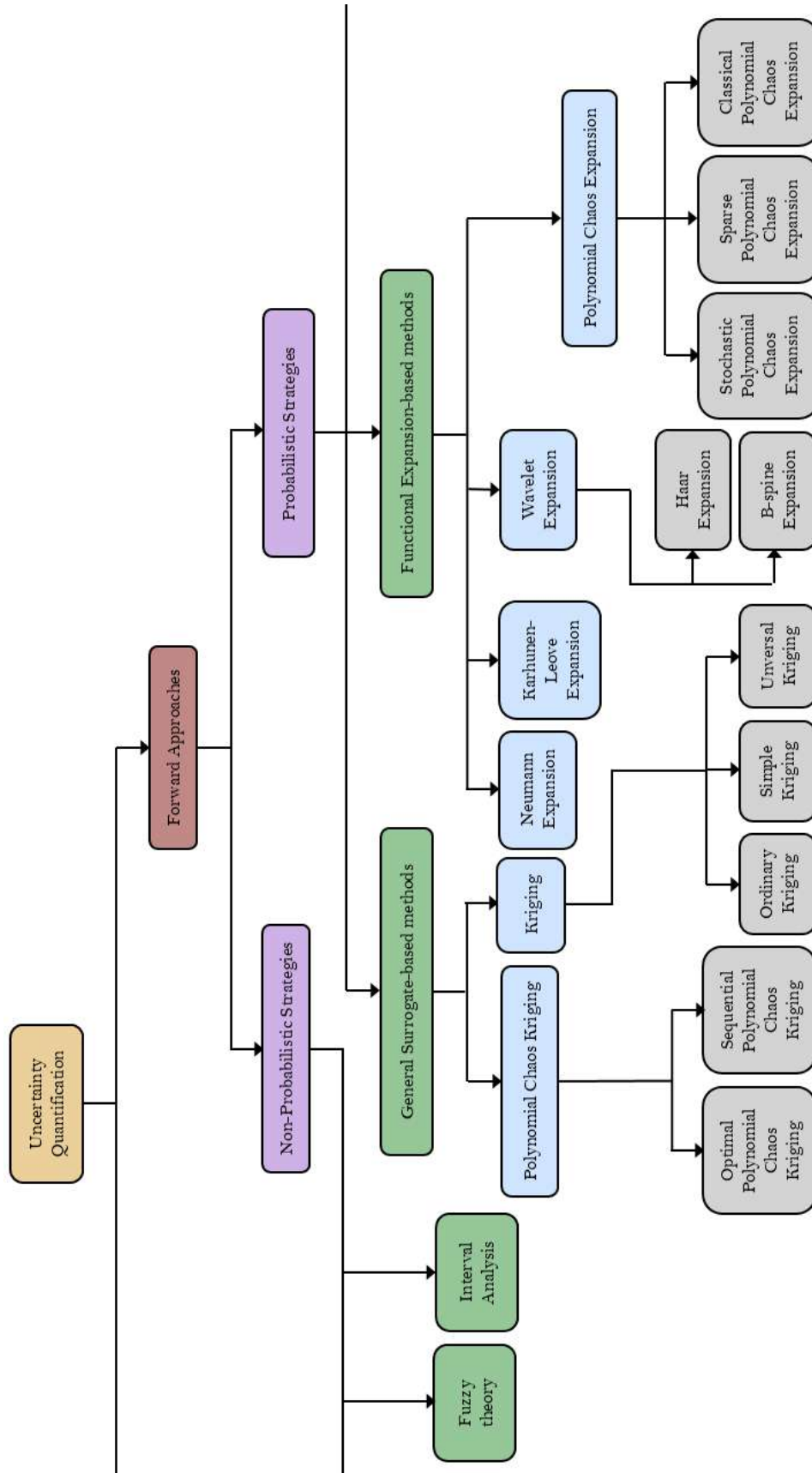


Figure 1.5: Uncertainty Quantification - part 2

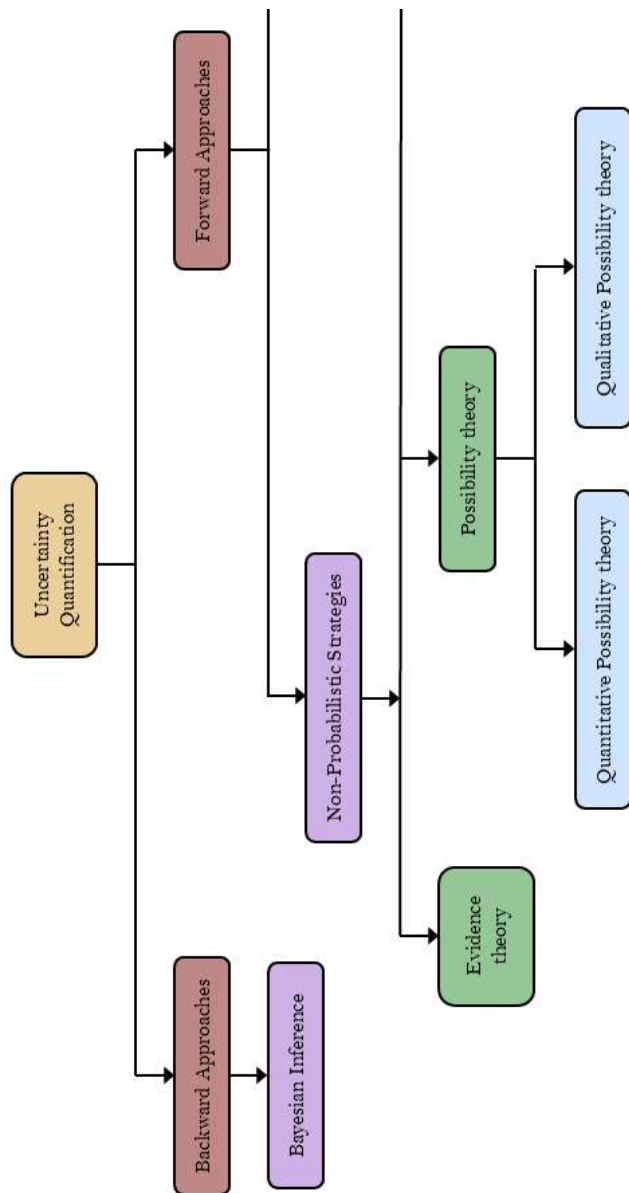


Figure 1.6: Uncertainty Quantification - part 3

Chapter 2

Sensitivity Analysis

2.1 Definition of Sensitivity Analysis

Sensitivity Analysis is a field of study coupled with the Uncertainty Quantification theory. As Uncertainty Quantification aims to evaluate the propagation of uncertainties through models to determine outputs or to construct input distributions for given responses, Sensitivity Analysis focuses on the impact of input parameters and their interactions on the output values of a mathematical model.

Each input parameter influences the output uncertainty in accordance with its importance in the system. It is noted that a mathematical model is defined by a series of independent variables; these variables weigh differently on the template and applying this methodology is possible to neglect the less important variables to simplify the given model. Controlling the most important variables is also possible to reduce the uncertainty and to improve the robustness of the model prediction or reduce the probability of failure of the structure system. The simplification of the model reduces computational time and effort.

Sensitivity Analysis is sub-classified into two groups, i.e., **Local Sensitivity Analysis** and **Global Sensitivity Analysis** [39, 40, 41, 42, 43]. In this chapter a complete Sensitivity Analysis review has been proposed.

2.1.1 Local Sensitivity Analysis

Local Sensitivity Analysis investigates the effects of local changes of a parameter in a system or investigates the variation of the response along a trajectory. The aim is to measure the local structure of a system. It is based on the computation of the gradient of the response with respect to its parameters around a nominal value.

2.1.2 Global Sensitivity Analysis

The aim of a global approach is to evaluate the entire parameter space and understand the contribution of input variables to the outputs. The application is treated in an average sense. In Global Sensitivity Analysis, the uncertainties of input parameters are random vectors (Local Sensitivity Analysis is a type of study based on a scalar approach, instead, Global Sensitivity Analysis is based on a vector approach). Moreover, input parameters are taken individually or in combination with others. Global Sensitivity Analysis is also finalized for the individuation of critical points as bifurcations, turning points and response extrema in the combined phase space formed by the parameters, state variables, and adjoint variables.

Following, a brief description about the methods used in the Sensitivity Analysis are given.

2.2 Local Sensitivity Analysis methods

As introduced, Local Sensitivity Analysis is applied to evaluate how local variations of initial variables influence the responses of a system. The principal methods applied are **Derivative method**, **Direct method**, **Green's function method** and **Adjoint method** [8, 40, 44, 45, 46].

2.3 Global Sensitivity Analysis methods

As explained, Global Sensitivity Analysis investigates the complete parameter space of a given problem and the methods applied to quantify the most important input quantities are classified based on whether the initial variables are independent or dependent. Globally, there exists **McDiarmid diameters** [8, 47], **Screening –based methods**, **ANOVA methods**, **Regression –based methods**, **Correlation –based methods**, **Moment – Independent Importance Measures methods**, **Metamodel –based methods**.

2.3.1 Screening-based methods

The Screening-based methods select a set of input factors among all system factors without reducing the system variance. These methods are employed when the interest is focused on a preliminary qualitative ranking of importance of variables without requiring a large number of samples. For more accurate information, other approaches are needed. Among others the most famous are **Morris method** and **Cotter method** [42, 48, 49, 50, 51].

2.3.2 ANOVA methods - ANalysis Of VAriance methods

ANOVA methods are based on the statistical inference to compare groups of data by analyzing the variability within groups and the variability among groups. The main characteristic of these methods is the use of variance to study main effects and higher-order effects of input variables on responses evaluations. This approach is suitable for complex nonlinear and non-additive systems and the main variance based methods are **Sobol decomposition** and **Fourier Amplitude Sensitivity Test** [41, 42, 49, 52, 53].

2.3.3 Regression-based methods

Regression methods are involved in statistical processes for estimating the relationship among the variables of a problem by applying regression techniques. Among others, the most used methods in Global Sensitivity Analysis are the **Standardized Regression Coefficient method**, **Standardized Rank Regression Coefficient method**, **Ordinary Regression Coefficient method**, **Normalized Regression Coefficient method** and the **Stepwise method** [42, 49, 54, 55, 56].

2.3.4 Correlation-based methods

Correlation-based methods identify the association between a variable ξ_i and the response $Y(\xi)$ through a measured relation. Among others we have **Linear Correlation Coefficient method**, **Partial Correlation Coefficient method**, **Partial Rank Correlation Coefficient method** and **Semi – Partial Correlation Coefficient method** [49, 55, 57].

2.3.5 Moment-Independent Importance Measures methods

Moment-Independent Importance Measures methods treat discrepancies between density functions, cumulative functions and value of information to quantify the sensitivity of the input variables with respect to response evaluations. In this class of methods, the study covers the change in the entire probability distribution of the output of interest and the principal scope is measuring the conditional distribution of a fixed variable and the unconditional distribution to quantify the influence of that variable on the output calculation. In this sector, the most famous Moment-Independent

Importance Measures are the **Borgonovo indices** and the **Cumulative Distribution – based Sensitivity Measures method** [40, 42].

2.3.6 Metamodel-based methods

The metamodeling Sensitivity Analysis is divided into two steps:

1. Firstly, a metamodel is generated by using a non-parametric regression method.
2. Secondly, the sensitivity indices are computed by involving variance-based approaches.

From a broad point of view, metamodel approaches are employed to reduce runtimes. Among others, there are **ACOSSO – Adaptive COmponent Selection and Smoothing Operator method**, **MARS – Multivariate Adaptive Regression Splines method**, **SVM – Support Vector Machine method**, **GP – Gaussian process method**, **TGP – Treed Gaussian process method** and **COSSO – Component Selection Shrinkage Operator method** [49, 58, 59, 60, 61].

In conclusion a graphical representation of the Sensitivity Analysis is given in figures 2.1 and 2.2.

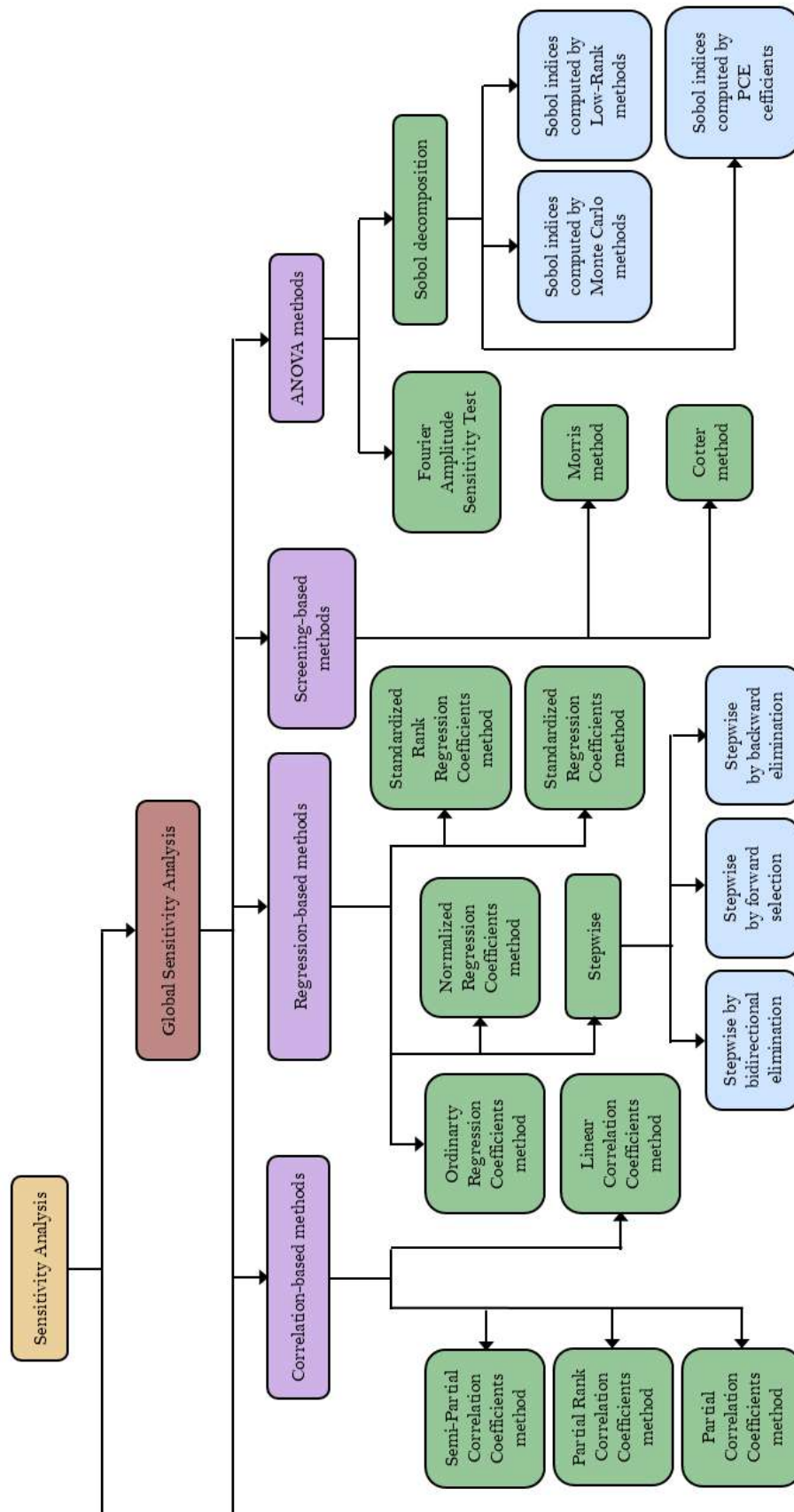


Figure 2.1: Sensitivity Analysis - part 1

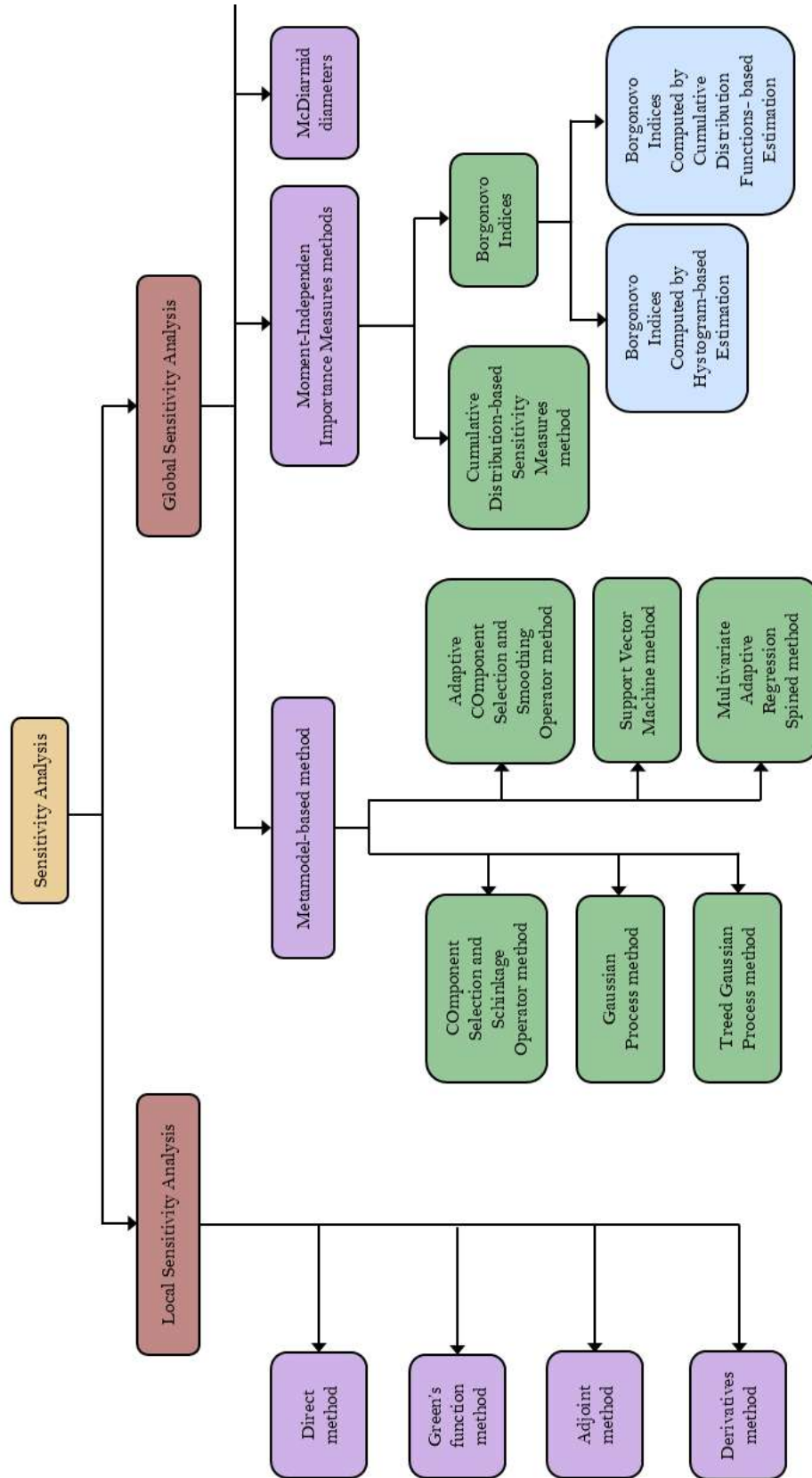


Figure 2.2: Sensitivity Analysis - part 2

Chapter 3

Problem of interest and state of art

The Uncertainty Quantification theory and the Sensitivity Analysis are widely employed tools in Fluid Dynamics. In this work, we have investigated the presence of uncertainties of particular classes of fluid flows which are associated with objects of naval interest.

In particular, Uncertainty Quantification and Sensitivity Analysis have been applied for a cavitating and a non-cavitating (fully wetted) flow regime on two geometries of naval interest: the first geometry is a two-dimensional test case, i.e. the NACA66(MOD) hydrofoil and the second one is a three dimensional test case, i.e. the Potsdam Propeller Test Case (PPTC). The hydrodynamic simulations have been carried out by applying a Reynolds-Averaged Navier-Stokes approach coupled with the two-equation $k - \varepsilon$ Turbulence model for both the flow regimes. The phenomenon of cavitation has been treated by using the Schnerr-Sauer cavitation model. Specifically, the sources of uncertainty in our problem have been the parametric uncertainties of input variables which are the five calibration constants of the $k - \varepsilon$ Turbulence model. These coefficients have been considered as epistemic uncertainties which propagates in the model by influencing the response evaluations. Specifically, the lift and drag coefficients have been the responses associated with the NACA66(MOD) hydrofoil while thrust and torque have been the outputs of the ship propeller.

We have applied a probabilistic strategy based on the family of Functional Expansion-based methods and general Surrogate-based methods; in particular, we have involved a Polynomial Chaos Expansion to quantify the mean value and the standard deviation of outputs. Furthermore, Polynomial Chaos Expansion has been compared with Polynomial Chaos-based kriging to assess differences in predictive performance. Additionally, the Global Sensitivity Analysis based on the ANOVA method of the Sobol decomposition has been employed to explore the entire parameter space of input variables and identify the most important coefficients for the response calculations.

The Uncertainty Quantification of these calibration constants has been addressed for different cases and for different aims over time. For example, Uncertainty Quantification has been employed in optimization or model reduction problems of the five calibration constants.

Turgeon et Al. [62] applied the $k - \varepsilon$ turbulence model coupled with wall functions to study the Sensitivity Analysis of turbulent flows for a backward facing step and a flat plate. In that study, the constants of the wall functions have been considered further sources of uncertainty. The governing equations have been re-written as sensitivity equations and they have been solved by an adaptive finite element method where the scaled sensitivities have been used to carry out the Sensitivity Analysis. For both the geometries, the output has been the skin friction coefficient. Analyzing the Backward facing step, the coefficients C_{ε_1} and C_{ε_2} seem to be the most important variables for the response determination while the friction coefficient of the flat plate is most influenced by the coefficient C_{ε_2} and by the Von Karman constant.

Bardow et Al. [63] analyzed a fully turbulent flow between two plates in a vertically oriented channel for two different Reynolds numbers in order to estimate the best $k - \varepsilon$ turbulence parameter by applying a least-squares optimization problem. They investigated the relations among the calibration constants by applying correlation coefficients and they studied what parameters were most suitable as free variables by using collinearity indices. From the results, C_{ε_1} and C_{ε_2} were the most important coefficients for the determination of the crosswise velocity distribution while σ_k had the least influence.

Platteuw et Al. [64] analyzed the uncertainties associated with the $k - \varepsilon$ Turbulence model coefficients and the wall functions parameters through the application of a probabilistic collocation method based on a chaos transformation applied to turbulent flat plate. The initial distribution functions of all coefficients were estimated by considering experimental results and numerical simulations. they were employed to determine the friction coefficient of the plate. Furthermore, the amplification factor was calculated to quantify the importance of each source of uncertainty in the problem. considering the results, the uncertainty in the friction coefficient is especially present at the beginning of the geometry and the most important parameters for the response calculation were the Von Karman and Wilcox constants of wall functions.

Furthermore, Dunn et Al. [65] investigated the propagation of uncertainties of the five coefficients of $k - \varepsilon$ model for a backward-facing step configuration. The numerical method of Latin Hypercube sampling was involved to treat the Uncertainty Quantification. Beyond the calibration coefficients of the turbulence model, the Von Karman and empirical constants of the wall velocity were taken into account as sources of uncertainties. The results highlighted a strong influence of uncertainties on of reattachment point, pressure and wall shear.

Oliver and Moser [66] applied a Bayesian Uncertainty Quantification to capture the uncertainties associated with model parameters and model inadequacy by employing four stochastic expansions of four eddy viscosity turbulent models. As a test case, a fully developed channel flow was applied and the mean velocity field was analyzed.

Edeling et Al. [67] applied a Bayesian approach to quantify the uncertainties inherent to the constants of the $k - \varepsilon$ model. They focused on the calibration of turbulence parameters to improve the predictability of the model for particular classes of fluids. The performance of the analysis was monitored by the model error and the Sobol indices were computed to evaluate the ranking of coefficients. In this work the coefficient C_{ε_2} seems to have the dominant contribution for the friction coefficient calculation while C_μ has the lowest importance for the response determination.

Margheri et Al. [68] studied the calibration constants from an analytical point of view. The test case considered was a turbulent channel flow at two low Reynolds numbers and the Polynomial Chaos Expansion together the Sobol decomposition were carried out to evaluate uncertainties. In this work, the Sensitivity Analysis showed as the dominant controbution, the production over dissipation in homogenelous turbulent shear flow with constant shear in the asymptotic exponential growth regime, for calculation of local error of the velocity field and the calculation of turbulent viscosity. the production over dissipation is associated to the coefficients C_{ε_1} and C_{ε_2} which are then the most important parameters of the $k - \varepsilon$ model for the outputs evaluations of the treated case.

Another work is based on the Guillas et Al study [69]; a Bayesian approach was employed for an airflow in a regular street canyon where the quantity of interest was the turbulent kinetic energy. Posterior Probability Distributions of the five parameters were evaluated considering the Prior distributions of initial variables.

Edeling et Al. [70] developed a study to estimate the posterior error in RANS simulations for a specific class of fluids. They applied a Bayesian model scenario averaging to calculate a stochastic estimate of the quantities of interest. They studied a class of turbulent boundary layers with different pressure gradients where friction coefficient and velocity field were analyzed as quantities

of interest. After, the Sobol decomposition was applied to establish the most important coefficients for the output evaluations. The variances of the problem were determined by a polynomial approximation of the third order and the results showed that the coefficient C_{ε_2} is the most important parameter.

Another work is based on the Hedberg et Al. [71] study. They analyzed uncertainties in turbulent flows by using sampling strategies, in particular, a deterministic sampling method was employed. Here, the continuous distribution of the calibration constants was replaced by an ensemble of discrete deterministic samples. The test case was a backward-facing step geometry and the quantities of interest were the velocity profile, the turbulent kinetic energy, the pressure coefficient on the wall and the reattachment length. For all outputs, mean value and standard deviation were computed.

Ray et Al [72] applied a Bayesian calibration of the constants of the $k - \varepsilon$ Turbulence model for a compressible jet-in-crossflow. The test cases were treated with a Mach number of 0.6, 0.7 and 0.8 where the associated momentum ratio were 10.2 and 16.2. The results proved that the greatest uncertainties were associated with C_μ and C_{ε_2} and then, they must be analyzed more carefully.

Zhang et Al. [73] investigated the Uncertainty Quantification of the five turbulence constants for a subcooled boiling in vertical pipe to calculate the void fraction and liquid temperature. Applying a Latin Hypercube Sampling, the probabilistic moments were determined, furthermore the ranking of coefficients showed that C_{ε_1} and C_{ε_2} had the dominant contribution.

Liu et Al. [74] applied a Non-Intrusive Polynomial Chaos and the Sobol decomposition for a high-speed train. The quantities of interest were the aerodynamics coefficients of pressure and drag and for both the responses, the parameter C_{ε_2} was the most important variable. Another important parameter was the coefficient σ_ε , whose particularly influenced the pressure coefficient evaluation.

Chapter 4

Polynomial Chaos Expansion

4.1 Introduction

As explained in the previous chapter, the main objective of the current work has been the application of Uncertainty Quantification of the five calibration constants of the Standard $k - \varepsilon$ turbulence model aimed at studying a class of fluids of interest by involving a RANS approach. It is possible to guess that the analysis has been focused on a Forward Approach of the Uncertainty Quantification in order to evaluate the lower order statistical moments of the outputs (i.e. mean value and standard deviation) starting from the Probability Distributions of the input parameters. The Forward Propagation of uncertainties has been investigated by applying a probabilistic strategy and, in reference of the first chapter, among the six methodologies used to study uncertainties from a probabilistic approach, a Functional Expansion-based method has been employed; in particular, the Polynomial Chaos Expansion has been applied [23, 75, 76, 77, 78, 79, 80]. In this chapter, the main theoretical foundations of that model have been described. Furthermore, the different ways to compute the Polynomial Chaos coefficients have been presented.

4.2 Definition and general properties

Let be $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}^T \in \mathbb{R}$ be the real-valued random vector of our problem (i.e. the vector composed by the five calibration constants of the $k - \varepsilon$ turbulence model) which are associated with a finite variance model $Y(\boldsymbol{\xi}) = \mathcal{M}(\boldsymbol{\xi})$. The response of our problem $Y(\boldsymbol{\xi})$ can be expressed in an infinite polynomial series:

$$Y(\boldsymbol{\xi}) = \mathcal{M}(\boldsymbol{\xi}) = \sum_{i=0}^{+\infty} \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}), \quad (4.1)$$

where α_{PCE_i} are Polynomial Chaos coefficients and φ_i are basis functions. In practical applications, (4.1) must be truncated to a finite polynomial expansion:

$$Y(\boldsymbol{\xi}) \approx \mathcal{M}_{\text{PCE}}(\boldsymbol{\xi}) = \sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) \quad (4.2)$$

where the extended expression of the compact form (4.2) is given by:

$$Y(\boldsymbol{\xi}) = \alpha_{\text{PCE}_0} \varphi_0 + \sum_{i=1}^n \alpha_{\text{PCE}_i} \varphi_1(\xi_i) + \sum_{i=1}^n \sum_{j=1}^i \alpha_{\text{PCE}_{ij}} \varphi_2(\xi_i, \xi_j) + \dots + \alpha_{\text{PCE}_{1, \dots, n}} \varphi(\xi_1, \dots, \xi_n). \quad (4.3)$$

An important property of basis functions is the orthogonality condition:

$$\langle \varphi_i(\boldsymbol{\xi}), \varphi_j(\boldsymbol{\xi}) \rangle = \int_{D_\xi} \varphi_i(\boldsymbol{\xi}) \varphi_j(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \gamma_{ij} \delta_{ij} \quad \text{for } i, j \in (1, \dots, M), \quad (4.4)$$

where $\langle \cdot, \cdot \rangle$ is the inner product, $W(\boldsymbol{\xi})$ is a weighting function with support $D_{\boldsymbol{\xi}}$, γ_{ij} is equal to 1 for orthonormal polynomials and is a real number for orthogonal polynomials and $D_{\boldsymbol{\xi}}$ is the parameters domain. The inner product in (4.4) is a multi-dimensional integral. It is important to note that a set of orthogonal basis functions can always be defined via standard normalization procedures. Polynomial Chaos Expansion is applied for complex systems without losing accuracy and efficiency. If the interest is directed to cumulative distribution functions or probability density functions, they can be determined via the sampling of (4.2). The first step of a simulation based on this expansion is to estimate the basis functions $\varphi_i(\boldsymbol{\xi})$. The basis functions are functions which are able to reproduce the change of response with a certain precision which depend on the form of approximate basis function used and are in general polynomial functions of $\boldsymbol{\xi}$. The main property of $\varphi_i(\boldsymbol{\xi})$ is the orthogonality relation (4.4) and observing that equation, several inner products can be obtained in accordance to the weighting function $W(\boldsymbol{\xi})$ used. It has been proved that the optimal convergence rate of a polynomial chaos model can be achieved when $W(\boldsymbol{\xi})$ is the joint probability density function of the random variables considered and expressed in standard form (normalization of $\boldsymbol{\xi}$). From a general point of view, the main polynomials and weighting functions are shown in Table 4.1.

Table 4.1: main polynomials and weighting functions

	Gaussian distr.	Uniform distr.	Gamma distr.	Beta distr.
Pol.	Hermite $He_n(\xi)$	Legendre $Le_n(\xi)$	Laguerre $La_n^{(\alpha)}(\xi)$	Jacobi $P_n^{(\alpha, \beta)}(\xi)$
PDF	$\frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}}$	$\frac{1}{2}$	$\frac{\xi^\alpha e^{-\xi}}{\Gamma(\alpha+1)}$	$\frac{(1-\xi)^\alpha (1+\xi)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}$
W(ξ)	$e^{-\frac{\xi^2}{2}}$	1	$\xi^\alpha e^{-\xi}$	$(1-\xi)^\alpha (1+\xi)^\beta$
Ortn. basis	$\frac{He_n(\xi)}{\sqrt{n!}}$	$\frac{Le_n(\xi)}{\sqrt{\frac{1}{2n+1}}}$	$\frac{La_n^{(\alpha)}(\xi)}{\sqrt{\frac{\Gamma(n+\alpha+1)}{n!}}}$	$\frac{P_n^{(\alpha, \beta)}}{\sqrt{\frac{2^{\alpha+\beta+1} \Gamma(n+\alpha+1) \Gamma(n+\beta+1)}{(2n+\alpha+\beta+1) \Gamma(n+\alpha+\beta+1) \Gamma(n+1)}}}$

At this point, it is clear that the choice of basis functions depends on the distribution of the initial variables ξ_i (more specifically on their joint probability density function). Under the assumption of independent initial variables, the probability density functions are equal to the product of the distributions of each random variable. Then, $\varphi_i(\boldsymbol{\xi})$ are calculated as product combinations of the orthogonal polynomials corresponding to each individual random variable. In other words, $\varphi_i(\boldsymbol{\xi})$ are multivariate orthogonal polynomials expressible as the tensor product of their univariate counterparts ϕ_{i_k} :

$$\varphi_i(\boldsymbol{\xi}) = \prod_{k=1}^n \phi_{i_k}(\xi_k) \quad \text{for } \sum_{k=1}^n i_k \leq p \text{ and } 0 \leq i \leq M. \quad (4.5)$$

Considering that basis functions are polynomials, a constant function corresponding to the zero-order polynomial is provided. Specifically, we have:

$$\varphi_0(\boldsymbol{\xi}) = 1 \quad (4.6)$$

when orthonormal polynomials are treated and:

$$\varphi_0(\boldsymbol{\xi}) = c \quad \text{for } c \in \mathbb{R} \quad (4.7)$$

when general orthogonal polynomials are applied. Considering (4.4) and let $W(\boldsymbol{\xi})$ be a probability density function, we have:

$$\langle \varphi_0(\boldsymbol{\xi}), \varphi_0(\boldsymbol{\xi}) \rangle = \int_{D_{\boldsymbol{\xi}}} \varphi_0(\boldsymbol{\xi}) \varphi_0(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int_{D_{\boldsymbol{\xi}}} W(\boldsymbol{\xi}) d\boldsymbol{\xi} = 1 \quad (4.8)$$

for orthonormal polynomials and:

$$\langle \varphi_0(\boldsymbol{\xi}), \varphi_0(\boldsymbol{\xi}) \rangle = \int_{D_{\boldsymbol{\xi}}} \varphi_0(\boldsymbol{\xi}) \varphi_0(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int_{D_{\boldsymbol{\xi}}} c^2 W(\boldsymbol{\xi}) d\boldsymbol{\xi} = c^2 \int_{D_{\boldsymbol{\xi}}} W(\boldsymbol{\xi}) d\boldsymbol{\xi} = c^2 \quad (4.9)$$

for general orthogonal polynomials.

4.3 Lower statistical moments

The Lower statistical moments of the Polynomial Chaos Expansion (i.e. mean values and standard deviation) are calculated by involving the Polynomial Chaos coefficients [79, 80]. Under the validity of 4.4 and 4.6, and considering the expression 4.2, the mean value is calculated as:

$$\begin{aligned} \mu_{\text{PCE}} &= \int_{D_{\boldsymbol{\xi}}} Y(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int_{D_{\boldsymbol{\xi}}} \sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \\ &= \int_{D_{\boldsymbol{\xi}}} \left[\alpha_{\text{PCE}_0} \varphi_0(\boldsymbol{\xi}) + \sum_{i=1}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) \right] W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int_{D_{\boldsymbol{\xi}}} \alpha_{\text{PCE}_0} \varphi_0(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} + \\ &+ \int_{D_{\boldsymbol{\xi}}} \sum_{i=1}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \alpha_{\text{PCE}_0} \varphi_0(\boldsymbol{\xi}) \underbrace{\int_{D_{\boldsymbol{\xi}}} W(\boldsymbol{\xi}) d\boldsymbol{\xi}}_{=1} + \\ &+ \underbrace{\sum_{i=1}^M \alpha_{\text{PCE}_i} \int_{D_{\boldsymbol{\xi}}} \varphi_0(\boldsymbol{\xi}) \varphi_i(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi}}_{=0} = \alpha_{\text{PCE}_0} \end{aligned} \quad (4.10)$$

while the variance is given by the following equation:

$$\begin{aligned} \sigma_{\text{PCE}}^2 &= \int_{D_{\boldsymbol{\xi}}} [Y(\boldsymbol{\xi}) - \mu_{\text{PCE}}]^2 W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \int_{D_{\boldsymbol{\xi}}} [Y^2(\boldsymbol{\xi}) + \mu_{\text{PCE}}^2 - 2Y(\boldsymbol{\xi})\mu_{\text{PCE}}] W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \\ &= \int_{D_{\boldsymbol{\xi}}} \left[\sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) \sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) + \alpha_{\text{PCE}_0}^2 - 2 \sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) \alpha_{\text{PCE}_0} \right] W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \\ &= \int_{D_{\boldsymbol{\xi}}} \left[\sum_{i=0}^M \alpha_{\text{PCE}_i}^2 \varphi_i^2(\boldsymbol{\xi}) + \alpha_{\text{PCE}_0}^2 \varphi_0^2(\boldsymbol{\xi}) - 2 \sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) \alpha_{\text{PCE}_0} \varphi_0(\boldsymbol{\xi}) \right] W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \\ &= \int_{D_{\boldsymbol{\xi}}} \left[\sum_{i=0}^M \alpha_{\text{PCE}_i}^2 \varphi_i^2(\boldsymbol{\xi}) - \alpha_{\text{PCE}_0}^2 \varphi_0^2(\boldsymbol{\xi}) \right] W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \sum_{i=0}^M \alpha_{\text{PCE}_i}^2 \int_{D_{\boldsymbol{\xi}}} \varphi_i^2(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} - \\ &- \alpha_{\text{PCE}_0}^2 \int_{D_{\boldsymbol{\xi}}} \varphi_0^2(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} = \sum_{i=0}^M \alpha_i^2 \underbrace{\int_{D_{\boldsymbol{\xi}}} \langle \varphi_i(\boldsymbol{\xi}), \varphi_i(\boldsymbol{\xi}) \rangle W(\boldsymbol{\xi}) d\boldsymbol{\xi}}_{=1} - \\ &- \alpha_0^2 \underbrace{\int_{D_{\boldsymbol{\xi}}} \langle \varphi_0(\boldsymbol{\xi}), \varphi_0(\boldsymbol{\xi}) \rangle W(\boldsymbol{\xi}) d\boldsymbol{\xi}}_{=1} = \sum_{i=1}^M \alpha_i^2 \end{aligned} \quad (4.11)$$

4.4 Number of terms of the polynomial series

As described in the first section, the polynomial series is truncated to a finite number of terms which are simply determined by [81, 82, 83]:

$$M + 1 = \frac{(p-1+1)!}{(p-1)!1!} + \dots + \frac{(p-1+n)!}{(p-1)!n!} = \frac{(n+p)!}{n!p!}, \quad (4.12)$$

where n is the number of initial variables and p is the Polynomial Chaos degree. This truncation is named "total order expansion". The main obstacle in a polynomial chaos expansion is to choose the exact polynomial order, but, alternatively, estimation of stochastic moments or also methods computing Sparse Polynomial Chaos models can be used, where only the most important terms among the $M + 1$ elements are employed. For most problems, using the number of sampling equal to the number of basis functions is not good enough to represent satisfactory the solution and then, a more substantial number of points is needed. As a consequence, an oversampling term n_p is introduced to generate a response surface with an appropriate set of collocation points K . Applying that consideration, K is given by:

$$K = n_p \frac{(n+p)!}{n!p!} > M + 1. \quad (4.13)$$

where for:

$$n_p = 2 \quad (4.14)$$

a robust solution is achieved.

4.5 Types of application of Polynomial Chaos Expansion

The computation of Polynomial Chaos is based on the formulation of Polynomial Chaos coefficients; in fact, basis functions are determined by the input probability distributions of the input quantities while the response vector is given by the treated problem. Basically, Polynomial Chaos can be applied by using an intrusive or non-intrusive strategy, which are following described.

4.5.1 Intrusive Polynomial Chaos Expansion

The application of an intrusive Polynomial Chaos requires the modification of governing equations of the model. In this approach, a new set of equations is generated where the unknown quantities are the polynomial coefficients.

4.5.2 Non-intrusive Polynomial Chaos Expansion

Non-intrusive Polynomial Chaos Expansion is coupled with a sampling method to solve the problem of interest. The strategy consists of selecting specific values of the initial variables and explicitly solving the problem with the specified parameters. Deterministic problems are thus solved for each value, although many computational iterations are required. Luckily the number of samples is limited. Non-intrusive approaches are simpler than intrusive approaches and then, they are the most commonly used.

In this work we applied a Polynomial Chaos Expansion based on a Non-intrusive strategy.

4.6 Computation of Polynomial Chaos coefficients

Taking as reference the Figure 4.1, Polynomial Chaos coefficients can be calculated in two main ways: we have polynomial coefficients computed by **classical methodologies** and polynomial coefficients calculated by considering **sparse approximation methodologies** [39, 41, 84, 85].

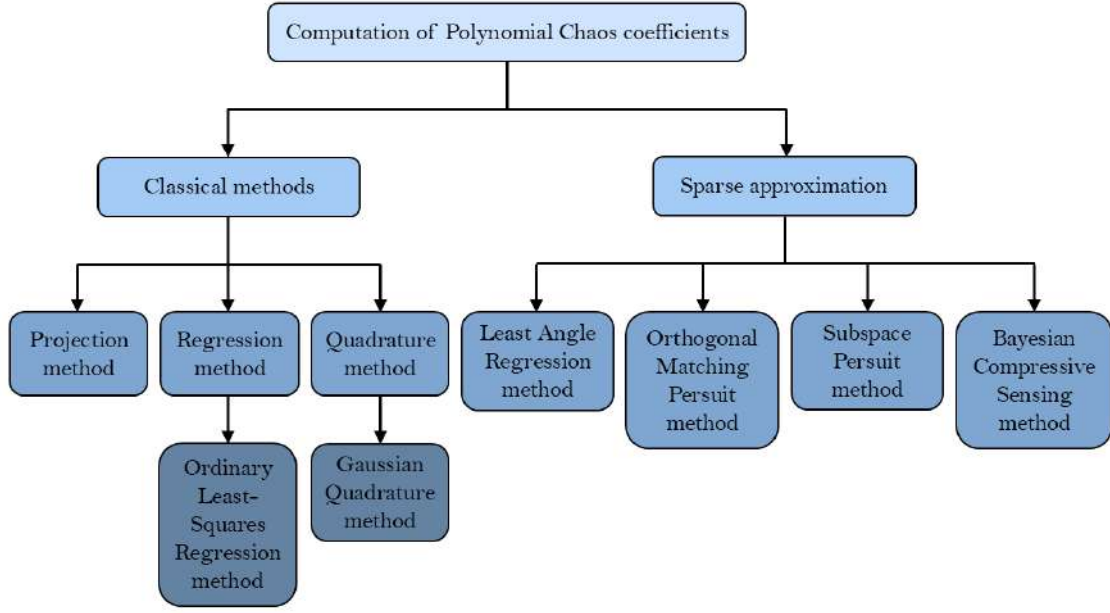


Figure 4.1: Computation of Polynomial of Polynomial Chaos coefficients

4.6.1 Classical methods to compute Polynomial Chaos coefficients

The classical methods preserve all mathematical elements to evaluate the polynomial coefficients and generally, they are more expensive than the methods based on the sparse approximation. The classical methods are **Projection method**, **Quadrature method** and **Regression method**.

Projection method

Polynomial Chaos coefficients can be directly determined by the definition of Polynomial Chaos expansion. using the expected values, we have:

$$\alpha_{\text{PCE}_i} = \mathbb{E}[\varphi_i(\boldsymbol{\xi}) Y(\boldsymbol{\xi})] \quad \text{for } i = 1, \dots, M. \quad (4.15)$$

(4.15) can be directly obtained by projecting the equation (4.2) onto each basis function φ_i for $i = 0, \dots, M$ and by the orthonormal relation (4.4).

Quadrature method

(4.15) can be rewritten in a multi-dimensional integral:

$$\alpha_{\text{PCE}_i} = \int_{D_{\boldsymbol{\xi}}} Y(\boldsymbol{\xi}) \varphi_i(\boldsymbol{\xi}) W(\boldsymbol{\xi}) d\boldsymbol{\xi} \quad \text{for } i = 0, \dots, M. \quad (4.16)$$

(4.16) is rarely solvable by directly applying analytic integrals and often numerical integration techniques are adopted. From this consideration a set of K sampling are obtained and $Y(\boldsymbol{\xi}^{(k)})$ is the deterministic solution of the k -th random variable model. It is possible to express (4.16) as:

$$\alpha_{\text{PCE}_i} \approx \sum_{k=1}^K Y(\boldsymbol{\xi}^{(k)}) \varphi_i(\boldsymbol{\xi}^{(k)}) W(\boldsymbol{\xi}^{(k)}) \quad \text{for } i = 0, \dots, M. \quad (4.17)$$

$\boldsymbol{\xi}^{(k)}$ are quadrature points of the problem where the weights $W(\boldsymbol{\xi})$ depend on the numerical method used and they are derived from Lagrange interpolations. Quadrature points are not selected arbitrarily. For example, the approximations of α_i are based on Gaussian quadrature schemes. In addition, quadrature points and weights are generated using the theory of orthogonal polynomials

with respect to the Gaussian measure and so for the k -th order scheme, the associated points are the roots of the k -th order Hermite Polynomial.

Regression method

The most common Regression method used in the Polynomial Chaos analysis is the **Ordinary Least – Squares Regression method**. The least-squares minimization problem is a non-intrusive approach used to determine the Polynomial Chaos coefficients. The infinite series (4.1) can be expressed as a sum of its truncated representation plus a residual term:

$$Y(\boldsymbol{\xi}) = \sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) + \epsilon \quad (4.18)$$

where the Polynomial Chaos coefficients are determined from (4.18) by solving the following Least-Squares regression problem:

$$\boldsymbol{\alpha}_{\text{PCE}} = \arg \left\{ \min \left\{ \mathbb{E} \left[\left[\sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}) - \mathcal{M}(\boldsymbol{\xi}) \right]^2 \right] \right\} \right\}. \quad (4.19)$$

The expected value $\mathbb{E}$ is evaluated by an empirical sample-based estimator. If we take into account K sampling points where for each point the initial vector $\boldsymbol{\xi}$ is defined, (4.19) can be rewritten as:

$$\boldsymbol{\alpha}_{\text{PCE}} = \arg \left\{ \min \left\{ \frac{1}{K} \sum_{k=1}^K \left[\sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi}^{(k)}) - \mathcal{M}(\boldsymbol{\xi}) \right]^2 \right\} \right\} \quad (4.20)$$

and can be solved by applying the following Ordinary Least Squares approach:

$$\boldsymbol{\alpha}_{\text{PCE}} = [\boldsymbol{\Psi}^T(\boldsymbol{\xi}) \boldsymbol{\Psi}(\boldsymbol{\xi})]^{-1} \boldsymbol{\Psi}(\boldsymbol{\xi})^T \mathbf{Y}(\boldsymbol{\xi}). \quad (4.21)$$

In extended form we have:

$$\begin{aligned} \begin{Bmatrix} \alpha_{\text{PCE}_0} \\ \vdots \\ \alpha_{\text{PCE}_M} \end{Bmatrix} &= \left(\begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \right)^{-1} \\ &\cdot \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix}^T \begin{Bmatrix} Y(\boldsymbol{\xi}^{(1)}) \\ \vdots \\ Y(\boldsymbol{\xi}^{(K)}) \end{Bmatrix} \end{aligned} \quad (4.22)$$

4.6.2 Computation of Polynomial Chaos coefficients by introducing Sparse Approximation

The main characteristic of the Sparse Approximation is the representation of most or all information contained in data by using weighted linear combinations of small number of elements which are chosen from an incomplete or redundant basis [86]. Then, we achieve a representation of the input data by minimizing the number of non-zero components. The Sparsity-based methods for the evaluation of the Polynomial Chaos coefficients are the **Orthogonal Matching Pursuit method**, the **Subspace Pursuit method**, the **Bayesian Compressive Sensing method** and the **Least Angle Regression method**.

Orthogonal Matching Pursuit method

The Orthogonal Matching Pursuit method works by retrieving the polynomial basis elements that are most correlated with the current approximation residual and adding them to the active set

of regressors. This approach minimizes the approximation residual at each iteration. The approximation residual for a polynomial basis with j elements can be projected onto a new polynomial by writing:

$$r_j(\boldsymbol{\xi}) = \langle r_j(\boldsymbol{\xi}), \varphi_{i_{j+1}}(\boldsymbol{\xi}) \rangle \varphi_{i_{j+1}}(\boldsymbol{\xi}) + r_{j+1}(\boldsymbol{\xi}) \quad \text{for } i = 1, \dots, M \quad (4.23)$$

where $r_{j+1}(\boldsymbol{\xi})$ is the approximation residual for a polynomial basis with $j + 1$ elements. Projecting (4.23) onto $r_j(\boldsymbol{\xi})$ we have:

$$\|r_j(\boldsymbol{\xi})\|^2 = |\langle r_j(\boldsymbol{\xi}), \varphi_{i_{j+1}}(\boldsymbol{\xi}) \rangle|^2 + \|r_{j+1}(\boldsymbol{\xi})\|^2 \quad \text{for } i = 1, \dots, M \quad (4.24)$$

where the minimization $r_{j+1}(\boldsymbol{\xi})$ is obtained by minimizing $|\langle r_j(\boldsymbol{\xi}), \varphi_{i_{j+1}}(\boldsymbol{\xi}) \rangle|$ such that the method is reduced to solve:

$$\varphi_{i_{j+1}}(\boldsymbol{\xi}) = \arg \left\{ \max_{i=0, \dots, M} \{ |r_j(\boldsymbol{\xi}), \varphi_i(\boldsymbol{\xi})| \} \right\}. \quad (4.25)$$

When $\varphi_{i_{j+1}}(\boldsymbol{\xi})$ is added to the active set of regressor, α_i are computed by using (4.21). Specifically, the problem is initialized by imposing the vector of polynomial coefficients equal to the null vector:

$$\boldsymbol{\alpha}_{\text{PCE}} = \boldsymbol{\alpha}_{\text{PCE}_0} = \{\alpha_{\text{PCE}_0}, \dots, \alpha_{\text{PCE}_M}\}^T = \{0, \dots, 0\}^T. \quad (4.26)$$

The first candidate set $\boldsymbol{\Psi}_0^C(\boldsymbol{\xi})$ is composed by the initial multivariate polynomials $\varphi_i(\boldsymbol{\xi})$:

$$\boldsymbol{\Psi}_0^C(\boldsymbol{\xi}) = \varphi_i(\boldsymbol{\xi}) \quad \text{for } i = 0, \dots, M \quad (4.27)$$

while the active set $\boldsymbol{\Psi}_0^A(\boldsymbol{\xi})$ is imposed to be the null set:

$$\boldsymbol{\Psi}_0^A(\boldsymbol{\xi}) = \emptyset. \quad (4.28)$$

The last initialization concerns the initial residual which is set to be the vector of the responses:

$$r_0(\boldsymbol{\xi}) = \mathbf{Y}(\boldsymbol{\xi}) = \left\{ Y(\boldsymbol{\xi}^{(1)}), \dots, Y(\boldsymbol{\xi}^{(K)}) \right\}^T. \quad (4.29)$$

The first step is based on finding the polynomial $\varphi_{i_j}(\boldsymbol{\xi})$ that is the most correlated with the current residual $r_{j-1}(\boldsymbol{\xi})$ so that it is added to the active set of polynomials:

$$\boldsymbol{\Psi}_j^A(\boldsymbol{\xi}) = \boldsymbol{\Psi}_{j-1}^A(\boldsymbol{\xi}) \cup \varphi_{i_j}(\boldsymbol{\xi}) \quad \text{for } i = 0, \dots, M. \quad (4.30)$$

At this point, the new vector of Polynomial Chaos coefficients $\boldsymbol{\alpha}_{\text{PCE}_j} = \{\alpha_{\text{PCE}_{0_j}}, \dots, \alpha_{\text{PCE}_{0_M}}\}$ is obtained by projecting the output vector $\{Y(\boldsymbol{\xi}^{(1)}), \dots, Y(\boldsymbol{\xi}^{(K)})\}^T$ onto the active set of polynomials and the new residual is determined by:

$$r_j(\boldsymbol{\xi}) = \mathbf{Y}(\boldsymbol{\xi}) - \boldsymbol{\Psi}_j^A(\boldsymbol{\xi}) \boldsymbol{\alpha}_{\text{PCE}_j} \quad (4.31)$$

whose extended form is:

$$r_j(\boldsymbol{\xi}) = \begin{Bmatrix} Y(\boldsymbol{\xi}^{(1)}) \\ \vdots \\ Y(\boldsymbol{\xi}^{(K)}) \end{Bmatrix} - \begin{bmatrix} \varphi_{0_j}(\boldsymbol{\xi}^{(1)}) & \dots & \varphi_{M_j}(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_{0_j}(\boldsymbol{\xi}^{(K)}) & \dots & \varphi_{M_j}(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \begin{Bmatrix} \alpha_{\text{PCE}_{0_j}} \\ \vdots \\ \alpha_{\text{PCE}_{M_j}} \end{Bmatrix}. \quad (4.32)$$

After that, the Leave-One-Out Cross-Validation error is determined for the current iteration and the complete cycle is repeated until the size of the active set is equal to:

$$m = \min \{M, K\}. \quad (4.33)$$

In conclusion the active set associated to the lowest Leave-One-Out Cross-Validation error is designated as the best sparse basis. The algorithm is graphically represented in Figure 4.2.

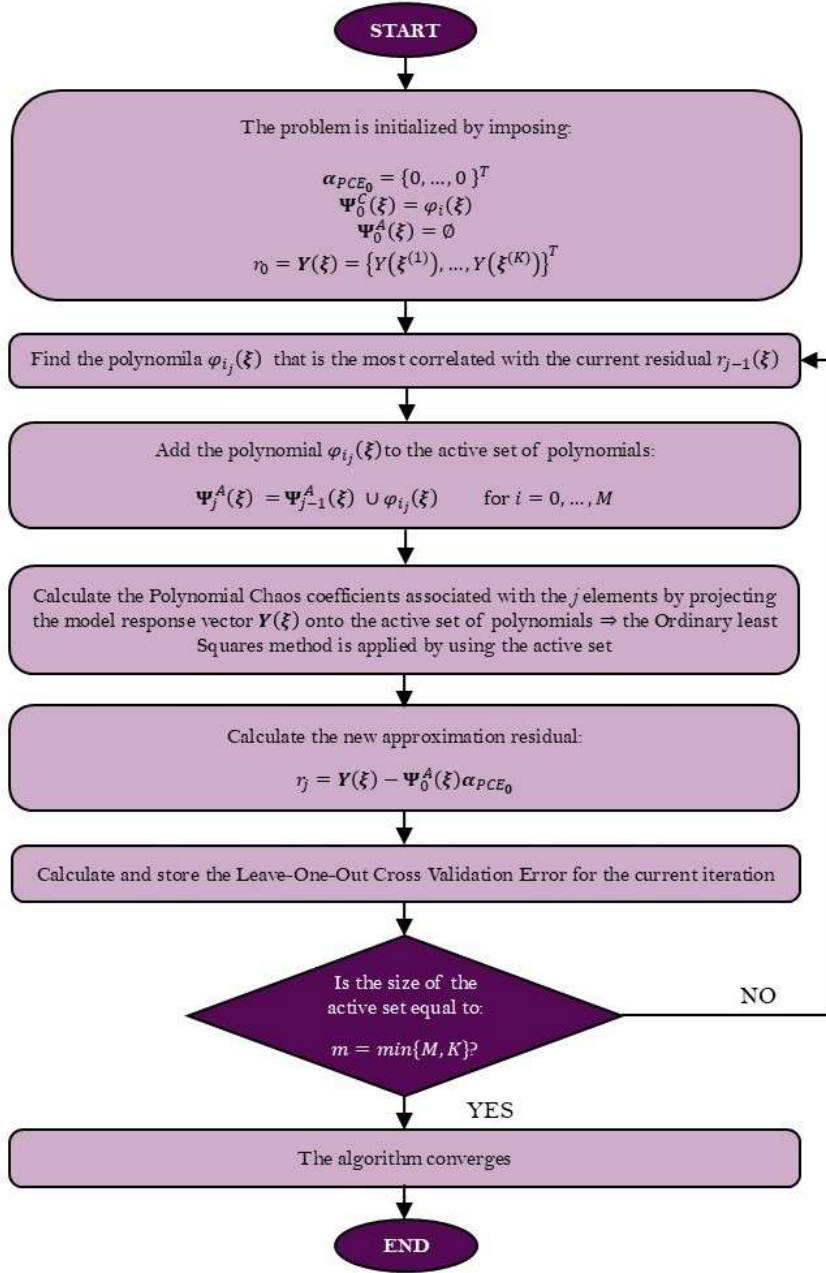


Figure 4.2: Orthogonal Matching Pursuit algorithm.

Subspace Pursuit method

The Subspace Pursuit method can be interpreted as a revisitation of the Least-Squares Regression method. The problem is characterized by a single hyperparameter $\overline{M}$ which is the number of nonzero elements in the coefficient vector. The process starts from $\overline{M}$ regressors which are used to calculate α_i with (4.21) and after, other $\overline{M}$ regressors are identified to calculate the new Polynomial Chaos coefficients with $2\overline{M}$ regressors. $\overline{M}$ regressors are removed with the smallest-in-magnitude coefficients and the process is repeated until convergence. Specifically, the problem is initialized by $\overline{M}$ number of nonzero coefficients such that:

$$2\overline{M} \leq \min \{K, M\}. \quad (4.34)$$

From the matrix of basis functions $\Psi(\xi)$, the candidate set A_0 is defined to consist of $\overline{M}$ indices corresponding to the largest-in-magnitude entries in $\Psi(\xi)^T Y(\xi)$ and the elements of this set are used to define the sub-matrix $\Psi_0^A(\xi)$ as:

$$\Psi_0^A(\xi) = \begin{bmatrix} \varphi_0(\xi^{(1)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(1)})_{A_0} \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(K)})_{A_0} \end{bmatrix}. \quad (4.35)$$

The initial residual is evaluated by using the initial candidate matrix so that:

$$\mathbf{r}_0(\xi) = Y(\xi) - \Psi_0^A(\xi) \left\{ [\Psi_0^A(\xi)]^T \Psi_0^A(\xi) \right\}^{-1} [\Psi_0^A(\xi)]^T Y(\xi) \quad (4.36)$$

where its extended form is:

$$\begin{aligned} \mathbf{r}_0(\xi) = & \begin{Bmatrix} Y(\xi^{(1)}) \\ \vdots \\ Y(\xi^{(K)}) \end{Bmatrix} - \begin{bmatrix} \varphi_0(\xi^{(1)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(1)})_{A_0} \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(K)})_{A_0} \end{bmatrix} \left(\begin{bmatrix} \varphi_0(\xi^{(1)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(1)})_{A_0} \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(K)})_{A_0} \end{bmatrix}^T \right. \\ & \cdot \left. \begin{bmatrix} \varphi_0(\xi^{(1)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(1)})_{A_0} \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(K)})_{A_0} \end{bmatrix} \right)^{-1} \begin{bmatrix} \varphi_0(\xi^{(1)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(1)})_{A_0} \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_{A_0} & \cdots & \varphi_{\overline{M}}(\xi^{(K)})_{A_0} \end{bmatrix}^T \begin{Bmatrix} Y(\xi^{(1)}) \\ \vdots \\ Y(\xi^{(K)}) \end{Bmatrix} \end{aligned} \quad (4.37)$$

After all initializations, a cycle of iterations is applied by defining a temporary set S composed of the active set of the previous step A_{j-1} and $\overline{M}$ regressors corresponding to the largest-in-magnitude entries in $\Psi(\xi)^T \mathbf{r}_{j-1}$. Then, the corresponding Polynomial Chaos coefficients are calculated as:

$$\alpha_{\text{PCE}_S} = \left\{ [\Psi^S(\xi)]^T \Psi^S(\xi) \right\}^{-1} [\Psi^S(\xi)]^T Y(\xi) \quad (4.38)$$

and in extended form:

$$\begin{aligned} \begin{Bmatrix} \alpha_{\text{PCE}_{0_S}} \\ \vdots \\ \alpha_{\text{PCE}_{2\overline{M}_S}} \end{Bmatrix} = & \left(\begin{bmatrix} \varphi_0(\xi^{(1)})_S & \cdots & \varphi_{2\overline{M}}(\xi^{(1)})_S \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_S & \cdots & \varphi_{2\overline{M}}(\xi^{(K)})_S \end{bmatrix}^T \begin{bmatrix} \varphi_0(\xi^{(1)})_S & \cdots & \varphi_{2\overline{M}}(\xi^{(1)})_S \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_S & \cdots & \varphi_{2\overline{M}}(\xi^{(K)})_S \end{bmatrix} \right)^{-1} \\ & \cdot \begin{bmatrix} \varphi_0(\xi^{(1)})_S & \cdots & \varphi_{2\overline{M}}(\xi^{(1)})_S \\ \vdots & \ddots & \vdots \\ \varphi_0(\xi^{(K)})_S & \cdots & \varphi_{2\overline{M}}(\xi^{(K)})_S \end{bmatrix}^T \begin{Bmatrix} Y(\xi^{(1)}) \\ \vdots \\ Y(\xi^{(K)}) \end{Bmatrix} \end{aligned} \quad (4.39)$$

From (4.38), $\overline{M}$ indices corresponding to the largest-in-magnitude are extrapolated and used for the actual active set A_j ; at this point, the actual residual is computed:

$$\mathbf{r}_j(\xi) = Y(\xi) - \Psi_j^A(\xi) \left\{ [\Psi_j^A(\xi)]^T \Psi_j^A(\xi) \right\}^{-1} [\Psi_j^A(\xi)]^T Y(\xi) \quad (4.40)$$

and in extended form:

$$\begin{aligned}
\mathbf{r}_j(\boldsymbol{\xi}) = & \begin{Bmatrix} Y(\boldsymbol{\xi}^{(1)}) \\ \vdots \\ Y(\boldsymbol{\xi}^{(K)}) \end{Bmatrix} - \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(1)})_{A_j} \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(K)})_{A_j} \end{bmatrix} \left(\begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(1)})_{A_j} \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(K)})_{A_j} \end{bmatrix}^T \right. \\
& \cdot \left. \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(1)})_{A_j} \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(K)})_{A_j} \end{bmatrix}^{-1} \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(1)})_{A_j} \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)})_{A_j} & \cdots & \varphi_{\overline{M}}(\boldsymbol{\xi}^{(K)})_{A_j} \end{bmatrix}^T \begin{Bmatrix} Y(\boldsymbol{\xi}^{(1)}) \\ \vdots \\ Y(\boldsymbol{\xi}^{(K)}) \end{Bmatrix} \right).
\end{aligned} \tag{4.41}$$

If the condition:

$$\|\mathbf{r}_j\|_2 \geq \|\mathbf{r}_{j-1}\|_2 \tag{4.42}$$

is satisfied, the algorithm converges and the calculus is stopped. The hyperparameter $\overline{M}$ is determined by the Leave-One-Out Cross-validation error and the final solution is associated to the lowest Leave-One-Out Cross-validation error. The algorithm is graphically represented in Figure 4.3.

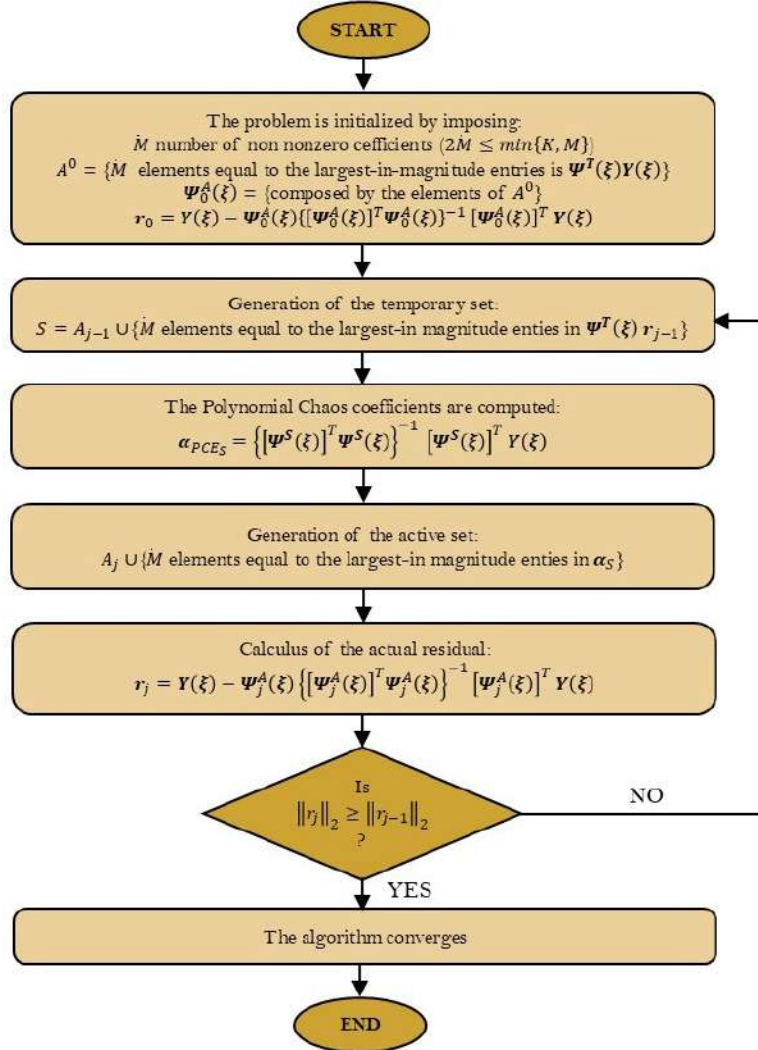


Figure 4.3: Subspace Pursuit algorithm.

Bayesian Compressive Sensing method

In this case, the regression problem is reformulated in a Bayesian framework as shown in Figure 4.4. The coefficients are computed to be the maximum-a-posteriori estimate in reference of the model evaluations. Each quantity and auxiliary variable is considered as a random variable, associated with a parametrized distribution (except for σ^2 and $\nu = 0$). The output vector $\mathbf{Y}(\boldsymbol{\xi})$ is assumed to consist of independent and identically distributed realizations of a random variable parametrized by $\boldsymbol{\alpha}_{\text{PCE}}$ and a noise variance parameter σ^2 such that:

$$\mathbb{P}[\mathbf{Y}(\boldsymbol{\xi}) | \boldsymbol{\alpha}_{\text{PCE}}, \sigma^2] = \mathcal{N}[\mathbf{Y}(\boldsymbol{\xi}) | \boldsymbol{\Psi}(\boldsymbol{\xi})\boldsymbol{\alpha}_{\text{PCE}}, \sigma^2 \mathbb{I}] \quad (4.43)$$

σ^2 is a known and fixed hyperparameter while α_{PCE_i} are considered normally distributed random variables with their own variance D_i such that:

$$\mathbb{P}[\alpha_{\text{PCE}_i} | D_i] = \mathcal{N}[\alpha_{\text{PCE}_i} | 0, D_i]. \quad (4.44)$$

The polynomial Chaos variances are independent and identically distributed random variables, following an exponential distribution weighted with the shared parameter λ :

$$\mathbb{P} = [D_i | \lambda] = e^{(D_i | \frac{\lambda}{2})} \quad (4.45)$$

λ is the last layer of the hierarchical framework, drawn from a gamma satisfying the following property:

$$\lim_{\nu \rightarrow 0} \mathbb{P}[\lambda | \nu] = \Gamma\left[\lambda \middle| \frac{\nu}{2}, \frac{\nu}{2}\right]. \quad (4.46)$$

The main aim of the algorithm is to determine the posterior distribution $\mathbb{P}[\boldsymbol{\alpha}_{\text{PCE}}, \mathbf{D}, \lambda | \mathbf{Y}(\boldsymbol{\xi})]$ for the output vector $\mathbf{Y}(\boldsymbol{\xi})$ such that the main estimate for $\boldsymbol{\alpha}_{\text{PCE}}$ can be calculated. Considering the variances associated with the polynomial coefficients, if $D_i = 0$, the corresponding polynomial coefficient is zero while if $D_i > 0$, the corresponding α_{PCE_i} is non-null. Based on this, for each iteration one regressor is selected and is added to the basis if the $D_i > 0$ condition is satisfied, is deleted if $D_i = 0$ and is reassessed by means of a re-estimation of the the variance D_i .

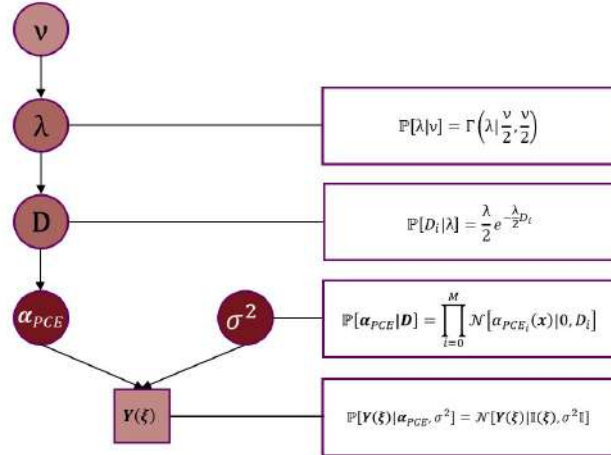


Figure 4.4: Bayesian algorithm

The algorithm is characterized by an objective function $\mathcal{L}$ which is the logarithm of $\mathbb{P}[\mathbf{D}, \lambda, \mathbf{Y}(\boldsymbol{\xi})]$. Specifically, the problem is initialized by knowing the vector of responses, the matrix of basis functions, the noise variance and the stopping threshold η . Furthermore the regressor associated with the largest correlation with the data is added to the model. Next, a partial variance D_i is computed for each of the regressors and if only him is updated and the associated hypothetical change in $\mathcal{L}(\mathbf{D})$. The regressor i which accounts for the largest increase in $\mathcal{L}$ is adopted. If no-one regressor shows an increase in $\mathcal{L}$ or the increase of $\mathcal{L}$ divided by the current value of $\mathcal{L}$ is less than η , the

algorithm converges; otherwise, the regressor is added, deleted or re-estimated in accordance with the value of D_i . All other quantities are updated accordingly. The algorithm is graphically represented in Figure 4.5. In this method, σ^2 is known by the application of the k-fold cross-validation. In few words, a number of noise variances are numerically created while the vector of responses is divided into k equally sized chunks. For each turn, a chunk is treated as a validation set while the others are the training data so that the averaging over the k validation errors can be used to evaluate the corresponding cross-validation error. This approach is applied for each estimated noise variance and the variance with the lowest Cross-Validation error is used for the Bayesian Compressive Sensing process.

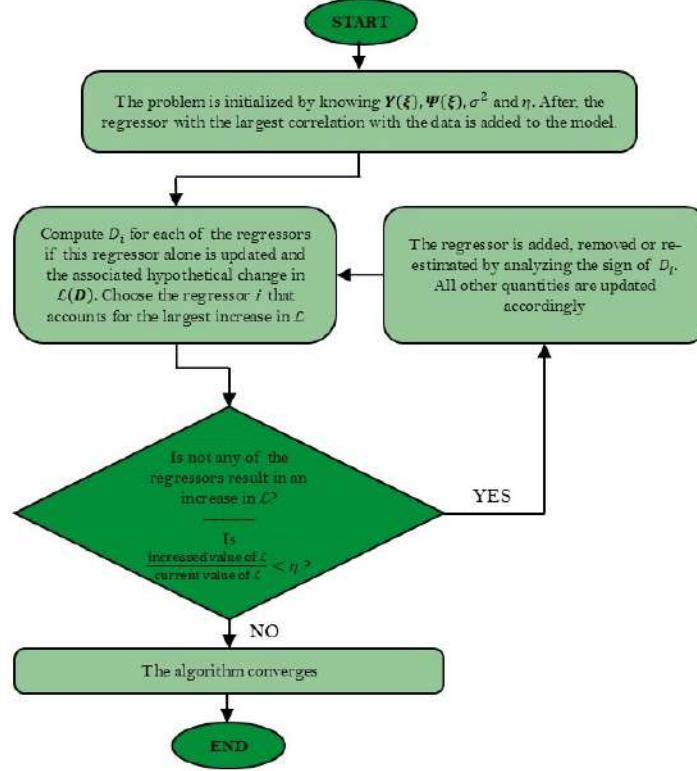


Figure 4.5: Bayesian Compressive Sensing algorithm.

Least Angle Regression method

The Least Angle regression method is a strategy applied in Sparse Polynomial Chaos approaches which is derived by modifying the Ordinary Least-Squares regression method (4.19). The Polynomial Chaos coefficients are calculated by using the equation shown below:

$$\alpha_{\text{PCE}} = \arg \left\{ \min \left\{ \mathbb{E} \left[\left[\sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\xi) - \mathcal{M}(\xi) \right]^2 \right] \right\} \right\} + \lambda \sum_{i=0}^M |\alpha_{\text{PCE}_i}|, \quad (4.47)$$

where $\lambda \sum_{i=0}^M |\alpha_{\text{PCE}_i}|$ is the regularization term. The resolution of (4.47) is led by the application of the LAR algorithm where the regressors are moved from a candidate set to an active set. At each step, the new regressor is selected by considering its correlation with the current residual and the best set of coefficients for the current active set is determined by imposing that the active regressors are equicorrelated with the current residual. The optimal number of predictors is established by using a suitable criterion. Specifically, the algorithm is initialized similarly to the Orthogonal Matching Pursuit algorithm: the Polynomial Chaos coefficients vector is imposed to be the null-vector, the candidate set is given by the initial multivariate polynomials, the active set is the null

set and the initial residual is the vector responses. The first step is to calculate the most correlated regressor $\varphi_i(\xi)$ with the current residual so that all coefficients of the current active set are moved towards their least square value until their associated regressors are equicorrelated to the residual as some other regressor inside the candidate set. This regressor is the most correlated regressor to the residual of the next iteration. Next, the Leave-One-Out Cross-Validation error of the current step is determined, the active coefficients are updated and the new regressions are moved from the candidate set to the active set. At this point, if the size of the active set becomes:

$$m = \min \{M, K - 1\}, \quad (4.48)$$

the algorithm converges, otherwise the complete process is repeated until the convergence. In conclusion, the best sparse candidate basis are associated with the lowest Leave-One-Out Cross-Validation error. The algorithm is graphically represented in Figure 4.6

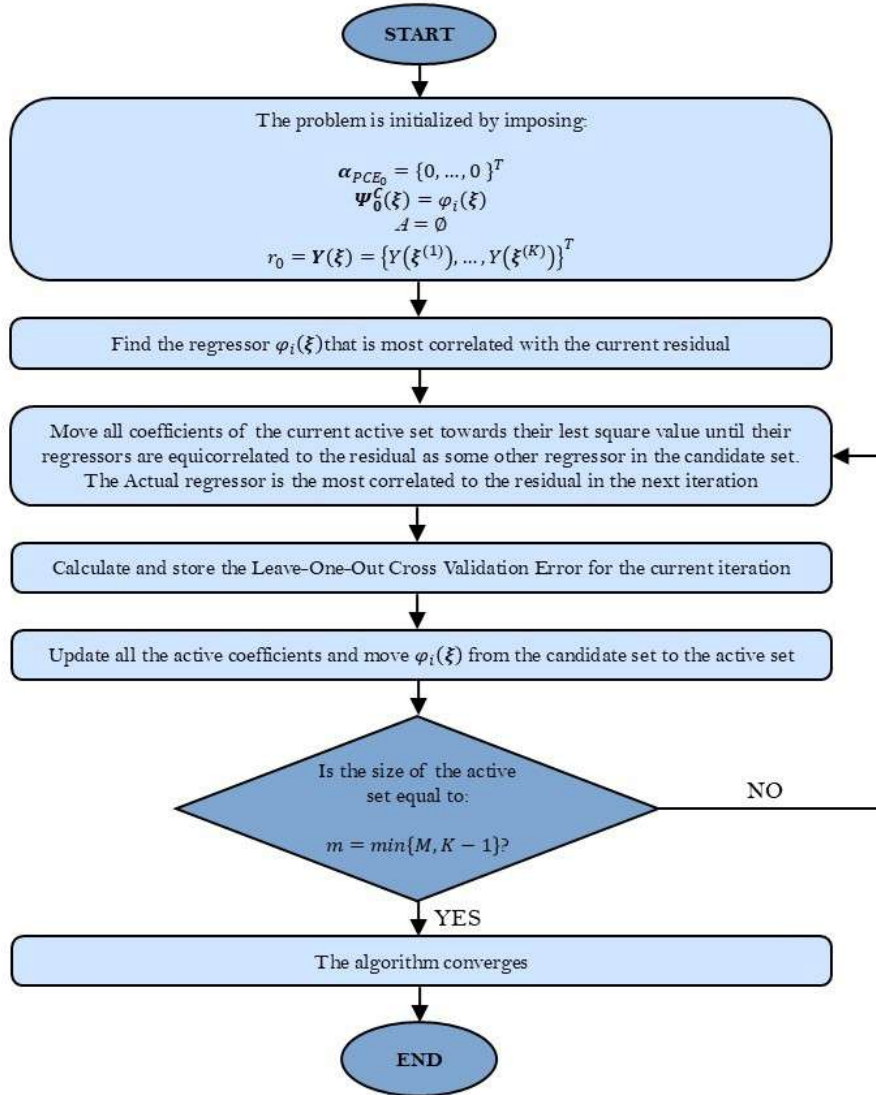


Figure 4.6: Least Angle Regression algorithm.

In this work, we applied the Least Angle Regression method to calculate the Polynomial Chaos coefficients.

4.7 Leave-One-Out Cross-validation error

The Leave-One-Out Cross-Validation error was introduced in statistical learning theory to quantify the local performance of metamodels in terms of predictability. Furthermore, the error was employed in several algorithms to compute the polynomial Chaos coefficients. The scope is to generate K Polynomial Chaos metamodels where each metamodel is built by excluding per turn a different sampling point such that the model is generated by involving $K - 1$ collocation points. In conclusion, the predictions of the reduced Polynomial Chaos Expansion models are compared with the prediction of the excluded points and the error is evaluated [85]. Mathematically we have:

$$\varepsilon_{\text{LOO}} = \frac{\sum_{i=1}^K [\mathcal{M}(\boldsymbol{\xi}^{(i)}) - \mathcal{M}_{\text{PCE}/i}(\boldsymbol{\xi}^{(i)})]^2}{\sum_{i=1}^K [\mathcal{M}(\boldsymbol{\xi}^{(i)}) - \mu_{\text{PCE}}]^2} \quad (4.49)$$

where $\mathcal{M}(\boldsymbol{\xi}^{(i)})$ is the response model of the $\boldsymbol{\xi}^{(i)}$ collocation point and $\mathcal{M}_{\text{PCE}/i}(\boldsymbol{\xi}^{(i)})$ is the PCE metamodel generated by excluding the $\boldsymbol{\xi}^{(i)}$ collocation point. The equation (4.49) is directly applied when the Orthogonal Matching Pursuit method, Bayesian Compressive Sensing method and the Least Angle Regression method are applied. When the Ordinary Least-Squares Regression method and the Subspace Pursuit method are employed, (4.49) can be modified as:

$$\varepsilon_{\text{LOO}} = \frac{\sum_{i=1}^K \left[\frac{\mathcal{M}(\boldsymbol{\xi}^{(i)}) - \mathcal{M}_{\text{PCE}}(\boldsymbol{\xi}^{(i)})}{1 - h_i} \right]^2}{\sum_{i=1}^K [\mathcal{M}(\boldsymbol{\xi}^{(i)}) - \mu_{\text{PCE}}]^2} \quad (4.50)$$

where:

$$\mathbf{h} = \text{diag} \left\{ \boldsymbol{\Psi}(\boldsymbol{\xi}) [\boldsymbol{\Psi}(\boldsymbol{\xi})^T \boldsymbol{\Psi}(\boldsymbol{\xi})]^{-1} \boldsymbol{\Psi}(\boldsymbol{\xi})^T \right\} \quad (4.51)$$

and in extended form:

$$\begin{aligned} \begin{Bmatrix} h_1 \\ \vdots \\ h_K \end{Bmatrix} &= \text{diag} \left\{ \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \left(\begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix}^T \right. \right. \\ &\quad \cdot \left. \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \right)^{-1} \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix}^T \left. \right\} \end{aligned} \quad (4.52)$$

Chapter 5

Polynomial Chaos-based Kriging

5.1 Introduction

Polynomial Chaos Kriging has been employed as the second surrogate model to investigate the propagation of uncertainty of the five calibration constants of the $k - \varepsilon$ turbulence model. Polynomial Chaos Kriging can be interpreted as an universal kriging where the global behaviour is modelled by the Polynomial Chaos Expansion. In this chapter, the main characteristics of this model have been discussed, in particular, the kernel configurations and the numerical implementation.

5.2 Definition and general properties

Given a model response $Y(\boldsymbol{\xi})$ generated by the initial random variables $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}^T$, the response can be expressed by using Kriging and Polynomial Chaos Expansion for:

- capturing the local behaviour of the phenomenon by the Kriging
- describing the global behaviour of the phenomenon by the Polynomial Chaos Expansion.

The response is expressible as:

$$Y(\boldsymbol{\xi}) = \underbrace{\sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\boldsymbol{\xi})}_{\text{global behavior}} + \underbrace{\sigma_S^2 Z(\boldsymbol{\xi})}_{\text{local behavior}} \quad (5.1)$$

where $\sum_{i=0}^M \alpha_i(\boldsymbol{x}) \varphi_i(\boldsymbol{\xi})$ is the Polynomial Chaos Expansion of $Y(\boldsymbol{\xi})$, $Z(\boldsymbol{\xi},)$ is a stationary Gaussian process characterized by the kernel $R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta})$, unitary variance and zero mean, σ_S^2 is the system variance and $\boldsymbol{\theta} = \{\theta_1, \dots, \theta_n\}$ are hyperparameters. The system variance can be calculated as:

$$\sigma_S^2 = \frac{1}{K} [\mathbf{Y}(\boldsymbol{\xi}) - \boldsymbol{\Psi}(\boldsymbol{\xi}) \boldsymbol{\alpha}_{\text{PCE}}]^T \mathbf{R}(\boldsymbol{\xi}, \boldsymbol{\theta})^{-1} [\mathbf{Y}(\boldsymbol{\xi}) - \boldsymbol{\Psi}(\boldsymbol{\xi}) \boldsymbol{\alpha}_{\text{PCE}}] \quad (5.2)$$

and in extended form:

$$\begin{aligned}
\sigma_S^2 = & \frac{1}{K} \left[\begin{Bmatrix} Y(\boldsymbol{\xi}^{(1)}) \\ \vdots \\ Y(\boldsymbol{\xi}^{(K)}) \end{Bmatrix} - \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \cdot \begin{Bmatrix} \alpha_{\text{PCE}_0} \\ \vdots \\ \alpha_{\text{PCE}_M} \end{Bmatrix} \right]^T \\
& \cdot \left[\begin{matrix} R(|\boldsymbol{\xi}^{(1)} - \boldsymbol{\xi}^{(1)}|, \boldsymbol{\theta}) & \cdots & R(|\boldsymbol{\xi}^{(1)} - \boldsymbol{\xi}^{(K)}|, \boldsymbol{\theta}) \\ \vdots & \ddots & \vdots \\ R(|\boldsymbol{\xi}^{(K)} - \boldsymbol{\xi}^{(1)}|, \boldsymbol{\theta}) & \cdots & R(|\boldsymbol{\xi}^{(K)} - \boldsymbol{\xi}^{(K)}|, \boldsymbol{\theta}) \end{matrix} \right]^{-1} \left(\begin{Bmatrix} Y(\boldsymbol{\xi}^{(1)}) \\ \vdots \\ Y(\boldsymbol{\xi}^{(K)}) \end{Bmatrix} - \right. \\
& \left. - \begin{bmatrix} \varphi_0(\boldsymbol{\xi}^{(1)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(1)}) \\ \vdots & \ddots & \vdots \\ \varphi_0(\boldsymbol{\xi}^{(K)}) & \cdots & \varphi_M(\boldsymbol{\xi}^{(K)}) \end{bmatrix} \begin{Bmatrix} \alpha_{\text{PCE}_0} \\ \vdots \\ \alpha_{\text{PCE}_M} \end{Bmatrix} \right). \quad (5.3)
\end{aligned}$$

5.3 Types of correlation functions

Correlation functions are also named kernel or covariance. They are semi-positive definite and symmetric functions which describe the mathematical relations among the collocation points of the model. Typical correlation function are:

- **Linear correlation functions:**

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}) = \prod_{i=1}^n \max \left\{ 0, 1 - \frac{|\xi_i - \xi'_i|}{\theta_i} \right\} \quad (5.4)$$

- **Exponential correlation functions:**

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}) = \prod_{i=1}^n e^{-\frac{|\xi_i - \xi'_i|}{\theta_i}} \quad (5.5)$$

- **Matern correlation functions:**

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}, h) = \prod_{i=1}^n \frac{1}{2^{h-1} \Gamma(h)} \left(2\sqrt{h} \frac{|\xi_i - \xi'_i|}{\theta_i} \right)^h \mathcal{K}_h \left(2\sqrt{h} \frac{|\xi_i - \xi'_i|}{\theta_i} \right), \quad (5.6)$$

where h is a shape parameter, Γ is the Euler's gamma function and $\mathcal{K}_h$ modified Bessel function of the II kind.

- **Gaussian correlation functions $\rightarrow h = +\infty$:**

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}, +\infty) = \prod_{i=1}^n e^{-\frac{1}{2} \left(\frac{|\xi_i - \xi'_i|}{\theta_i} \right)^2} \quad (5.7)$$

- **Matern $\frac{3}{2}$ correlation functions $\rightarrow h = \frac{3}{2}$:**

$$R\left(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}, \frac{3}{2}\right) = \prod_{i=1}^n \left[1 + \sqrt{3} \left(\frac{|\xi_i - \xi'_i|}{\theta_i} \right) \right] e^{-\sqrt{3} \left(\frac{|\xi_i - \xi'_i|}{\theta_i} \right)} \quad (5.8)$$

- **Matern $\frac{5}{2}$ correlation functions $\rightarrow h = \frac{5}{2}$:**

$$R\left(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}, \frac{5}{2}\right) = \prod_{i=1}^n \left[1 + \sqrt{5} \left(\frac{|\xi_i - \xi'_i|}{\theta_i} \right) + \frac{5}{3} \left(\frac{|\xi_i - \xi'_i|}{\theta_i} \right)^2 \right] e^{-\sqrt{5} \left(\frac{|\xi_i - \xi'_i|}{\theta_i} \right)} \quad (5.9)$$

5.4 Types of Polynomial Chaos-based Kriging

Polynomial Chaos Kriging can be generated by following a sequential or optimal approach. The two approaches are described below.

5.4.1 Sequential Polynomial Chaos Kriging

In sequential Polynomial Chaos Kriging, the set of polynomials are determined sequentially. The original set of polynomials:

$$\mathcal{A} = M + 1 \quad (5.10)$$

is selected by Sparse Polynomial Chaos Expansion based on Least Angle Regression method. The optimal set is implemented in the PCK model as a trend of:

$$P = |M + 1| = |\mathcal{A}| \quad (5.11)$$

regressors. Finally, the model is calibrated in the same way as universal Kriging (including for the polynomial coefficients) and the local mean value and variance of a new point (which does not belong to the Design Of Experiments) can be calculated by applying:

$$\mu_{\hat{Y}} = \boldsymbol{\varphi}(\boldsymbol{\xi})^T \boldsymbol{\alpha}_{\text{PCE}} + \mathbf{r}(\boldsymbol{\xi}, \boldsymbol{\theta})^T \mathbf{R}^{-1}(\boldsymbol{\xi}, \boldsymbol{\theta}) [\mathbf{Y}(\boldsymbol{\xi}) - \boldsymbol{\Psi}(\boldsymbol{\xi}) \boldsymbol{\alpha}_{\text{PCE}}] \quad (5.12)$$

and:

$$\sigma_{\hat{Y}}^2 = \sigma^2 \left\{ 1 - \mathbf{r}(\boldsymbol{\xi}, \boldsymbol{\theta})^T \mathbf{R}^{-1}(\boldsymbol{\xi}, \boldsymbol{\theta}) \mathbf{r}(\boldsymbol{\xi}, \boldsymbol{\theta}) + \left[\boldsymbol{\Psi}(\boldsymbol{\xi})^T \mathbf{R}^{-1}(\boldsymbol{\xi}, \boldsymbol{\theta}) \mathbf{r}(\boldsymbol{\xi}, \boldsymbol{\theta}) - \boldsymbol{\varphi}(\boldsymbol{\xi}) \right]^T \cdot \left[\boldsymbol{\Psi}(\boldsymbol{\xi})^T \mathbf{R}^{-1}(\boldsymbol{\xi}, \boldsymbol{\theta}) \boldsymbol{\Psi}(\boldsymbol{\xi}) \right]^{-1} \left[\boldsymbol{\Psi}(\boldsymbol{\xi})^T \mathbf{R}^{-1}(\boldsymbol{\xi}, \boldsymbol{\theta}) \mathbf{r}(\boldsymbol{\xi}, \boldsymbol{\theta}) - \boldsymbol{\varphi}(\boldsymbol{\xi}) \right] \right\} \quad (5.13)$$

where:

$$r_i(\boldsymbol{\xi}) = R \left(\left| \boldsymbol{\xi} - \boldsymbol{\xi}^{(i)} \right|, \boldsymbol{\theta} \right) \quad (5.14)$$

$$\boldsymbol{\varphi}(\boldsymbol{\xi}) = [\varphi_0(\boldsymbol{\xi}), \dots, \varphi_M(\boldsymbol{\xi})]^T. \quad (5.15)$$

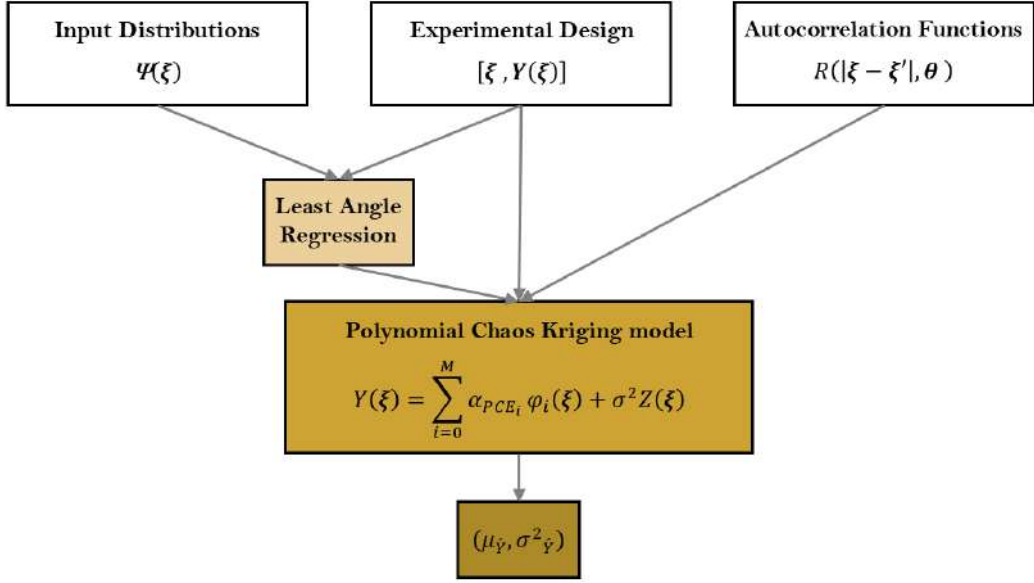


Figure 5.1: Sequential Polynomial Chaos Kriging.

5.4.2 Optimal Polynomial Chaos Kriging

In Optimal Polynomial Chaos Kriging, the Polynomial Chaos Kriging model is obtained iteratively. The original set of polynomials $\mathcal{A} = M + 1$ is selected by Sparse Polynomial Chaos Expansion based on the Least Angle Regression Selection method. The set of polynomials is ranked according to their correlation with the current residual at each Least Angle Regression Selection iteration. Each polynomial is added to the trend of the Polynomial Chaos kriging model so that the Polynomial Chaos Kriging model is updated with the new information. In each iteration, the Polynomial Chaos coefficients and the parameters of the auto-correlation functions are calibrated. Finally, we obtain:

$$P = |M + 1| = |\mathcal{A}| \quad (5.16)$$

models and the best one minimizes:

$$\varepsilon_{\text{LOO}} = \frac{1}{K} \left\{ \frac{\sum_{k=1}^K \left[\sum_{i=0}^M \alpha_{\text{PCE}_i} \varphi_i(\xi^{(k)}) + \sigma^2 Z(\xi^{(k)}) - \mu_{\hat{Y} \sim \xi^{(k)}}(\xi^{(k)}) \right]^2}{\text{Var}\{\mathbf{Y}(\xi)\}} \right\}, \quad (5.17)$$

where:

$$\mu_{\hat{Y} \sim \xi^{(k)}}(\xi^{(k)}) = \left\{ \varphi(\xi^{(k)})^T \alpha_{\text{PCE}} + \mathbf{r}(\xi^{(k)}, \theta)^T \mathbf{R}(\xi, \theta)^{-1} [\mathbf{Y}(\xi) - \Psi(\xi) \alpha_{\text{PCE}}] \right\}_{\sim \xi^{(k)}}. \quad (5.18)$$

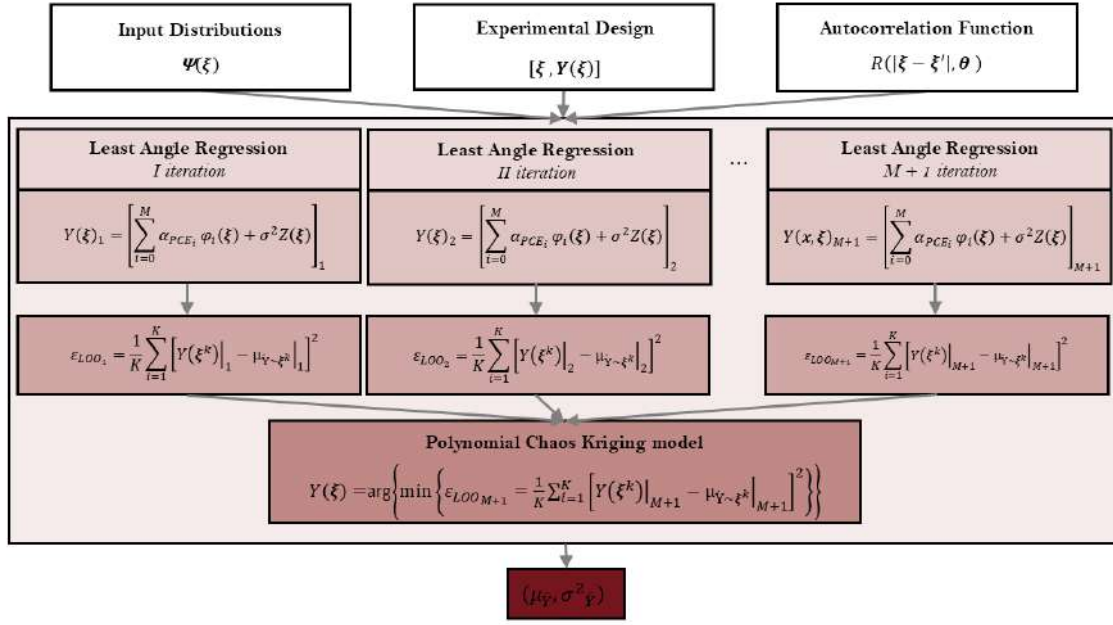


Figure 5.2: Optimal polynomial Chaos Kriging.

Chapter 6

Sobol Decomposition

6.1 Introduction

In addition to the Forward Propagation of Uncertainties of the calibration constants of the $k - \varepsilon$ Turbulence model, the Sensitivity Analysis of these quantities over the responses of the problem has been conducted. As written in the second chapter, we have been interested in an approach based on the Global Sensitivity Analysis in order to examine the sensitivity across the entire parameter space of the initial variables and among the developed methodology, we have applied the ANOVA method about the Sobol decomposition [39, 40, 41, 87, 88, 89, 90]. In the present section, we describe the characteristics and properties of the Sobol decomposition. Furthermore, the procedures of computing the Sobol indices are explained.

6.2 Definition and general properties

Let $Y(\boldsymbol{\xi})$ be the response of interest and $\boldsymbol{\xi}$ the initial variables of the problem. In accordance with Sobol, if outputs are associated with finite variance models $\mathcal{M}(\boldsymbol{\xi})$, it is possible to rewrite that model as composition of submodels which depend on the various combinations of initial variables:

$$Y(\boldsymbol{\xi}) = \mathcal{M}_0 + \sum_{i=1}^n \mathcal{M}_i(\xi_i) + \sum_{i=1}^n \sum_{j=1}^j \mathcal{M}_{ij}(\xi_i, \xi_j) + \cdots + \mathcal{M}_{1,\dots,n}(\xi_1, \dots, \xi_n). \quad (6.1)$$

whose components are mathematically calculated as:

$$\mathcal{M}_0 = \mathbb{E}[Y(\boldsymbol{\xi})] = \int_{D_{\boldsymbol{\xi}}} \mathcal{M}(\boldsymbol{\xi}) d\boldsymbol{\xi} \quad (6.2)$$

$$\mathcal{M}_i(\xi_i) = \mathbb{E}[Y(\boldsymbol{\xi})|\xi_i] - \mathcal{M}_0 = \int_{\mathbb{K}^{n-1}} \mathcal{M}(\boldsymbol{\xi}) d\boldsymbol{\xi}_{\sim i} - \mathcal{M}_0 \quad (6.3)$$

$$\mathcal{M}_{ij}(\xi_i, \xi_j) = \mathbb{E}[Y|\xi_i, \xi_j] - \mathcal{M}_i(\xi_i) - \mathcal{M}_j(\xi_j) - \mathcal{M}_0 = \int_{\mathbb{K}^{n-2}} \mathcal{M}(\boldsymbol{\xi}) d\boldsymbol{\xi}_{\sim ij} - \mathcal{M}_i(\xi_i) - \mathcal{M}_j(\xi_j) - \mathcal{M}_0 \quad (6.4)$$

$$\boldsymbol{\xi}_{\sim i} = (\xi_1, \dots, \xi_{i-1}, \xi_{i+1}, \dots, \xi_n) \quad (6.5)$$

$$\boldsymbol{\xi}_{\sim ij} = (\xi_1, \dots, \xi_{i-1}, \xi_{i+1}, \dots, \xi_{j-1}, \xi_{j+1}, \dots, \xi_n). \quad (6.6)$$

$$\mathbb{K}^n = \{\boldsymbol{\xi} : 0 \leq \xi_i \leq 1 : i = 1, \dots, n\}. \quad (6.7)$$

The previously described decomposition satisfies the following properties:

1. The integrals of the summands with respect to their own variables $\mathcal{M}_{i_1, \dots, i_s}$ vanish:

$$\int_0^1 \mathcal{M}_{i_1, \dots, i_s}(\xi_{i_1}, \dots, \xi_{i_s}) d\xi_{i_k} = 0 \quad \text{for } 1 \leq k \leq s. \quad (6.8)$$

2. The sum contains a number of summands equal to:

$$\sum_{i=1}^n \binom{n}{i} = 2^n - 1 \quad (6.9)$$

3. The summands are orthogonal to each other:

$$\int_{\mathbb{K}^n} \mathcal{M}_{i_1, \dots, i_s}(\xi_{i_1}, \dots, \xi_{i_s}) \mathcal{M}_{j_1, \dots, j_t}(\xi_{j_1}, \dots, \xi_{j_t}) d\boldsymbol{\xi} = 0 \quad \text{for } (i_1, \dots, i_s) \neq (j_1, \dots, j_t). \quad (6.10)$$

The decomposition (6.1) can be extended to the total variance of the system D such that it can be represented as sum of partial variances $D_{i_1, \dots, i_s}$ as:

$$D = \sum_{i=1}^n D_i + \sum_{i=1}^n \sum_{j=1}^i D_{ij} + \dots + D_{1, \dots, n}, \quad (6.11)$$

where:

$$D = \text{Var} \{Y(\boldsymbol{\xi})\} = \int_{D_{\boldsymbol{\xi}}} \mathcal{M}^2(\boldsymbol{\xi}) d\boldsymbol{\xi} - \mathcal{M}_0^2 \quad (6.12)$$

$$D_{i_1, \dots, i_s} = \int_{\mathbb{K}^s} \mathcal{M}_{i_1, \dots, i_s}^2(\xi_{i_1}, \dots, \xi_{i_s}) d\xi_{i_1} \dots d\xi_{i_s} \quad \text{for } 1 \leq i_1 < \dots < i_s \leq n \text{ and } s = 1, \dots, n. \quad (6.13)$$

At this point, Sobol indices are computed as the ratio among partial variances and the total variance of the system:

$$S_{i_1, \dots, i_s} = \frac{D_{i_1, \dots, i_s}}{D} \quad (6.14)$$

Sobol indices measure the importance of random variables $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}^T$ on the response $Y(\boldsymbol{\xi})$. In particular, the Sobol index S_i associated with the variable ξ_i determines the weight of ξ_i in the evaluation of $Y(\boldsymbol{\xi})$ and the Sobol index S_{ij} associated with the variables ξ_i and ξ_j determines the weight of the interaction $\xi_i - \xi_j$ in the evaluation of $Y(\boldsymbol{\xi})$ and so on. All indices satisfy the following property:

$$\sum_{i=1}^n S_i + \sum_{i=1}^n \sum_{j=1}^i S_{ij} + \dots + S_{1, \dots, n} = 1 \quad (6.15)$$

and in conclusion, to analyze the complete contribution of a random variable ξ_i , the total Sobol index, which takes into consideration the contributions of main Sobol index and all Sobol indices of higher orders of ξ_i , is calculated as follows:

$$S_{T_i} = \sum_{i \subset (i_1, \dots, i_s)} S_{i_1, \dots, i_s}. \quad (6.16)$$

6.3 Computation of Sobol Indices

The computation of Sobol indices can be performed by using three main strategies: they can be calculated by applying **Monte Carlo methods**, **Low – Rank Approximation methods** or **PCE coefficients** [42].

6.3.1 Computation of Sobol Indices by using Monte Carlo methods

The variances described in (6.12) and (6.13) can be computed by means of Monte Carlo simulations with the following estimators:

$$\mathcal{M}_{0\text{MC}} = \frac{1}{K} \sum_{k=1}^K \mathcal{M}(\xi^{(k)}) \quad (6.17)$$

$$D_{\text{MC}} = \frac{1}{K} \sum_{k=1}^K \mathcal{M}^2(\xi^{(k)}) - \mathcal{M}_{0\text{MC}} \quad (6.18)$$

$$D_{i\text{MC}} = \frac{1}{K} \sum_{k=1}^K \mathcal{M}(\xi_i^{(k)}, \xi_{\sim i}^{(k)}) \mathcal{M}(\xi_i^{(k)}, \tilde{\xi}_{\sim i}^{(k)}) - \mathcal{M}_{0\text{MC}} \quad (6.19)$$

where:

$$\tilde{\xi} : \text{realization of } \xi \text{ independent of } \left\{ \xi_i^{(k)}, \xi_{\sim i}^{(k)} \right\}^T \quad (6.20)$$

such that, for example, the main Sobol Indices can be computed as:

$$S_i = \frac{\frac{1}{K} \sum_{k=1}^K \mathcal{M}(\xi_i^{(k)}, \xi_{\sim i}^{(k)}) \mathcal{M}(\xi_i^{(k)}, \tilde{\xi}_{\sim i}^{(k)}) - \mathcal{M}_{0\text{MC}}}{\frac{1}{K} \sum_{k=1}^K \mathcal{M}^2(\xi^{(k)}) - \mathcal{M}_{0\text{MC}}} \quad (6.21)$$

6.3.2 Computation of Sobol Indices by using Low-Rank Approximation methods

Sobol Indices can be also calculated by executing Canonical Low-Rank Approximation meta-models. In this case, the response $Y(\xi)$ is approximated by:

$$Y(\xi) = \mathcal{M}_{\text{LRA}} = \sum_{k=1}^R W_k \left\{ \prod_{j=1}^n \left[\sum_{i=0}^p \alpha_{\text{LRA}_{ik}}^{(j)} \phi_i^{(j)}(\xi_j) \right] \right\}, \quad (6.22)$$

where $\phi_i^{(j)}$ is a univariate polynomial of degree i in the j input variable, $\alpha_{\text{LRA}_{ik}}^{(j)}$ are polynomial coefficients and W_k are weighting functions. The mean value and the total variance of the response can be approximated by using the following approximators:

$$\mu_{\text{LRA}} = \sum_{k=1}^R W_k \left[\prod_{j=1}^n \alpha_{\text{LRA}_{0k}}^{(j)} \right] \quad (6.23)$$

$$D_{\text{LRA}} = \sum_{k=1}^R \sum_{k'=1}^R W_k W_{k'} \left\{ \prod_{j=1}^n \left[\sum_{i=0}^p \alpha_{\text{LRA}_{ik}}^{(j)} \alpha_{\text{LRA}_{ik'}}^{(j)} \right] - \prod_{j=1}^n \alpha_{\text{LRA}_{0k}}^{(j)} \alpha_{\text{LRA}_{0k'}}^{(j)} \right\} \quad (6.24)$$

such that, the main Sobol Indices, for example, can be computed as:

$$S_i = \frac{\mathbb{E} \left[\mathbb{E}[Y(\xi) | \xi_i]^2 \right] - \mu_{\text{LRA}}^2}{D_{\text{LRA}}}, \quad (6.25)$$

where:

$$\mathbb{E} \left[\mathbb{E}[Y(\xi) | \xi_i]^2 \right] = \sum_{k=1}^R \sum_{k'=1}^R W_k W_{k'} \left[\prod_{\substack{j'=1 \\ j' \neq j}}^n \alpha_{\text{LRA}_{0k}}^{(j')} \alpha_{\text{LRA}_{0k'}}^{(j')} \right] \sum_{i=0}^M \alpha_{\text{LRA}_{ik}}^{(j)} \alpha_{\text{LRA}_{ik'}}^{(j)}. \quad (6.26)$$

and then:

$$S_i = \frac{\sum_{k=1}^R \sum_{k'=1}^R W_k W_{k'} \left[\prod_{\substack{j'=1 \\ j' \neq j}}^n \alpha_{\text{LRA}_{0k}}^{(j')} \alpha_{\text{LRA}_{0k}}^{(j')} \right] \sum_{i=0}^M \alpha_{\text{LRA}_{ik}}^{(j)} \alpha_{\text{LRA}_{ik'}}^{(j)} - \left\{ \sum_{k=1}^R W_k \left[\prod_{j=1}^n \alpha_{\text{LRA}_{0k}}^{(j)} \right] \right\}^2}{\sum_{k=1}^R \sum_{k'=1}^R W_k W_{k'} \left\{ \prod_{j=1}^n \left[\sum_{i=0}^M \alpha_{\text{LRA}_{ik}}^{(j)} \alpha_{\text{LRA}_{ik'}}^{(j)} \right] - \prod_{j=1}^n \alpha_{\text{LRA}_{0k}}^{(j)} \alpha_{\text{LRA}_{0k'}}^{(j)} \right\}}. \quad (6.27)$$

6.3.3 Computation of Sobol Indices by using Polynomial Chaos coefficients

Sobol indices can be also computed by applying the Polynomial Chaos Expansion. The mean value and the total variance of the system are determined by directly applying (4.10) and (4.11). Similarly, partial variances are computed as follows:

$$D_{i_{\text{PCE}}} = \sum_{\mathbf{m} \in \mathcal{A}_i} \alpha_{\text{PCE}_{\mathbf{m}}}^2, \quad (6.28)$$

where:

$$\mathcal{A}_i = \{ \mathbf{m} \in \mathcal{A} \in \mathbb{N}^n \mid j \in i \Leftrightarrow m_j \neq 0, j = 1, \dots, n \}. \quad (6.29)$$

As example, the main Sobol indices can be computed as:

$$S_i = \frac{D_{i_{\text{PCE}}}}{D_{\text{PCE}}} = \frac{D_{i_{\text{PCE}}}}{\sigma_{\text{PCE}}^2} = \frac{\sum_{\mathbf{m} \in \mathcal{M}_i} \alpha_{\text{PCE}_{\mathbf{m}}}^2}{\sum_{i=1}^M \alpha_{\text{PCE}_i}^2} \quad (6.30)$$

In this work, we have determined the Sobol indices by using the Polynomial Chaos coefficients. Since the Sobol decomposition of the system variance is based on the Polynomial Chaos construction, the higher variances in the variance decomposition correspond to the order of the Polynomial Chaos.

Chapter 7

Fluid Dynamics background

7.1 Introduction

As described, the scope of this work has been to analyze how the uncertainty in certain quantities, i.e. Parametric Uncertainties of the $k - \varepsilon$ Turbulence model, propagates through the applied model to influence the determination of the outputs.

In Fluid Dynamics, flow fields are studied by the application of the Navier-Stokes equations. Navier-Stokes equations are a set of partial differential equations that describe the motion of viscous fluids. They arise from the application of Newton's second law of fluid motion and consist specifically of three laws: **conservation of mass**, **linear momentum equation** and **energy equation**, under particular conditions. The three laws can fully describe the dynamics of fluids and are characterized by the same basic hypothesis: they are developed for a simply connected volume $V \in \mathbb{R}^n$ where the time evolution is described by the time variable $t \in \mathbb{R}$ which is defined over the time interval $T_{\text{ime}} \in \mathbb{R}$ where the two main fields are the velocity field $\mathbf{v} = \{v_1, \dots, v_n\}^T \in \mathbb{R}^n$ and the density function $\rho : V \times T_{\text{ime}} \rightarrow \mathbb{R} \in C^1(V \times T_{\text{ime}})$. In the majority of practical applications, only two-dimensional and three-dimensional flows are treated.

Navier-Stokes equations have been derived from an Eulerian description where the properties of fluids are described by considering a control volume at a spatially fixed point over the time variable. In this manner, velocity field, pressure field and temperature field are analyzed within that volume as time progresses. In this chapter, the derivation of the Navier-Stokes have been shown. Subsequently, there have been described the strategy to deal the turbulence modelling and a review about the turbulence model employed in RANS simulations has been proposed. In particular, the Standard $k - \varepsilon$ Turbulence model is described in detail.

7.2 The three conservation laws of Fluid Dynamics

From a general point of view, the three conservation laws of Fluid Dynamics (i.e: equation of conservation of mass, equation of linear momentum and equation of energy) are applicable to any type of fluids and when some assumptions are satisfied they take the name of Navier-Stokes equations. In the following sections, the general conservation laws of Fluid Dynamics are discussed and after, their particular application is described in order to derive the Navier-Stokes equations [91, 92, 93].

7.2.1 Conservation of mass

The general definition of mass m is given by the integral of the density over the control volume at a given instant of time:

$$m = \iiint_{V(t)} \rho dV. \quad (7.1)$$

During the time evolution of the system from the instant t to the instant $t + \Delta t$, there is a variation of the mass into the system of study where the total change of the mass $\frac{dm}{dt}$ is expressed as:

$$\frac{dm}{dt} = \frac{d}{dt} \left(\iiint_{V(t)} \rho dV \right) = \lim_{\Delta t \rightarrow 0} \frac{\iiint_{V(t+\Delta t)} \rho|_{t+\Delta t} dV - \iiint_{V(t)} \rho dV}{\Delta t} \quad (7.2)$$

where $V(t + \Delta t)$ and $\rho(t + \Delta t)$ are respectively the volume and the density at the time $t + \Delta t$. Writing:

$$V(t + \Delta t) = V + \Delta V, \quad (7.3)$$

the equation (7.2) is decomposed as:

$$\frac{dm}{dt} = \underbrace{\lim_{\Delta t \rightarrow 0} \frac{\iiint_{V(t)} (\rho|_{t+\Delta t} - \rho) dV}{\Delta t}}_{\text{I block}} + \underbrace{\lim_{\Delta t \rightarrow 0} \frac{\iiint_{\Delta V} \rho|_{t+\Delta t} dV}{\Delta t}}_{\text{II block}} \quad (7.4)$$

and considering the definition of differentiability, the I block of (7.4) is equal to:

$$\lim_{\Delta t \rightarrow 0} \frac{\iiint_{V(t)} (\rho|_{t+\Delta t} - \rho) dV}{\Delta t} = \lim_{\Delta t \rightarrow 0} \iiint_{V(t)} \left(\frac{\rho|_{t+\Delta t} - \rho}{\Delta t} \right) dV = \iiint_{V(t)} \frac{\partial \rho}{\partial t} dV \quad (7.5)$$

and by:

$$dV = \mathbf{v} \Delta t \hat{\mathbf{n}} dS, \quad (7.6)$$

the II block of (7.4) is equivalent to:

$$\lim_{\Delta t \rightarrow 0} \frac{\iiint_{\Delta V} \rho|_{t+\Delta t} dV}{\Delta t} = \lim_{\Delta t \rightarrow 0} \iint_{S(t)} \frac{\rho|_{t+\Delta t} \mathbf{v} \Delta t \hat{\mathbf{n}} dS}{\Delta t} = \iint_{S(t)} \rho \mathbf{v} \hat{\mathbf{n}} dS \quad (7.7)$$

where $\hat{\mathbf{n}}$ is the normal vector and S is the surface of control. Then, the Reynolds transport theorem states that the total change of mass is equal to the sum of the mass change inside $V(t)$ and the net flow of m through the surface $S(t)$:

$$\frac{dm}{dt} = \iiint_{V(t)} \frac{\partial \rho}{\partial t} dV + \iint_{S(t)} \rho \mathbf{v} \hat{\mathbf{n}} dS. \quad (7.8)$$

Applying the divergence theorem for the surface integral:

$$\iint_{S(t)} \rho \mathbf{v} \hat{\mathbf{n}} dS = \iiint_{V(t)} \nabla \cdot (\rho \mathbf{v}) dV, \quad (7.9)$$

and taking into account the validity of absence of mass sources and sinks, the fluid region conserves its mass such that the variation of total mass is equal to zero:

$$\frac{dm}{dt} = \iiint_{V(t)} \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV = 0 \Rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (7.10)$$

If the phenomenon is stationary, the density is independent of time and the continuity equation is simplified as:

$$\nabla \cdot (\rho \mathbf{v}) = 0. \quad (7.11)$$

and in conclusion, if the flow is also incompressible, the density assumes a constant value and the continuity equation is further simplified:

$$\nabla \cdot (\rho \mathbf{v}) = \rho \nabla \cdot \mathbf{v} = 0 \Rightarrow \nabla \cdot \mathbf{v} = 0. \quad (7.12)$$

Conservation of mass for a two-dimensional flow

For a two-dimensional flow, the flow field is imposed as $\mathbf{v} = \{u, v\}^T$ and the continuity equation in scalar component is given by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0 \quad (7.13)$$

$$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) = 0 \quad (7.14)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0. \quad (7.15)$$

Conservation of mass for a three-dimensional flow

For a three-dimensional flow, the flow field is imposed as $\mathbf{v} = \{u, v, w\}^T$ and the continuity equation in scalar component is given by:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0 \quad (7.16)$$

$$\frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0 \quad (7.17)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (7.18)$$

7.2.2 Conservation of linear momentum

Applying the Newton's second law (second cardinal equation of dynamics), the linear momentum can change if and only if there are external acting forces on the body. If this happens, it is possible to express the variation of linear momentum as:

$$\frac{d}{dt}(m\mathbf{v}) = m \frac{d\mathbf{v}}{dt} = \mathbf{F}_V + \mathbf{F}_S = \iiint_{V(t)} \mathbf{f}_V dV + \iint_{S(t)} \mathbf{f}_S dS, \quad (7.19)$$

where:

$$\mathbf{F}_V = \iiint_{V(t)} \mathbf{f}_V dV : \text{total volume forces} \quad (7.20)$$

$$\mathbf{F}_S = \iint_{S(t)} \mathbf{f}_S dS : \text{total surface forces.} \quad (7.21)$$

Taking into account the definition of mass and the Reynolds transport theorem, is rewritten as:

$$\iiint_{V(t)} \left[\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) \right] dV = \iiint_{V(t)} \mathbf{f}_V dV + \iint_{S(t)} \mathbf{f}_S dS. \quad (7.22)$$

Now, surface forces can be expressed in terms of the stress tensor $\mathbf{T}$:

$$\iint_{S(t)} \mathbf{f}_S dS = \iint_{S(t)} \mathbf{T} \hat{\mathbf{n}} dS = \iiint_{V(t)} \nabla \cdot \mathbf{T} dV \quad (7.23)$$

and (7.22) is modified as:

$$\begin{aligned} \iiint_{V(t)} \left[\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) \right] dV &= \iiint_{V(t)} \left[\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \mathbf{f}_V - \nabla \cdot \mathbf{T} \right] dV = 0 \Rightarrow \\ &\Rightarrow \frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \mathbf{f}_V - \nabla \cdot \mathbf{T} = 0. \end{aligned} \quad (7.24)$$

Considering that the stress tensor is given by the sum of normal stresses generated by the pressure $p\mathbf{I}$ and tangential stresses $\boldsymbol{\tau}$, we have:

$$\mathbf{T} = -p\mathbf{I} + \boldsymbol{\tau} \Rightarrow \nabla \cdot \mathbf{T} = -\nabla p + \nabla \cdot \boldsymbol{\tau} \quad (7.25)$$

and considering (7.24) and (7.25), the conservation of linear momentum applied in Fluid Dynamics is:

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \mathbf{f}_V + \nabla p - \nabla \cdot \boldsymbol{\tau} = 0. \quad (7.26)$$

In this work, the heat transfer has not been treated, as consequence, the energy equation has not discussed.

7.3 Navier-Stokes equations

7.3.1 The fluid stress tensor

As introduced, the Navier-Stokes equations are the conservation laws of fluid dynamics under specific conditions; in few words, the Navier-Stokes equations are the Navier equations when the Stokes laws are valid. In general, we consider Newtonian and incompressible fluids so that the tangential fluid stress tensor can be expressed in terms of velocity field and dynamic viscosity μ :

$$\boldsymbol{\tau} = \begin{bmatrix} 2\mu \frac{\partial u}{\partial x} & \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & 2\mu \frac{\partial v}{\partial y} & \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) & \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) & 2\mu \frac{\partial w}{\partial z} \end{bmatrix} = \mu \left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right] \quad (7.27)$$

and its divergence:

$$\nabla \cdot \boldsymbol{\tau} = \begin{bmatrix} \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \\ \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \\ \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] \end{bmatrix} = \begin{bmatrix} \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \\ \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \\ \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) \end{bmatrix} = \mu \nabla^2 \mathbf{v} \quad (7.28)$$

(7.28) is used to complete the conservation of mass, conservation of linear momentum. For two-dimensional flows, (7.27) and (7.28) are reduced to:

$$\boldsymbol{\tau} = \begin{bmatrix} 2\mu \dot{\epsilon}_{xx} & \mu \dot{\gamma}_{xy} \\ \mu \dot{\gamma}_{yx} & 2\mu \dot{\epsilon}_{yy} \end{bmatrix} = \begin{bmatrix} 2\mu \frac{\partial u}{\partial x} & \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & 2\mu \frac{\partial v}{\partial y} \end{bmatrix} \quad (7.29)$$

$$\nabla \cdot \boldsymbol{\tau} = \begin{bmatrix} \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \\ \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \end{bmatrix}. \quad (7.30)$$

7.3.2 Conservation of mass in Navier-Stokes equations

The equation of conservation of mass in Navier-Stokes equations is the same as previously presented as the fluid stress tensor does not influence this equation.

7.3.3 Linear momentum in Navier-Stokes equations

As a first point, the applied volume forces in Fluid Dynamics simulations are generally only gravitational forces by their dominant contribution over the control volume of reference. In fact, other volume forces are often neglected. From that consideration, it is written:

$$\mathbf{f}_V = \rho \mathbf{g}, \quad (7.31)$$

where:

$$\mathbf{g} = (0, -g, 0) : \text{gravity vector} \quad (7.32)$$

Considering (7.28) and (7.31), the equation (7.26) becomes:

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \mu \nabla^2 \mathbf{v} + \rho \mathbf{g}. \quad (7.33)$$

Linear momentum in Navier-Stokes equations for two-dimensional flows

For two-dimensional flows, the scalar components of (7.33) are respectively:

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u u) + \frac{\partial}{\partial y}(\rho v u) = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \quad (7.34)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho u v) + \frac{\partial}{\partial y}(\rho v v) = -\frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - \rho g. \quad (7.35)$$

Linear momentum in Navier-Stokes equations for three-dimensional flows

For three-dimensional flows, the scalar components of (7.33) are respectively:

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u u) + \frac{\partial}{\partial y}(\rho v u) + \frac{\partial}{\partial z}(\rho w u) = -\frac{\partial p}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \quad (7.36)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho u v) + \frac{\partial}{\partial y}(\rho v v) + \frac{\partial}{\partial z}(\rho w v) = -\frac{\partial p}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) - \rho g \quad (7.37)$$

$$\frac{\partial}{\partial t}(\rho w) + \frac{\partial}{\partial x}(\rho u w) + \frac{\partial}{\partial y}(\rho v w) + \frac{\partial}{\partial z}(\rho w w) = -\frac{\partial p}{\partial z} + \mu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right). \quad (7.38)$$

7.4 Turbulent flows

Navier-Stokes equations are involved to study the fluid behaviours for any flow regime (i.e. **laminar flows**, **transitional flows** and **turbulent flows**). In particular, we have paid attention to turbulent flows. They are identified by a Reynolds number greater than 4000 and are characterized by a chaotic behaviour without a clear definition of streamlines; in that case, mass exchanges and vorticity fluctuations are present. Analytic solutions of Navier-Stokes equations for turbulent flows are not possible. Each aspect of turbulence is not analyzable and then, people are content with studying global aspect of turbulence by introducing other strategies. In general, the main accepted turbulence theory is based on the "energy cascade" developed by Kolmogorov which is still considered valid for the turbulence modelling used nowadays.



Figure 7.1: Streamlines and velocity profile for turbulent regime flows.

Energy cascade is implemented in the classical approaches of turbulence: **Direct Numerical Simulations**, **Large Energy Cascade** and **Reynolds – Averaged Navier – Stokes equations**.

7.5 Energy cascade theory of Kolmogorov

The graphical representation of the Kolmogorov's theory is shown in Figure 7.2. According to Kolmogorov, a turbulent flow can be considered as a set composed of eddies of different sizes where each eddy has a certain amount of energy. The quantity of energy depends on the size of the eddy, the greater the size, the greater the transported energy. When the larger eddies break up, they give their energy to the smaller eddies "which in turn break up and pass their energy to the smaller and so on. All the chain process continues until the smallest possible eddy size.

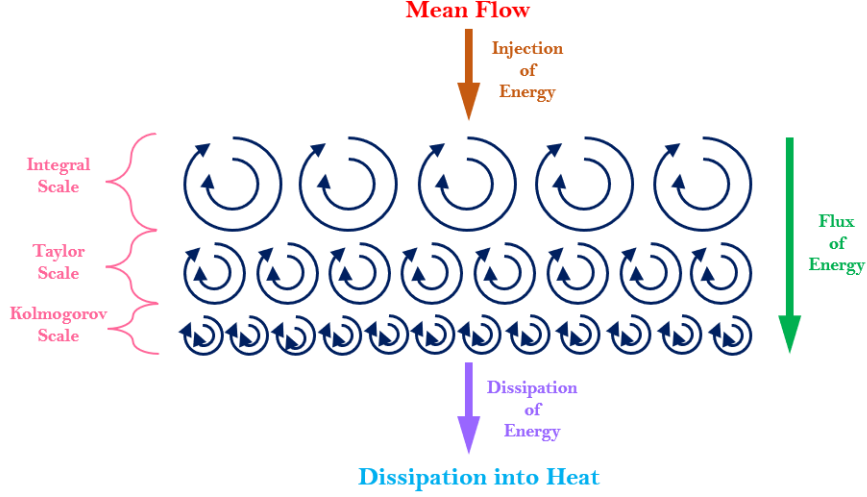


Figure 7.2: Energy cascade theory of Kolmogorov.

"which in turn break up and pass their energy

$$l = \frac{\bar{\nu}^{\frac{3}{2}}}{\varepsilon} : \text{integral length scale [m]} \quad (7.39)$$

$$t = \frac{\bar{\nu}}{\varepsilon} : \text{integral time scale [s]} \quad (7.40)$$

$$v = \bar{\nu}^{\frac{1}{2}} : \text{integral velocity scale } \left[\frac{\text{m}}{\text{s}} \right], \quad (7.41)$$

where $\bar{\nu}$ is the wave number in m^{-1} and ε is the turbulent kinetic energy dissipation rate in $\frac{\text{m}^2}{\text{s}^3}$. Among the largest and the smallest eddies, there are intermediate eddies, identified by the Taylor microscale. In this region, the majority of the energy cascade occurs. Finally, the smallest turbulent eddies are characterized by the following Kolmogorov scales:

$$\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} : \text{Kolmogorov length scale [m]} \quad (7.42)$$

$$\tau_\eta = \left(\frac{\nu}{\varepsilon} \right)^{\frac{1}{2}} : \text{Kolmogorov time scale [s]} \quad (7.43)$$

$$v_\eta = (\nu\varepsilon)^{\frac{1}{4}} : \text{Kolmogorov velocity scale } \left[\frac{\text{m}}{\text{s}} \right], \quad (7.44)$$

where ν represents the kinematic viscosity. These eddies are isotropic because the diffusive actions of strong viscosity smear out anisotropic characteristics of the large eddies and here, the turbulent kinetic energy is dissipated into heat.

7.5.1 DNS - Direct Numerical Simulations

In DNS, the Navier-Stokes equations are directly computed and all temporal and spatial scales are solved. The selection of mesh is chosen to be able to capture the Kolmogorov scales.

7.5.2 LES - Large Energy Cascade

In this strategy, turbulent structures are directly modeled by using sub-grid scale models where the main aim is to filter the Navier-Stokes equations by applying spatial averaging techniques in order to determine which scales to keep and which scales to neglect. This methodology was born from the fact that the largest eddies structures cannot be accurately modeled by general approaches because they are strongly anisotropic. Those large scales are the most cause of convective effects, turbulent kinetic energy and the smallest eddies scales are isotropic and can be analyzed by general methods (in general they are neglected) [94].

7.6 RANS - Reynolds Averaged Navier-Stokes

The most popular approach for treating turbulent flows (particularly in industrial fields) is the application of RANS approach. The main difference between the LES approach and the RANS approach is the averaging technique applied: LES simulations are based on spatial averaging rules which are integrated over the time domain while RANS simulations are based on time averaging rules which are integrated over the space of reference. Let $\phi(\mathbf{x}, t)$ be a general variable of state of governing equations which is function of the space $\mathbf{x}$ and the time t ; it is decomposed as the sum of a time-mean value component $\bar{\phi}(\mathbf{x}, t)$ and a fluctuating component $\phi'(\mathbf{x}, t)$:

$$\phi(\mathbf{x}, t) = \bar{\phi}(\mathbf{x}, t) + \phi'(\mathbf{x}, t). \quad (7.45)$$

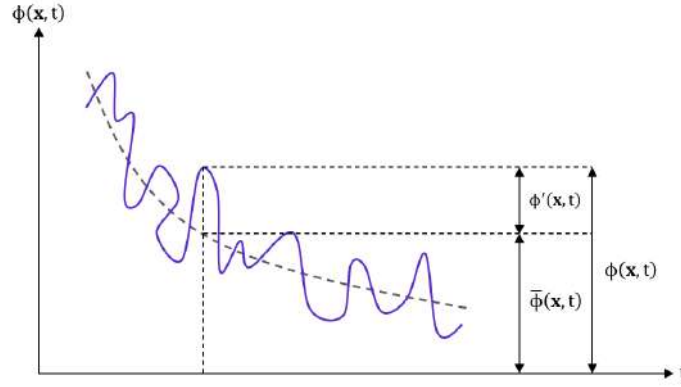


Figure 7.3: Reynolds time averaging approach.

The intention is to model all scales of turbulent flows so that the mesh size limitation is not as constraining as in DNS and LES simulations. It is important to remember that the flow is globally stationary and the time averaged component represents the average of the interested quantity over a time interval T_{ime} such that:

$$\bar{\phi}(\mathbf{x}, t) = \lim_{t \rightarrow +\infty} \frac{1}{T_{\text{ime}}} \int_t^{t+T_{\text{ime}}} \phi(\mathbf{x}, t) dt. \quad (7.46)$$

Globally, the Reynolds averaging rules are:

$$\overline{\bar{\phi}} = \bar{\phi} \Rightarrow \frac{\partial \bar{\phi}}{\partial s} = \frac{\partial \bar{\phi}}{\partial s} = \frac{\partial \bar{\phi}}{\partial s} \quad (7.47)$$

$$\overline{\phi'} = 0 \Rightarrow \frac{\partial \phi'}{\partial s} = \frac{\partial \phi'}{\partial s} = 0, \quad (7.48)$$

$$\overline{\bar{\phi} \cdot \phi'} = \bar{\phi} \cdot \overline{\phi'} = \bar{\phi} \cdot 0 = 0 \Rightarrow \frac{\partial}{\partial s} (\bar{\phi} \cdot \phi') = \frac{\partial}{\partial s} (\bar{\phi} \cdot \phi') = \frac{\partial}{\partial s} (\bar{\phi} \cdot \phi') = \frac{\partial}{\partial s} (\bar{\phi} \cdot \phi') = 0 \quad (7.49)$$

$$\begin{aligned}
\overline{\phi \cdot \varphi} &= \overline{(\bar{\phi} + \phi')(\bar{\varphi} + \varphi')} = \overline{\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \bar{\phi} + \phi' \cdot \bar{\varphi} + \phi' \cdot \varphi'} = \overline{\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \bar{\phi} + \phi' \cdot \bar{\varphi} + \phi' \cdot \varphi'} = \overline{\bar{\phi} \cdot \bar{\varphi} +} \\
&+ \overline{\phi' \cdot \bar{\phi} + \phi' \cdot \bar{\varphi} + \phi' \cdot \varphi'} = \overline{\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \varphi'} \Rightarrow \overline{\frac{\partial}{\partial s}(\phi \cdot \varphi)} = \frac{\partial}{\partial s}(\overline{\phi \cdot \varphi}) = \frac{\partial}{\partial s}(\overline{(\bar{\phi} + \phi')(\bar{\varphi} + \varphi')}) = \\
&= \frac{\partial}{\partial s}(\overline{\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \bar{\phi} + \phi' \cdot \bar{\varphi} + \phi' \cdot \varphi'}) = \frac{\partial}{\partial s}(\overline{\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \bar{\phi} + \phi' \cdot \bar{\varphi} + \phi' \cdot \varphi'}) = \\
&= \frac{\partial}{\partial s}(\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \bar{\phi} + \phi' \cdot \bar{\varphi} + \phi' \cdot \varphi') = \frac{\partial}{\partial s}(\bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \varphi') = \frac{\partial}{\partial s}(\bar{\phi} \cdot \bar{\varphi}) + \frac{\partial}{\partial s}(\phi' \cdot \varphi')
\end{aligned} \tag{7.50}$$

$$\begin{aligned}
\overline{\phi + \varphi} &= \overline{(\bar{\phi} + \phi') + (\bar{\varphi} + \varphi')} = \overline{\bar{\phi} + \phi' + \bar{\varphi} + \varphi'} = \overline{\bar{\phi} + \bar{\varphi} + \phi' + \varphi'} = \overline{\bar{\phi} + \bar{\varphi}} \Rightarrow \overline{\frac{\partial}{\partial s}(\phi + \varphi)} = \frac{\partial}{\partial s}(\overline{\phi + \varphi}) = \\
&= \frac{\partial}{\partial s}[\overline{(\bar{\phi} + \phi') + (\bar{\varphi} + \varphi')}] = \frac{\partial}{\partial s}(\bar{\phi} + \bar{\varphi} + \phi' + \varphi') = \frac{\partial}{\partial s}(\bar{\phi} + \bar{\varphi}) = \frac{\partial \bar{\phi}}{\partial s} + \frac{\partial \bar{\varphi}}{\partial s}
\end{aligned} \tag{7.51}$$

and:

$$\begin{aligned}
\overline{\phi \cdot \varphi} &= \overline{\bar{\phi} \cdot (\bar{\varphi} + \varphi')} = \overline{\bar{\phi} \cdot \bar{\varphi} + \bar{\phi} \cdot \varphi'} = \overline{\bar{\phi} \cdot \bar{\varphi} + \bar{\phi} \cdot \varphi'} = \overline{\bar{\phi} \cdot \bar{\varphi}} \Rightarrow \overline{\frac{\partial}{\partial s}(\phi \cdot \varphi)} = \frac{\partial}{\partial s}(\overline{\phi \cdot \varphi}) = \\
&= \frac{\partial}{\partial s}[\overline{\bar{\phi} \cdot (\bar{\varphi} + \varphi')}] = \frac{\partial}{\partial s}(\bar{\phi} \cdot \bar{\varphi} + \bar{\phi} \cdot \varphi') = \frac{\partial}{\partial s}(\bar{\phi} \cdot \bar{\varphi} + \bar{\phi} \cdot \varphi') = \frac{\partial}{\partial s}(\bar{\phi} \cdot \bar{\varphi}).
\end{aligned} \tag{7.52}$$

At this points, taking into consideration a three-dimensional flow, (7.18), (7.36), (7.37), (7.38) and (??) are mediated in accordance with Reynolds as:

$$\overline{\frac{\partial}{\partial x}(\bar{u} + u') + \frac{\partial}{\partial y}(\bar{v} + v') + \frac{\partial}{\partial z}(\bar{w} + w')} = \frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0 \tag{7.53}$$

$$\begin{aligned}
&\overline{\frac{\partial}{\partial t}[\rho(\bar{u} + u')] + \frac{\partial}{\partial x}[\rho(\bar{u} + u')(\bar{u} + u')] + \frac{\partial}{\partial y}[\rho(\bar{v} + v')(\bar{u} + u')] + \frac{\partial}{\partial z}[\rho(\bar{w} + w')(\bar{u} + u')]} = \\
&= -\frac{\partial}{\partial x}(\bar{p} + p') + \mu \left[\frac{\partial^2}{\partial x^2}(\bar{u} + u') + \frac{\partial^2}{\partial y^2}(\bar{u} + u') + \frac{\partial^2}{\partial z^2}(\bar{u} + u') \right] \Rightarrow \frac{\partial}{\partial t}(\rho \bar{u}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{u}) + \\
&+ \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{u}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{u}) = -\frac{\partial \bar{p}}{\partial x} + \mu \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) - \left[\frac{\partial}{\partial x}(\rho \bar{u}' \cdot \bar{u}') + \frac{\partial}{\partial y}(\rho \bar{v}' \cdot \bar{u}') + \right. \\
&+ \left. \frac{\partial}{\partial z}(\rho \bar{w}' \cdot \bar{u}') \right] \Rightarrow \frac{\partial}{\partial t}(\rho \bar{u}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{u}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{u}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{u}) = -\frac{\partial \bar{p}}{\partial x} + \mu \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \right. \\
&+ \left. \frac{\partial^2 \bar{u}}{\partial z^2} \right) - \underbrace{\left\{ \frac{\partial}{\partial x}[\rho(\bar{u}\bar{u}' - \bar{u}' \cdot \bar{u})] + \frac{\partial}{\partial y}[\rho(\bar{v}\bar{u}' - \bar{v}' \cdot \bar{u})] + \frac{\partial}{\partial z}[\rho(\bar{w}\bar{u}' - \bar{w}' \cdot \bar{u})] \right\}}_{\text{from } \phi\varphi = \bar{\phi} \cdot \bar{\varphi} + \phi' \cdot \bar{\varphi}'}
\end{aligned} \tag{7.54}$$

$$\begin{aligned}
&\overline{\frac{\partial}{\partial t}[\rho(\bar{v} + v')] + \frac{\partial}{\partial x}[\rho(\bar{u} + u')(\bar{v} + v')] + \frac{\partial}{\partial y}[\rho(\bar{v} + v')(\bar{v} + v')] + \frac{\partial}{\partial z}[\rho(\bar{w} + w')(\bar{v} + v')]} = \\
&= -\frac{\partial}{\partial y}(\bar{p} + p') + \mu \left[\frac{\partial^2}{\partial x^2}(\bar{v} + v') + \frac{\partial^2}{\partial y^2}(\bar{v} + v') + \frac{\partial^2}{\partial z^2}(\bar{v} + v') \right] - \rho g \Rightarrow \frac{\partial}{\partial t}(\rho \bar{v}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{v}) + \\
&+ \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{v}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{v}) = -\frac{\partial \bar{p}}{\partial y} + \mu \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} + \frac{\partial^2 \bar{v}}{\partial z^2} \right) - \left[\frac{\partial}{\partial x}(\rho \bar{u}' \cdot \bar{v}') + \frac{\partial}{\partial y}(\rho \bar{v}' \cdot \bar{v}') + \right. \\
&+ \left. \frac{\partial}{\partial z}(\rho \bar{w}' \cdot \bar{v}') \right] - \rho g \Rightarrow \frac{\partial}{\partial t}(\rho \bar{v}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{v}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{v}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{v}) = -\frac{\partial \bar{p}}{\partial y} + \mu \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \right. \\
&+ \left. \frac{\partial^2 \bar{v}}{\partial y^2} + \frac{\partial^2 \bar{v}}{\partial z^2} \right) - \rho g - \left\{ \frac{\partial}{\partial x}[\rho(\bar{u}\bar{v}' - \bar{u}' \cdot \bar{v})] + \frac{\partial}{\partial y}[\rho(\bar{v}\bar{v}' - \bar{v}' \cdot \bar{v})] + \frac{\partial}{\partial z}[\rho(\bar{w}\bar{v}' - \bar{w}' \cdot \bar{v})] \right\}
\end{aligned} \tag{7.55}$$

$$\begin{aligned}
& \overline{\frac{\partial}{\partial t} [\rho (\bar{w} + w')] + \frac{\partial}{\partial x} [\rho (\bar{u} + u') (\bar{w} + w')] + \frac{\partial}{\partial y} [\rho (\bar{v} + v') (\bar{w} + w')] + \frac{\partial}{\partial z} [\rho (\bar{w} + w') (\bar{w} + w')]} = \\
& = -\frac{\partial}{\partial z} (\bar{p} + p') + \mu \left[\frac{\partial^2}{\partial x^2} (\bar{w} + w') + \frac{\partial^2}{\partial y^2} (\bar{w} + w') + \frac{\partial^2}{\partial z^2} (\bar{w} + w') \right] \Rightarrow \frac{\partial}{\partial t} (\rho \bar{w}) + \frac{\partial}{\partial x} (\rho \bar{u} \cdot \bar{w}) + \\
& + \frac{\partial}{\partial y} (\rho \bar{v} \cdot \bar{w}) + \frac{\partial}{\partial z} (\rho \bar{w} \cdot \bar{w}) = -\frac{\partial \bar{p}}{\partial z} + \mu \left(\frac{\partial^2 \bar{w}}{\partial x^2} + \frac{\partial^2 \bar{w}}{\partial y^2} + \frac{\partial^2 \bar{w}}{\partial z^2} \right) - \left[\frac{\partial}{\partial x} (\rho \bar{u}' \cdot \bar{w}') + \frac{\partial}{\partial y} (\rho \bar{v}' \cdot \bar{w}') + \right. \\
& + \left. \frac{\partial}{\partial z} (\rho \bar{w}' \cdot \bar{w}') \right] \Rightarrow \frac{\partial}{\partial t} (\rho \bar{w}) + \frac{\partial}{\partial x} (\rho \bar{u} \cdot \bar{w}) + \frac{\partial}{\partial y} (\rho \bar{v} \cdot \bar{w}) + \frac{\partial}{\partial z} (\rho \bar{w} \cdot \bar{w}) = -\frac{\partial \bar{p}}{\partial z} + \mu \left(\frac{\partial^2 \bar{w}}{\partial x^2} + \frac{\partial^2 \bar{w}}{\partial y^2} + \right. \\
& + \left. \frac{\partial^2 \bar{w}}{\partial z^2} \right) - \left\{ \frac{\partial}{\partial x} [\rho (\bar{u}\bar{w} - \bar{u} \cdot \bar{w})] + \frac{\partial}{\partial y} [\rho (\bar{v}\bar{w} - \bar{v} \cdot \bar{w})] + \frac{\partial}{\partial z} [\rho (\bar{w}\bar{w} - \bar{w} \cdot \bar{w})] \right\}
\end{aligned} \tag{7.56}$$

Analyzing the above equations, a series of new unknowns are introduced: we have a further stress tensor τ_R in linear momentum equation:

$$\tau_R = -\rho \begin{bmatrix} \frac{\overline{u' \cdot u'}}{\overline{u' \cdot v'}} & \frac{\overline{v' \cdot u'}}{\overline{v' \cdot v'}} & \frac{\overline{w' \cdot u'}}{\overline{w' \cdot v'}} \\ \frac{\overline{u' \cdot v'}}{\overline{u' \cdot w'}} & \frac{\overline{v' \cdot v'}}{\overline{v' \cdot w'}} & \frac{\overline{w' \cdot v'}}{\overline{w' \cdot w'}} \end{bmatrix} \tag{7.57}$$

named Reynolds stress tensor. The Reynolds stress tensor comes from the non-linear convective terms of momentum, confirming that the turbulence is the effect of a non-linear phenomenon highly sensitive to any perturbation. These quantities need to be modeled to close the RANS approach. In particular, the closure of RANS equations is based on the Boussinesq hypothesis.

7.6.1 Boussinesq hypothesis for the direct modelling of the Reynolds stress tensor

Similarly to (7.27), Boussinesq assumed that the Reynolds stress tensor be proportional to the mean velocity gradient through turbulent eddy viscosity μ_t in order to rewrite τ_R as:

$$\tau_R = \mu_t \left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right] - \left(\frac{2}{3} \rho k + \mu_t \nabla \cdot \mathbf{v} \right) \mathbf{I} \tag{7.58}$$

where:

$$k = \frac{1}{2} \overline{\mathbf{v} \cdot \mathbf{v}} = \frac{1}{2} \left(\overline{u'^2 + v'^2 + w'^2} \right) : \text{turbulent kinetic energy.} \tag{7.59}$$

For incompressible flows, the continuity equation (7.12) can be applied to reduce (7.58) as:

$$\tau_R = \mu_t \left[\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right] - \frac{2}{3} \rho k \mathbf{I} \tag{7.60}$$

and can be further simplified implementing the term $-\frac{2}{3} \rho k \mathbf{I}$ into the pressure:

$$\bar{p}_R = \bar{p} - \frac{2}{3} \rho k. \tag{7.61}$$

7.6.2 RANS equations for two-dimensional flows

Applying the Reynolds averaging rules and the Boussinesq hypothesis previously explained, the derived RANS equations for a two-dimensional flow are given by the following equations:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} = 0 \tag{7.62}$$

$$\frac{\partial}{\partial t}(\rho \bar{u}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{u}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{u}) = -\frac{\partial \bar{p}_R}{\partial x} + (\mu + \mu_t) \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} \right) \quad (7.63)$$

$$\frac{\partial}{\partial t}(\rho \bar{v}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{v}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{v}) = -\frac{\partial \bar{p}_R}{\partial y} + (\mu + \mu_t) \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} \right) - \rho g \quad (7.64)$$

7.6.3 RANS equations for three-dimensional flows

Applying the Reynolds averaging rules and the Boussinesq hypothesis previously explained, the derived RANS equations for a three-dimensional flow are given by the following equations:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0 \quad (7.65)$$

$$\frac{\partial}{\partial t}(\rho \bar{u}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{u}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{u}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{u}) = -\frac{\partial \bar{p}_R}{\partial x} + (\mu + \mu_t) \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \frac{\partial^2 \bar{u}}{\partial z^2} \right) \quad (7.66)$$

$$\frac{\partial}{\partial t}(\rho \bar{v}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{v}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{v}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{v}) = -\frac{\partial \bar{p}_R}{\partial y} + (\mu + \mu_t) \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} + \frac{\partial^2 \bar{v}}{\partial z^2} \right) - \rho g \quad (7.67)$$

$$\frac{\partial}{\partial t}(\rho \bar{w}) + \frac{\partial}{\partial x}(\rho \bar{u} \cdot \bar{w}) + \frac{\partial}{\partial y}(\rho \bar{v} \cdot \bar{w}) + \frac{\partial}{\partial z}(\rho \bar{w} \cdot \bar{w}) = -\frac{\partial \bar{p}_R}{\partial z} + (\mu + \mu_t) \left(\frac{\partial^2 \bar{w}}{\partial x^2} + \frac{\partial^2 \bar{w}}{\partial y^2} + \frac{\partial^2 \bar{w}}{\partial z^2} \right). \quad (7.68)$$

7.6.4 Turbulence models

The use of turbulence models is based on the need to express μ_t and k_t by considering the validity of the Boussinesq hypothesis in order to close the RANS equations. The turbulent viscosity is considered proportional to the fluid density, multiplied by a length scale ℓ and a velocity term $\sqrt{k}$:

$$\mu_t = \rho \ell \sqrt{k} \quad (7.69)$$

while the turbulent thermal diffusivity is considered to be proportional to μ_t through the equation:

$$k_{T_t} = \frac{c_p \mu_t}{\text{Pr}_t}, \quad (7.70)$$

where Pr_t is the turbulent Prandtl number. In accordance with the number of additional equations introduced, turbulence models are grouped into five categories: **(Algebraic) Zero – equation models**, **One – equation models**, **Two – equation models**, **three – equation models** and **four – equation models**, Figure 7.4.

(Algebraic) Zero-equation models

Zero-equation models use an algebraic equation to compute μ_t without solving any additional differential equation. Some zero-equation models are **Prandtl mixing length model**, **Cebeci – Smith model** and **Baldwin – Lomax model** [95, 96, 97].

One-equation models

One-equation models use one further partial differential equation to solve the RANS equations by computing the turbulent eddy viscosity. Some one-equation models are: **Prandtl's one equation model**, **Baldwin – Barth model**, **Spalart – Allmaras model**, **Rahman – Siikonen – Agarwal model**, **Wray – Agarwal model** and **Shuai – Agarwal model** [98, 99, 100, 101, 102, 103].

Two-equation models

Two-equation models involve two further partial differential equations to run RANS simulations. Some models are the **$k - \varepsilon$ models**, **$k - \omega$ models**, **$k - \tau$ model** and **$k - kL$ model** [92, 104, 105, 106].

Three-equation models

Three equation models involve three transport equations for the closure of the RANS approach. A model of this type is the **$k - \varepsilon - R_t$ model** [107].

Four-equation models

This class of turbulence model use four transport equations and among others we have **$\overline{v^2} - f$ model** and **$\zeta - f$ model** [108, 109].

7.6.5 $k - \varepsilon$ Turbulence model

The $k - \varepsilon$ Turbulence model has been the chosen turbulent model to run the hydrodynamics RANS simulations of the problem where the inherent calibration constants have been sources of uncertainty in the output calculations. The model was formulated by Jones and Launder who expressed the turbulent viscosity and the thermal diffusivity as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (7.71)$$

and:

$$k_t = \frac{c_p \mu_t}{Pr_t}, \quad (7.72)$$

where the rate of dissipation of turbulent kinetic energy per unit mass due to viscous stresses is calculated by considering the fluctuating components of the velocity field:

$$\varepsilon = \frac{1}{2} \frac{\mu}{\rho} \overline{[\nabla \mathbf{v}' + (\nabla \mathbf{v}')^T] : [\nabla \mathbf{v}' + (\nabla \mathbf{v}')^T]}. \quad (7.73)$$

Specifically, for a two-dimensional flow, ε is determined as:

$$\varepsilon = \frac{\mu}{\rho} \overline{\left\{ 2 \left[\left(\frac{\partial u'}{\partial x} \right)^2 + \left(\frac{\partial v'}{\partial y} \right)^2 + \frac{\partial u'}{\partial y} \frac{\partial v'}{\partial x} \right] + \left(\frac{\partial u'}{\partial y} \right)^2 + \left(\frac{\partial v'}{\partial x} \right)^2 \right\}} \quad (7.74)$$

and for a three-dimensional flow we have:

$$\begin{aligned} \varepsilon = \frac{\mu}{\rho} \overline{\left\{ 2 \left[\left(\frac{\partial u'}{\partial x} \right)^2 + \left(\frac{\partial v'}{\partial y} \right)^2 + \left(\frac{\partial w'}{\partial z} \right)^2 + \frac{\partial u'}{\partial y} \frac{\partial v'}{\partial x} + \frac{\partial u'}{\partial z} \frac{\partial w'}{\partial x} + \frac{\partial v'}{\partial z} \frac{\partial w'}{\partial y} \right] + \left(\frac{\partial u'}{\partial y} \right)^2 + \right.} \\ \left. + \left(\frac{\partial v'}{\partial x} \right)^2 + \left(\frac{\partial u'}{\partial z} \right)^2 + \left(\frac{\partial w'}{\partial x} \right)^2 + \left(\frac{\partial v'}{\partial z} \right)^2 + \left(\frac{\partial w'}{\partial y} \right)^2 \right\}}. \end{aligned} \quad (7.75)$$

At this point, the transport equations of the turbulence models are:

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{\mathbf{v}} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon \quad (7.76)$$

and:

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \cdot (\rho \bar{\mathbf{v}} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + C_{\varepsilon_1} \frac{\varepsilon}{k} P_k - C_{\varepsilon_2} \rho \frac{\varepsilon^2}{k}, \quad (7.77)$$

where the production of turbulent kinetic energy P_k is determined by:

$$P_k = \boldsymbol{\tau}_R : \nabla \bar{\mathbf{v}} \quad (7.78)$$

which is equivalent to:

$$P_k = \mu_t \overline{\left\{ 2 \left[\left(\frac{\partial \bar{u}}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}}{\partial y} \right)^2 + \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{v}}{\partial x} \right] + \left(\frac{\partial \bar{u}}{\partial y} \right)^2 + \left(\frac{\partial \bar{v}}{\partial x} \right)^2 \right\}} \quad (7.79)$$

for a two-dimensional flow field, while is equivalent to:

$$\begin{aligned} P_k = \mu_t \overline{\left\{ 2 \left[\left(\frac{\partial \bar{u}}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}}{\partial y} \right)^2 + \left(\frac{\partial \bar{w}}{\partial z} \right)^2 + \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{v}}{\partial x} + \frac{\partial \bar{u}}{\partial z} \frac{\partial \bar{w}}{\partial x} + \frac{\partial \bar{v}}{\partial z} \frac{\partial \bar{w}}{\partial y} \right] + \left(\frac{\partial \bar{u}}{\partial y} \right)^2 + \left(\frac{\partial \bar{u}}{\partial z} \right)^2 + \right.} \\ \left. + \left(\frac{\partial \bar{v}}{\partial x} \right)^2 + \left(\frac{\partial \bar{v}}{\partial z} \right)^2 + \left(\frac{\partial \bar{w}}{\partial x} \right)^2 + \left(\frac{\partial \bar{w}}{\partial y} \right)^2 \right\}} \end{aligned} \quad (7.80)$$

for a three-dimensional flow. In conclusion, the standard values of the calibration constants of the $k - \varepsilon$ model are shown in Table 7.1

Table 7.1: Calibration constants of the $k - \varepsilon$ turbulence model

C_μ	C_{ε_1}	C_{ε_2}	σ_ε	σ_k
0.09	1.44	1.92	1.30	1.00

$k - \varepsilon$ Turbulence model for two-dimensional flows

Considering an extended representation, (7.76) and (7.77) for a bi-dimensiona flow are:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x}(\rho \bar{u}k) + \frac{\partial}{\partial x}(\rho \bar{v}k) &= \left(\mu + \frac{\mu_t}{\sigma_k}\right) \left(\frac{\partial^2 k}{\partial x^2} + \frac{\partial^2 k}{\partial y^2}\right) + \mu_t \left\{ 2 \left[\left(\frac{\partial \bar{u}}{\partial x}\right)^2 + \left(\frac{\partial \bar{v}}{\partial y}\right)^2 + \right. \right. \\ &\quad \left. \left. + \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{v}}{\partial x} \right] + \left(\frac{\partial \bar{u}}{\partial y}\right)^2 + \left(\frac{\partial \bar{v}}{\partial x}\right)^2 \right\} - \rho \varepsilon \end{aligned} \quad (7.81)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x}(\rho \bar{u} \varepsilon) + \frac{\partial}{\partial x}(\rho \bar{v} \varepsilon) &= \left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right) \left(\frac{\partial^2 \varepsilon}{\partial x^2} + \frac{\partial^2 \varepsilon}{\partial y^2}\right) + C_{\varepsilon_1} \frac{\varepsilon}{k} \mu_t \left\{ 2 \left[\left(\frac{\partial \bar{u}}{\partial x}\right)^2 + \left(\frac{\partial \bar{v}}{\partial y}\right)^2 + \right. \right. \\ &\quad \left. \left. + \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{v}}{\partial x} \right] + \left(\frac{\partial \bar{u}}{\partial y}\right)^2 + \left(\frac{\partial \bar{v}}{\partial x}\right)^2 \right\} - C_{\varepsilon_2} \rho \frac{\varepsilon^2}{k} \end{aligned} \quad (7.82)$$

$k - \varepsilon$ Turbulence model for three-dimensional flows

Considering an extended representation, (7.76) and (7.77) for a three-dimensiona flow are:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x}(\rho \bar{u}k) + \frac{\partial}{\partial x}(\rho \bar{v}k) + \frac{\partial}{\partial z}(\rho \bar{w}k) &= \left(\mu + \frac{\mu_t}{\sigma_k}\right) \left(\frac{\partial^2 k}{\partial x^2} + \frac{\partial^2 k}{\partial y^2} + \frac{\partial^2 k}{\partial z^2}\right) + \mu_t \left\{ 2 \left[\left(\frac{\partial \bar{u}}{\partial x}\right)^2 + \right. \right. \\ &\quad \left. \left. + \left(\frac{\partial \bar{v}}{\partial y}\right)^2 + \left(\frac{\partial \bar{w}}{\partial z}\right)^2 + \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{v}}{\partial x} + \frac{\partial \bar{u}}{\partial z} \frac{\partial \bar{w}}{\partial x} + \frac{\partial \bar{v}}{\partial z} \frac{\partial \bar{w}}{\partial y} \right] + \left(\frac{\partial \bar{u}}{\partial y}\right)^2 + \left(\frac{\partial \bar{u}}{\partial z}\right)^2 + \left(\frac{\partial \bar{v}}{\partial x}\right)^2 + \left(\frac{\partial \bar{v}}{\partial z}\right)^2 + \right. \\ &\quad \left. \left. + \left(\frac{\partial \bar{w}}{\partial x}\right)^2 + \left(\frac{\partial \bar{w}}{\partial y}\right)^2 \right\} - \rho \varepsilon \end{aligned} \quad (7.83)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x}(\rho \bar{u} \varepsilon) + \frac{\partial}{\partial x}(\rho \bar{v} \varepsilon) + \frac{\partial}{\partial z}(\rho \bar{w} \varepsilon) &= \left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right) \left(\frac{\partial^2 \varepsilon}{\partial x^2} + \frac{\partial^2 \varepsilon}{\partial y^2} + \frac{\partial^2 \varepsilon}{\partial z^2}\right) + \\ &\quad + C_{\varepsilon_1} \frac{\varepsilon}{k} \mu_t \left\{ 2 \left[\left(\frac{\partial \bar{u}}{\partial x}\right)^2 + \left(\frac{\partial \bar{v}}{\partial y}\right)^2 + \left(\frac{\partial \bar{w}}{\partial z}\right)^2 + \frac{\partial \bar{u}}{\partial y} \frac{\partial \bar{v}}{\partial x} + \frac{\partial \bar{u}}{\partial z} \frac{\partial \bar{w}}{\partial x} + \frac{\partial \bar{v}}{\partial z} \frac{\partial \bar{w}}{\partial y} \right] + \left(\frac{\partial \bar{u}}{\partial y}\right)^2 + \left(\frac{\partial \bar{u}}{\partial z}\right)^2 + \right. \\ &\quad \left. \left. + \left(\frac{\partial \bar{v}}{\partial x}\right)^2 + \left(\frac{\partial \bar{v}}{\partial z}\right)^2 + \left(\frac{\partial \bar{w}}{\partial x}\right)^2 + \left(\frac{\partial \bar{w}}{\partial y}\right)^2 \right\} - C_{\varepsilon_2} \rho \frac{\varepsilon^2}{k}. \end{aligned} \quad (7.84)$$

Chapter 8

Cavitation

8.1 Basic features of cavitation

Cavitation can also occur in a static or nearly static liquid when an oscillating pressure field is applied over the free surface of a liquid contained in a reservoir and it can appear within the liquid bulk under large oscillations [110]. In this chapter, the main physical characteristics of the phenomenon of cavitation are discussed; subsequently, there have been explained the dynamics of cavities by considering the Rayleigh-Plesset equation and a review of the most famous cavitation models has been applied. Finally, the Schnner-Sauer cavitation model, which is the cavitation model employed in this study, is described.

8.2 Basic features of cavitation

Considering water, for example, the fluid is represented by a phase diagram to describe their states of matter related to pressure and temperature, Figure 8.1.

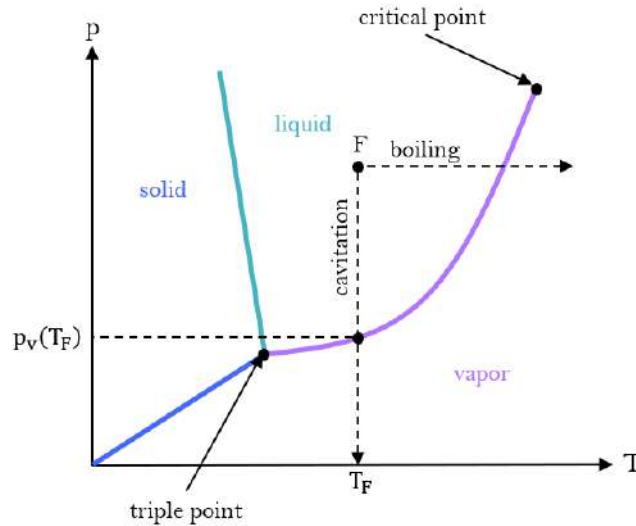


Figure 8.1: Diagram phase of liquids

Considering a point F where the substance is a liquid, the cavitation arises when the pressure decreases below the vapor pressure p_v at a constant temperature. The behaviour of cavitation is similar to fluids boiling. Theoretically, cavitation consists of the three steps: breakdown or void creation, filling of void with vapor and eventual saturation with vapor, which occur simultaneously

in real fluids. In fluids with rapid phase change, the p_v curve is not an absolute boundary between liquid and vapor states and the phase change may do not occur for $p < p_v$.

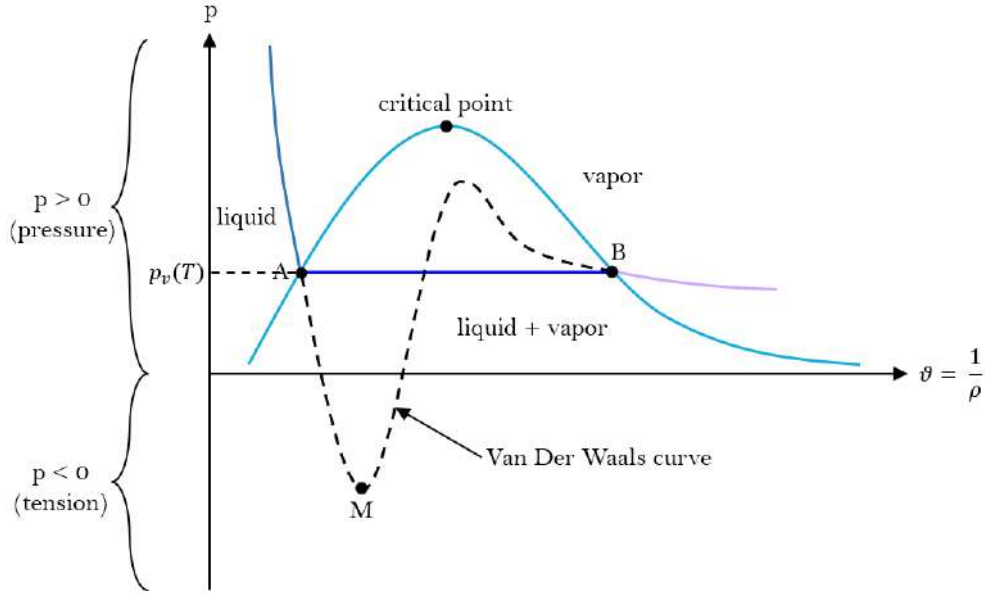


Figure 8.2: Diagram phase of liquids

For example, taking into account the Andrew-Isotherms curve, Figure 8.2, we can use the Van Der Waals equation of state:

$$\left(p + \frac{a}{\vartheta^2}\right)(\vartheta - b) = RT \quad (8.1)$$

to identify the domains of liquid and vapor phases. The transformation from liquid to vapor along the path AM can be avoided; along this path the liquid is in metastable equilibrium having at $p < 0$ without phase changes and then, even if $p < p_v$, cavitation does not occur. Initially, cavities are strongly influenced by the main flow structure but during the growing, they tend to disturb and modify the basic flow. Cavitation patterns are divided into three groups:

- **Transient isolated bubbles** where the presence of cavitation is localized in the region of low pressure. These bubbles disappear when they enter in regions of high pressure.
- **Attached or sheet cavities** where cavities are attached to the leading edge of solid bodies.
- **Cavitating vortices** where cavities manifest in low pressure regions of vortices in turbulent wakes or as a regular pattern in tip vortices of 3D wings or propeller blades.

In particular studies, cavitation is classified into:

- **Cavitation inception:** cavitation appears and disappears in the regime between the non-cavitating and the cavitating flow.
- **Developed cavitation:** cavitation is persistent.

Cavitation can arise from particular geometries in which the local velocity grows up and the local pressure decreases consistently. Cavitation can arise for the presence of large turbulent pressure fluctuations and unsteady nature of some flows. Furthermore, cavitation can occur for surface roughness and vibratory motions of walls.

8.2.1 Cavitation numbers

Cavitation numbers are dimensionless number used for quantifying the cavitation in a hydrodynamic system with reference to the cavitation region and cavitation nature. Cavitation numbers are classified into: **cavitation number σ_v** , **cavitation number at inception σ_{v_i}** and **cavitation number at inception σ_c** .

Cavitation number σ_v

The cavitation number is used to predict the hydrodynamic cavitation; it is defined as:

$$\sigma_v = \frac{p_r - p_v(T)}{\Delta p}, \quad (8.2)$$

where p_r is the local absolute pressure and $p_v(T)$ is the vapor pressure of the fluid at the operating temperature T . In accordance with the case of study, the cavitation number is expressible as:

$$\sigma_v = \begin{cases} \frac{p_{\text{downstream}} - p_v(T)}{p_{\text{upstream}} - p_{\text{downstream}}} & \text{for a gate} \\ \frac{p_0 + \rho gh - p_v(T)}{\frac{1}{2} \rho V^2} & \text{for a foil placed at a submersion depth } h \text{ in a} \\ & \text{horizontal free surface at surface pressure } p_0 \\ & \text{and velocity flow } V \\ \frac{p_{\text{inlet}} - p_v(T)}{\rho V_p^2} & \text{for a pump with periphery velocity } V_p \end{cases} \quad (8.3)$$

The lower the cavitation number, the higher the probability of cavitation.

Cavitation number at inception σ_{v_i}

σ_{v_i} is the value of σ_v corresponding to cavitation inception at any point of the flow system. In non-cavitating flows we have:

$$\sigma_v > \sigma_{v_i} \quad (8.4)$$

and the smallest σ_{v_i} , the better behaved the flow is. In numerical modeling of cavitating flows, the following restriction is typically considered:

$$\sigma_{v_i} = - \left. \frac{p_M - p_r}{\Delta p} \right|_{\min} \quad (8.5)$$

where p_M is the pressure at the point M . The formulation of σ_{v_i} lies two potentially restrictive assumptions: cavitation occurs at the point of minimum pressure and pressure threshold value is that of the vapor pressure.

Cavitation number at inception σ_c

The relative underpressure of a cavity is a dimensionless parameter introduced for an attached developed cavity or for a large number of bubbles in the flow so that the pressure p_c in the region covered by the cavity is assumed to be uniform. The coefficient is expressed as:

$$\sigma_c = \frac{p_r - p_c}{\Delta p} \quad (8.6)$$

This number is used in numerical modeling of developed cavitation. Generally, the pressure p_c is the sum of p_v and p_g which is the partial pressure due to the presence of non-condensable gas within the cavity.

8.2.2 Nuclei

In real fluids, it is possible to have pressures lower than the vapor pressure without the appearance of vaporization. Real fluids are not fully homogeneous but they contain points of small gas and vapor inclusions which operate as starting points for the liquid breakdown (by assumption). These points are named cavitation nuclei. Their size is between a few micrometers and some hundreds of micrometers and are the cause of generation of cavitation. Nuclei are produced by reducing the pressure of a saturated liquid and their evolutions are influenced by the gravity. There are free nuclei where which are not attached to any wall and in general, nuclei are described by their equilibrium conditions and gas diffusion behaviour.

Nuclei equilibrium

For hypothesis, the mass diffusion is considered and the mass of the enclosed gas is assumed to be constant. It is considered a spherical microbubble with radius R containing gas with pressure p_g and vapor with pressure p_v such that the total pressure p_{tot} is given by (Figure 8.3):

$$p_{\text{tot}} = p_g + p_v. \quad (8.7)$$

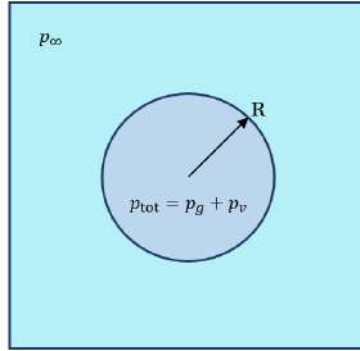


Figure 8.3: Bubble of vapor.

The bubble is enough small to neglect the effects of the hydrostatic pressure which is given by the condition:

$$R < \sqrt{\frac{\mathcal{S}}{\rho g}}, \quad (8.8)$$

where $\mathcal{S}$ is the surface tension. The liquid pressure around the bubble is denoted as p_{∞} and the equilibrium of the interface is given by:

$$p_{\infty} = p_g + p_v - \frac{2\mathcal{S}}{R}. \quad (8.9)$$

It is assumed that the pressure changes slowly enough such that the mechanical equilibrium is satisfied and heat transfer between gas and liquid is possible but the change must be sufficiently rapid to neglect the gas diffusion at the interface. For these reasons, the process is considered isothermal and the gas mass is assumed constant. For the initial state, where p_{∞_0} is the initial liquid pressure, p_{g_0} is the initial gas pressure and R_0 is the initial bubble radius, we have:

$$p_{\infty_0} = p_{g_0} + p_v - \frac{2\mathcal{S}}{R_0}. \quad (8.10)$$

and supposing an isothermal transformation:

$$p_{\infty} = p_{g_0} \left(\frac{R_0}{R} \right)^3 + p_v - \frac{2\mathcal{S}}{R}. \quad (8.11)$$

Thanks to (8.11), we have an expression for the curve of $p_{\infty} = f(R)$ represented in Figure 8.4.

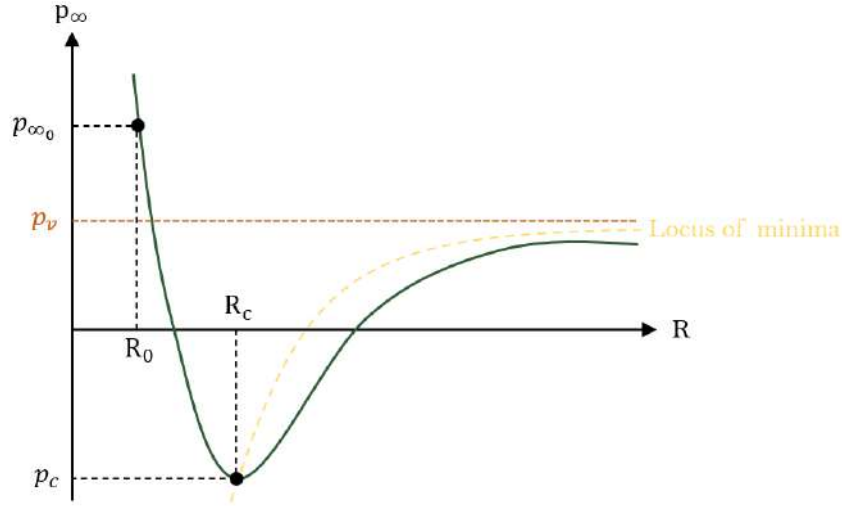


Figure 8.4: p_∞ as function of R

The bubble is subject to an internal pressure effect, which tends to increase the bubble size and a surface tension effect which acts in the opposite direction. The equilibrium of these two effects leads to the existence of a minimum given by:

$$\begin{cases} R_c = R_0 \sqrt{\frac{3p_{g0}}{\frac{2S}{R_0}}} \\ p_c = p_v - \frac{4S}{3R_c} \end{cases} \quad (8.12)$$

Equilibrium of spherical nuclei is stable on the branch of the curve that has a negative slope. Figure 8.4 takes into account also the unstable domain (where $p_\infty < 0$) but in practice, only stable domains are treated (where $p_\infty > 0$) and then, another expression of p_∞ is needed. Using $p_v - p_c$ (static delay to cavitation) and (8.11) with (8.12), we can rewrite p_∞ as a function of $p_v - p_c$:

$$p_\infty = p_{g0} \left(\underbrace{\frac{16S^2}{9(p_v - p_c)^2 \frac{3p_{g0}}{2S}}}_{=R_0^3} \right) \frac{1}{R^3} + p_v - \frac{2S}{R} = \frac{4}{27} \frac{\left(\frac{2S}{R}\right)^3}{(p_v - p_c)^2} + p_v - \frac{2S}{R}. \quad (8.13)$$

In conclusion, the larger nuclei, (which are more likely to generate a breakdown of the liquid medium), the smaller the static decay.

8.3 Dynamics of spherical bubbles

8.3.1 Hypothesis

The dynamic of spherical bubbles is described by the Rayleigh-Plesset differential equation. We consider the dynamic evolution of spherical bubbles with fixed centers that undergo uniform pressure variations at infinity. For hypothesis we have that the liquid is incompressible or Newtonian or inviscid, gravity is neglected, the air inside the bubble is constant, the air inertia is neglected, the exchange of heat is neglected, the adiabaticity is assumed for large bubbles and the bubble is saturated with vapor whose partial pressure is the vapor pressure at the liquid bulk temperature. As shown in Figure (8.5), the equations are solved for $r \leq R(t)$ where $u(r, t)$ and $p(r, t)$ are the velocity and the pressure at the point r .

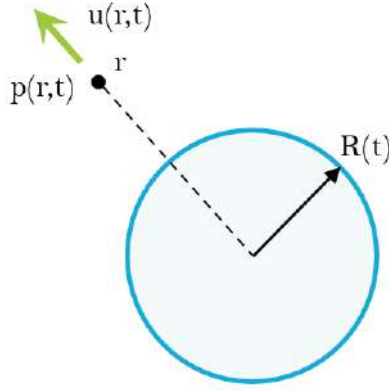


Figure 8.5: model of bubble

8.3.2 Boundary and initial conditions

Boundary and initial conditions imposed to describe the Rayleigh-Plesset equation are following discussed. Firstly, the mass transfer is neglected:

$$\dot{m} = 0, \quad (8.14)$$

the liquid velocity at the interface is equal to the interface velocity:

$$u(r, t) = \frac{dR}{dt}, \quad (8.15)$$

the normal stress is expressed as:

$$\tau_{rr}(R, t) = -p(R, t) + 2\mu \left. \frac{\partial u}{\partial r} \right|_{r=R}, \quad (8.16)$$

the balance of normal forces is:

$$-\tau_{rr}(R, t) = p_v + p_g(t) - \frac{2S}{R}, \quad (8.17)$$

and after, under the assumption of adiabatic transformation of gas, the instantaneous gas pressure is:

$$p_g(t) = p_{g0} \left(\frac{R_0}{R} \right)^{3\gamma}, \quad (8.18)$$

where:

$$\gamma = \frac{c_p}{c_v}. \quad (8.19)$$

At this point, the pressure on the cavity interface is:

$$p(R, t) = p_v + p_{g0} \left(\frac{R_0}{R} \right)^{3\gamma} - \frac{2S}{R} + 2\mu \left. \frac{\partial u}{\partial r} \right|_{r=R}, \quad (8.20)$$

the velocity tends to zero at the infinity:

$$\lim_{R \rightarrow +\infty} u(r, t) \rightarrow 0, \quad (8.21)$$

the pressure is posed equal to a known value at the infinity:

$$\lim_{R \rightarrow +\infty} p(R, t) = p_\infty(t) \quad (8.22)$$

and in conclusion the bubble is initially in an equilibrium state:

$$\begin{cases} \frac{dR}{dt}(0) = 0 \\ p_\infty(0) = p_{\infty_0} = p_{g_0} + p_v - \frac{2\mathcal{S}}{R_0} \end{cases} \quad (8.23)$$

8.3.3 Rayleigh-Plesset equation

As first consideration, taking into account the spherical symmetry of bubble, the fluid has an irrotational behaviour such that the curl of the velocity field is null:

$$\nabla \times \mathbf{v} = 0 \quad (8.24)$$

and for the incompressible condition we have:

$$\nabla \cdot \mathbf{v} = 0. \quad (8.25)$$

At this point, the mass conservation equation is expressed as:

$$u(r, t) = \frac{dR}{dt} \frac{R^2}{r^2} \quad (8.26)$$

and the linear momentum equation in spherical coordinates is given by the expression:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial r} = -\frac{1}{\rho} \frac{\partial p}{\partial r} \quad (8.27)$$

which is coupled with the equation (8.26):

$$\frac{\partial}{\partial t} \left(\frac{dR}{dt} \frac{R^2}{r^2} \right) + \left(\frac{dR}{dt} \frac{R^2}{r^2} \right) \frac{\partial}{\partial r} \left(\frac{dR}{dt} \frac{R^2}{r^2} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial r} \Rightarrow \frac{d^2 R}{dt^2} \frac{R^2}{r^2} + 2 \left(\frac{dR}{dt} \right)^2 \left(\frac{R}{r} - \frac{R^4}{r^5} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial r}. \quad (8.28)$$

Integrating (8.28) from r to $+\infty$, one obtains:

$$\begin{aligned} \int_r^{+\infty} \left[\frac{d^2 R}{dt^2} \frac{R^2}{\tilde{r}^2} + 2 \left(\frac{dR}{dt} \right)^2 \left(\frac{R}{\tilde{r}} - \frac{R^4}{\tilde{r}^5} \right) \right] d\tilde{r} &= - \int_r^{+\infty} \frac{1}{\rho} \frac{\partial p}{\partial \tilde{r}} d\tilde{r} \Rightarrow \frac{d^2 R}{dt^2} R^2 \left(-\underbrace{\frac{1}{r_\infty}}_{=0} + \frac{1}{r} \right) + \\ &+ 2 \left(\frac{dR}{dt} \right)^2 R \left(-\underbrace{\frac{1}{r_\infty}}_{=0} + \frac{1}{r} \right) - 2 \left(\frac{dR}{dt} \right)^2 R^4 \left(-\underbrace{\frac{1}{4r_\infty^4}}_{=0} + \frac{1}{4r^4} \right) = -\frac{1}{\rho} [p_\infty(t) - p(r, t)] \Rightarrow \frac{d^2 R}{dt^2} \frac{R^2}{r} + \\ &+ 2 \left(\frac{dR}{dt} \right)^2 \left(\frac{R}{r} - \frac{R^4}{4r^4} \right) = \frac{p(r, t) - p_\infty(t)}{\rho} \end{aligned} \quad (8.29)$$

which is equivalent to the Bernoulli equation for a variable in an unsteady flow of non-viscous liquid. Now, on the interface we have:

$$r = R \quad (8.30)$$

so that, (8.29) becomes:

$$\frac{d^2 R}{dt^2} R + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 = \frac{p(R, t) - p_\infty(t)}{\rho}. \quad (8.31)$$

Futhermore, from (8.26), we have:

$$\frac{\partial u}{\partial r} = -2 \frac{dR}{dt} \frac{R^2}{r^3} \Rightarrow \frac{\partial u}{\partial r} \Big|_{r=R} = -2 \frac{dR}{dt} \frac{1}{R}. \quad (8.32)$$

Putting together (8.20), (8.31) and (8.32) we have the Rayleigh-Plesset equation:

$$\rho \left[R \frac{d^2 R}{dt^2} + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 \right] = p_v - p_\infty(t) + p_{g0} \left(\frac{R_0}{R} \right)^{3\gamma} - \frac{2\mathcal{S}}{R} - 4\mu \frac{dR}{dt} \frac{1}{R} \quad (8.33)$$

which allows to determine the temporal evolution of the radius R and the pressure field when $p_\infty(t)$ is known. For non-viscous flows there is:

$$\rho \left[R \frac{d^2 R}{dt^2} + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 \right] = p_v - p_\infty(t) + p_{g0} \left(\frac{R_0}{R} \right)^{3\gamma} - \frac{2\mathcal{S}}{R} \quad (8.34)$$

which is simply named Rayleigh equation.

8.4 Cavitation modeling

The modeling of cavitation in numerical simulations has been found many challenges due to the fact that the treatment of cavitation involves a multiphase flow and consequently, both Navier-Stokes equations (specifically the RANS equations) and cavitation models (which describes the formation, growth, motion, shape and collapse of cavities) must be satisfied at the same time. Formally, two main modeling approaches have been applied in Fluid Dynamics to study cavitation: **homogeneous mixture approach** and **homogeneous mixture with further cavitating effects approach** which are described below[111].

8.4.1 Homogeneous mixture approach

Homogeneous mixture approach is the most commonly used in cavitation models. The main physical hypothesis is based on the thermal and mechanical equilibrium between the two vapour and liquid phases. Both phases have the same velocity and pressure fields and are locally defined in a homogeneous mixture. So, the mixture density ρ_m and the mixture dynamic viscosity μ_m are calculated as:

$$\rho_m = \rho = \alpha \rho_v + \gamma \rho_l = \alpha \rho_v + (1 - \alpha) \rho_l \quad (8.35)$$

$$\mu_m = \mu = \alpha \mu_v + \gamma \mu_l = \alpha \mu_v + (1 - \alpha) \mu_l \quad (8.36)$$

where ρ_v is vapour density, ρ_l is the liquid density, μ_v is the vapour dynamic viscosity and μ_l is the liquid dynamic viscosity and:

$$\alpha = \frac{V_{\text{vapour}}}{V_{\text{total}}} : \text{vapour fraction} \quad (8.37)$$

$$\gamma = \frac{V_{\text{liquid}}}{V_{\text{total}}} : \text{liquid fraction} \quad (8.38)$$

$$\alpha + \gamma = 1. \quad (8.39)$$

8.4.2 Homogeneous mixture with further cavitating effects approach

If one wishes to describe cavitation from a more comprehensive and refined perspective, the homogeneous mixture approach can be extended by incorporating additional effects that are typically neglected to simplify the study of cavitation.

8.4.3 Model categories for homogeneous mixture flows

As introduced, the cavitation modeling based on the application of a homogeneous mixture approach is the most commonly developed in practical applications. This macro family of models can be sub-classified into five categories: **Category of Transport Equation Model (TEM)**, **Category of Rayleigh – Plesset Equation (RPE)**, **Category of Equation Of State (EOS)**, **Category of Interface Tracking Model (ITM)** and **Category of Multiscale (MUL)** [111].

Category of Transport Equation Model (TEM)

One of the most important implementations in cavitation modeling is the application of a modified volume-of-fluid approach in order to describe the dynamic of the system by a modified transport equation:

$$\nabla \cdot \bar{\mathbf{v}} = \dot{m} \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \quad (8.40)$$

in reference to the vapour fraction:

$$\frac{\partial}{\partial t} (\rho_v \alpha) + \nabla \cdot (\rho_v \alpha \bar{\mathbf{v}}) = \dot{m} \quad (8.41)$$

or in reference to the liquid fraction:

$$\frac{\partial}{\partial t} (\rho_l \gamma) + \nabla \cdot (\rho_l \gamma \bar{\mathbf{v}}) = \dot{m} \quad (8.42)$$

where $\dot{m}$ is the mass transport rate. Cavitation models employed in Category of Transport of Transport Equation Model define an expression for the mass transfer rate. It is important to note that if the transport equations are evaluated in terms of vapour fraction (8.41), the mixture physical greatness are expressed in terms of vapour fraction as in (8.35) and (8.36), otherwise, if the transport equations are evaluated in terms of liquid fraction (8.42), the mixture physical quantities are given in terms of liquid fraction [112]:

$$\rho_m = \rho = (1 - \gamma)\rho_v + \gamma\rho_l \quad (8.43)$$

$$\mu_m = \mu = (1 - \gamma)\mu_v + \gamma\mu_l. \quad (8.44)$$

To formulate a right expression for $\dot{m}$, additional assumptions are required. The most commonly used approach is to consider that in each computational cell, the vapour fraction quantity is equal to the amount of volume of the cell occupied by bubbles of vapour (nuclei) which grow and collapse in accordance with the local pressure.

Category of Rayleigh-Plesset Equation (RPE)

Category of Rayleigh Plesset equation is introduced to express the growth and collapse of vapour nuclei by using the equation (8.33). Some cavitation models which are simply based on that equation and cavitation models of Category of transport Equation Model which formulate the appropriate expression for $\dot{m}$ by considering the theory of Rayleigh-Plesset. As known, the Rayleigh-Plesset equation can evaluate the evolution of radius of spherical bubbles under the effect of an environmental pressure p_∞ where the internal pressure of bubbles are p_v . Often, the surface tension and internal effects are neglected so that the simplified rayleigh equation is implemented.

Category of Equation Of State (EOS)

This Category is focused on defying an equation of state to describe the thermodynamic behaviour of cavitating flows such that it is possible to model a quantity of reference which represent the two phase flows. Often, that quantity is the density. The methods based on this category need less hypothesis to be used and they can be also employed for cryogenic flows due to the inclusion of thermodynamic effects.

Category of Interface Tracking Model (ITM)

All models within this category employ a scheme that directly track the interface between the liquid and the vapour phases.

Category of Multiscale (MUL)

Models about Category of Multiscale apply several schemes to simulate the growth and collapse of cavities. cavities are modelled by using different length scales.

8.4.4 Model categories for homogeneous mixture with further cavitating effects flows

A second categorization of cavitation models was developed to describe the presence of additional phenomena involved in the onset and evolution of cavitation. The four new categories are exactly: **Category of Turbulence (TUR)**, **Category of Population Balance (POP)**, **Category of Empirical (EMP)** and **Category of Non – condensable Gas (NCG)**.

Category of Turbulence (TUR)

This category of cavitation models takes into consideration the effects of local fluctuations of pressure induced by turbulent flow. These turbulence effects feed the cavitation inception where the generated cavities are bombarded by the eddies of the turbulent flow, causing deformations on cavity surfaces which are destroyed into smaller cavities.

Category of Population Balance (POP)

Category of population balance takes into account cavity populations changes by analyzing the bubble number distribution. For example, the population change can be due to the turbulence effects of flows.

Category of Empirical (EMP)

The models of this category include empirical constants to improve simulations of characteristic flows.

Category of Non-condensable Gas (NCG)

In this category, the effect of non-condensable gas are taken into account. In this manner, the cavitation is manipulated from a two phase model to a three phase model and the mixture density and the mixture dynamic viscosity are re-written as:

$$\rho_m = \rho = \alpha\rho_v + \alpha_{ng}\rho_{ng} + \gamma\rho_l = \alpha\rho_v + \alpha_{ng}\rho_{ng} + (1 - \alpha - \alpha_{ng})\rho_l \quad (8.45)$$

$$\mu_m = \mu = \alpha\mu_v + \alpha_{ng}\mu_{ng} + \gamma\mu_l = \alpha\mu_v + \alpha_{ng}\mu_{ng} + (1 - \alpha - \alpha_{ng})\mu_l \quad (8.46)$$

where ρ_{ng} is the non-condensable gas density, μ_{ng} is the non-condensable gas dynamic viscosity and:

$$\alpha_{ng} = \frac{V_{\text{non-gas}}}{V_{\text{total}}} : \text{non-condensable gas fraction} \quad (8.47)$$

$$\alpha + \gamma + \alpha_{ng} = 1. \quad (8.48)$$

8.4.5 Cavitation models in numerical simulations

The Cavitation models developed for numerical simulations have been constructed to treat homogeneous mixture flows without and with additional cavitating effects in accordance with the mentioned categories. The methods are calibrated by following initial hypothesis of problem of interest. The most famous cavitation models are **Zwart et Al. model** [113], **Kunz et Al. model** [114], **Denner et Al. model** [115], **Ghahramani et Al. model** [116], **Hsiao et Al. model** [117], **Li and Carrica model** [118], **Kubota et Al. model** [119], **Shi et Al. model** [120], **Deshpande et Al. model** [121], **Huang and Wang model** [122], **Konstantinov et Al. model** [123], **Goncalves and Charriere model** [124], **Ventikos and Tzabiras model** [125], **Banerjee and Satitha model** [126], **Shingal et Al. model** [127], **Senocak and Shyy model** [128], **Liu et At. model** [129] and **Schnerr and Sauer model** [130] which is the turbulene model employed to investigate the cavitating flow around the NACA66(MOD) hydrofoil and the PPTC propeller.

Schnerr and Sauer model - The Bubble Density Liquid Volume Coupling Model

The Schnerr-Sauer model follows the Singhal model approach. The transport equation for the vapour fraction is expressed in the form shown below:

$$\frac{\partial}{\partial t} (\rho_v \alpha) + \nabla \cdot (\rho_v \alpha \mathbf{v}) = \frac{\rho_v \rho_l}{\rho} \frac{d\alpha}{dt} = \dot{m} \quad (8.49)$$

The model writes α :

$$\alpha = \frac{n_b V_b}{1 + n_b V_b} = \frac{n_b \frac{4}{3} \pi R^3}{1 + n_b \frac{4}{3} \pi R^3} \quad (8.50)$$

and considering the Right Hand Side of (8.50) and (8.50) we have:

$$\begin{aligned} \dot{m} &= \frac{\rho_v \rho_l}{\rho} \frac{d}{dt} \left(\frac{n_b \frac{4}{3} \pi R^3}{1 + n_b \frac{4}{3} \pi R^3} \right) = \frac{\rho_v \rho_l}{\rho} \left[\frac{(n_b 4\pi R^2 \frac{dR}{dt}) (1 + n_b \frac{4}{3} \pi R^3) - (n_b \frac{4}{3} \pi R^3) (n_b 4\pi R^2 \frac{dR}{dt})}{(1 + n_b \frac{4}{3} \pi R^3)^2} \right] = \\ &= \frac{\rho_v \rho_l}{\rho} \left[\frac{n_b 4\pi R^2 \frac{dR}{dt}}{(1 + n_b \frac{4}{3} \pi R^3)^2} \right] = \frac{\rho_v \rho_l}{\rho} \left(\frac{\alpha}{1 + n_b \frac{4}{3} \pi R^3} \right) \frac{3}{R} \frac{dR}{dt} = \frac{\rho_v \rho_l}{\rho} \alpha (1 - \alpha) \frac{3}{R} \frac{dR}{dt}. \end{aligned} \quad (8.51)$$

In conclusion, the same assumptions of the Rayleigh-Plesset equation in the Zwart model (equation (E.1)) have been applied to express the mass transport rate as:

$$\dot{m} = \begin{cases} \frac{\rho_v \rho_l}{\rho} \alpha (1 - \alpha) \frac{3}{R} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} & \text{for } p \leq p_v \\ \frac{\rho_v \rho_l}{\rho} \alpha (1 - \alpha) \frac{3}{R} \sqrt{\frac{2}{3} \left(\frac{p - p_v}{\rho_l} \right)} & \text{for } p > p_v \end{cases} \quad (8.52)$$

The Schneer-Sauer cavitation model is the natural cavitation model of Simcenter Star CCM+ and it has been the model used in the current work.

All cavitation models can be associated with one or more categories. In Figure 8.6, the categories corresponding to each cavitation model from the first classification, i.e. models based on homogeneous mixture flows are presented while in Figure 8.7 illustrates the second classification, which includes homogeneous mixture flows with additional cavitating effects.

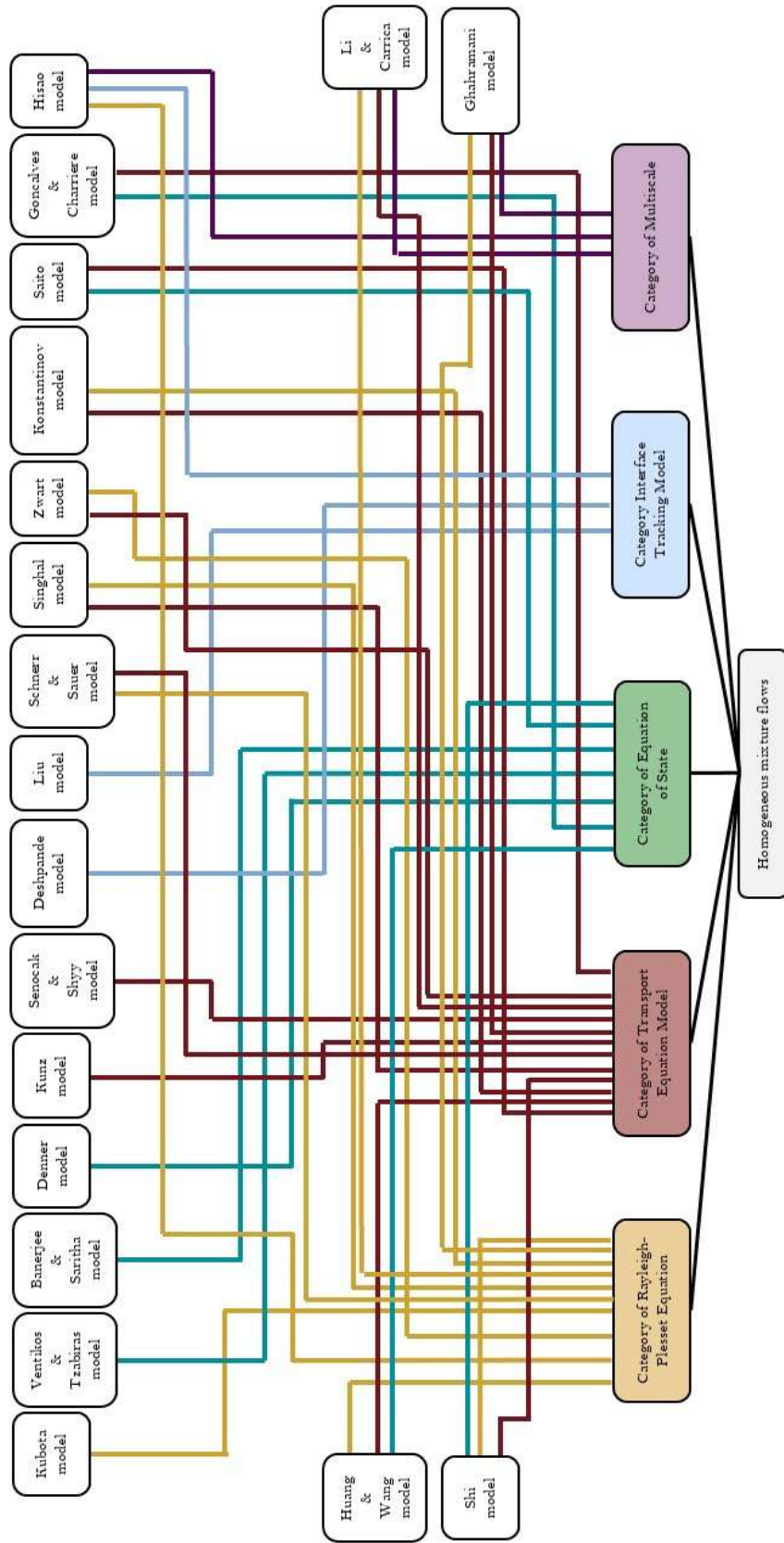


Figure 8.6: Classification of cavitation models for homogeneous mixture flows.

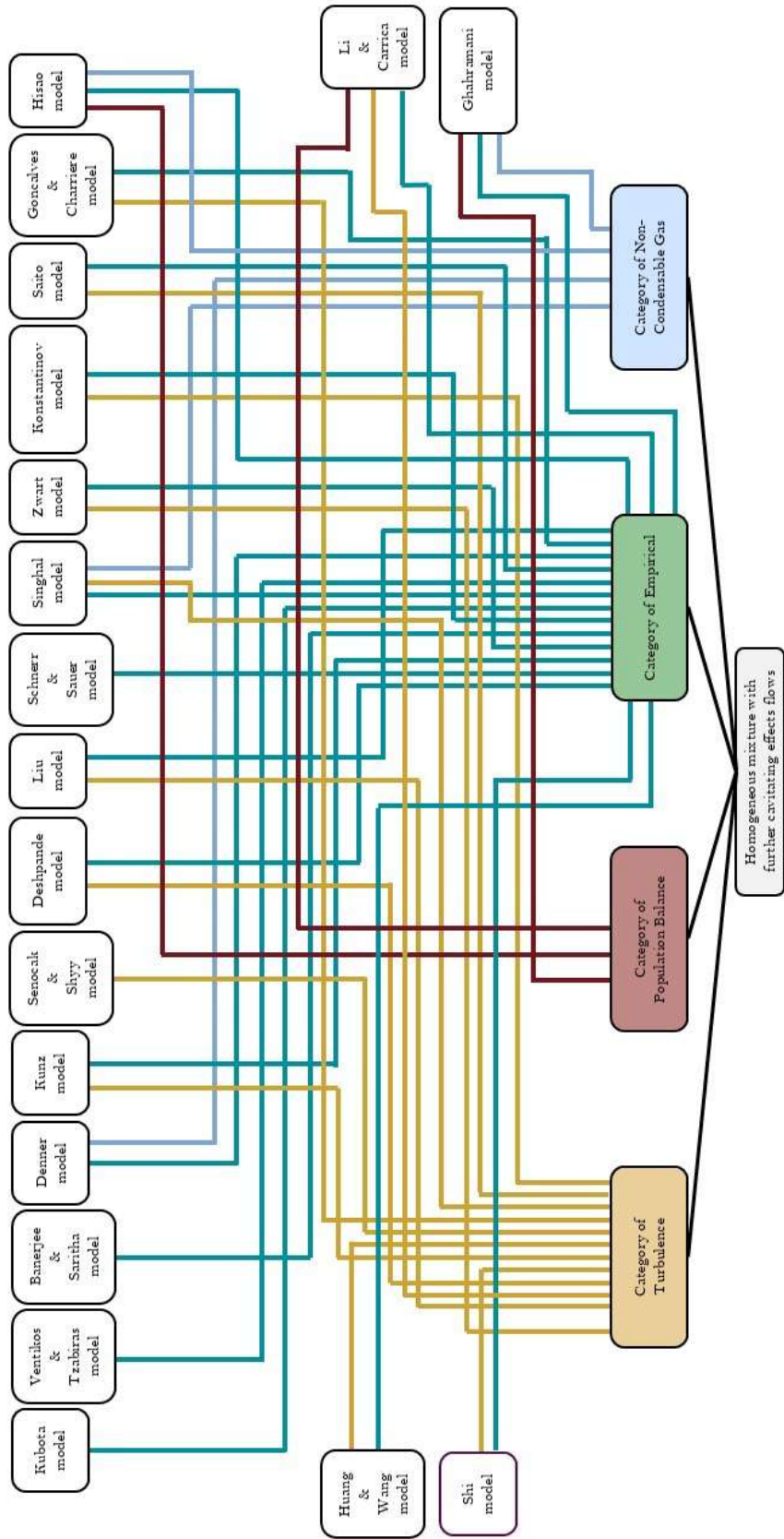


Figure 8.7: Classification of cavitation models for homogeneous mixture flows with further cavitating effects.

Chapter 9

NACA66(MOD) hydrofoil

9.1 Introduction

The first object of interest of the following work has been a two-dimensional geometry lapped by a cavitating and non cavitating flow. In this chapter, the numerical framework, mesh and boundary and initial conditions of the hydrodynamic simulations of the NACA66(MOD) hydrofoil have been described. Furthermore, the geometry of NACA66(MOD) has been described.

9.2 Numerical framework

Numerical simulations have been initialized from the setting of $k - \varepsilon$ Turbulence model coefficients. All parameters have been considered linearly independent in order to ensure the validity of orthogonal expansion and Sobol decomposition. The calibration constants have been setted as uniformly distributed random variables as consequence of lack of knowledge about preferential numerical values of these quantities. Their random domains (sensitivity intervals) are shown in Table 9.1 and their choice has been in line with descriptions in [135] at exception for the sensitivity interval of σ_ε which has been determined by taking into account the Pope equation [136]:

$$\sigma_\varepsilon = \frac{k_{VK}^2}{C_\mu^{\frac{1}{2}} (C_{\varepsilon_2} - C_{\varepsilon_1})} \rightarrow \begin{cases} \sigma_\varepsilon|_{\min} = \frac{k_{VK}^2}{C_\mu^{\frac{1}{2}}|_{\max} (C_{\varepsilon_2}|_{\max} - C_{\varepsilon_1}|_{\max})} \\ \sigma_\varepsilon|_{\max} = \frac{k_{VK}^2}{C_\mu^{\frac{1}{2}}|_{\min} (C_{\varepsilon_2}|_{\min} - C_{\varepsilon_1}|_{\min})} \end{cases} \quad (9.1)$$

Table 9.1: Sensitivity intervals of $k - \varepsilon$ turbulence model coefficients

Coefficient	Lower Bound	Upper Bound	Interval	Standard Value
C_μ	0.050	0.150	0.100	0.090
C_{ε_1}	1.000	1.500	0.500	1.440
C_{ε_2}	1.500	3.000	1.500	1.920
σ_ε	0.290	1.500	1.210	1.300
σ_k	0.800	1.400	0.600	1.000

Applying (4.13) to quantify the number of samplings and considering an oversampling ratio of 2 (4.14), a Polynomial Chaos Expansion of the 2nd, 3rd, 4th and 5th order has been employed to investigate the Forward Propagation of Uncertainty and the Global Sensitivity Analysis of the five turbulent parameters with respect to the hydrodynamic coefficients of lift and drag.

A further study has been conducted by applying a second order polynomial chaos expansion and the Sobol decomposition with respect to pressure and friction coefficients.

In conclusion, a comparison between the Polynomial Chaos Expansion and the Polynomial Chaos-based Kriging has been employed to investigate the performance of both metamodels by fixing the number of samples. The choice is justified by the fact that in some Uncertainty Quantification studies, it is not possible to generate a Design Of Experiment by employing an arbitrary set of points but it could be limited to a fixed set of collocation points. For this reason, It is important to evaluate the best adaptable surrogate model for the problem of interest.

Taking into account the DOE of 42 collocation points named "few points" and 504 collocation points named "many points", Polynomial Chaos Expansion and Polynomial Chaos Kriging have been generated for both the sets by increasing the polynomial order from a second to a tenth. Specifically, the Polynomial Chaos-based Kriging has been constructed by applying an optimal approach. Matern $\frac{5}{2}$ correlation functions have been applied and the hyperparameters have been computed by using a hybrid genetic algorithm. For each polynomial expansion, the Leave-One-Out Cross-Validation error has been computed to evaluate the performance of these surrogate model and Sobol indices have been determined. Sobol indices of first and total order, which is associated with Polynomial Chaos Kriging have been evaluated by using Monte Carlo approaches for the lift and drag coefficients.

The Design Of Experiment (DOE) has been generated by applying a Latin Hypercube Sampling strategy imposing an uniform probability distribution for each initial variable of the problem. In order to use a Non-Intrusive Polynomial Chaos approach, the number of collocation points required to generate the response surfaces are:

$$K = \begin{cases} K = 42 & \text{for a second polynomial order} \\ K = 112 & \text{for a third polynomial order} \\ K = 252 & \text{for a fourth polynomial order} \\ K = 504 & \text{for a fifth polynomial order} \end{cases} \quad (9.2)$$

and in Figures 9.1, 9.2, 9.3 and 9.4, the sampled domains of the five calibration constants of the Standard $k - \varepsilon$ model are shown.

After that, the numerical simulations for each collocation has been carried out through the commercial Simcenter Star CCM+ [137]. The results obtained by the numerical calculus (i.e. lift coefficient, drag coefficient, friction coefficient and pressure coefficient), has been used to generate the Polynomial Chaos and Polynomial Chaos Kriging. The computation of polynomial coefficients for both the models has been performed by the application of the Sparse approach based on the Least Angle Regression (LAR) method. The computed coefficients have been employed to compute mean values, standard deviations, confidence Intervals of outputs and Sobol indices of the initial parameters for the Polynomial Chaos Expansion. A graphical representation of the numerical strategy is shown in Figure 9.5

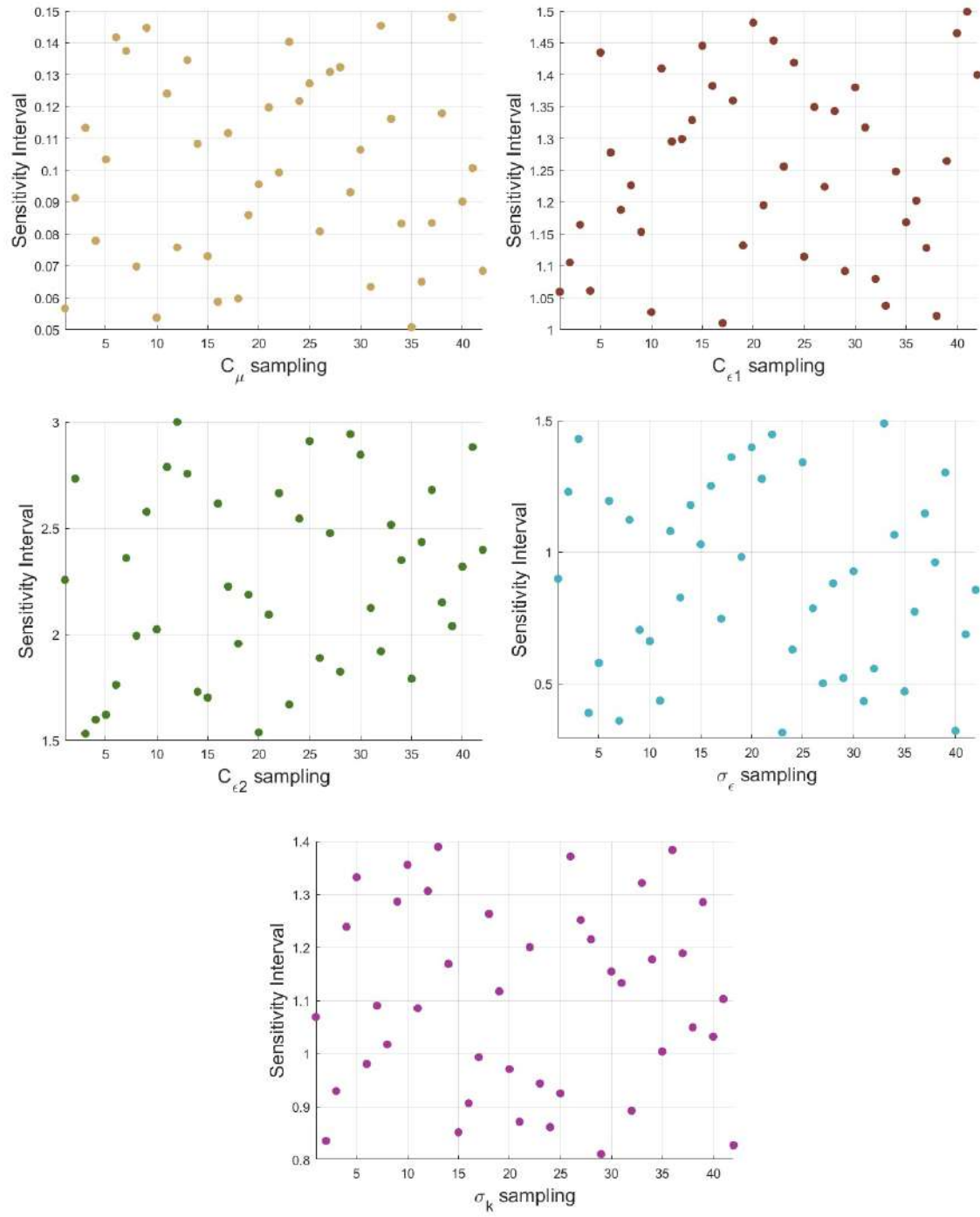


Figure 9.1: Design of Experiment for the Polynomial Chaos of the second degree.

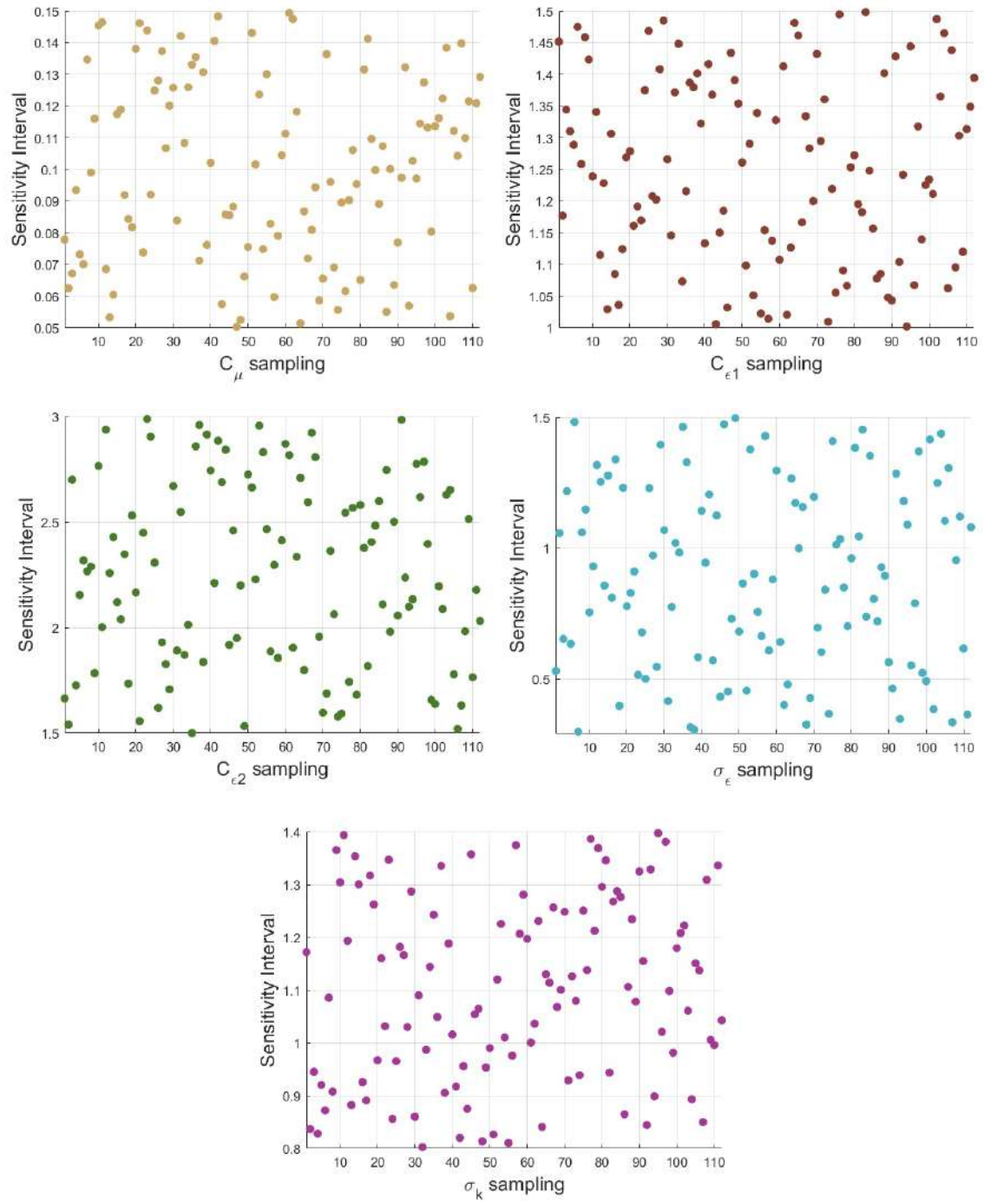


Figure 9.2: Design of Experiment for the Polynomial Chaos of the third degree.

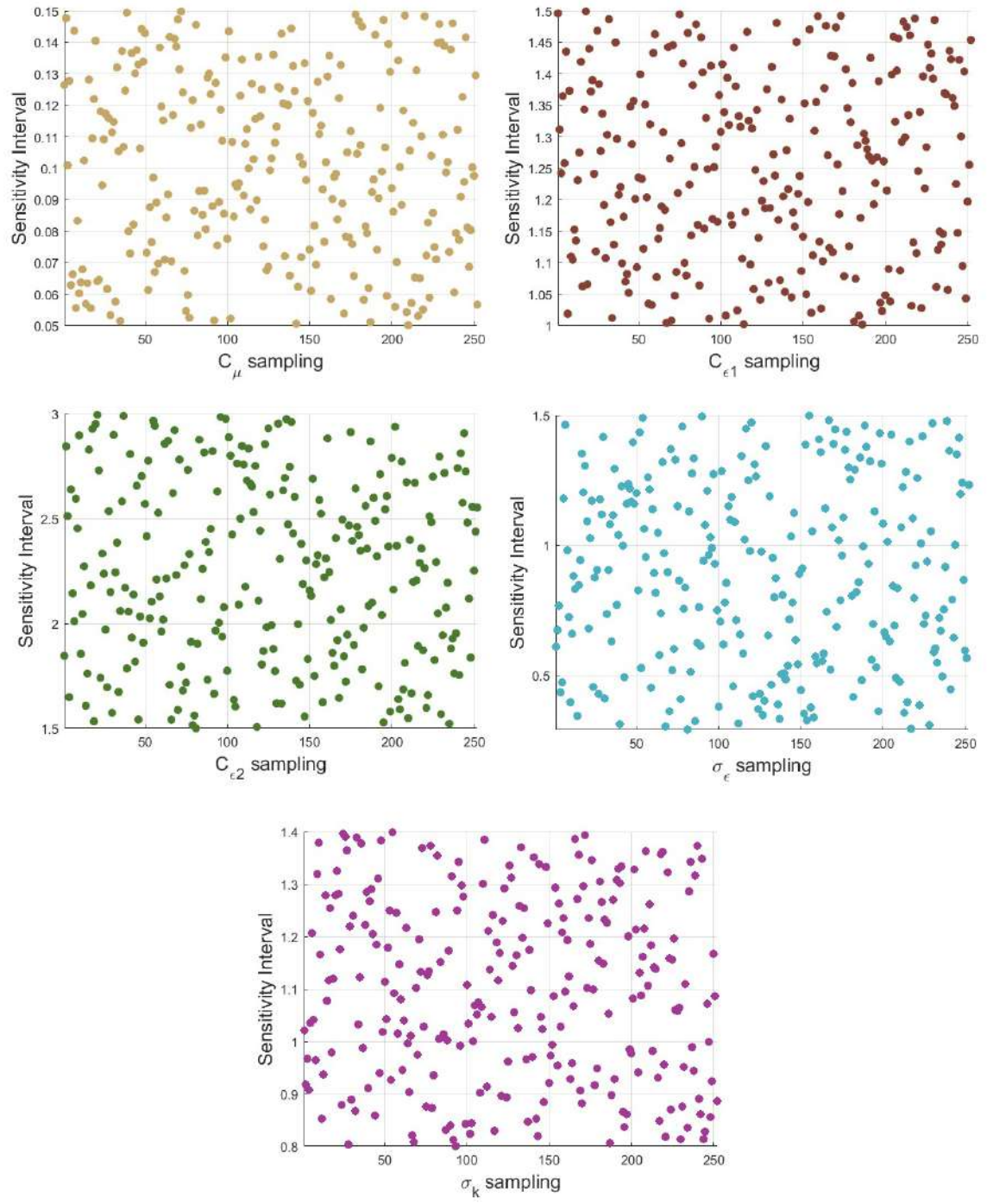


Figure 9.3: Design of Experiment for the Polynomial Chaos of the fourth degree.

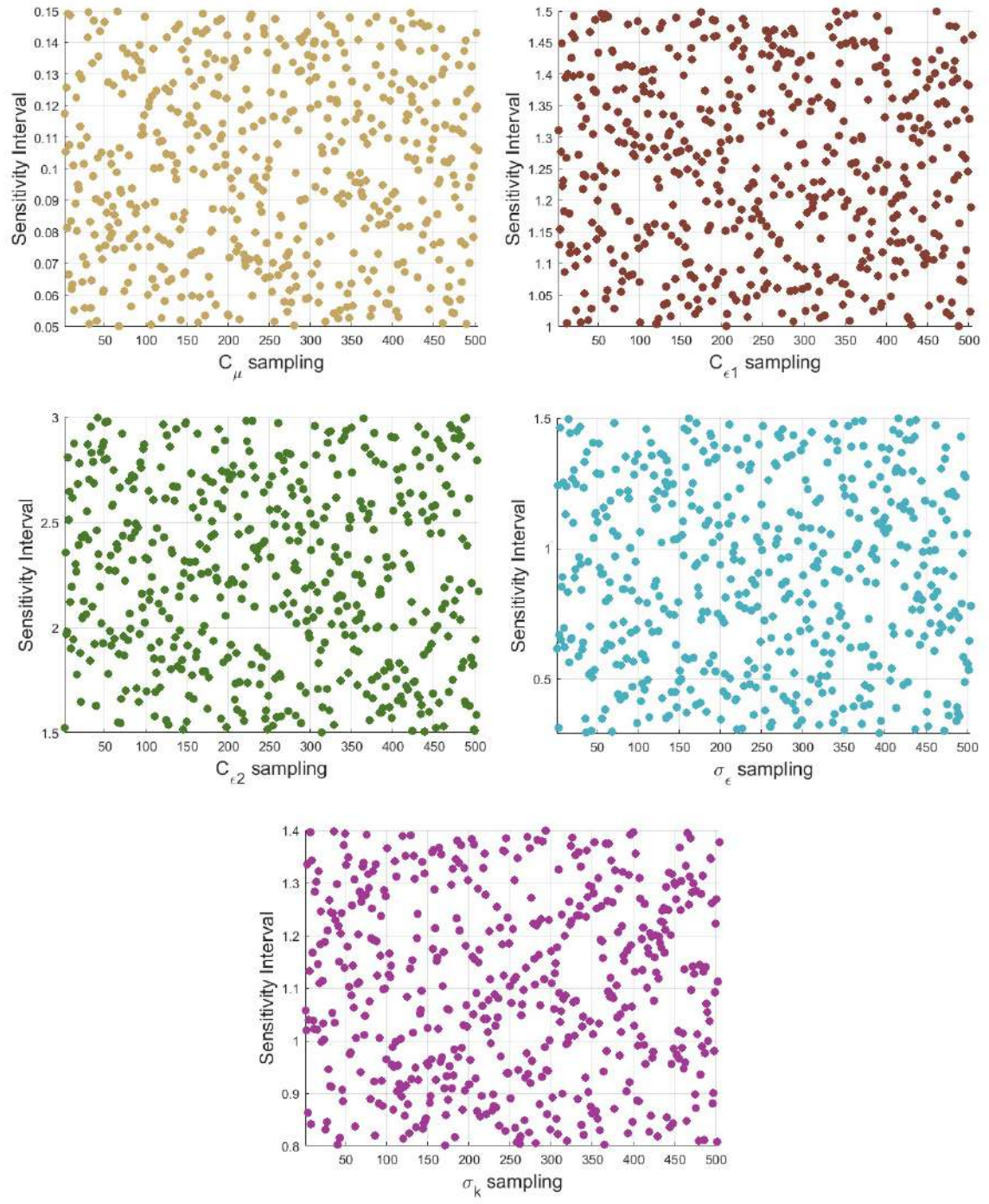


Figure 9.4: Design of Experiment for the Polynomial Chaos of the fifth degree.

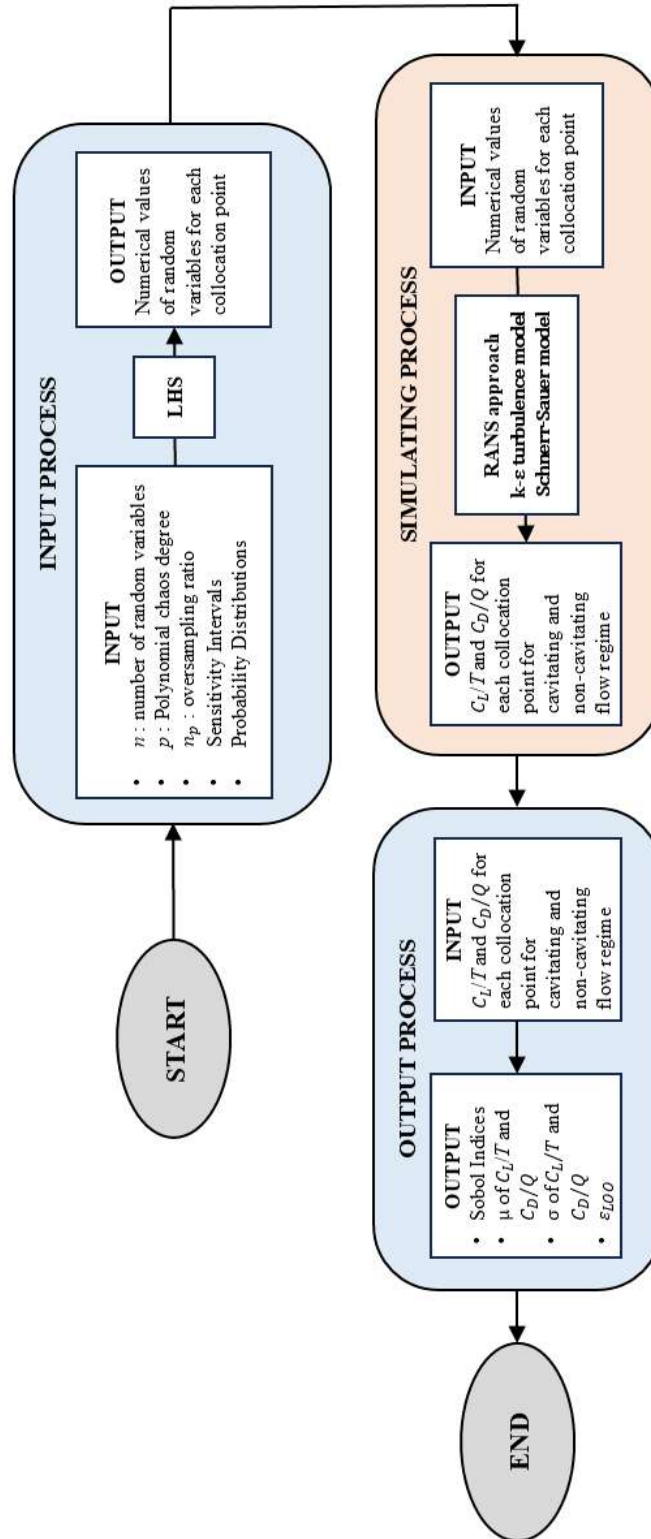


Figure 9.5: Logical diagram of simulations

9.3 The geometry of NACA66(MOD) hydrofoil

The Forward Propagation of Uncertainty based on the Sparse Polynomial Chaos Expansion and the Global Sensitivity Analysis based on the Sobol decomposition for the five calibration constants of the $k - \varepsilon$ Turbulence model have been applied for cavitating and non cavitating flows around objects of naval interest. The first test case employed in the study has been the two-dimensional NACA66(MOD) hydrofoil where the main technical data about the chord c , the maximum thickness t and the maximum bending f have been shown in Table 9.2.

Table 9.2: Technical data of NACA66(MOD) hydrofoil

f/c	a	t/c	c
[/]	[m]	[/]	[m]
0.02	0.5	0.09	0.15

The NACA66(MOD) hydrofoil is known to have good characteristics for inception of cavitation whose development was around 1940 by the National Advisory Committee for Aeronautics (NACA) [131]. The relative maximum thickness of the hydrofoil is 12% at 45% chord length from the leading edge and the relative maximum chamber ratio is 2% at 50% chord length from the leading edge [132].

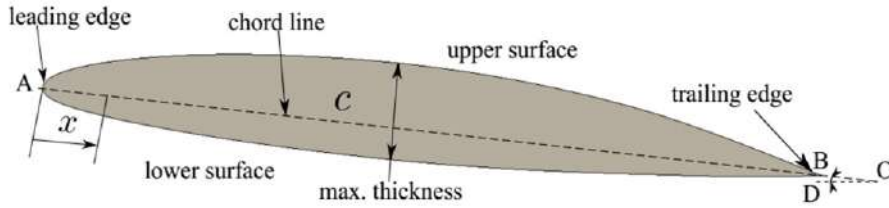


Figure 9.6: NACA66(MOD) hydrofoil.

In this context, two types of analysis have been applied: the first one has been a global study where the outputs of interest have been respectively the lift

$$C_l = \frac{L}{\frac{1}{2}\rho U_\infty^2 A} \quad (9.3)$$

and drag:

$$C_d = \frac{D}{\frac{1}{2}\rho U_\infty^2 A} \quad (9.4)$$

hydrodynamics coefficients, where D is the drag force, L is the lift force, U_∞ is the free-stream velocity and A is the foil area and the second one has been a local analysis based where the responses have been the friction coefficient:

$$C_f = \frac{\tau}{\frac{1}{2}\rho U_\infty^2} \quad (9.5)$$

and the pressure coefficient:

$$C_p = \frac{|p_{\text{local}}| - p_{\text{ref}}}{\frac{1}{2}\rho U_\infty^2} \quad (9.6)$$

where τ is the wall shear stress. Then, the aim has been the evaluation of the propagation of uncertainties of the five turbulence coefficients for the determination of lift and drag coefficients (calculation of mean value and standard deviation) and the evaluation of the ranking of importance of the five parameters for the fully-wetted and cavitating flow regimes.

9.4 Mesh

To simulate the flow around the hydrofoil, the two-dimensional domain represented in Figure 9.7 has been used.

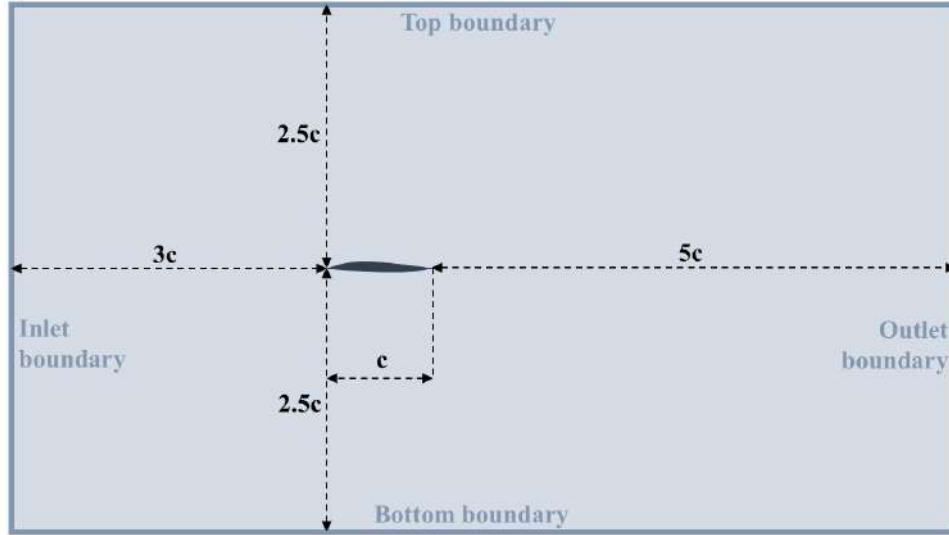


Figure 9.7: Computational domain.

It has been spatially discretized by using a 2D unstructured polygonal mesher in Simcenter STAR-CCM+ with a layer of prismatic cells inflated from the surface of the hydrofoil. The mesh-generation process has been automated and parametrized, so that all the refinement steps, adopted by the current meshing strategy, are linked in relative terms to a given cell base-size. A mesh-sensitivity study has been carried out considering the fully wetted flow condition and using progressively refined meshes, generated using different values of the cell base-size as reported in Table 9.3. For reasons of computational efficiency, the uncertainty quantification study relies on the coarse mesh [133].

Table 9.3: Mesh data - hydrofoil

mesh	mesh nodes on hydrofoil	number of cells	base size for mesh generation	min y^+ (max y^+)	C_d	C_l
coarse (C)	663	32874	10	2.7 (11)	0.0218	0.6151
medium (M)	1268	81425	5	1.2 (6.2)	0.0242	0.6010
fine (F)	2477	226455	2.5	0.47 (3.4)	0.0254	0.5949

For the sake of completeness, in Figures 9.8, 9.9, 9.10 and ?? the adopted mesh is shown.

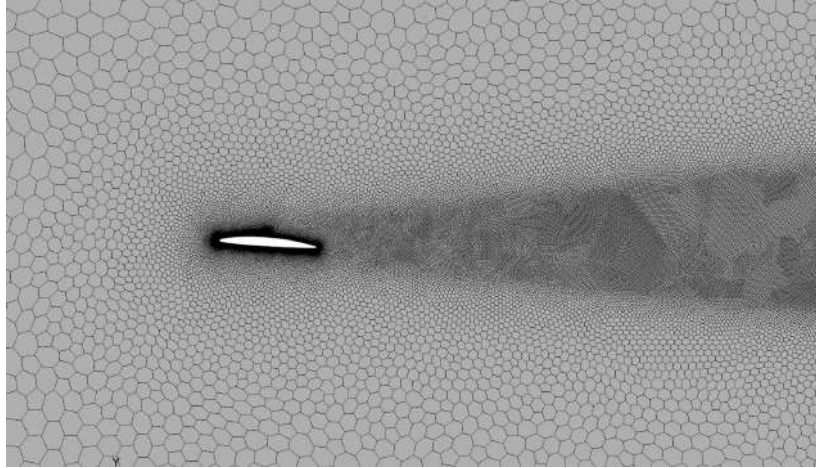


Figure 9.8: Hydrofoil mesh detail - 1.

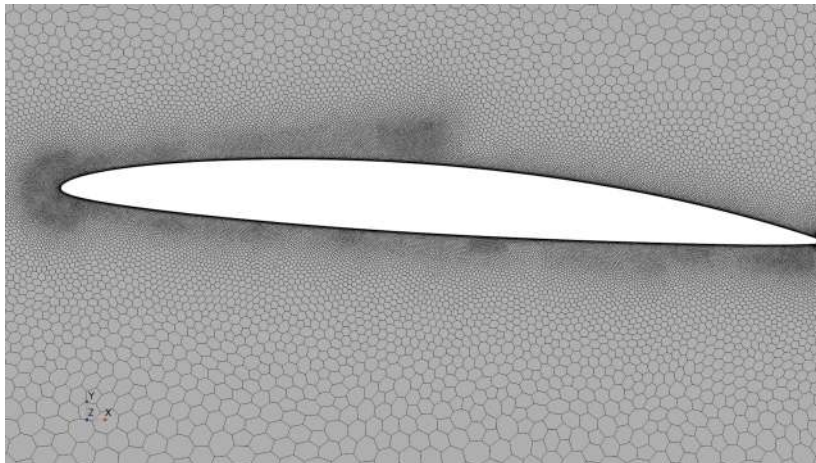


Figure 9.9: Hydrofoil mesh detail - 2.

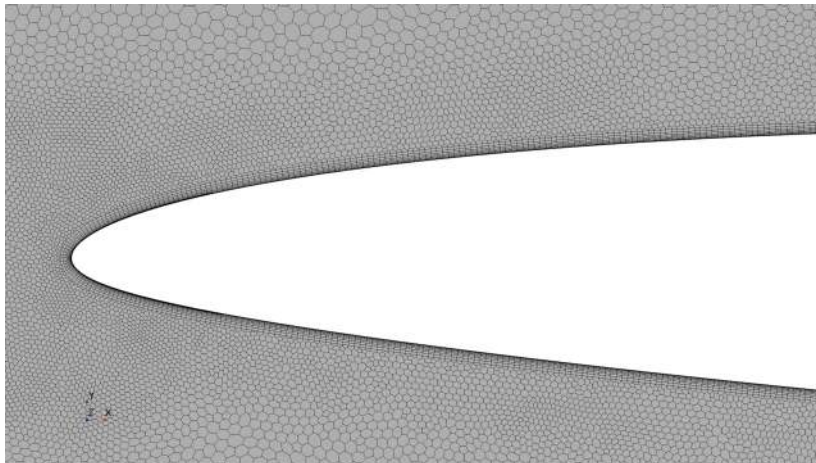


Figure 9.10: Hydrofoil mesh detail - 3.

9.5 Boundary and initial conditions

The study has been carried out for an angle of attack equal to 4 degree for both the fully-wetted and cavitating flows by using a boundary layer thickness of $y^+ = 1$ where:

$$y^+ = \frac{U_\tau}{\nu} y \quad (9.7)$$

$$U_\tau : \text{friction velocity} \quad (9.8)$$

The free-stream velocity has been kept equal to $12.2 \frac{\text{m}}{\text{s}}$ at the inlet boundary, as well as the turbulent kinetic energy has been imposed equal to $0.0223 \left(\frac{\text{m}}{\text{s}}\right)^2$ and the turbulent kinetic energy dissipation rate has been selected equal to $0.1837 \frac{\text{m}^2}{\text{s}^3}$. The numerical value of the pressure at the outlet boundary has been imposed constant at a value of 202650 pa [134]. On the solid surfaces of the hydrofoil, as well as the top and the bottom boundaries of the domain, a no-slip boundary condition has been imposed. The flow has been considered incompressible without the presence of bouyancy terms and heat transfer so that the governing equations for the fully-wetted condition have been (7.62), (7.63), (7.64), (7.71), (7.81) and (7.82). The cavitating flow has been considered as a homogeneous mixture flow where the continuity equation has been modified as (8.40) where its expression in scalar components for two-dimensional problems is:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} = \dot{m} \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right). \quad (9.9)$$

Furthermore, the transport equation of the vapour fraction (8.41) has been used to close the problem equations where its extended expression for a two-dimensional flow is given by:

$$\frac{\partial}{\partial t} (\rho_v \alpha) + \frac{\partial}{\partial x} (\rho_v \alpha \bar{u}) + \frac{\partial}{\partial y} (\rho_v \alpha \bar{v}) = \dot{m} \quad (9.10)$$

and the mixture physical greatneses have been given in terms of vapour fraction ((8.35) and (8.36)). The magnitude on the vapour fraction has been initialized as 0 in simulations and as mentioned, the Schnerr-Sauer cavitation model (8.52) has been employed to model the mass transfer rate. For the water and water-vapour fluids, the following values have been set: $\rho_l = 997 \frac{\text{kg}}{\text{m}^3}$, $\mu_l = 8.89324 \cdot 10^{-4} \text{ pa} \cdot \text{s}$, $\rho_v = 0.023084 \frac{\text{kg}}{\text{m}^3}$, $\mu_v = 9.055 \cdot 10^{-6} \text{ pa} \cdot \text{s}$. The fixed cavitation number (8.3) of the work has been 0.91 [133].

Chapter 10

Potsdam Propeller Test Case - PPTC

10.1 Introduction

The second object of interest in this study has been a three-dimensional geometry lapped by a cavitating and non cavitating flow. In this chapter, the numerical framework, mesh and boundary and initial conditions of the hydrodynamic simulations of the Potsdam Propeller Test Case have been presented. Furthermore, the geometry of PPTC propeller has been described.

10.2 Numerical framework

Numerical simulations and Uncertainty Quantification analysis have been initialized and carried out in the same way of the process employed for the NACA66(MOD) hydrofoil. A Polynomial Chaos Expansion of the second order has been used and the coherence between the hydrofoil and the propeller has been kept by involving the same collocation points for generating the response surfaces. The initial variables have been considered uniformly distributed random variables as described in Table 9.1. Furthermore, the propeller analysis has been conducted by considering a constant RPM n (revolutions per minute) and an advance velocity V_a to guarantee an advance ratio J :

$$J = \frac{V_a}{nD} \quad (10.1)$$

equal to 1.019 and 1.408. The analysis has been conducted for a cavitating and non cavitating flow regime and for these two operating points, Polynomial Chaos Expansion has been generated to evaluate the Leave-One-Out Cross-Validation error, the lower statistical moments, the posterior probability distributions and Sobol indices have been calculated. In conclusion, a reduced model order analysis based on the Polynomial Chaos Expansion has been applied. In this case, only three coefficients have been employed for the generation of the metamodel ($C_{\varepsilon_1}, C_{\varepsilon_2}$ and σ_ε) so that the number of collocation points needed to generate a Polynomial Chaos Expansion of the third order by using three initial variables have been:

$$K = 40. \quad (10.2)$$

The Design of Experiment has been obtained by using a Latin Hypercube sampling strategy and it is given in Figure 10.1. A comparison between the Polynomial Chaos Expansion and the Polynomial Chaos Kriging has been applied for the set of few points (42 collocation points) for $J = 1.019$ for both the flow regimes as for the NACA66(MOD) hydrofoil.

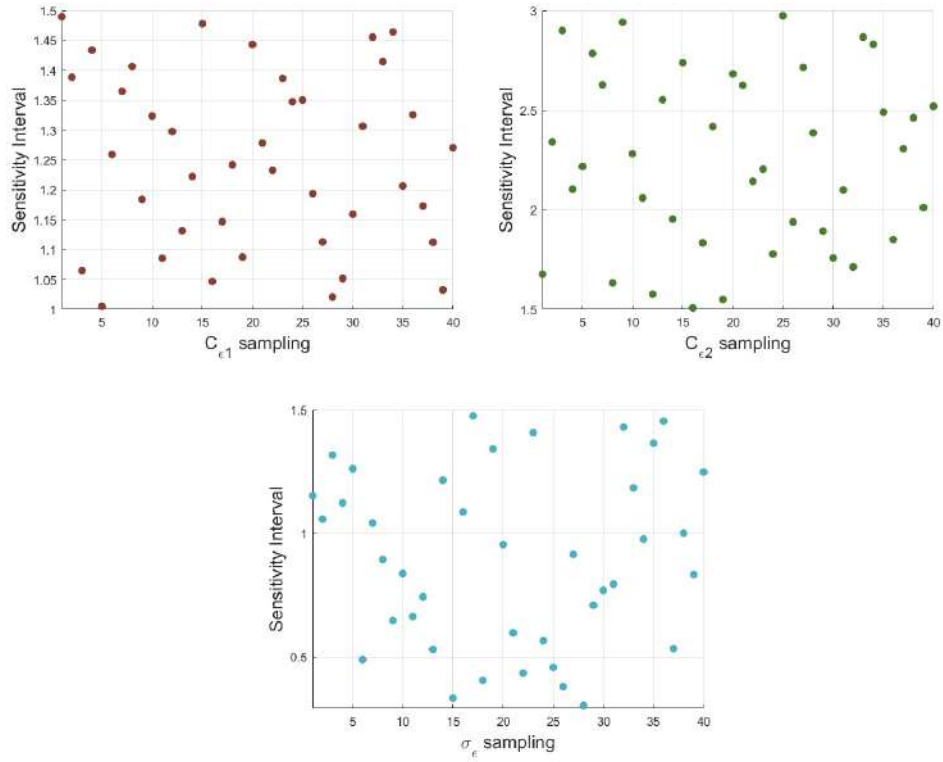


Figure 10.1: Design of Experiment for the reduced Polynomial Chaos analysis of the third degree.

10.3 The geometry of Potsdam Propeller Test Case - PPTC

After the analysis of the Uncertainty Quantification of the $k - \epsilon$ Turbulence model applied to the NACA66(MOD) hydrofoil, the study has been extended to the Potsdam Propeller Test Case PPTC in order to verify if there exists a direct correlation between the two-dimensional flow and the three-dimensional flow in terms of ranking of importance of the five calibration constants for both the flow regimes employed. As for NACA66(MOD) hydrofoil, the Polynomial Chaos Expansion has been employed to determine the mean value and the standard deviation of the two PPTC outputs of thrust T and torque Q while Sobol indices have been applied to evaluate the ranking of importance of the turbulence constants for these two responses. The adopted propeller is represented in Figure 10.2.



Figure 10.2: Potsdam Propeller Test Case

The propeller is characterized by five blades and it is a controllable pitch propeller. This effects the propeller blade design near the hub and results in a 0.3 mm gap between hub and propeller blade near the leading and trailing edge of the propeller. Furthermore, the trailing edge for the upper propeller radii is sharp and it is designed to create a tip vorcer [138]. In table 10.1, there are shown the main geometrical properties of the PPTC.

Table 10.1: Geometrical data of Potsdam Propeller Test Case

	Symbol	Measure	Value
propeller diameter	D	[mm]	250.0000
pitch at $\frac{r}{R} = 0.7$	$P_{0.7}$	[mm]	408.7500
pitch at $\frac{r}{R} = 0.75$	$P_{0.75}$	[mm]	407.3804
mean pitch	P_{mean}	[mm]	391.8812
chord length at $\frac{r}{R} = 0.7$	$C_{0.7}$	[mm]	104.1670
chord length at $\frac{r}{R} = 0.75$	$C_{0.7}$	[mm]	106.3476
thickness at $\frac{r}{R} = 0.75$	$t_{0.75}$	[mm]	3.7916
pitch ratio	$\frac{P_{0.7}}{D}$	[/]	1.6350
mean pitch ratio	$\frac{P_{\text{mean}}}{D}$	[/]	1.5675
area ratio	$\frac{A_E}{A_0}$	[/]	0.7790
skew	θ_{eff}	[°]	18.8000
hub diameter ratio	$\frac{d_h}{D}$	[/]	0.1500
number of blades	z	[/]	5
direction of rotation			right-handed (SCS)

and the geometrical representation of the blade is given in Figure 10.3.

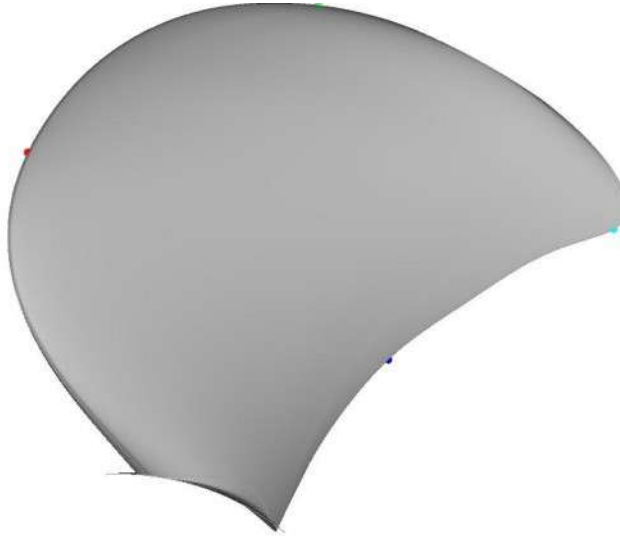


Figure 10.3: Blade of Potsdam Propeller Test Case

10.4 Mesh

To simulate the flow around the PPTC, a three dimensional domain has been used. The domain has been characterized by a stationary "global" zone which is represented in Figure 10.4 within which a rotating "local" zone around the propeller has been defined, which is represented in Figure 10.5. It is important to note that only one blade has been considered so as to reduce the computational cost of work.

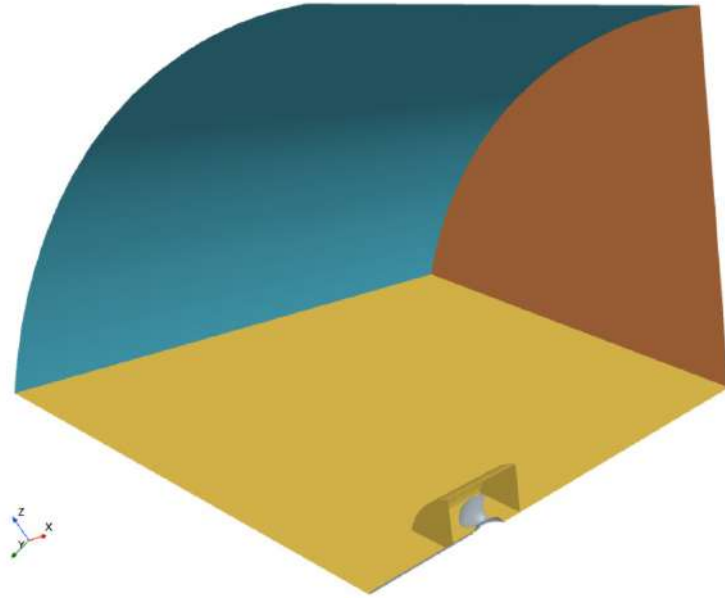


Figure 10.4: Propeller domain - 1.

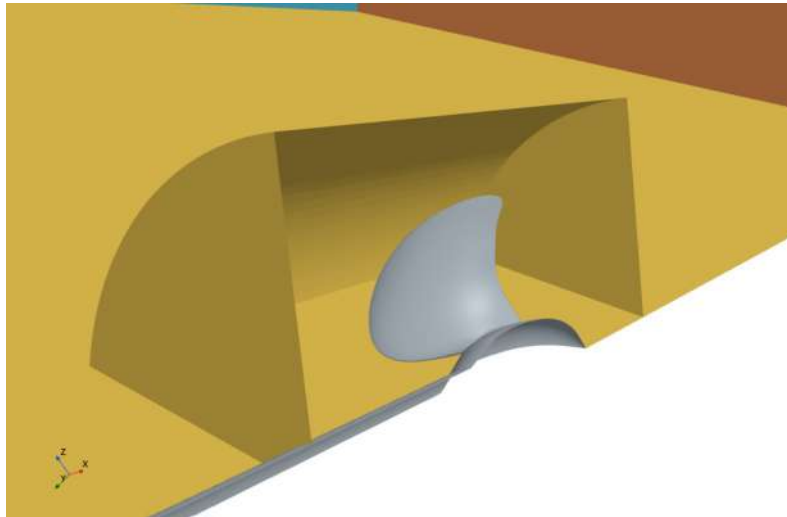


Figure 10.5: Propeller domain - 2.

The domain has been spatially discretized using a 2D trained cell mesher in Simcenter STAR CCM+; specifically, the mesh has been generated by a Parts-Based Meshing (PBM) approach where the two zones have been differently meshed. A mesh sensitivity study has been carried out by considering the fully wetted flow condition and progressively refined meshes, generated using different values of the cell base-size reported in Table 10.2.

Table 10.2: Mesh data - propeller

mesh	number of cells of fixed zone	number of cells of rotating zone	T [N]
coarse (C)	417071	778274	180.8
medium (M)	528409	849145	181.2
fine (F)	1216412	1397446	181.7

To ensure a good approximation of the fluid field, the medium mesh has been employed to carry

out the computational simulations and in Figures 10.6, 10.7, 10.8, 10.9 and 10.10, some detail of the adopted mesh is shown.

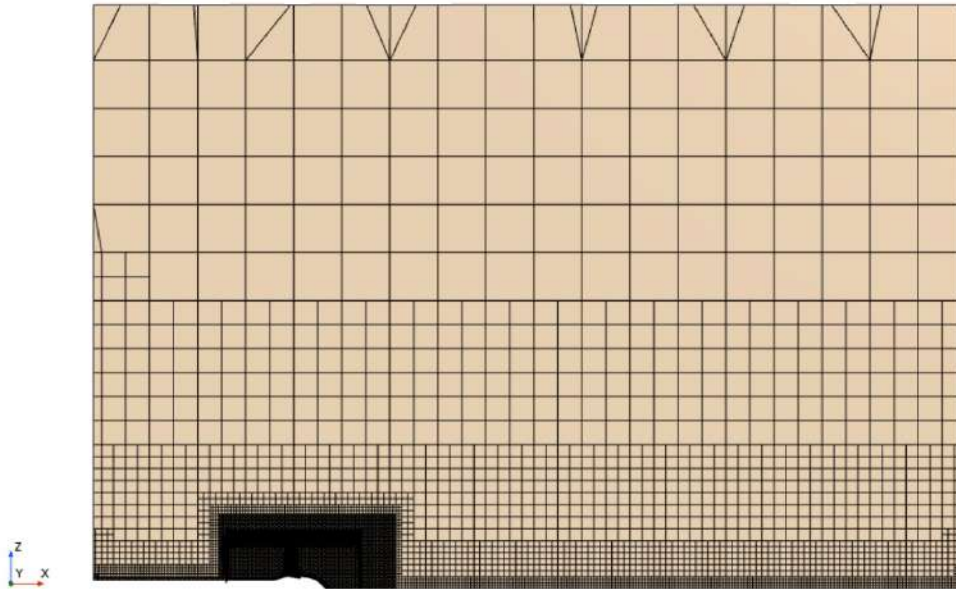


Figure 10.6: Propeller mesh detail - 1.

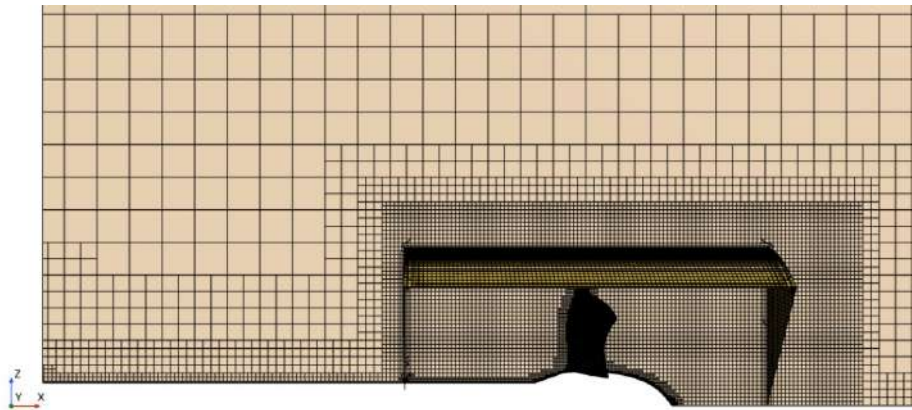


Figure 10.7: Propeller mesh detail - 2.

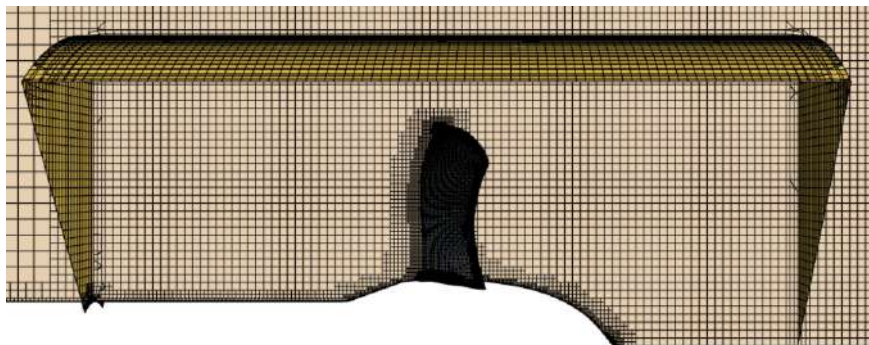


Figure 10.8: Propeller mesh detail - 3.

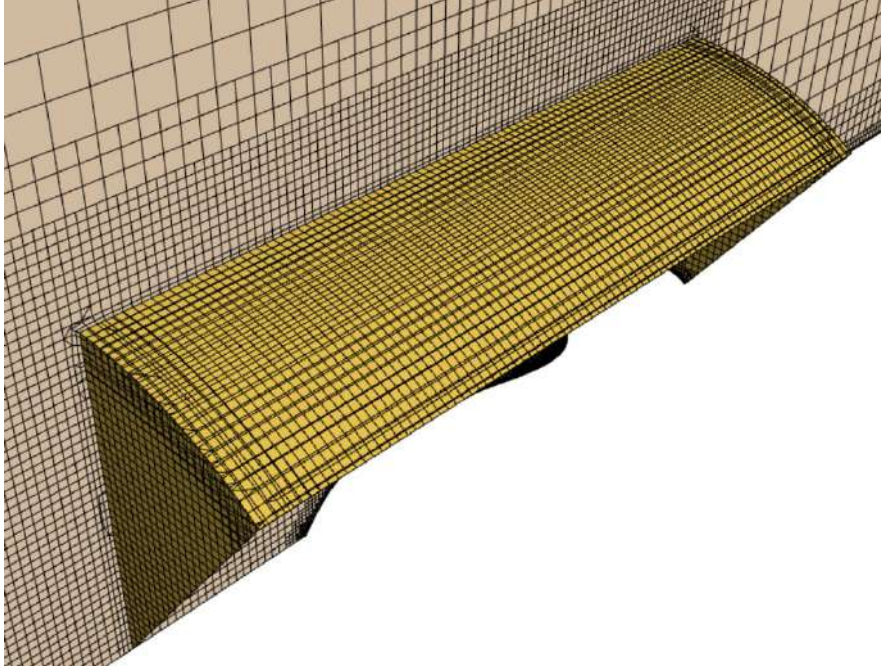


Figure 10.9: Propeller mesh detail - 4.

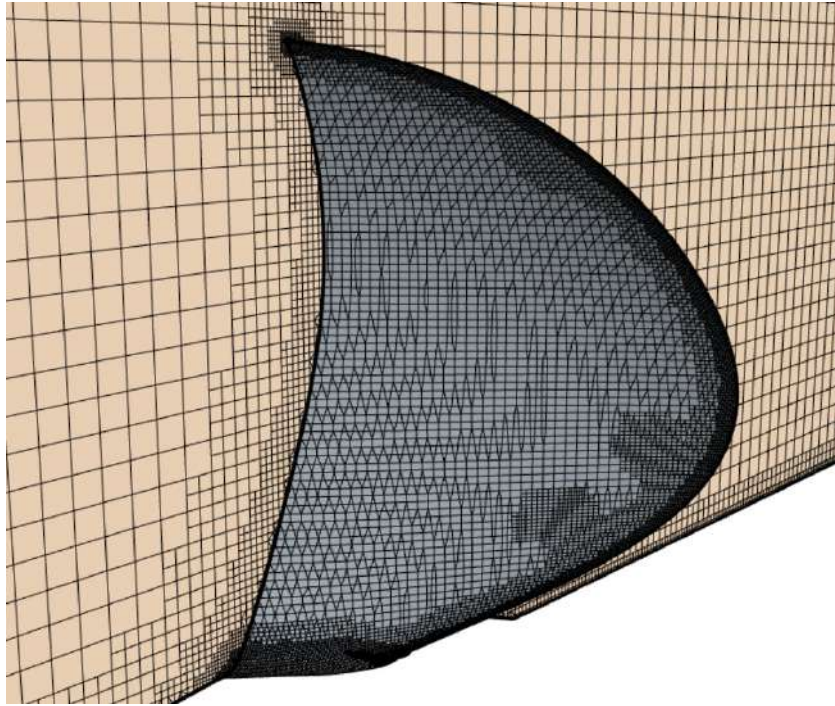


Figure 10.10: Propeller mesh detail - 5.

10.5 Boundary and initial conditions

Taking into account the initial conditions, the free-stream velocity has been fixed equal to $6.365 \frac{\text{m}}{\text{s}}$ along the x-axis of the domain, the turbulent kinetic energy, as well as its dissipation rate have been kept equal to $0.0223 \left(\frac{\text{m}}{\text{s}}\right)^2$ and $0.1837 \frac{\text{m}^2}{\text{s}^3}$. Furthermore, simulations have been executed by

setting $y^+ = 28$. The RPM n (revolutions per minute) have been kept constant. A pressure equal to 202650 pa has been imposed as initial condition of the flow field. A no-slip condition has been applied on the blade and top surfaces and the rotating zone has been simulated by the Moving Reference Frame (MRF) method. Also in this case, the flow has been considered incompressible without buoyancy and heat transfer terms; the governing equations for the fully-wetted flow have been (7.65), (7.66), (7.67), (7.68), (7.83) and (7.84) while for the cavitating flow, a cavitation number of $\sigma = 2$ has been taken into account and the following equations:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = \dot{m} \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \quad (10.3)$$

$$\frac{\partial}{\partial t} (\rho_v \alpha) + \frac{\partial}{\partial x} (\rho_v \alpha \bar{u}) + \frac{\partial}{\partial y} (\rho_v \alpha \bar{v}) + \frac{\partial}{\partial z} (\rho_v \alpha \bar{w}) = \dot{m} \quad (10.4)$$

have been adopted. The mass transfer term has been determined by applying the Schnerr-Sauer model and the physical quantities of the flow phases have been selected as follows: $\rho_l = 997.561 \frac{\text{kg}}{\text{m}^3}$, $\mu_l = 8.88871 \cdot 10^{-4} \text{ pa} \cdot \text{s}$, $p_s = 61931 \text{ pa}$, $\rho_v = 0.59531 \frac{\text{kg}}{\text{m}^3}$, $\mu_v = 12.7 \cdot 10^{-6} \text{ pa} \cdot \text{s}$. Furthermore in the mixture mode, seed density and seed diameter have been respectively imposed equal to $1 \cdot 10^{12} \frac{1}{\text{m}^3}$ and $1 \cdot 10^{-6} \text{ m}$, the turbulent intensity has been fixed to 0.01, the turbulent viscosity ratio has been chosen as 10 and the turbulent velocity scale has been equal to $1 \frac{\text{m}}{\text{s}}$.

Chapter 11

NACA66(MOD) hydrofoil results

11.1 Summary of results

In the following chapter, results of NACA66(MOD) hydrofoil are shown. Results can be divided into two main typologies: results about a **Global Analysis** where outputs have been the lift and drag coefficients of the entire hydrofoil and a **Local Analysis** where responses have been the pressure and friction coefficients along the longitudinal development of the NACA66(MOD) hydrofoil.

Considering the Global Analysis, a **Forward Propagation of Uncertainty** has been conducted by introducing a **Non – Intrusive Polynomial Chaos Expansion** generated by a **Sparsity Approach** based on a **Least Angle Regression** method and a **Global Sensitivity Analysis** has been applied by involving the **Sobol decomposition**. For both the lift and drag coefficients four polynomial expansions have been applied; specifically, a Polynomial Chaos from the **second** to the **fifth** order expansions have been created to compute the Sobol indices of the **first, second, third, fourth, fifth** and **total** orders. Furthermore, for each polynomial expansion, **Leave–One–Out Cross–Validation error**, **Lower Statistical Moments** and **Posterior Distributions** have been calculated. The analysis has been applied for a cavitating and non-cavitating flow regime.

In conclusion, a comparison between the Polynomial Chaos Expansion and an **Optimal Polynomial Chaos–based Kriging** has been applied to identify the most performant metamodel for this type of study. Taking into account a set of 42 points and a set of 504 points, Polynomial Chaos and Polynomial Chaos Kriging have been generated from a **second** to a **tenth** order where, for each polynomial degree, the Leave-One-Out Cross-Validation error, and the main and total Sobol indices have been computed. The kernel of Polynomial Chaos Kriging has been considered to be modelled by Matern $\frac{5}{2}$ correlation functions. The Global analysis has been done for both a cavitating and non-cavitating flow regime.

After, the application of Local Analysis has been conducted by applying a **Polynomial Chaos Expansion** for the variation of pressure and friction coefficients along the hydrofoil. A Polynomial Chaos Expansion of the **second order** has been employed to evaluate trends of **Leave–One–Out Cross–Validation error** and **total, first** and **second** orders Sobol indices. Furthermore, the variation of **mean value** and **condidence interval** along the NACA66(MOD) hydrofoil has been investigated. The analysis has been applied for the fully wetted flow since the fact that when the cavity occurs, the pressure inside the bubble is equal to the vapour pressure of water.

In Figures 11.1, 11.2 and 11.3, there is represented the scheme of the obtained results with respect to the NACA66(MOD) hydrofoil.

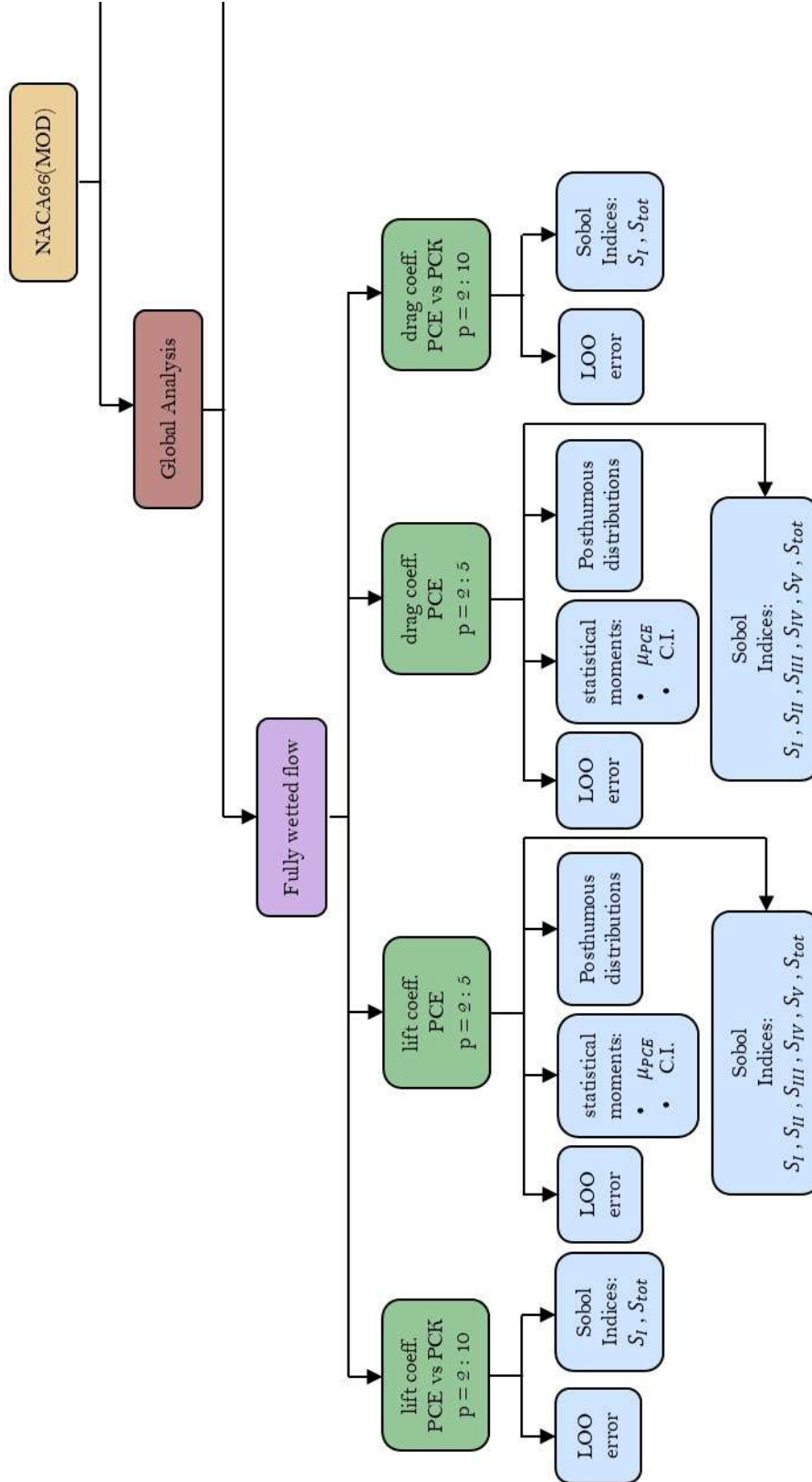


Figure 11.1: Results scheme of NACA66(MOD) hydrofoil - 1.

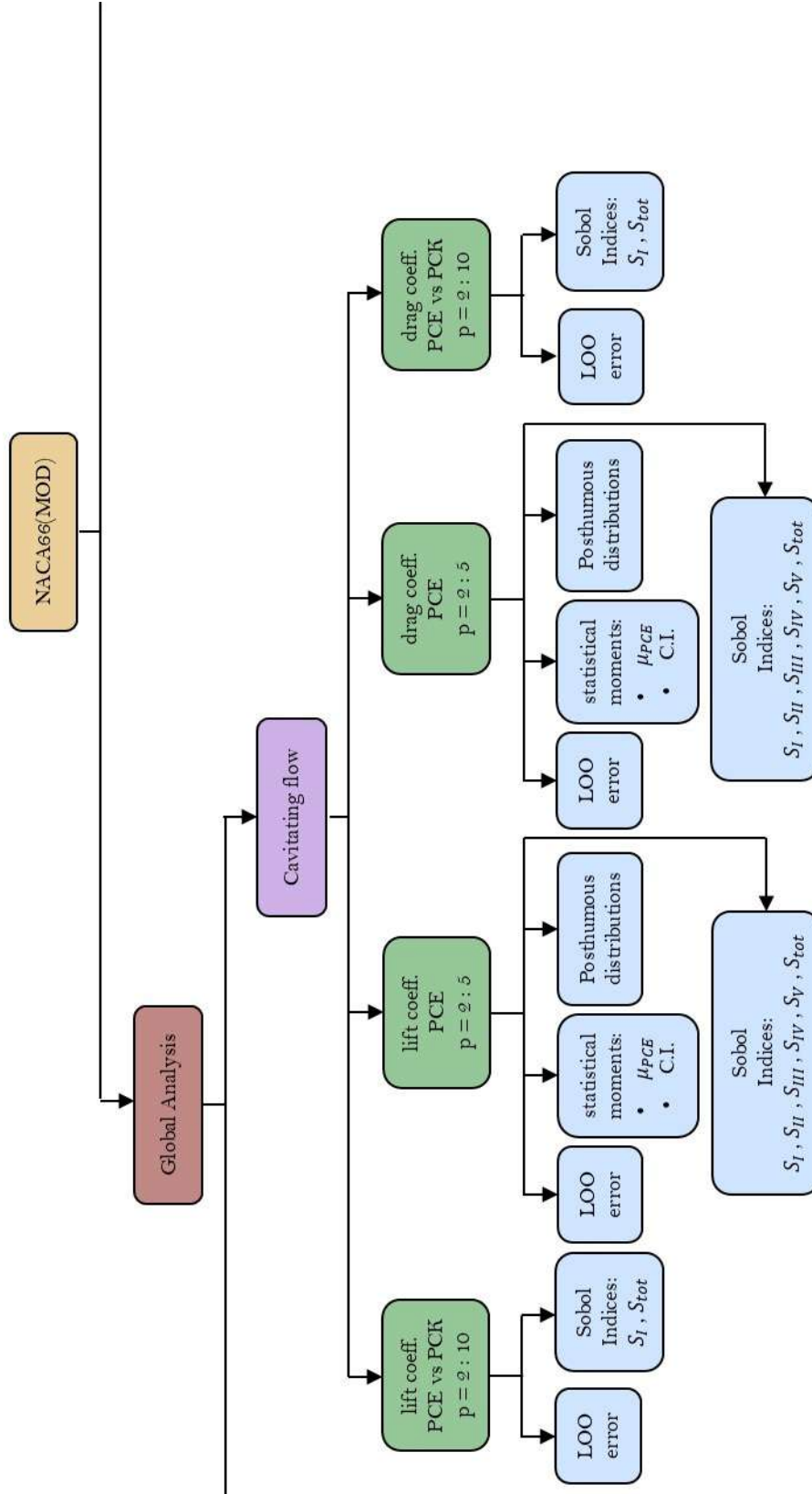


Figure 11.2: Results scheme of NACA66(MOD) hydrofoil - 2.

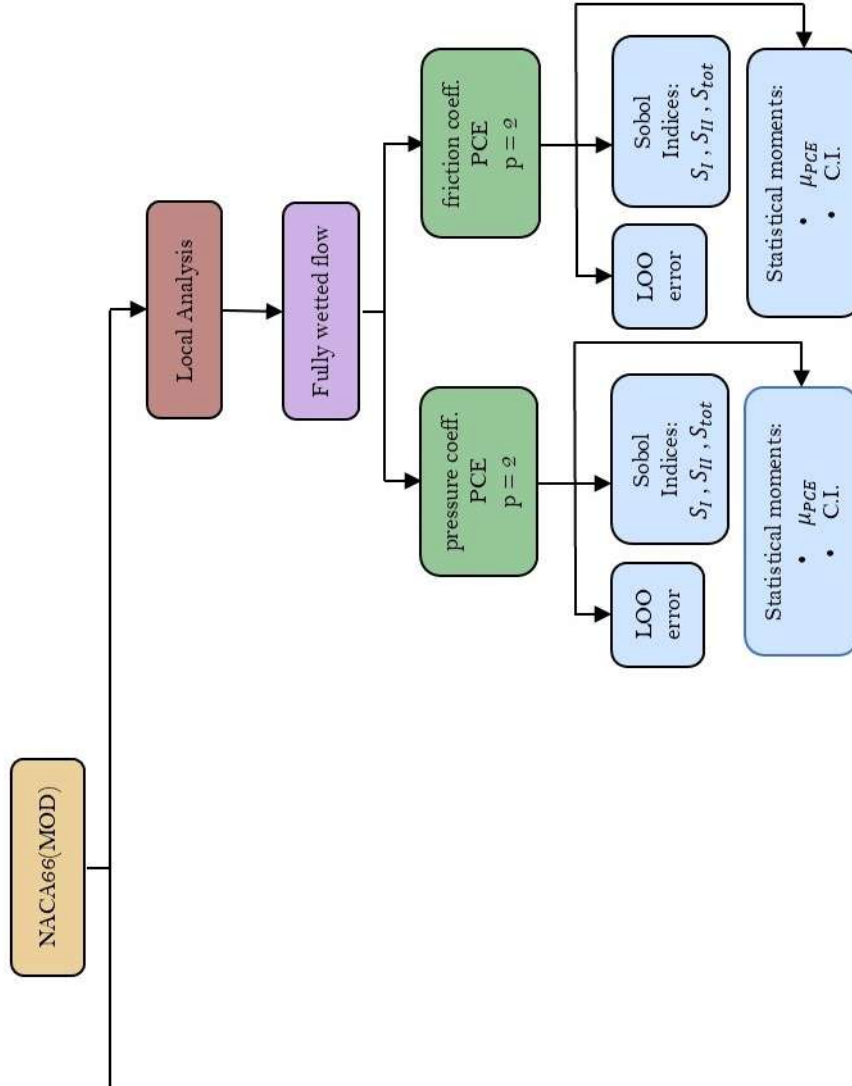


Figure 11.3: Results scheme of NACA66(MOD) hydrofoil - 3.

11.2 Global Analysis

11.2.1 Fully wetted flow regime

Leave-One-Out Cross-Validation error

In Figures 11.4 and 11.5 are respectively shown the Leave-One-Our Cross Validation errors for the drag and lift coefficients for a fully wetted flow. For both the hydrodynamics coefficients, the error decreases monotonically by increasing the polynomial order (and consequentially also the number of collocation points); this behaviour suggests that, in this case of study, the polynomial increase can improve the predictability of the phenomenon (which is not always true).

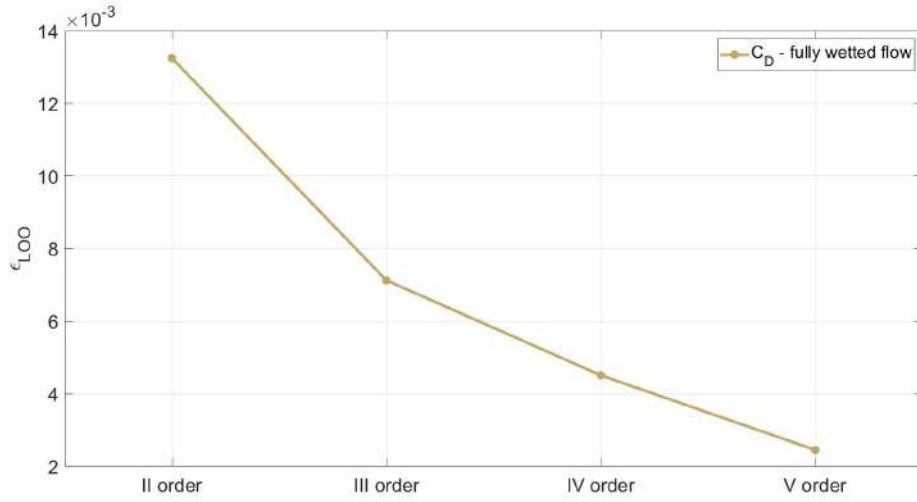


Figure 11.4: Leave-One-Out Cross-validation error trend of the drag coefficient in the fully wetted flow condition - NACA66(MOD).



Figure 11.5: Leave-One-Out Cross-validation error trend of the lift coefficient in the fully wetted flow condition - NACA66(MOD).

Statistical moments

In Figures 11.6 and 11.7 the mean values and the confidence Intervals trends of the outputs are shown. Taken into account the calculated standard deviations, the confidence intervals CI have been calculated by applying the following equation:

$$CI = \mu_{PCE} \pm MOE \quad (11.1)$$

where:

$$MOE \equiv 1.96 \left(\frac{\sigma_{PCE}}{\sqrt{K}} \right) : \text{Margin Of Error of 95\%} \quad (11.2)$$

Analyzing the results, a convergent trend of the mean value for both the drag and lift coefficients is reached when the polynomial order increases. Finally, it is also possible to note that confidence intervals decrease with the increment of the polynomial order showing the expected trend, i.e., the calculation error of the uncertainty reduces by increasing the polynomial degree.

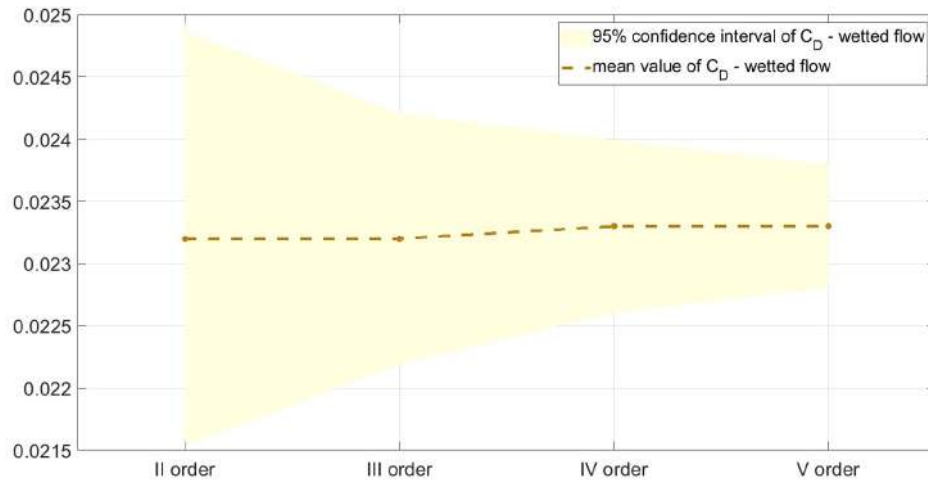


Figure 11.6: Mean values and Confidence Intervals of the drag coefficient in the fully wetted flow condition - NACA66(MOD).

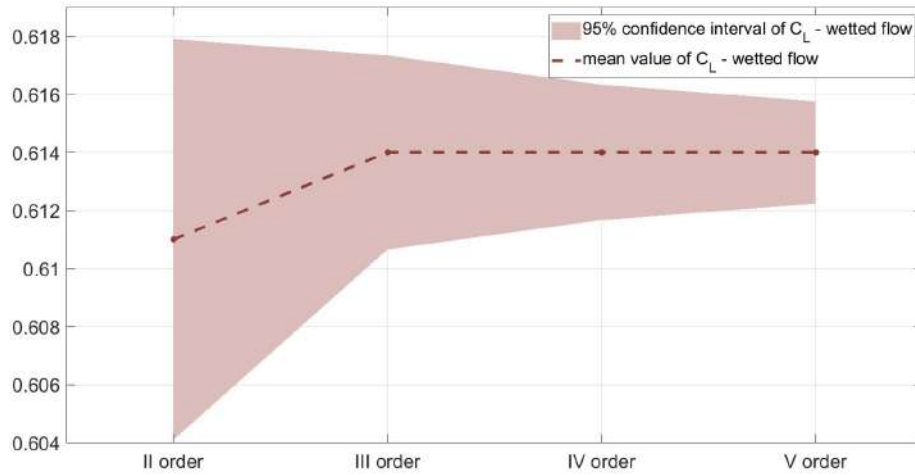


Figure 11.7: Mean values and Confidence Intervals of the lift coefficient in the fully wetted flow condition - NACA66(MOD).

Posterior probability distributions

In Figure 11.8 and 11.9, it is possible to observe the posterior probability distributions of lift and drag coefficients for each polynomial expansion. All distributions have been obtained by applying a Latin Hypercube Sampling strategy on the response surfaces generated by the Polynomial Chaos Expansions. In addition to distributions, mean values, standard deviations, modes and medians are shown in Table 11.1 and Figures 11.8 and 11.9.

Table 11.1: Data of posterior distribution functions of wetted flow regime - NACA66(MOD).

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
C_d	II	0.0232	0.00549	0.0210	0.0288
C_d	III	0.0233	0.00542	0.0212	0.0288
C_d	IV	0.0233	0.00559	0.0213	0.0335
C_d	V	0.0233	0.00557	0.0209	0.0334
C_l	II	0.611	0.0228	0.634	0.578
C_l	III	0.614	0.0180	0.616,0.627	0.583
C_l	IV	0.614	0.0188	0.623	0.564
C_l	V	0.614	0.0201	0.625	0.554

Paying attention to the probability distributions of drag, all distributions (for the different polynomial orders) have a similar behaviour. There is a modest reduction in uncertainty by increasing the Polynomial Expansion, due to the thinning of the probability distribution curve as the polynomial degree increases and analyzing the evolution of distributions, a Polynomial Chaos Expansion of the second order seems to be sufficiently accurate to predict the drag coefficient. Drag distributions show a skewness behaviour with analogous kurtosis where most of the values are positioned on the right side of the mode, suggesting then, an overestimate of some output values. All distributions are unimodal distributions and mode and mean value differ due to the presence of these overestimated responses. On the other hand, the probability distributions associated with the lift coefficient are very different to each others. Firstly, the uncertainty associated with outputs seems to have a discrete reduction when the polynomial expansion varies from the second to the third degree. This improvement in uncertainty is less pronounced for the other higher polynomial orders.

Generally, distributions of lift are unimodal even though the probability distribution for the Polynomial chaos of the third order shows a bi-modal attitude (maybe due to numerical approximations). Unlike the skewness characteristic of drag, the lift coefficient has an asymmetric probability distribution where most of the numerical values are on the left side of the mode value, suggesting an underestimation of some computational values. In this case, it is hard to understand which polynomial order converges in terms of posterior probability distribution and further Polynomial Chaos Expansion (than the fifth degree) may help the analysis. Nevertheless, it is possible to observe that distributions of the fourth and fifth orders are similar, except for the spike in the fourth order Polynomial Chaos probability distribution. Observing the two figures, kurtosis associated with the lift is higher than kurtosis associated with the drag and therefore the drag response seems to be more sensitive to the variations of the $k - \epsilon$ Turbulence model coefficients than the lift.

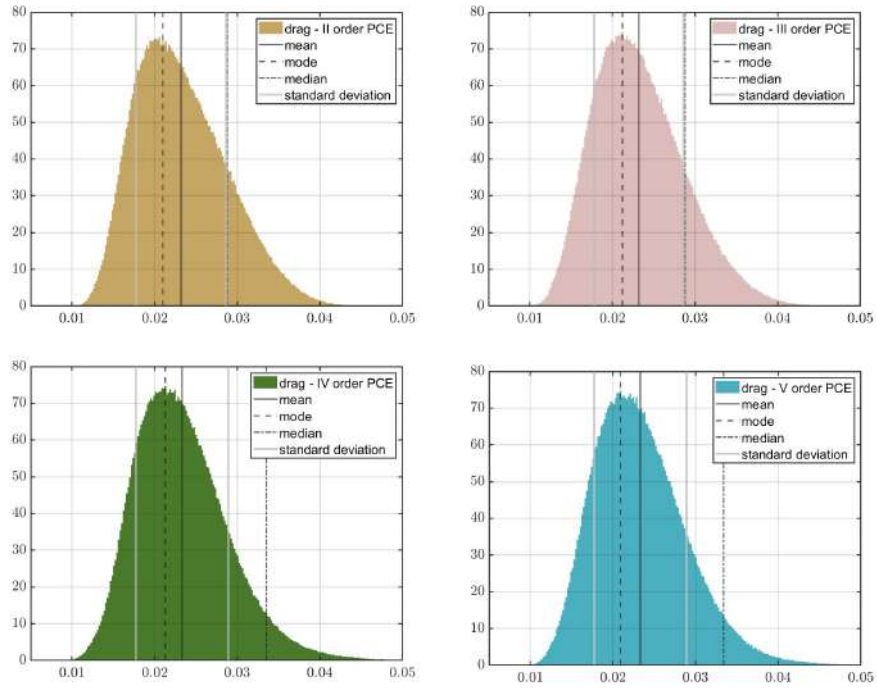


Figure 11.8: Posterior probability distributions of the drag coefficient for the fully wetted flow - NACA66(MOD).

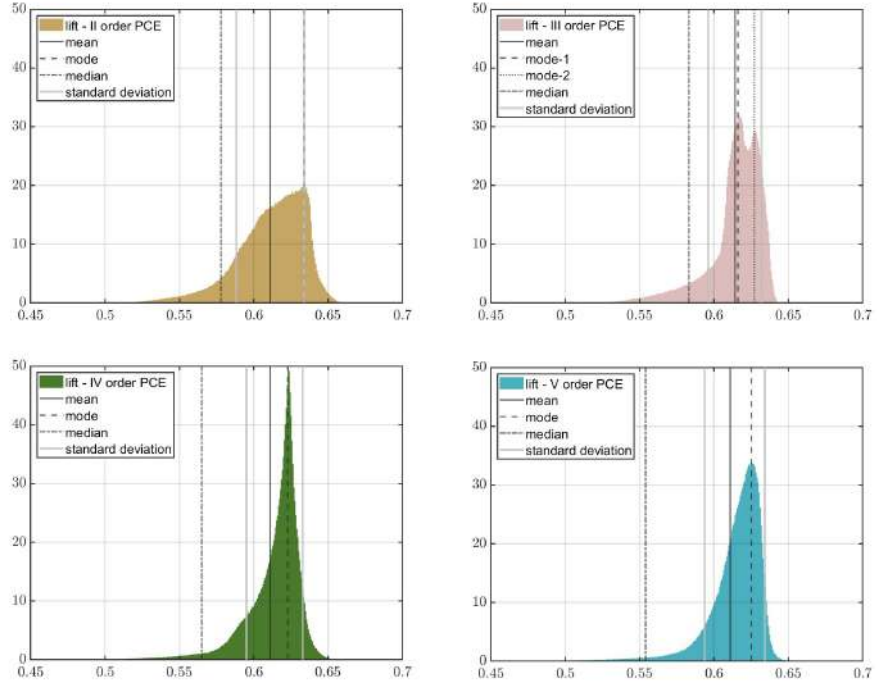


Figure 11.9: Posterior probability distributions of the lift coefficient for the fully wetted flow - NACA66(MOD).

Sobol indices

In the current section, the Sobol indices obtained by the Global Sensitivity Analysis are shown. Specifically, in Figures 11.10, 11.11, 11.12, 11.13 and 11.14 there are represented the Sobol indices of drag and in Figures 11.15, 11.16, 11.17, 11.18 and 11.19 there are shown the Sobol indices of lift.

If we pay attention to Figure 11.10, the main and total Sobol indices of the five calibration parameters for the drag are given. It is possible to note that the same ranking of indices has been obtained for each polynomial expansion, proving that the analysis of uncertainty has been not influenced by metamodel characteristics. The highest parameter corresponds to the σ_ε and it is interested to point out that the value of σ_ε is at least double compared to the other constants, showing that most of the uncertainty in the calculation of the drag originates from the model for the turbulent transport of the turbulent dissipation rate. From a general point of view, the most of uncertainty is associated to the main Sobol indices while the higher indices much less weights on the output evaluation.

However, as for the ranking of two-way interactions, from Figure 11.11, it is possible to observe that, in this case, the pair which seems to mostly influence the prediction of drag is $C_{\varepsilon_1} - \sigma_\varepsilon$ and the ranking of the most intense interactions is $C_{\varepsilon_1} - \sigma_\varepsilon$ and $\sigma_\varepsilon - \sigma_k$.

Even for the Sobol indices of second order, the ranking of indices is consistent for each polynomial expansion. After, in Figure 11.12, the Sobol indices of triplets are represented and the dominant combination of turbulence coefficients for all polynomial orders is $C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$.

In conclusion, observing Figure 11.13, Sobol indices of fourth order do not preserve the congruence of ranking when the polynomial order change. In fact, the combination $C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$ is the most important interaction when a polynomial chaos of the fourth order is employed while the combination $C_\mu - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$ is the most important interaction for a polynomial chaos of the fifth order. This situation may be justified by the fact it is hard to investigate the uncertainty of many interactions due to the presence of high non-linearities.

Taking into account the drag coefficient, the main Sobol indices have magnitude $\propto 10^{-1}$, the second order Sobol indices have magnitude $\propto 10^{-2}$, the third order Sobol indices have magnitude $\propto 10^{-3}$, the fourth order Sobol indices have magnitude $\propto 10^{-5}$, the fifth order Sobol indices have magnitude $\propto 10^{-5}$ and as consequence, the Sensitivity Analysis for the drag response in a fully wetted flow regime can be limited to the investigation of main indices.

Considering now the results related to the lift coefficient, from Figure 11.15, it is possible to note that, in this case, the turbulence model coefficient which seems to have the highest impact on the prediction of lift is C_{ε_2} . Similarly to the drag, the ranking of coefficients associated to the lift is not influenced by the increase of the polynomial degree. In this context, almost all uncertainty is incorporated in this parameter.

Considering the results related to the pairs presented in Figure 11.16, the couple $C_{\varepsilon_1} - C_{\varepsilon_2}$ is dominant with respect to the others interactions between pairs. Accordingly, the uncertainty on the lift coefficient is mostly affected by the uncertainty on the modelling of the production (by mean flow) and of the dissipation (by viscous effects) of the turbulent dissipation rate.

Analyzing the Figure 11.17, the combination $C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_k$ seems to be the most important interaction about the Sobol indices of third order and in Figure 11.18, the most important Sobol index of fourth order $C_\mu - C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon$.

Considering that the main Sobol indices have magnitude $\propto 10^{-1}$, the Sobol indices of second order have magnitude $\propto 10^{-1}$, the Sobol indices of third order have magnitude $\propto 10^{-2}/10^{-3}$, the Sobol indices of fourth order have magnitude $\propto 10^{-4}$ and the Sobol indices of fifth order have

magnitude $\propto 10^{-4}$, the study of the lift can be limited only to the analyzing of the first two-order Sobol indices even if the main Sobol indices are much more influent.

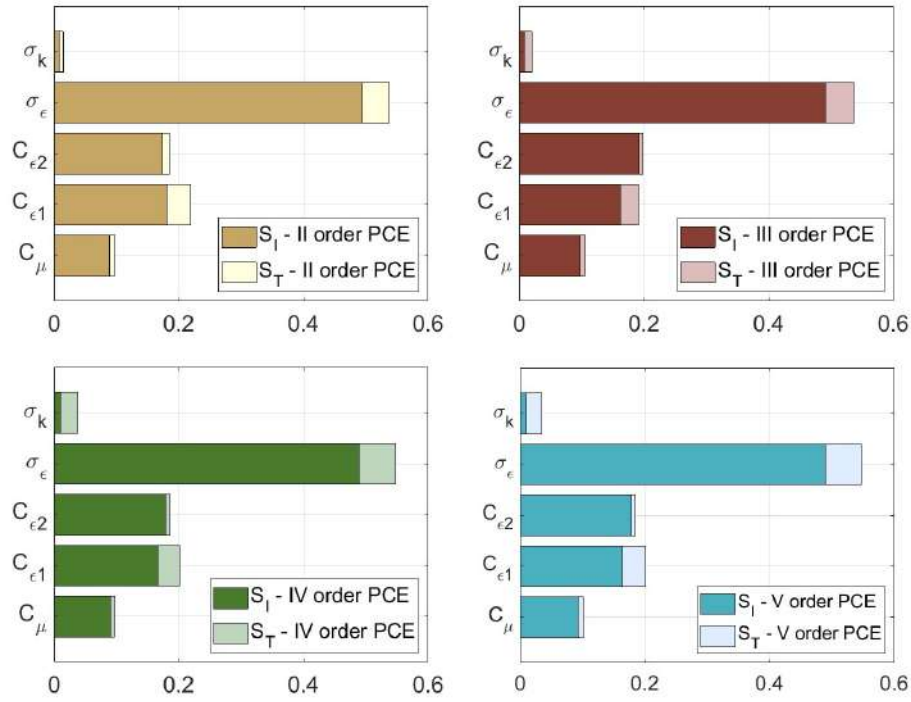


Figure 11.10: First and total order Sobol indices of the drag coefficient for the fully wetted flow regime - NACA66(MOD).

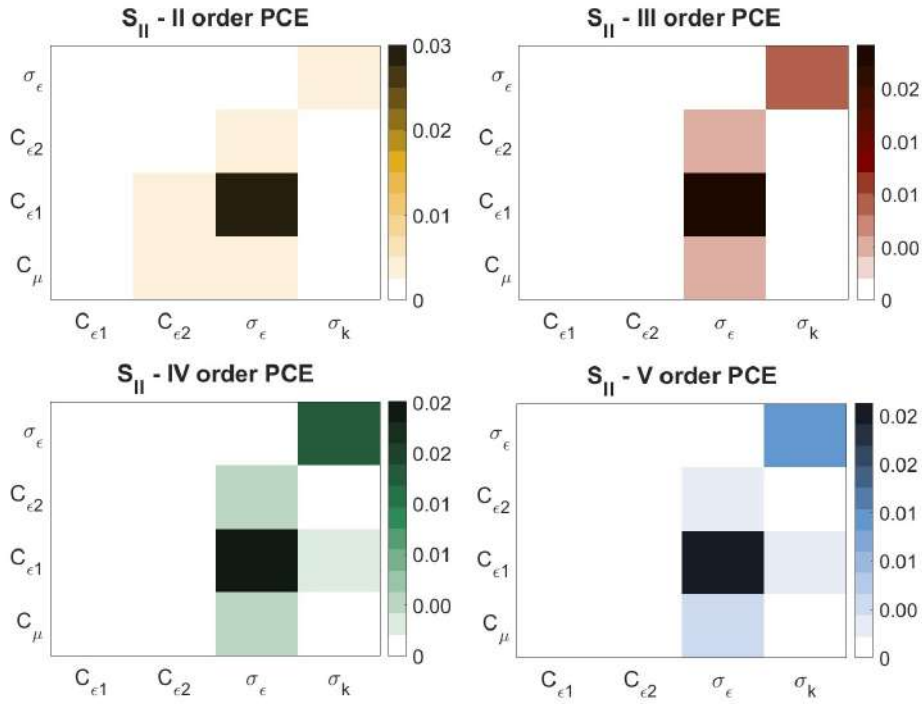


Figure 11.11: Second order Sobol indices of the drag coefficient for the fully wetted flow regime - NACA66(MOD).

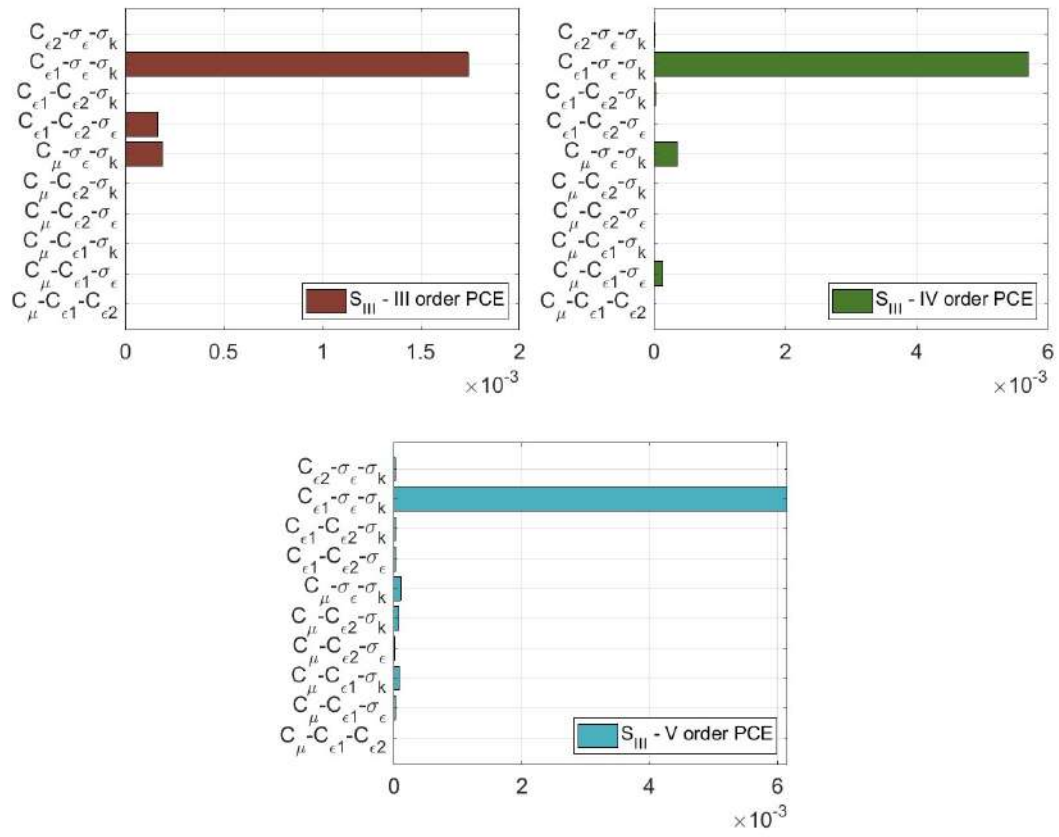


Figure 11.12: Third order Sobol indices of the drag coefficient for the fully wetted flow regime - NACA66(MOD).

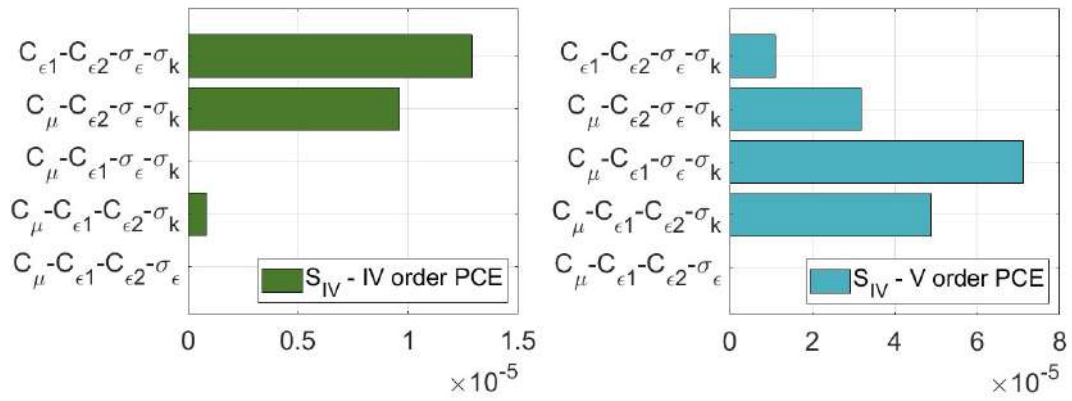


Figure 11.13: Fourth order Sobol indices of the drag coefficient for the fully wetted flow regime - NACA66(MOD).

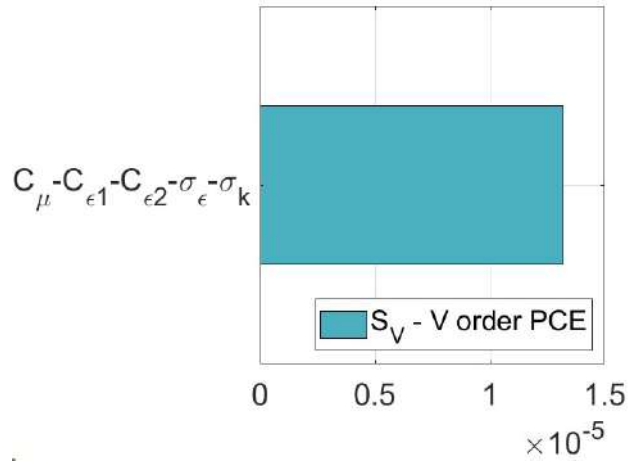


Figure 11.14: Fifth order Sobol indices of the drag coefficient for the fully wetted flow regime - NACA66(MOD).

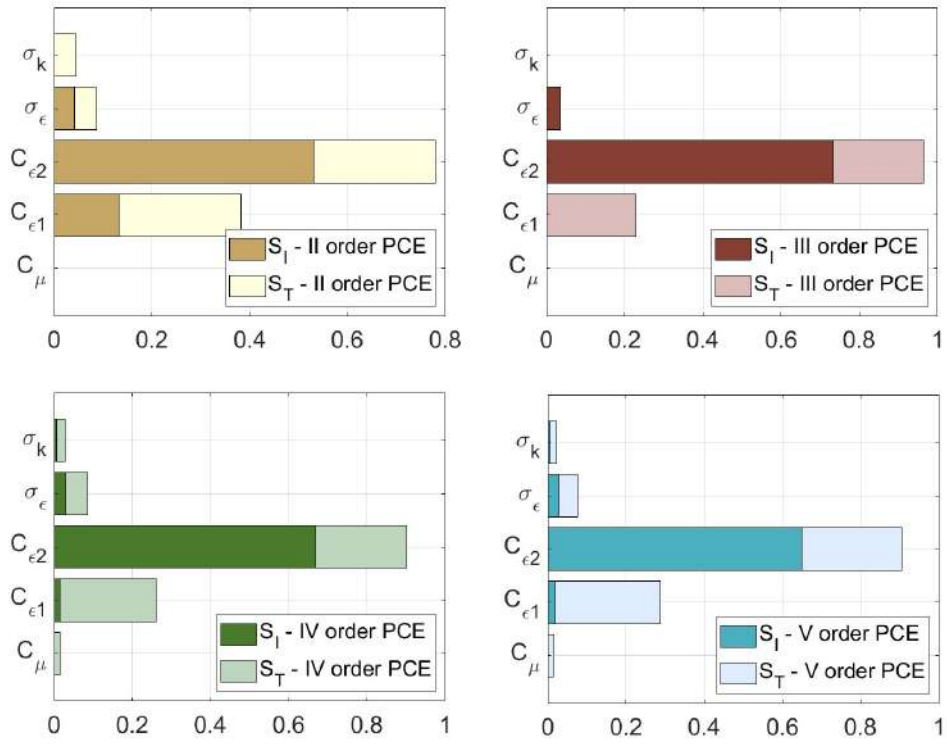


Figure 11.15: First and total order Sobol indices of the lift coefficient for the fully wetted flow regime - NACA66(MOD).

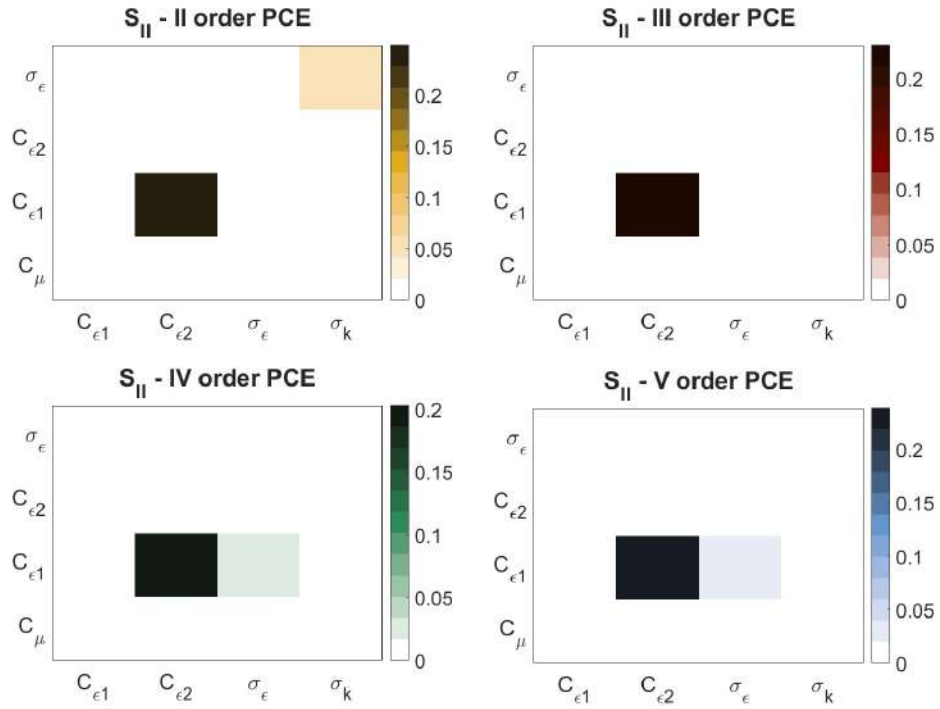


Figure 11.16: Second order Sobol indices of the lift coefficient for the fully wetted flow regime - NACA66(MOD).

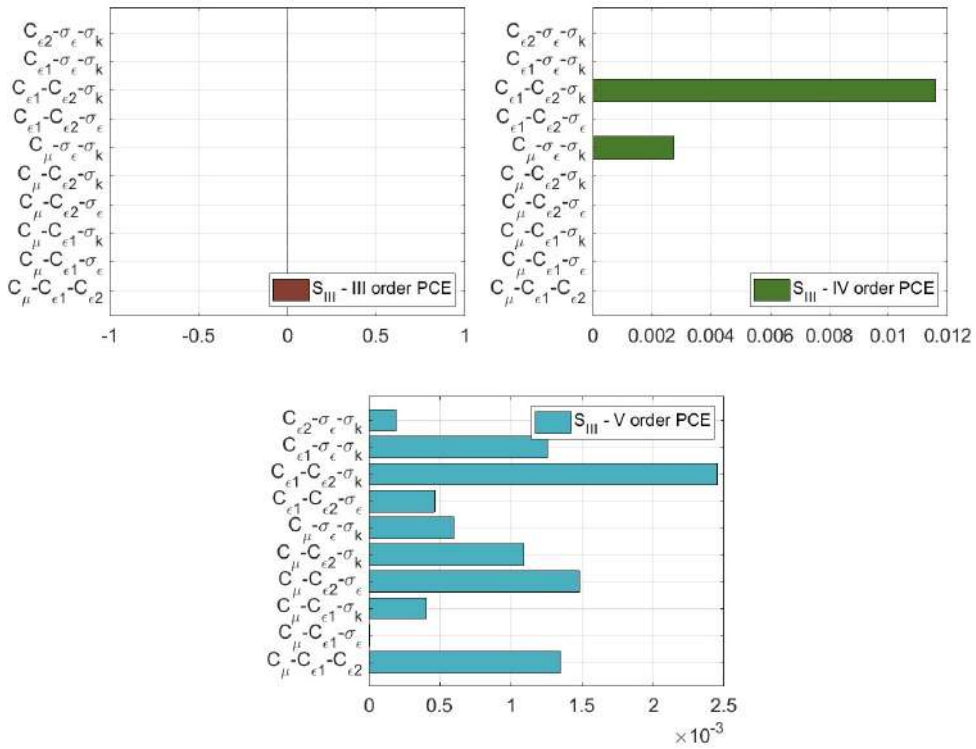


Figure 11.17: Third order Sobol indices of the lift coefficient for the fully wetted flow regime - NACA66(MOD).

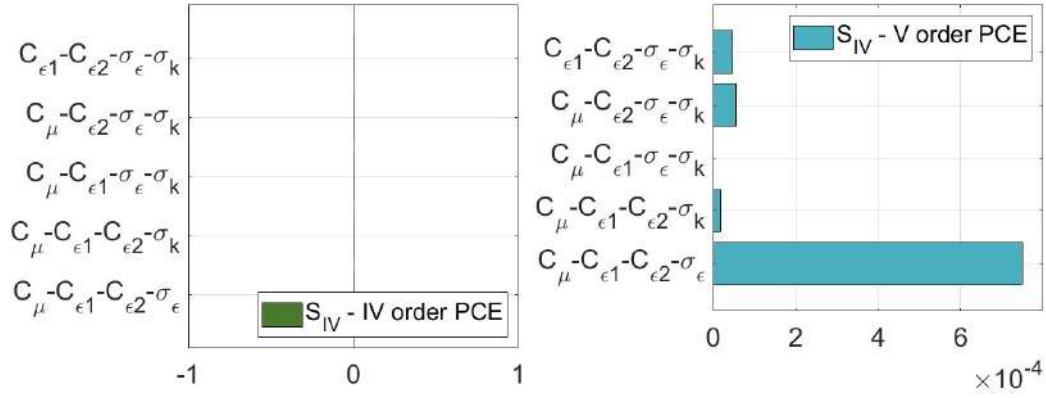


Figure 11.18: Fourth order Sobol indices of the lift coefficient for the fully wetted flow regime - NACA66(MOD).

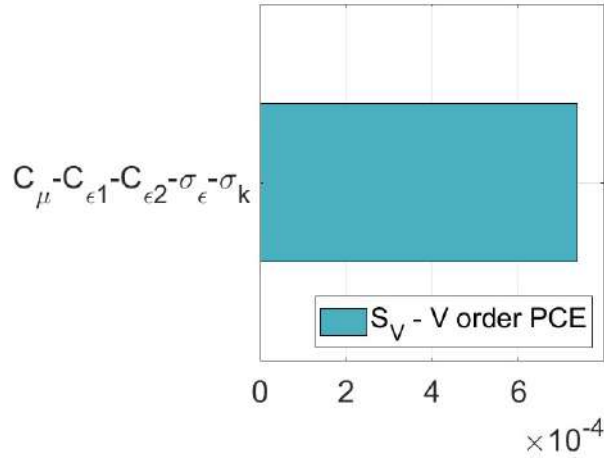


Figure 11.19: Fifth order Sobol indices of the lift coefficient for the fully wetted flow regime - NACA66(MOD).

Comparison between PCE and PCK for NACA66(MOD) hydrofoil

In some Uncertainty Quantification studies, it is not possible to generate a Design Of Experiment by employing an arbitrary set of points but it could be limited to a fixed set of collocation points. For this reason, it is important to evaluate the best suitable surrogate model for the problem of interest. In this section, a comparison between the Polynomial Chaos Expansion and the Polynomial Chaos-based Kriging has been conducted to evaluate the performance of these two metamodels. Specifically, we applied two set of points cataloged as "few points" and "many points" which correspond to the 42 sampling points of the Polynomial Chaos of the second order and by the 504 sampling points of the Polynomial Chaos of the fifth order.

- **Leave – One – Out Cross – Validation error:** Considering Figures 11.20, 11.21, 11.22 and 11.23, the Leave-One-Out Cross-Validation errors for the two set of points are shown.

Paying attention to Figure 11.20, we note a great difference between the trends of the two surrogate models for the prediction of drag when 42 collocation points are employed. In this context, the error of Polynomial Chaos Kriging seems to be more performant than the

error of Polynomial Chaos Expansion and the Polynomial Chaos Kriging stabilizes almost instantaneously.

Considering the lift output in Figure 11.21, the error has a mean decreasing behaviour as the polynomial degree increases for both Polynomial Chaos Expansion and Polynomial Chaos-based Kriging; from a general point of view, also in this case the Polynomial Chaos Kriging is a bit more performant than the classical Polynomial Chaos Expansion.

Taking into account now the errors associated with the set of many points (Figures 11.22 and 11.23), the Polynomial Chaos Kriging error converges from the first polynomial degrees (for both outputs) while the Polynomial Chaos Expansion errors decrease until they reach the Polynomial Chaos Kriging error trends. In this case, Polynomial Chaos Expansion and Polynomial Chaos-based Kriging show overlapping error trends.

In this context, if we apply a study which involves many points coupled with high polynomial expansion, a Polynomial Chaos Expansion could be favored due to its easier implementation while we can use a Polynomial Chaos Kriging for the lower polynomial orders. Summarizing, at least for this study, Polynomial Chaos Kriging is preferred for small sets of points for its capability of approximating the response surface through the presence of correlation functions among points (kernel) and it is also preferred for sets of many points for low polynomial orders. For analysis where many points and high polynomial orders are applied, the two metamodels have the same behaviour in terms of predictability and Polynomial Chaos Expansion may be preferred due to its simpler application.

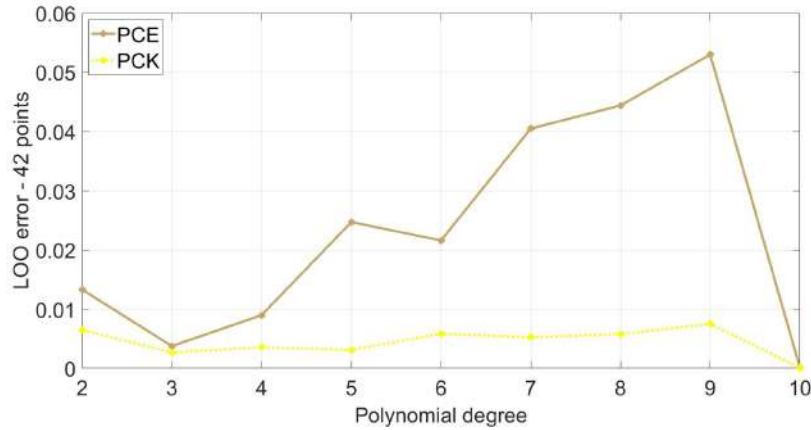


Figure 11.20: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response for 42 collocation points for a fully wetted flow - NACA66(MOD).

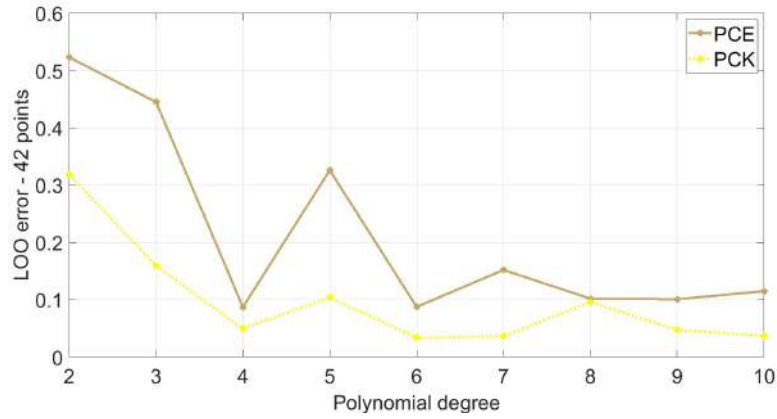


Figure 11.21: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response for 42 collocation points for a fully wetted flow - NACA66(MOD).

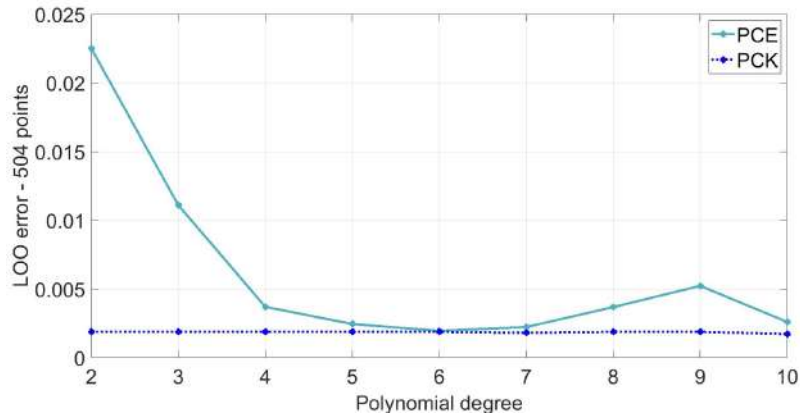


Figure 11.22: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response for 504 collocation points for a fully wetted flow - NACA66(MOD).

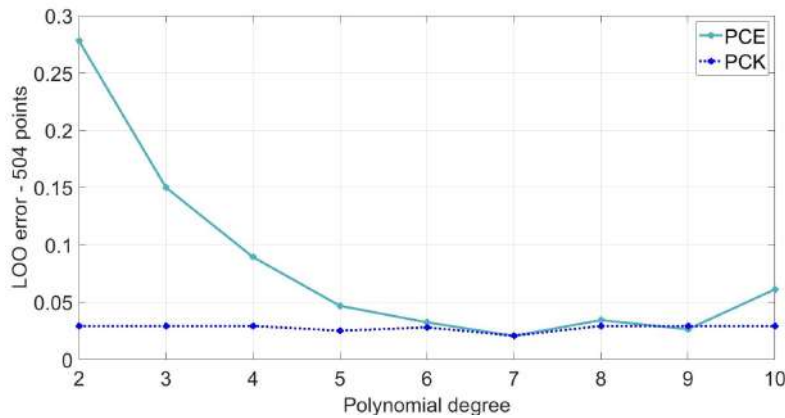


Figure 11.23: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response for 504 collocation points for a fully wetted flow - NACA66(MOD).

- **Sobol indices:** Following, results obtained by the application of the Global Sensitivity Analysis based on the ANOVA method of the Sobol decomposition for the Polynomial Chaos and Polynomial Chaos Kriging at each polynomial expansion of the two metamodels are discussed.

As known, Sobol indices are calculated by using Polynomial Chaos coefficients when Polynomial Chaos Expansion is employed for an Uncertainty Quantification analysis, but, when Polynomial Chaos-based Kriging is applied, it is not possible to involve Polynomial Chaos Kriging coefficients for determining the ranking of importance of the five calibration constants of the $k - \epsilon$ Turbulence model because there does not exist a closed form for the statistical moments of this surrogate model. To get around this problem, Sobol indices have been calculated by employing Monte Carlo sampling on the response surfaces generated by the Polynomial Chaos Kriging. The application of Monte Carlo strategies for Sobol indices computations is less robust than the application of Polynomial Chaos Expansions; in fact, the right computation of higher Sobol indices requires a very high computational cost (which can reach 10^9 samplings [42]) and then, only main and total Sobol indices have been calculated in this context. However, information contained in main and total Sobol indices is sufficient to achieve a good level of knowledge of a problem of this type.

Observing Figures 11.24, 11.25, 11.26 and 11.27 we have the results of sensitivity associated to the set of few points while in 11.28, 11.29, 11.30 and 11.31 there are the results inherent to the set of many points.

Observing all trends of Sobol indices is interesting to note that the ranking of coefficients does not change by varying the metamodel; in fact, the coefficient σ_ϵ is "still" the most important coefficient for the calculation of drag and the coefficient C_{ϵ_2} is the most influential parameter for the evaluation of lift. In conclusion, the weights of coefficients seem to be constant or almost stable when response surfaces are generated by applying 504 sampling points while the sensitivity coefficients show more numerical oscillations for the Design Of Experiment of 42 collocation points.

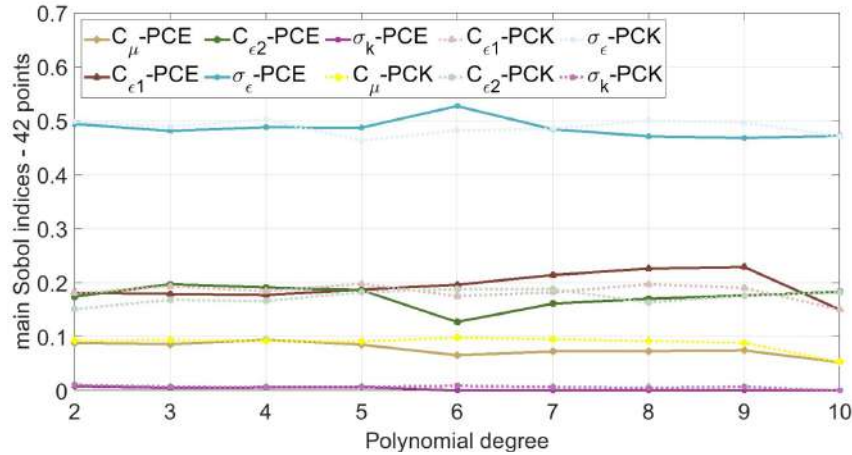


Figure 11.24: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 42 collocation points in a wetted flow condition - NACA66(MOD).

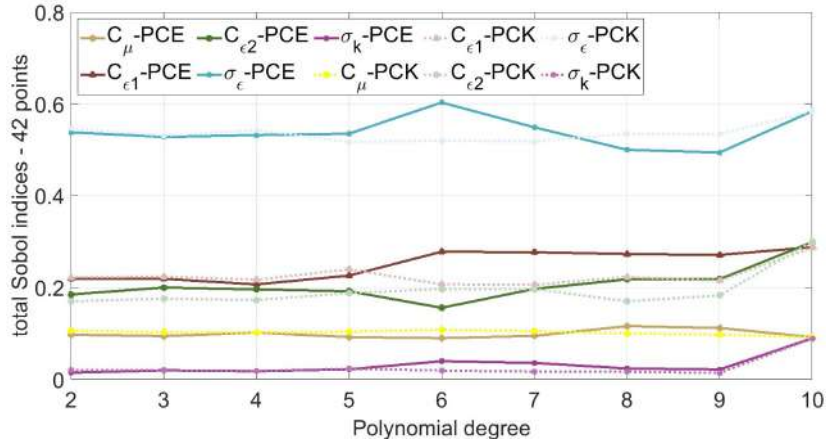


Figure 11.25: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 42 collocation points in a wetted flow condition - NACA66(MOD).

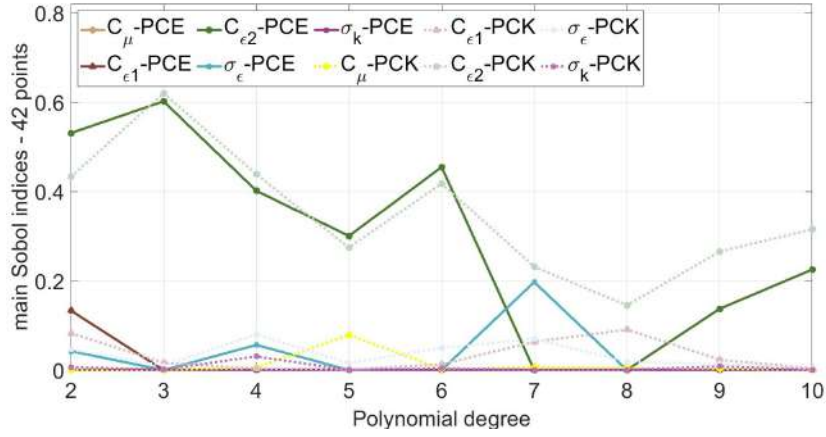


Figure 11.26: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 42 collocation points in a wetted flow condition - NACA66(MOD).

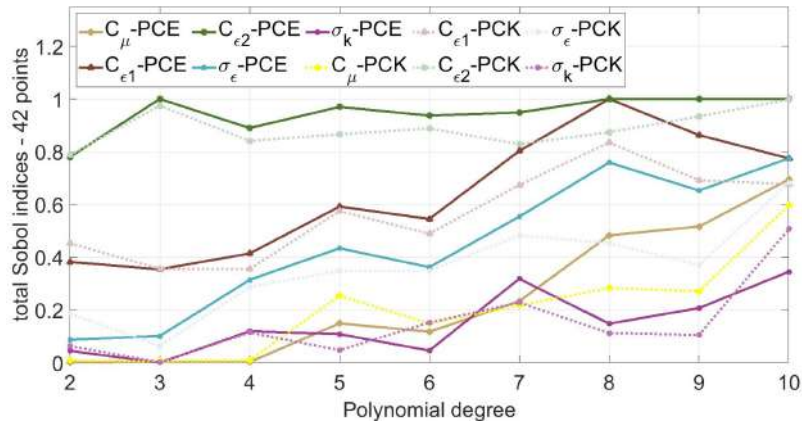


Figure 11.27: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 42 collocation points in a wetted flow condition - NACA66(MOD).

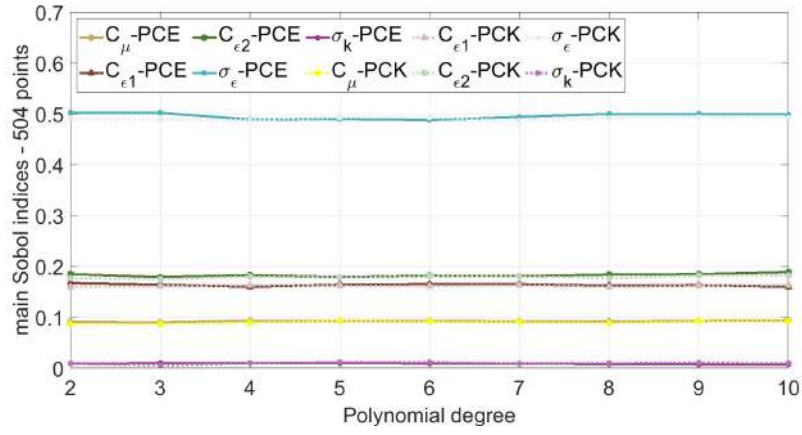


Figure 11.28: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 504 collocation points in a wetted flow condition - NACA66(MOD).

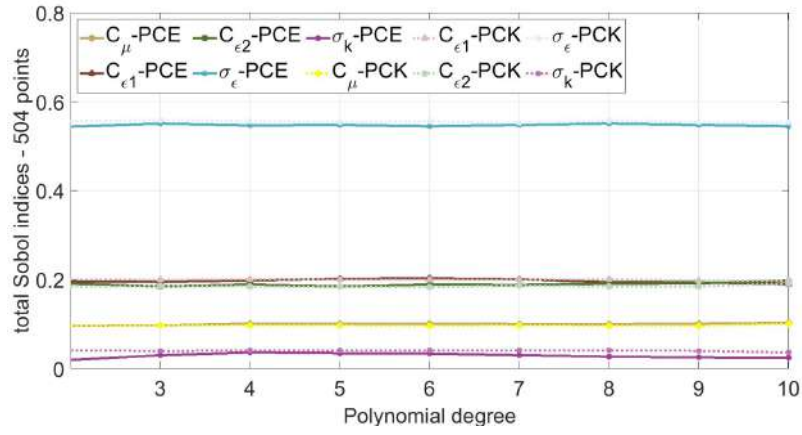


Figure 11.29: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 504 collocation points in a wetted flow condition - NACA66(MOD).

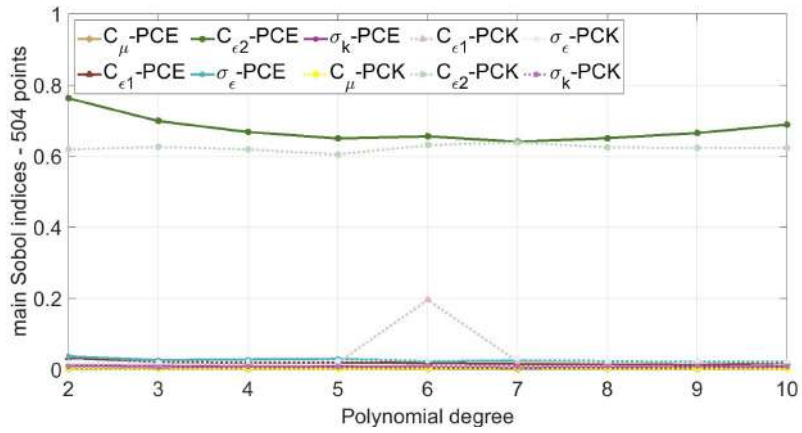


Figure 11.30: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 504 collocation points in a wetted flow condition - NACA66(MOD).

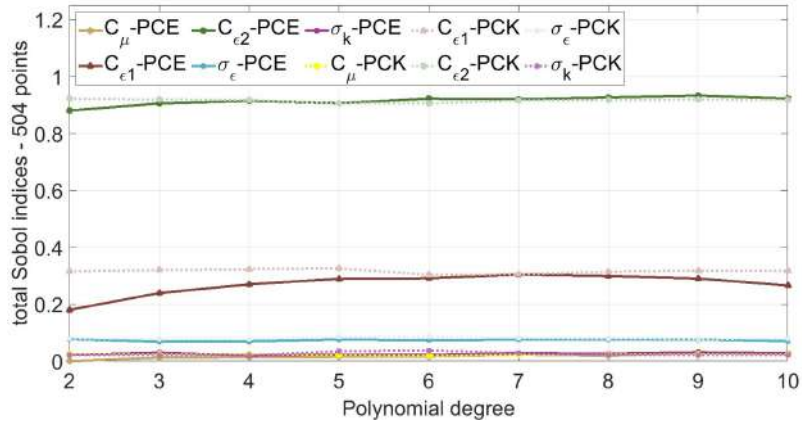


Figure 11.31: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 504 collocation points in a wetted flow condition - NACA66(MOD).

11.2.2 Cavitating flow regime

Leave-One-Out Cross-Validation error

Taking into account Figures 11.32 and 11.33, the Leave-One-Out Cross-Validation error trends for the cavitating flow regime are discussed. Likewise to the fully wetted flow condition, the errors for the two outputs preserve a convergence attitude when the Polynomial Chaos degree increases and observing the magnitude of errors for the lift and drag coefficient for both the flow regimes, we have that the LOO error curve associated to the cavitating flow (for the lift and drag respectively) is higher than the LOO error curve of the fully wetted flow (for the lift and drag respectively). This means that the response surface for the cavitating flow has less capability of predictability with respect to the response surface of the wetted flow (proving that cavitation is a phenomenon a bit more complicated to study).

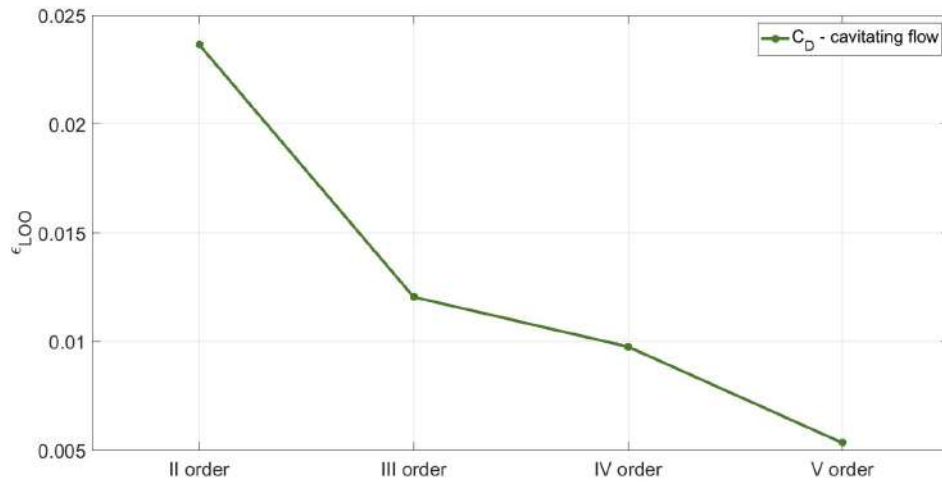


Figure 11.32: Leave-One-Out Cross-validation error trend of the drag coefficient in the cavitating flow condition - NACA66(MOD).



Figure 11.33: Leave-One-Out Cross-validation error trend of the lift coefficient in the cavitating flow condition - NACA66(MOD).

Statistical moments

In Figures 11.34 and 11.35 are shown mean values and confidence intervals at the 95 % margine of error for the drag and lift coefficients in a cavitating condition. Similarly to the fully wetted flow, confidence intervals reduce by increasing the Polynomial Chaos order and then, the the uncertainty can be reduced by increasing the degree of the Polynomial Chaos Expansion. Contrarily to the wetted flow, mean value trends of lift and drag do not converge to a specific numerical value but the magnitude of oscillations are very low.

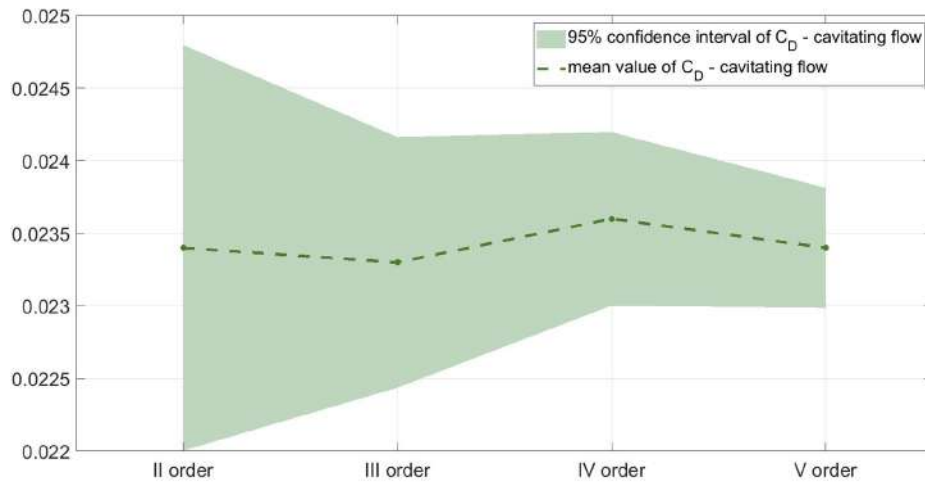


Figure 11.34: Mean values and Confidence Intervals of the drag coefficient in the cavitating flow condition - NACA66(MOD).

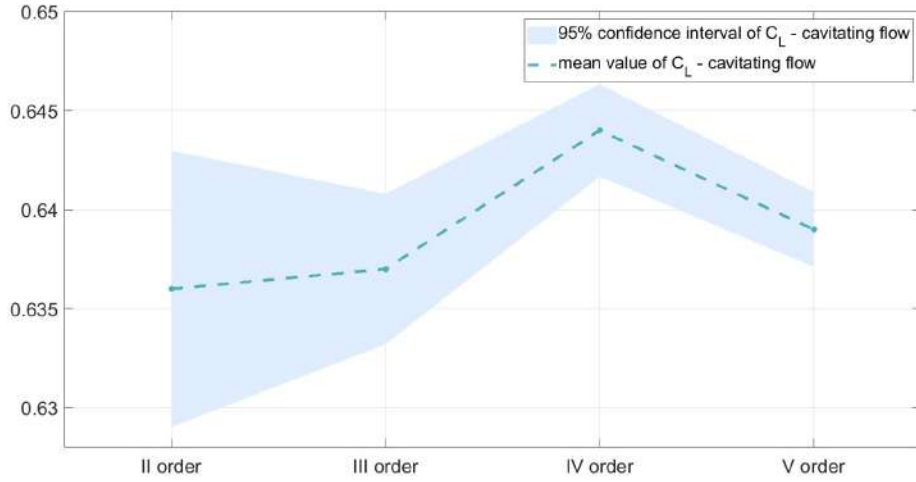


Figure 11.35: Mean values and Confidence Intervals of the lift coefficient in the cavitating flow condition - NACA66(MOD).

Posterior probability distributions

In the following paragraph, posterior probability distributions of drag in Figure 11.36 and posterior probability distributions of lift in Figure 11.37 for the cavitating flow regime are represented. The probability distributions have been generated by applying the same methodology used for the fully wetted flow scenario and as further information, mean values, standard deviations, modes and medians for the two hydrodynamics coefficients are tabulated in Table 11.2.

Considering the drag response, the probability distributions show a very modest uncertainty reduction by increasing the polynomial order, subjecting that a low degree of the Polynomial Chaos (i.e. second or third) is sufficient to predict that output. Probability distribution of drag for the fully wetted and cavitating flow regimes have very similar characteristics.

Considering now the lift coefficient, the associated probability distributions have different profiles for each polynomial expansion (i.e. the distributions change when the polynomial order changes) but those differences are less marked than the differences obtained in case study of the fully wetted flow. In this context, distributions of Polynomial Chaos of the fourth and fifth order seem to have a similar behaviour but further polynomial expansions could be useful to determine the best lower Polynomial Chaos order for the lift prediction in the cavitating regime.

As for the fully wetted flow, the probability distributions of drag show a skewed behaviour indicating a set of underestimated values while the probability distributions of lift show a skewness behaviour which represent a set of overestimated values.

Table 11.2: Data of posterior distribution functions of cavitating flow regime - NACA66(MOD).

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
C_d	II	0.0233	0.00465	0.0209	0.0275
C_d	III	0.0233	0.00466	0.0222	0.0286
C_d	IV	0.0236	0.00499	0.0224	0.0342
C_d	V	0.0234	0.00478	0.0217	0.0342
C_l	II	0.636	0.0253	0.653	0.607
C_l	III	0.637	0.0239	0.637	0.628
C_l	IV	0.644	0.0221	0.652	0.631
C_l	V	0.638	0.0265	0.644	0.621

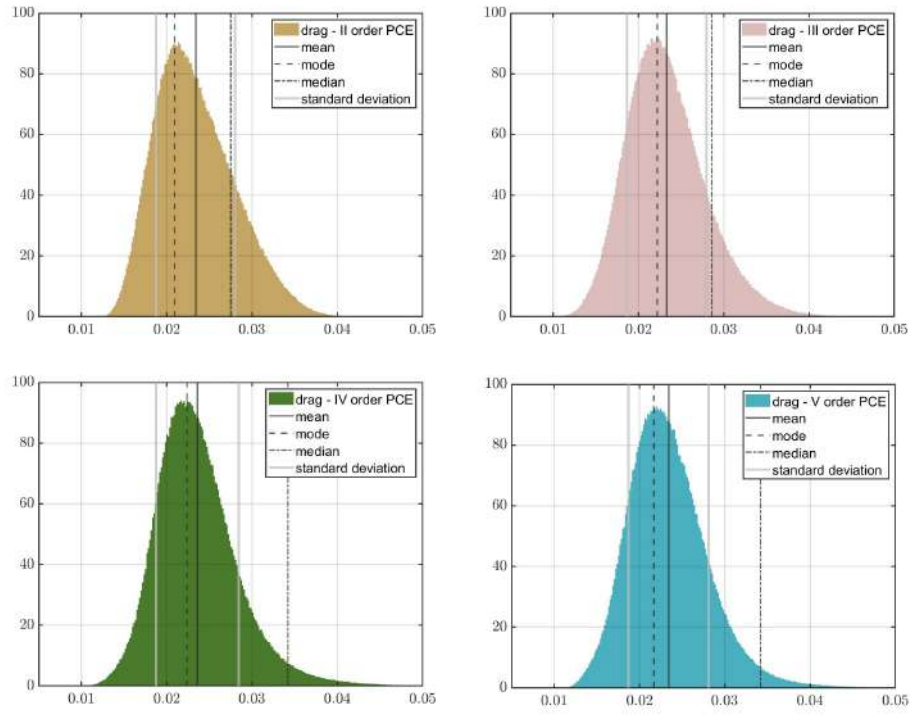


Figure 11.36: Posterior probability distributions of the drag coefficient for the cavitating flow - NACA66(MOD).

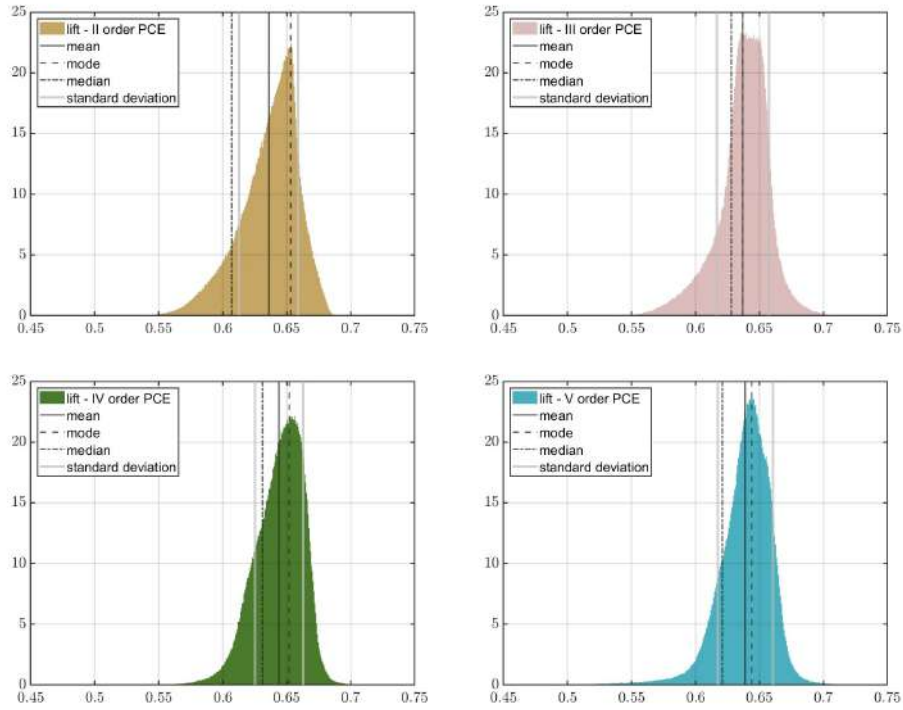


Figure 11.37: Posterior probability distributions of the lift coefficient for the cavitating flow - NACA66(MOD).

Sobol indices

In the following section, we show the Sobol indices obtained by taking into account the cavitating flow regime. In Figures 11.38, 11.39, 11.40, 11.41 and 11.42 there are the Sobol indices of drag and in Figures 11.43, 11.44, 11.45, 11.46 and 11.47 there are the Sobol indices of lift.

Considering the results presented in Figure 11.38, it is possible to observe that, also for the cavitating flow regime, the parameter with the highest weight on the drag evaluation is σ_ε and analyzing the results in Figures 11.39 and 11.40, the pair and the triplet interactions which seems to influence most the results are $C_{\varepsilon_1} - \sigma_\varepsilon$ and $C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$.

At the contrary of the fully wetted flow condition and observing the Figure 11.41, we have that the ranking of the Sobol indices of fourth order is preserved and the most influential triplet for the drag seems to be $C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$. As the matter of fact, it seems that the ranking of the model constants is not influenced by the presence of the attached sheet cavity.

Taking into account the lift coefficient instead, Figures 11.43, 11.44 and 11.46 show that the ranking of the turbulence parameters is very similar to the results about the fully wetted flow; in fact, the coefficient and interactions C_{ε_2} , $C_{\varepsilon_1} - C_{\varepsilon_2}$ and $C_\mu - C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon$ seems to be the most important constants for the lift calculation at any polynomial expansion. As difference, the ranking of triplets is not preserved when the Polynomial degree changes: the interaction $C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_k$ is the most important when a fourth order is employed and the interaction $C_\mu - C_{\varepsilon_2} - \sigma_\varepsilon$ is the most important when a fifth polynomial degree is adopted.

In conclusion, from a broadly point of view, the ranking of coefficients for the lift output do not vary by the presence of cavitation. Taking into account the magnitude of all Sobol indices for both the responses, only the Sobol indices of the first two order are relevant for the Global Sensitivity Analysis of this problem of interest.

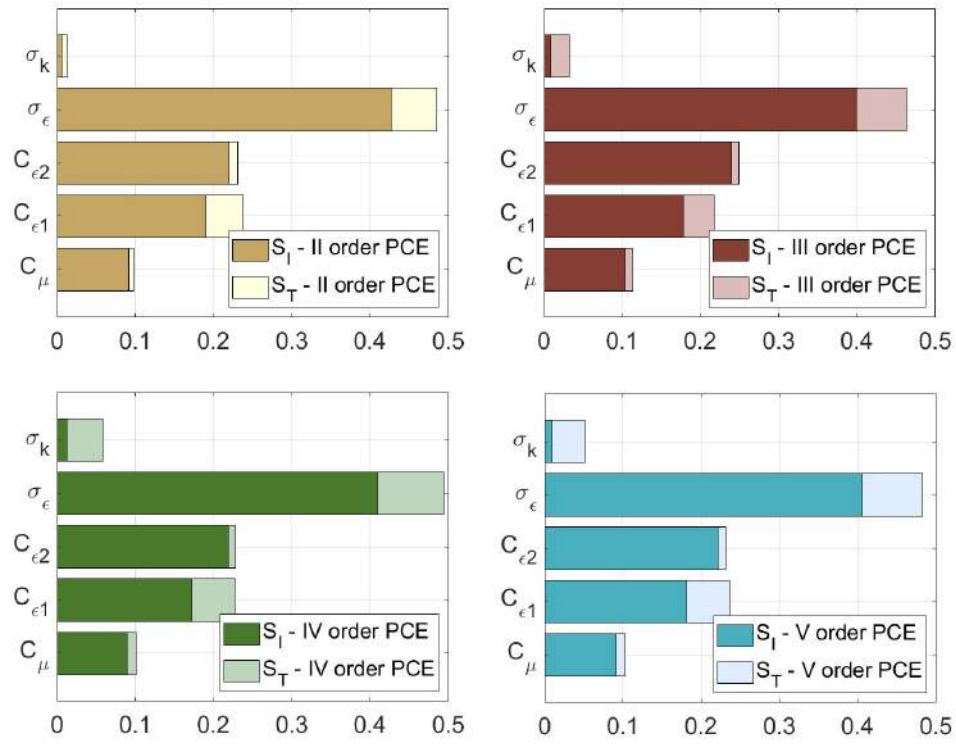


Figure 11.38: First and total order Sobol indices of the drag coefficient for the cavitating flow regime - NACA66(MOD).

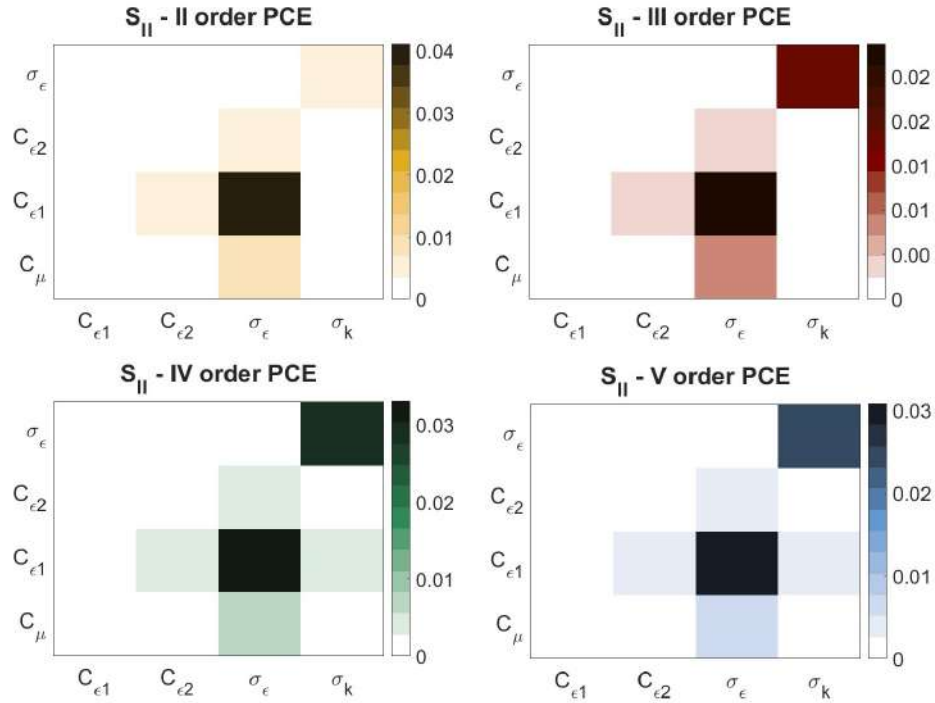


Figure 11.39: Second order Sobol indices of the drag coefficient for the cavitating flow regime - NACA66(MOD).

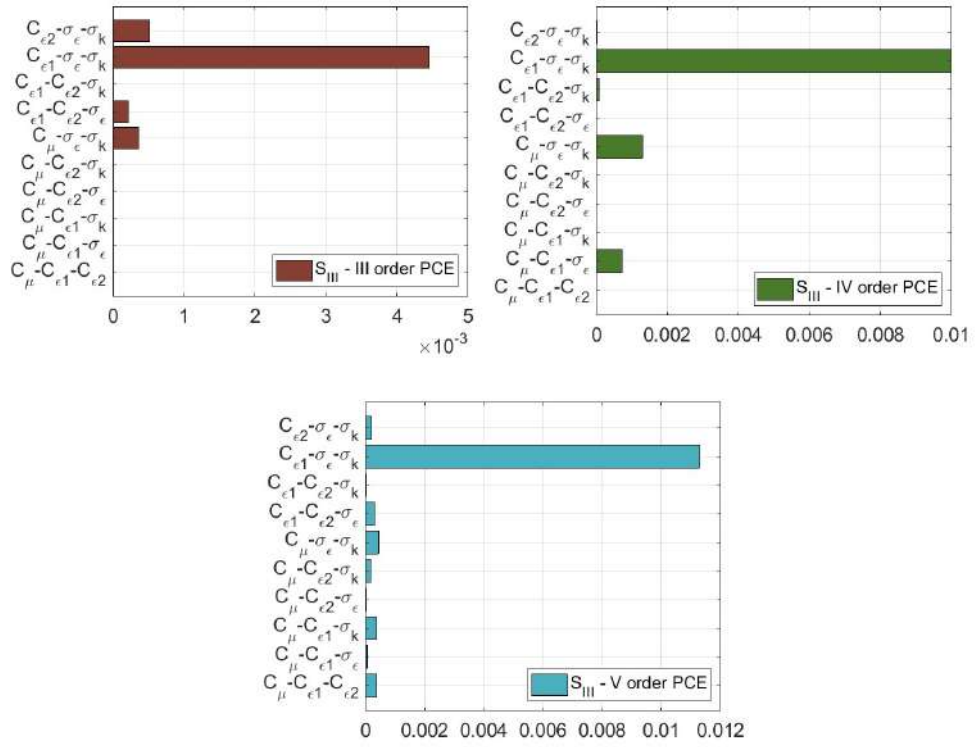


Figure 11.40: Third order Sobol indices of the drag coefficient for the cavitating flow regime - NACA66(MOD).

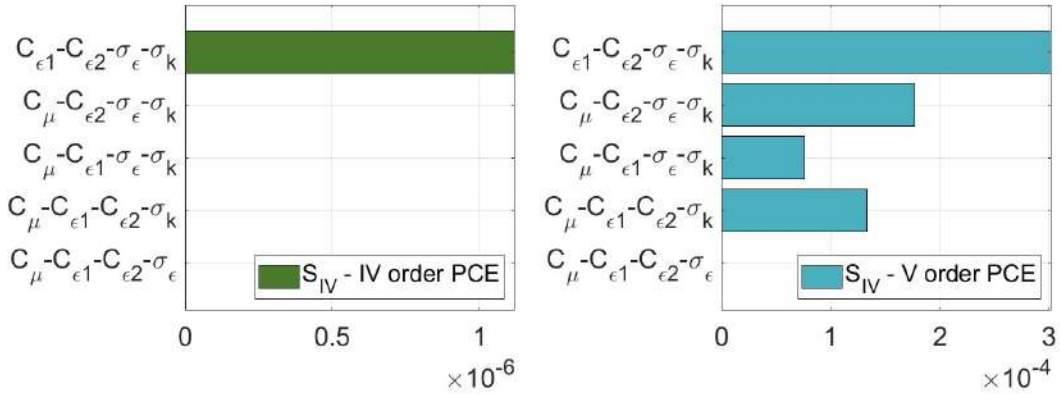


Figure 11.41: Fourth order Sobol indices of the drag coefficient for the cavitating flow regime - NACA66(MOD).

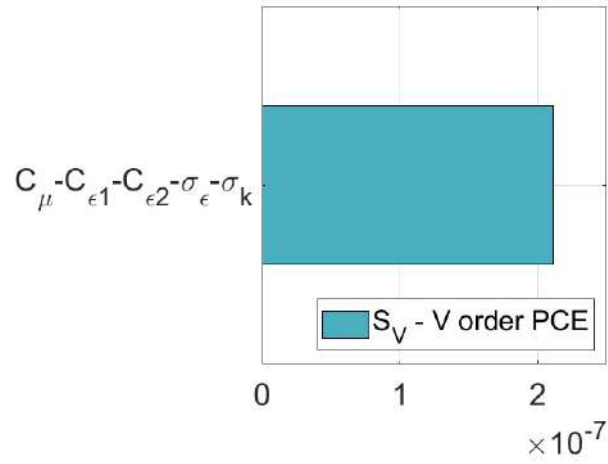


Figure 11.42: Fifth order Sobol indices of the drag coefficient for the cavitating flow regime - NACA66(MOD).

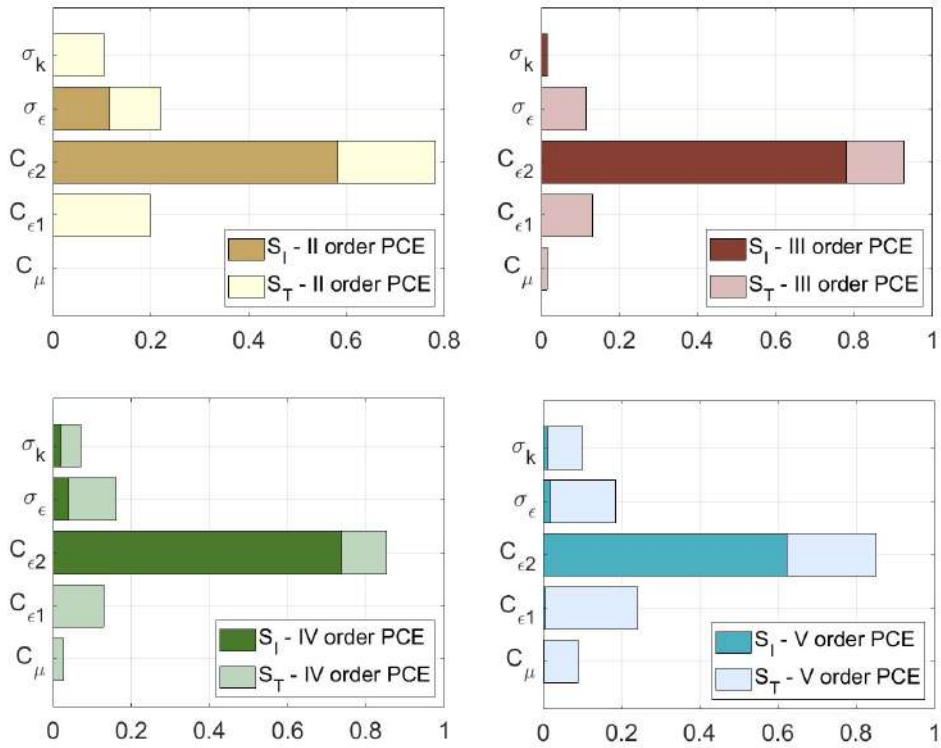


Figure 11.43: First and total order Sobol indices of the lift coefficient for the cavitating flow regime - NACA66(MOD).

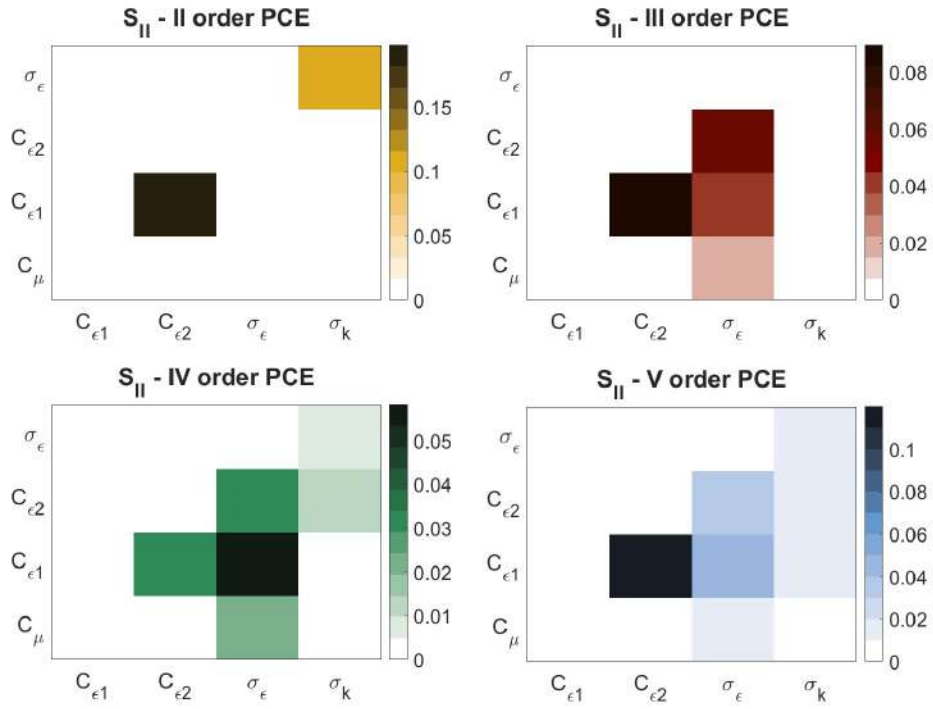


Figure 11.44: Second order Sobol indices of the lift coefficient for the cavitating flow regime - NACA66(MOD).

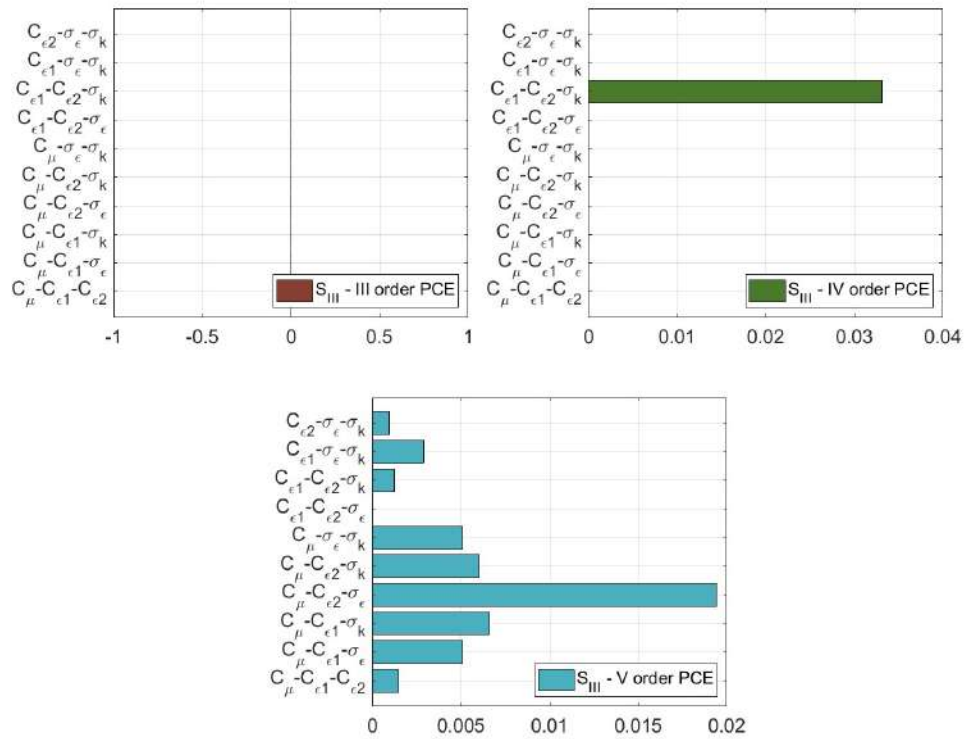


Figure 11.45: Third order Sobol indices of the lift coefficient for the cavitating flow regime - NACA66(MOD).

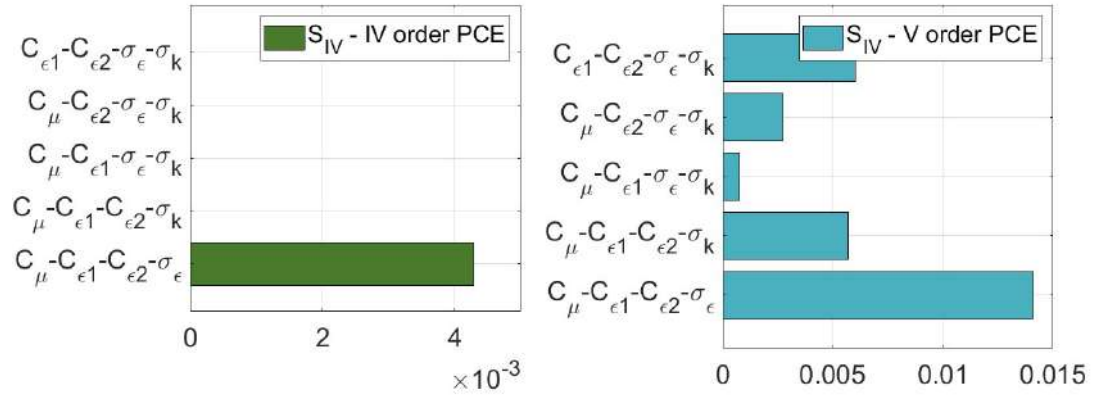


Figure 11.46: Fourth order Sobol indices of the lift coefficient for the cavitating flow regime - NACA66(MOD).

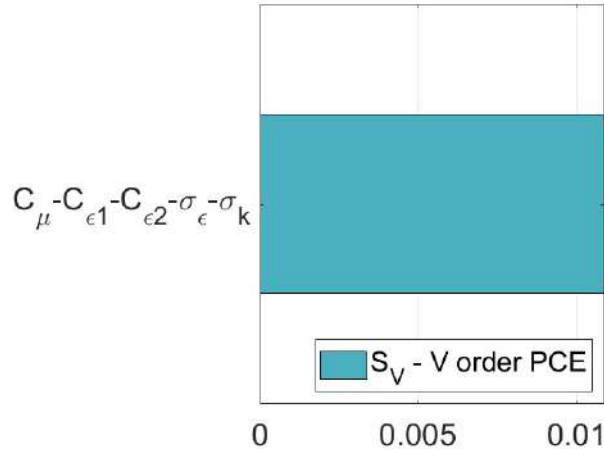


Figure 11.47: Fifth order Sobol indices of the lift coefficient for the cavitating flow regime - NACA66(MOD).

Comparison between PCE and PCK for NACA66(MOD) hydrofoil

- **Leave – One – Out Cross – Validation error:** the errors of prediction obtained for the cavitating flow are graphically represented in Figures 11.48, 11.49, 11.50 and 11.51. Paying attention to the drag output associated with the set of 42 points, we have that the Polynomial Chaos Kriging error has a stable trend while the Leave-One-Out Cross-Validation error of Polynomial Chaos has a more oscillatory behaviour. In this context, The Polynomial Chaos Kriging is more performant. After, observing the lift errors in 11.49, these two metamodels have a very similar and close behaviour, the polynomial Chaos Kriging is able to predict the lift output with slightly higher accuracy than the Polynomial Chaos Expansion but the second may be favorite by its simpler implementation.

In conclusion, analyzing the results about the set of many points, LOO errors of PCE and PCK have similar predictability for both the responses from the fifth/sixth polynomial order and they differ for the lower polynomial orders. the choice of the best surrogate models seem,s to be strictly connected to the polynomial expansion; however, the error of the Polynomial Chaos-based Kriging shows a more stable evolution than Polynomial Chaos error.

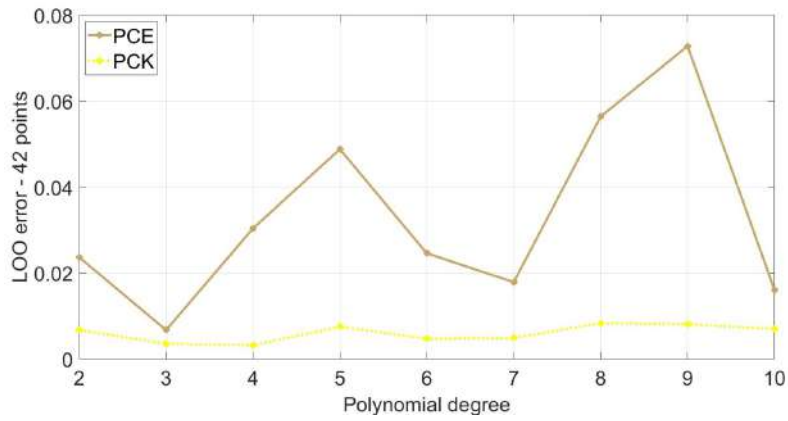


Figure 11.48: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response for 42 collocation points for a cavitating flow - NACA66(MOD).

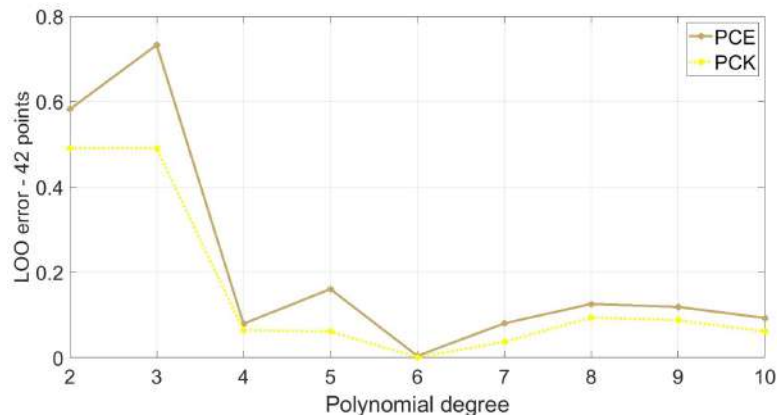


Figure 11.49: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response for 42 collocation points for a cavitating flow - NACA66(MOD).

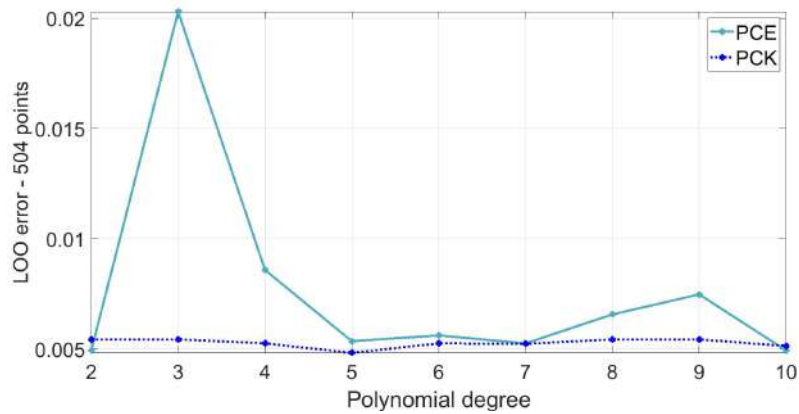


Figure 11.50: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response for 504 collocation points for a cavitating flow - NACA66(MOD).

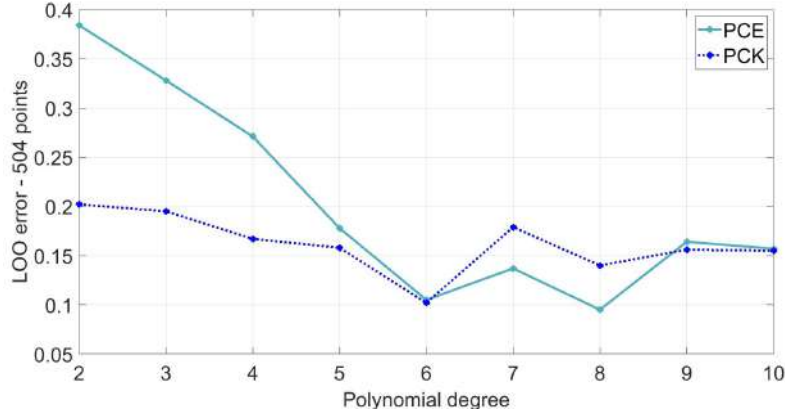


Figure 11.51: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response for 504 collocation points for a cavitating flow - NACA66(MOD).

- **Sobol indices:** in the current section, the Sobol indices obtained for the Polynomial Chaos and Polynomial Chaos Kriging in a cavitating flow regime are shown in Figures 11.52, 11.53, 11.54, 11.55, 11.56, 11.57, 11.58 and 11.59. Analyzing all graphs, it is interesting to note that, even for the cavitating flow, the ranking of turbulence parameters is not influenced by the choice of the surrogate model employed and the coefficients σ_ϵ and C_{ϵ_2} remain the most important constants for each polynomial expansion. From a general point of view, the weights of turbulent constants remain stable for the set of many points, suggesting a simpler variance-based analysis due to the presence of a bigger amount of points.

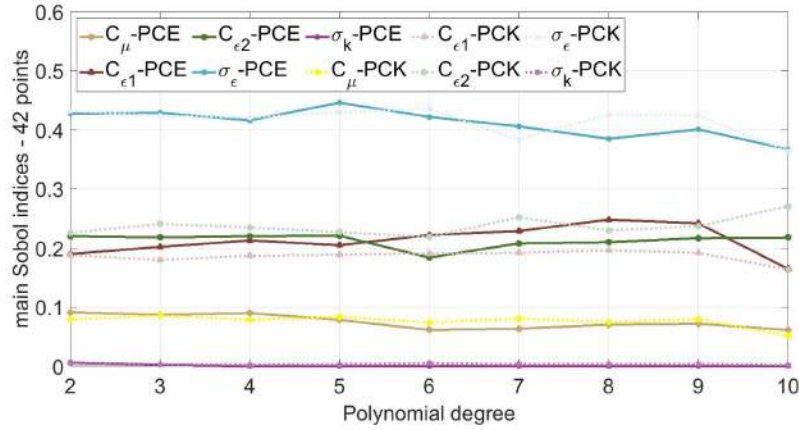


Figure 11.52: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 42 collocation points in a cavitating flow condition - NACA66(MOD).

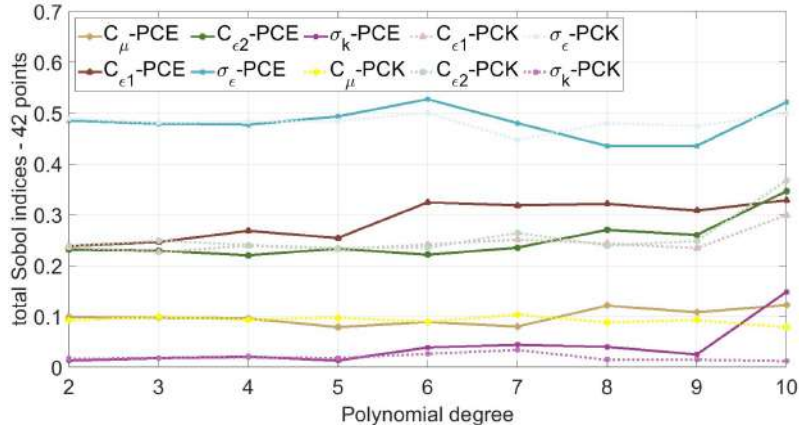


Figure 11.53: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 42 collocation points in a cavitating flow condition - NACA66(MOD).

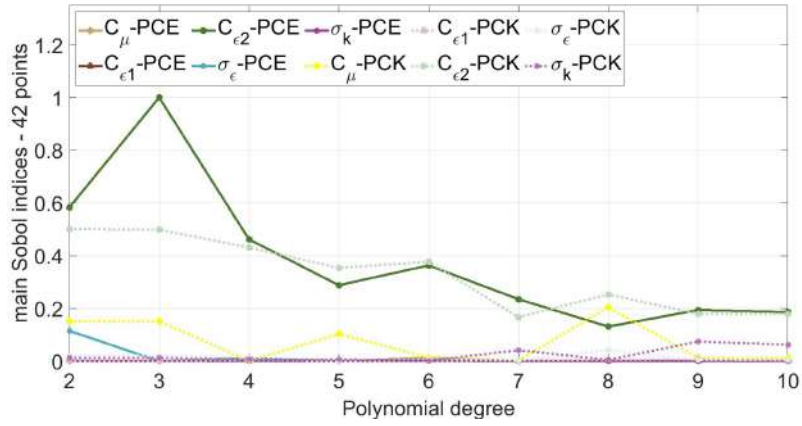


Figure 11.54: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 42 collocation points in a cavitating flow condition - NACA66(MOD).

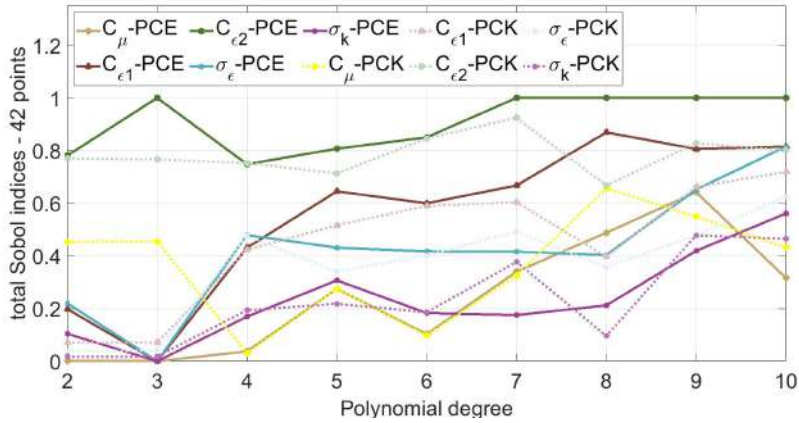


Figure 11.55: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 42 collocation points in a cavitating flow condition - NACA66(MOD).

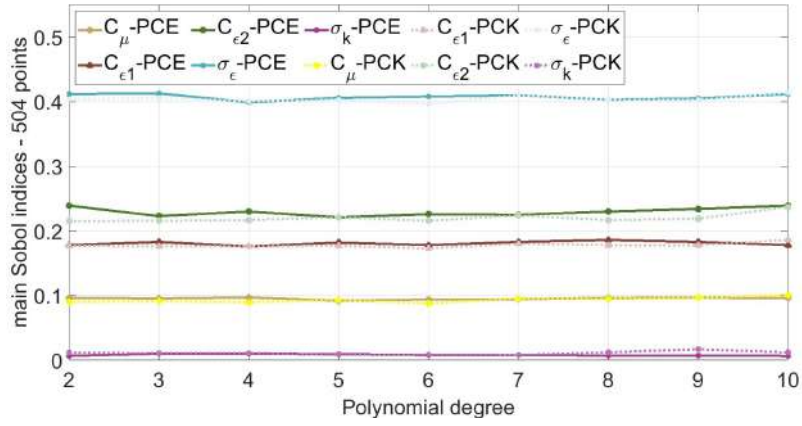


Figure 11.56: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 504 collocation points in a cavitating flow condition - NACA66(MOD).

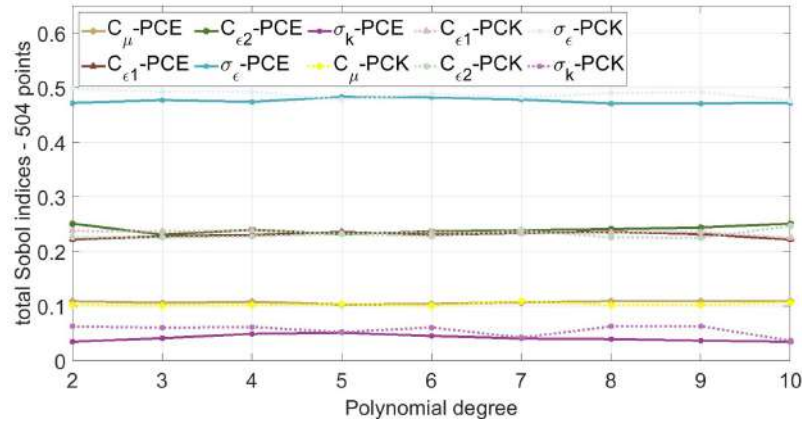


Figure 11.57: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the drag response by involving 504 collocation points in a cavitating flow condition - NACA66(MOD).

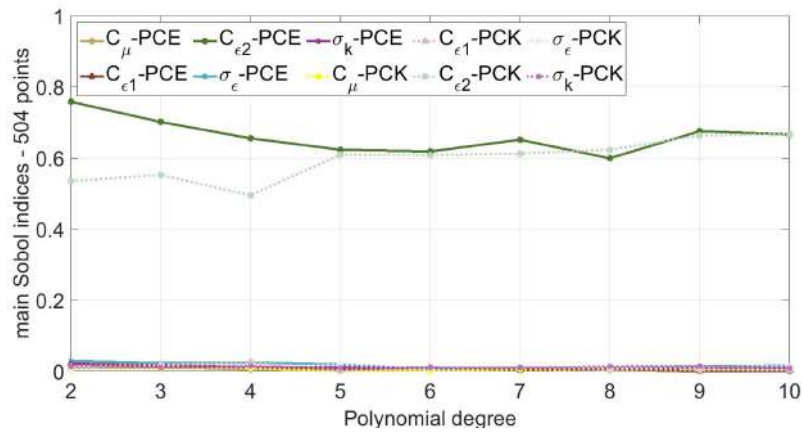


Figure 11.58: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 504 collocation points in a cavitating flow condition - NACA66(MOD).

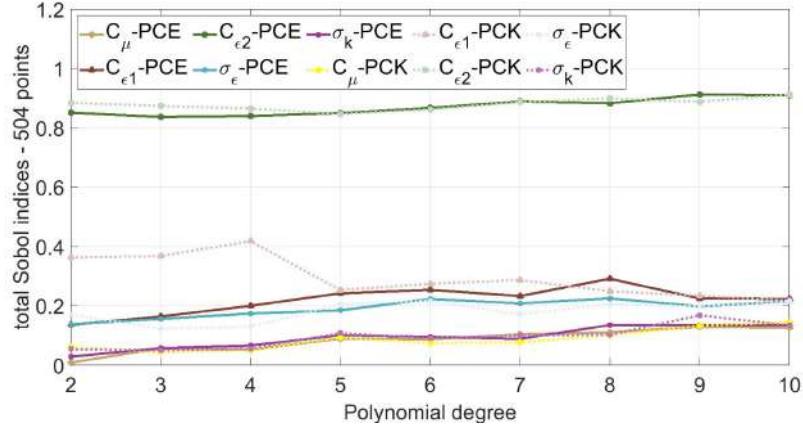


Figure 11.59: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the lift response by involving 504 collocation points in a cavitating flow condition - NACA66(MOD).

11.3 Local Analysis

In the following section, the results obtained from the local analysis of the NACA66(MOD) hydrofoil are discussed; in this work each result is determined with respect the upper surface of the hydrofoil.

11.3.1 Fully wetted flow regime

Leave-One-Out Cross-Validation error

In Figures 11.60 and 11.61 the Leave-One-Out Cross-Validation error trends along the NACA66(MOD) hydrofoil are described. Considering the pressure coefficient (Figure 11.60), the LOO error tends to zero near the leading edge of NACA. After that, the error increases at the 1/4 of the hydrofoil. This variation seems to be associated to the rapid increase of the pressure at this zone and subsequently, the error keeps his trend enough stable along the hydrofoil. In conclusion, there is a strong decrease and increase of the error at the trailing edge of the NACA(66)MOD hydrofoil.

Taking into account the LOO error of the friction coefficient (Figure 11.61), the error has a peak at the leading edge of the hydrofoil for then decrease instantly. Afterward, the error increases almost linearly and decreases at the trailing edge.

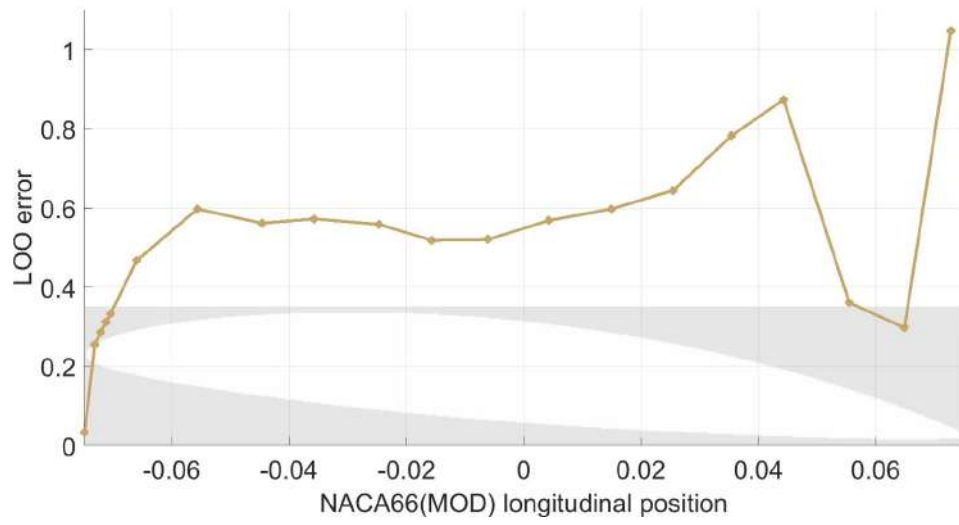


Figure 11.60: Trend of Leave-One-Out Cross-Validation error along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of pressure coefficient.

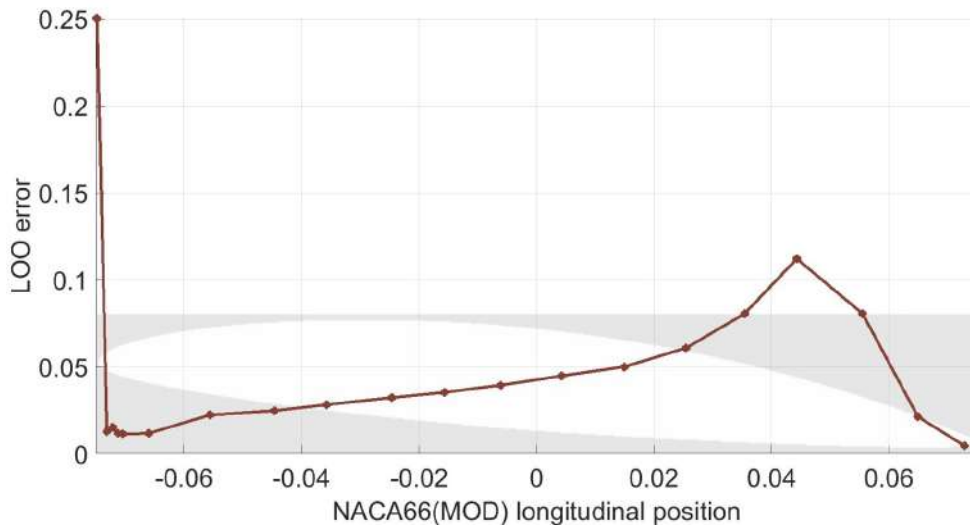


Figure 11.61: Trend of Leave-One-Out Cross-Validation error along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of the friction coefficient.

Statistical moments

In the following paragraph, mean value and confidence interval trends of c_p and c_f along the NACA66(MOD) hydrofoil are given. Observing the confidence intervals for both the responses, their values are very low, suggesting a low uncertainty about variations of the five calibration constants of the $k - \varepsilon$ turbulence model.

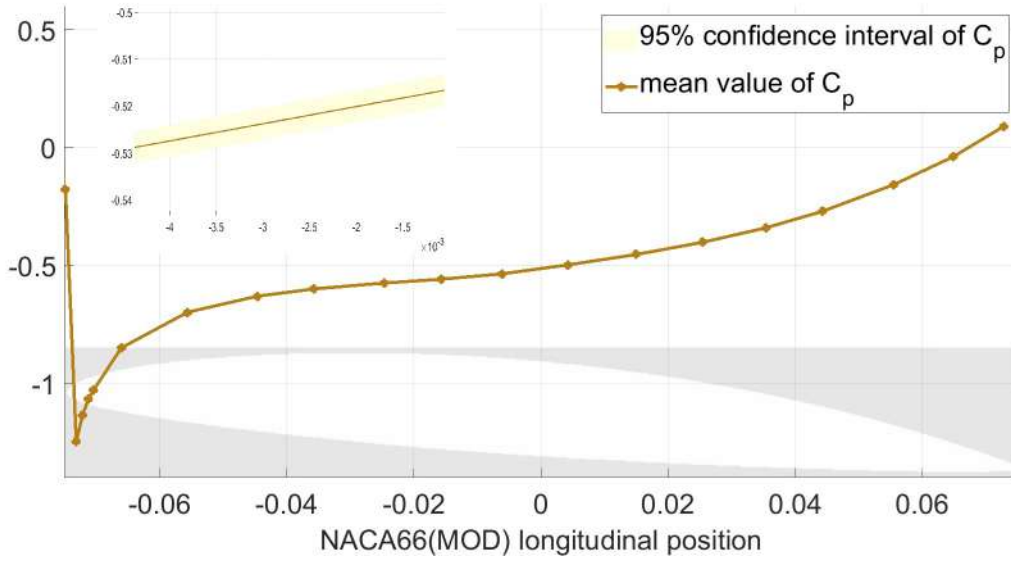


Figure 11.62: Trend of mean value and confidence interval along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of pressure coefficient.

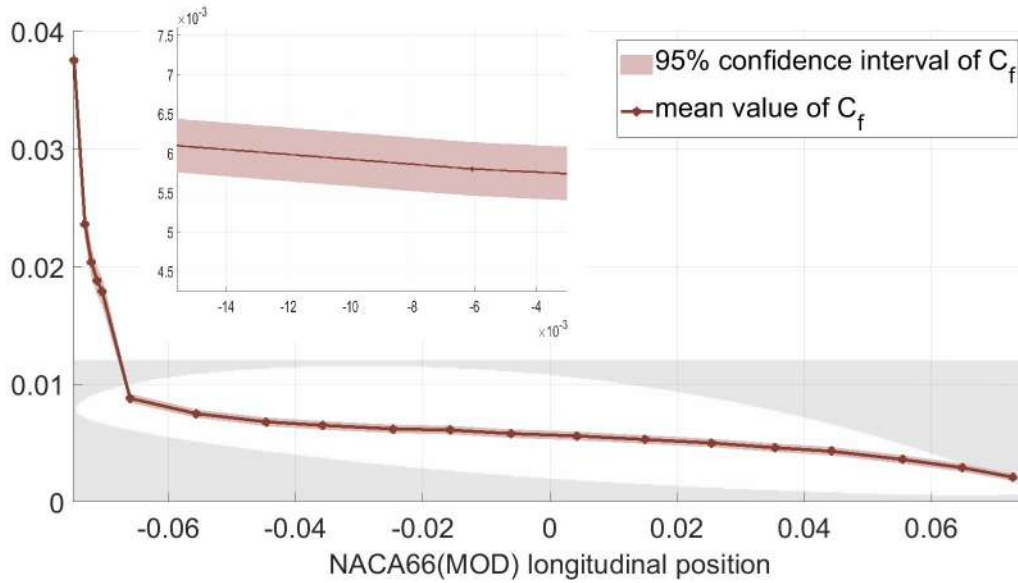


Figure 11.63: Trend of mean value and confidence interval along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of friction coefficient.

Sobol indices

Considering the Sobol indices obtained for the C_p output (Figures 11.64, 11.65 and 11.66), we observe that σ_ε is the most important coefficient at the leading edge of the hydrofoil while all others have a negligible contribution to the uncertainty in the pressure coefficient. Moving along the longitudinal position of the NACA66(MOD), the ranking of coefficients changes; the most important coefficient becomes C_{ε_2} while the second most important constant is the coefficient C_{ε_1} . The second and third positions of influence change at the trailing edge of the geometry. In this case, the second coefficient (in terms of importance) is σ_ε and the third becomes C_{ε_1} .

It is interesting to note that the parameters C_μ and σ_k remain the less important constant for each point of the hydrofoil. From a general point of view, C_{ϵ_2} is the most contribution on the uncertainty associated to c_p and it need to be taken into particular account when the lift force is determined. However, if cavitation occurs the pressure at the leading edge is the main quantity of interest which influence that phenomenon and then, if we are interested on the evolution of cavitation along the NACA, σ_ϵ is the coefficient which must be considered as first contribution of uncertainty. After, if the interest is about the uncertainty of separation point, σ_ϵ needs to be considered as the principal main source of uncertainty. From a general point of view, $C_{\epsilon_1} - C_{\epsilon_2}$ is the most influential non-linear effect between coefficients.

Comparing the results obtained in Figures 11.67 11.68 and 11.69 for the friction coefficient with the results of pressure coefficient, an analogous behaviour is observed. The most important parameter is the coefficient C_{ϵ_2} and the second one is the coefficient σ_ϵ . The ranking of C_{ϵ_2} and σ_ϵ is preserved at the leading edge while C_μ and σ_k are negligible. In conclusion, the pair $C_{\epsilon_1} - C_{\epsilon_2}$ is the most important interaction for C_f .

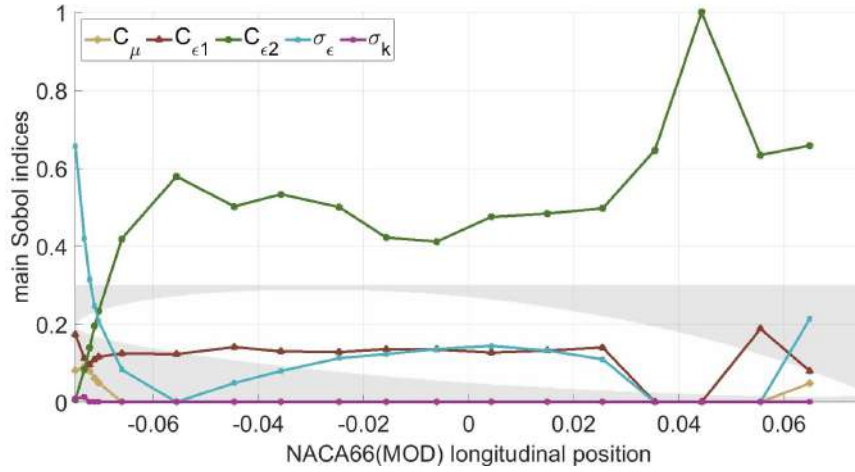


Figure 11.64: Trend of main Sobol indices along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of pressure coefficient.

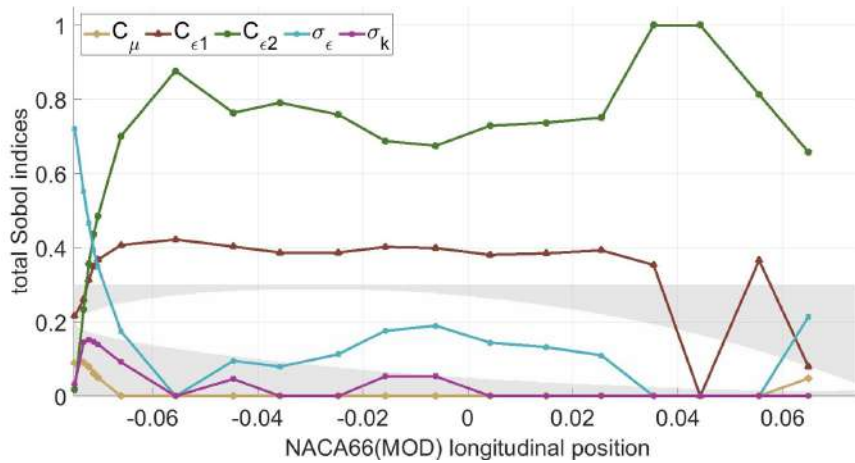


Figure 11.65: Trend of total Sobol indices along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of pressure coefficient.

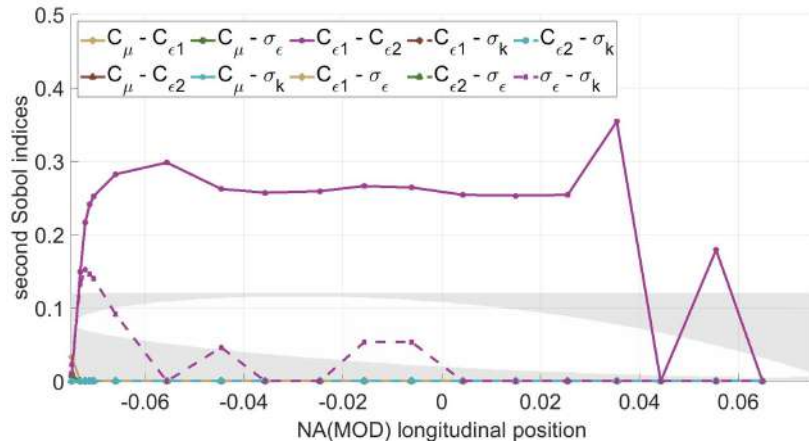


Figure 11.66: Trend of second Sobol indices along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of pressure coefficient.

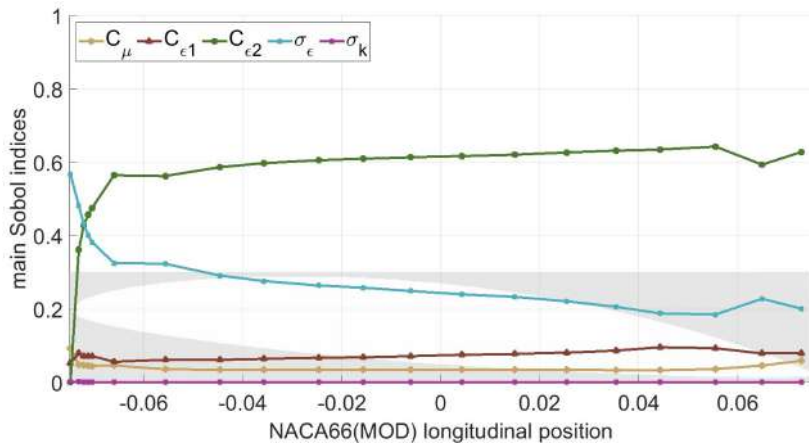


Figure 11.67: Trend of main Sobol indices along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of friction coefficient.

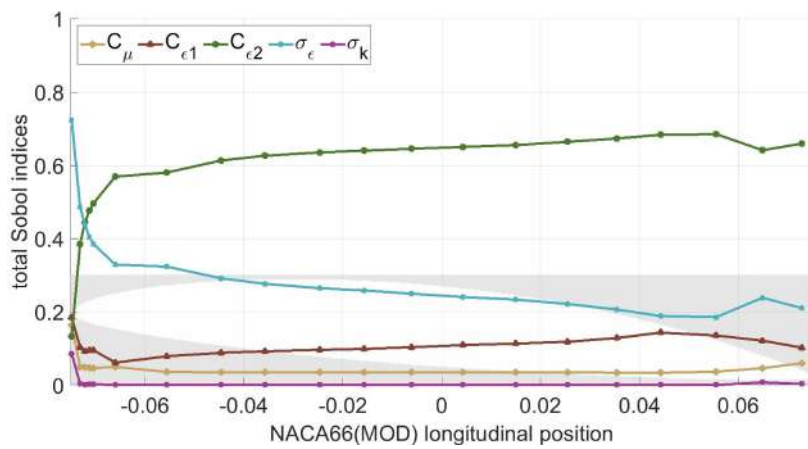


Figure 11.68: Trend of total Sobol indices along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of friction coefficient.

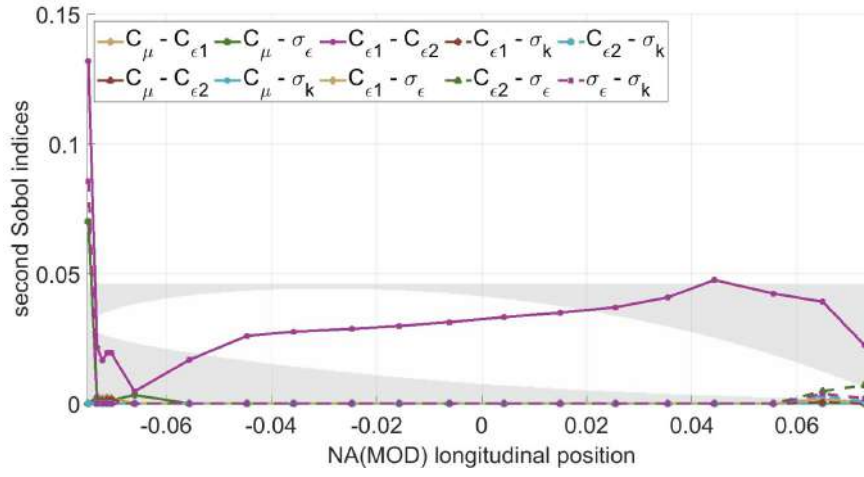


Figure 11.69: Trend of second Sobol indices along the NACA66(MOD) hydrofoil for a fully wetted flow by applying a Polynomial Chaos of II order of friction coefficient.

Chapter 12

Potsdam Propeller Test Case results

12.1 Summary of results

In the current chapter, the results of the Potsdam Propeller Test Case are shown. Results can be associated with two main groups: results about an advance ratio of $\mathbf{J} = \mathbf{1.019}$ and results for an advance ratio of $\mathbf{J} = \mathbf{1.408}$. For both configurations, responses of interest have been thrust and torque of the propeller and outputs have been calculated for both cavitating and non-cavitating flow regimes.

Considering $J = 1.019$, a **Non– Intrusive Polynomial Chaos Expansion** and the **Sobol decomposition** have been employed to investigate the **Forward Propagation of Uncertainty** and the **Global Sensitivity Analysis** of the thrust and torque with respect to $k - \varepsilon$ Turbulence model constants. A Polynomial Chaos Expansion of the **second order** has been applied to investigate the uncertainty of the entire parameter space of the five calibration constants and a reduced Polynomial Chaos Expansion of the **third degree** has been employed to only investigate the uncertainty of the most important turbulence parameters. For these two polynomial expansions, **Leave–One–Out Cross–Validation error**, **Lower Statistical Moments**, **Posterior Distributions** and **main, second, third and total** Sobol indices have been calculated.

A further analysis has been conducted by involving an **Optimal Polynomial Chaos–based Kriging**; this surrogate model and the Polynomial Chaos, as for the NACA66(MOD) hydrofoil, have been developed from a **second order** polynomial expansion to a **tenth order** polynomial expansion to investigate the best-performing model by fixing the number of collocation points to 42. In this case the Leave-One-Out Cross-Validation error and first and total orders of Sobol indices have been analyzed.

Finally, the same study has been employed for the working point of $J = 1.408$ except for the reduced Polynomial Chaos of the third order.

In Figures 12.1, 12.2, 12.3, 12.4 and 12.5 there is represented the scheme of the obtained results with respect to the PPTC propeller.

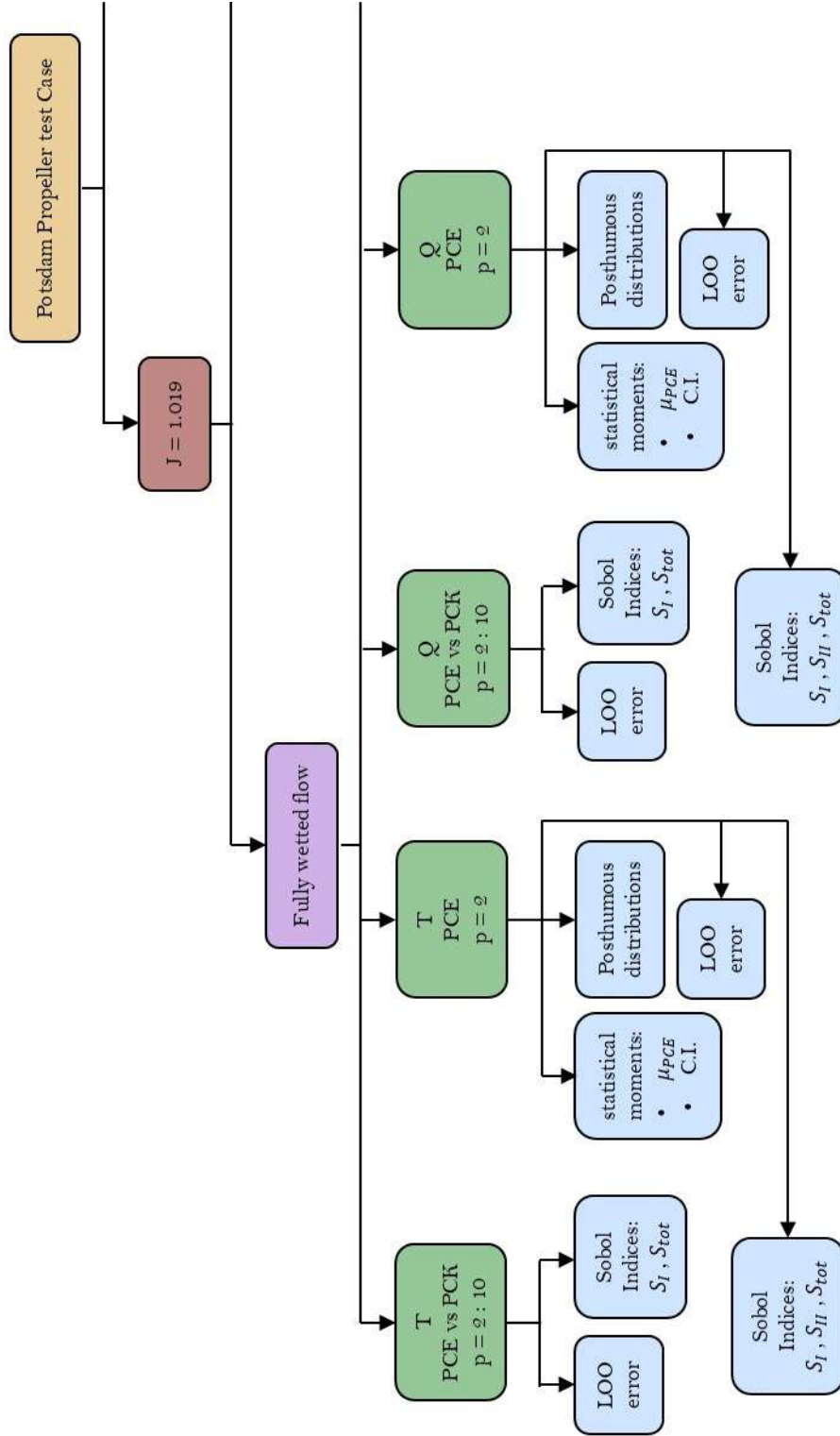


Figure 12.1: Results scheme of PPTC propeller - 1.

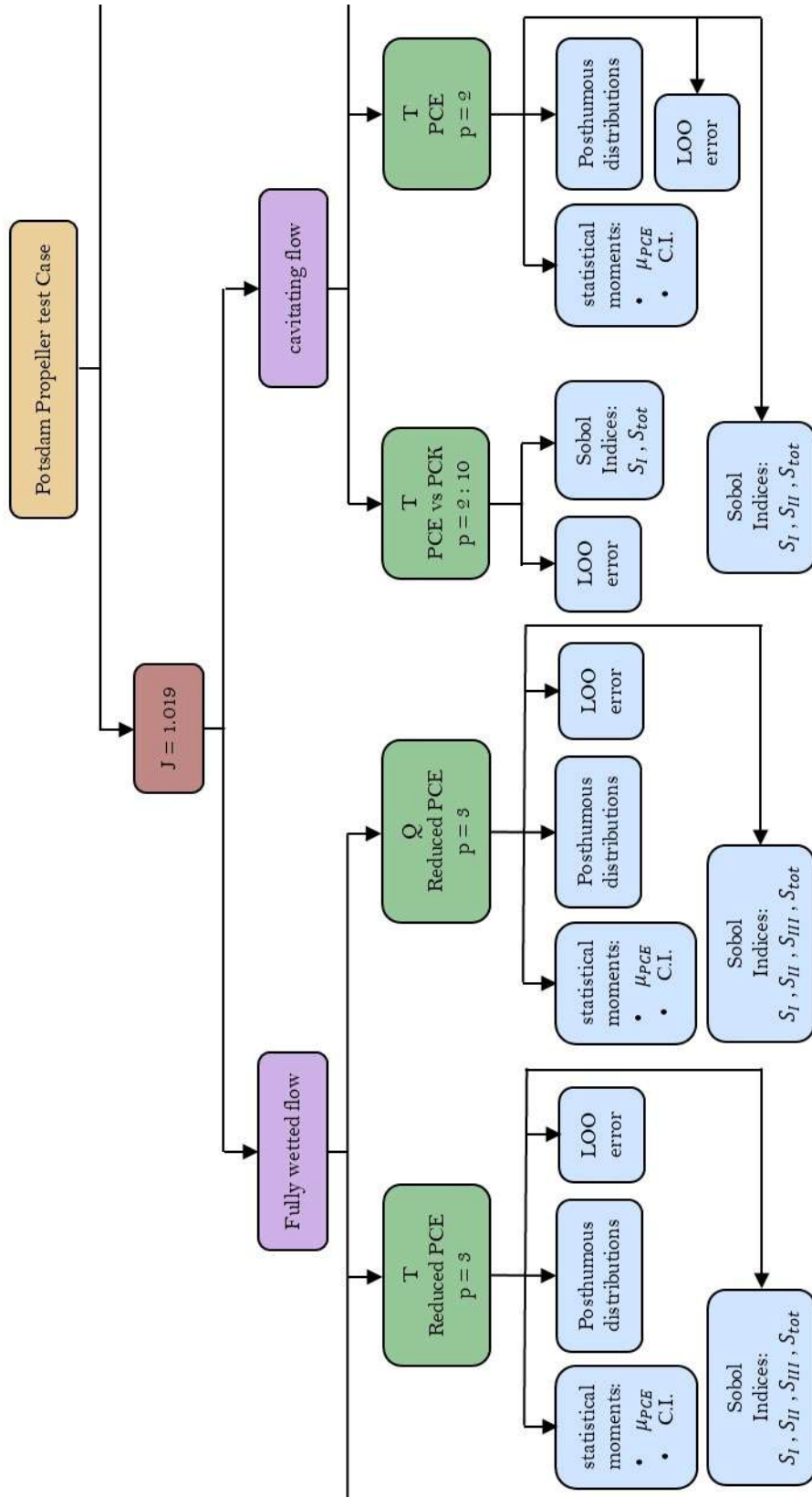


Figure 12.2: Results scheme of PPTC propeller - 2.

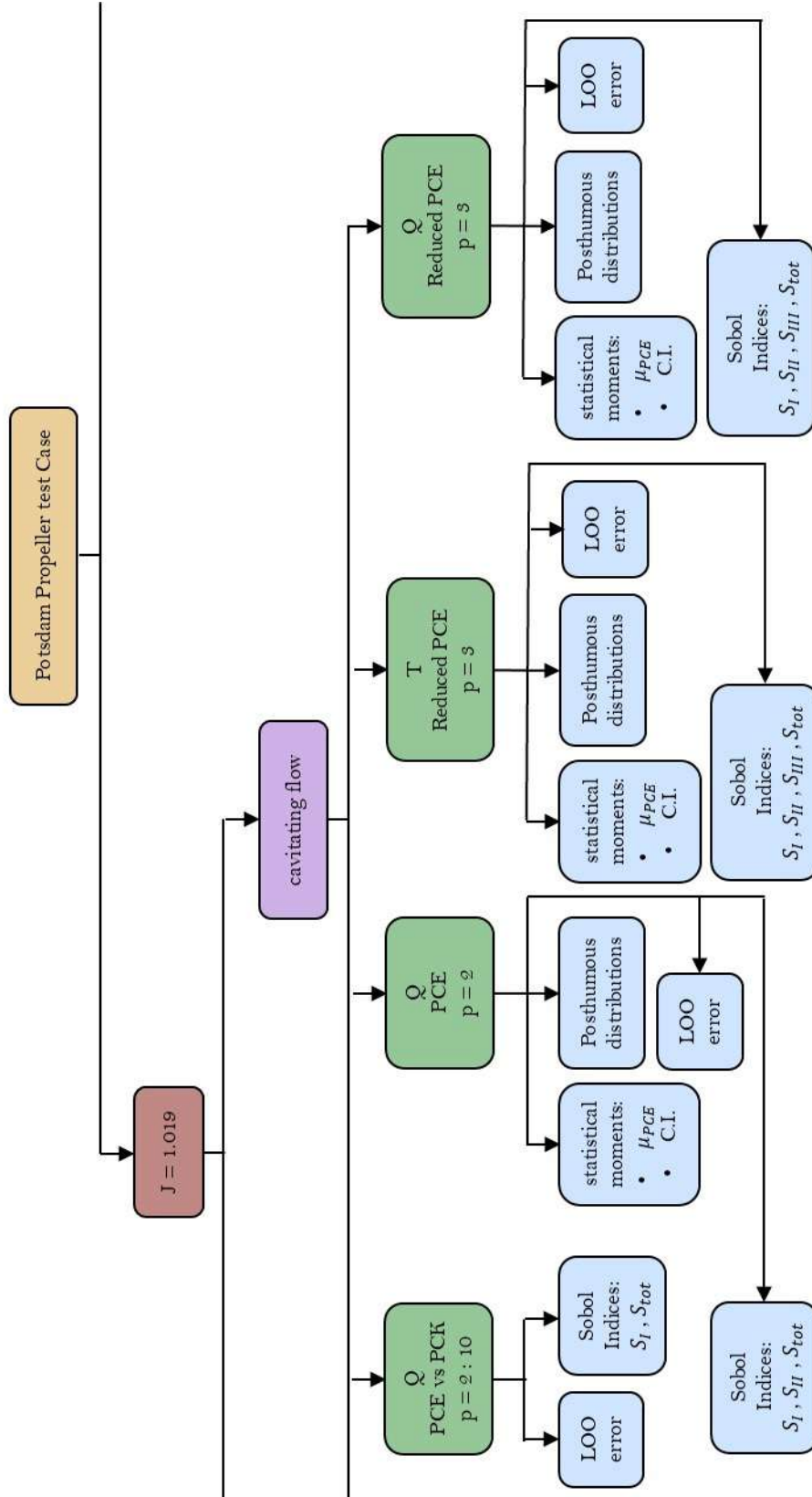


Figure 12.3: Results scheme of PPTC propeller - 3.

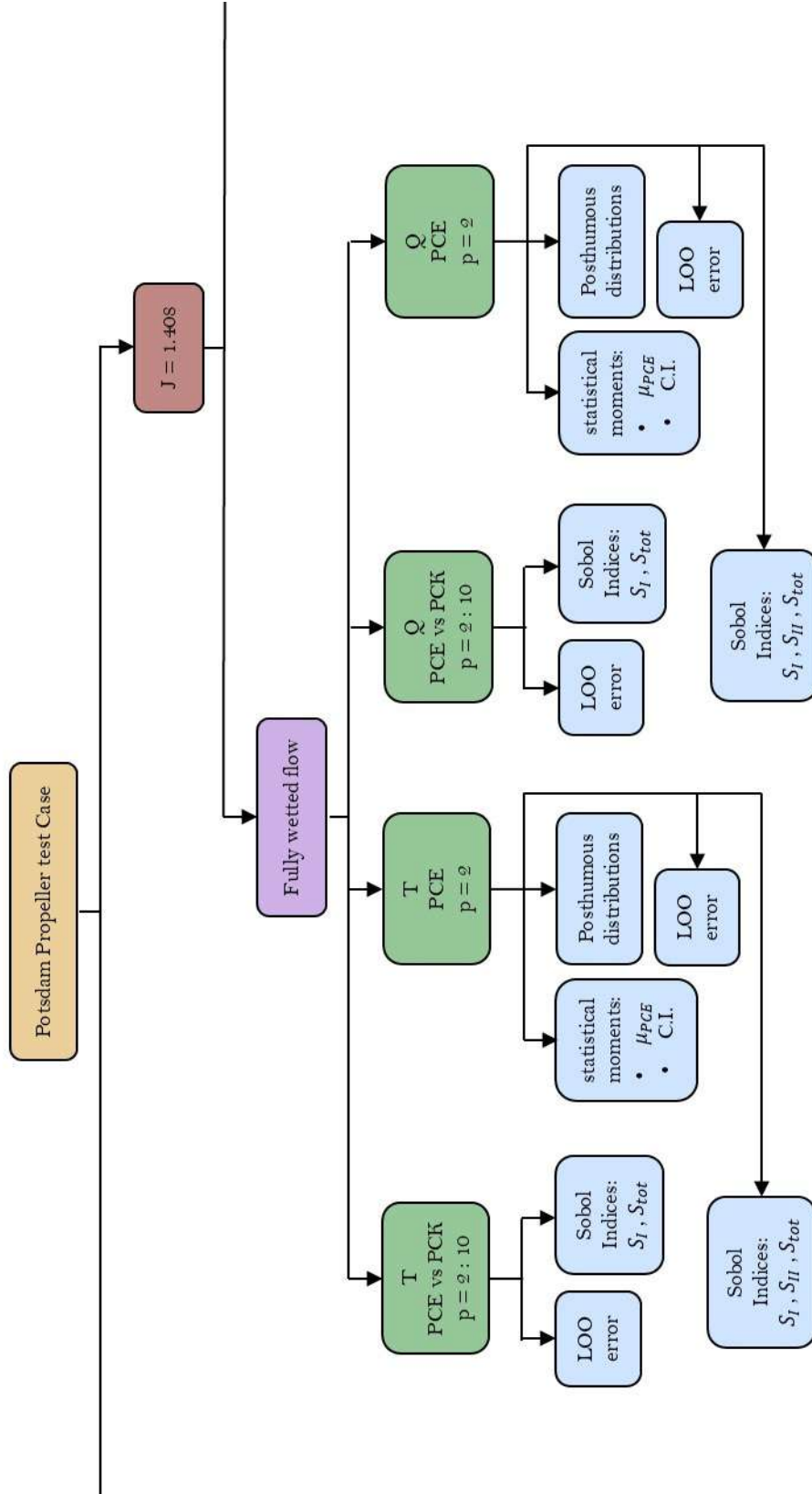


Figure 12.4: Results scheme of PPTC propeller - 4.

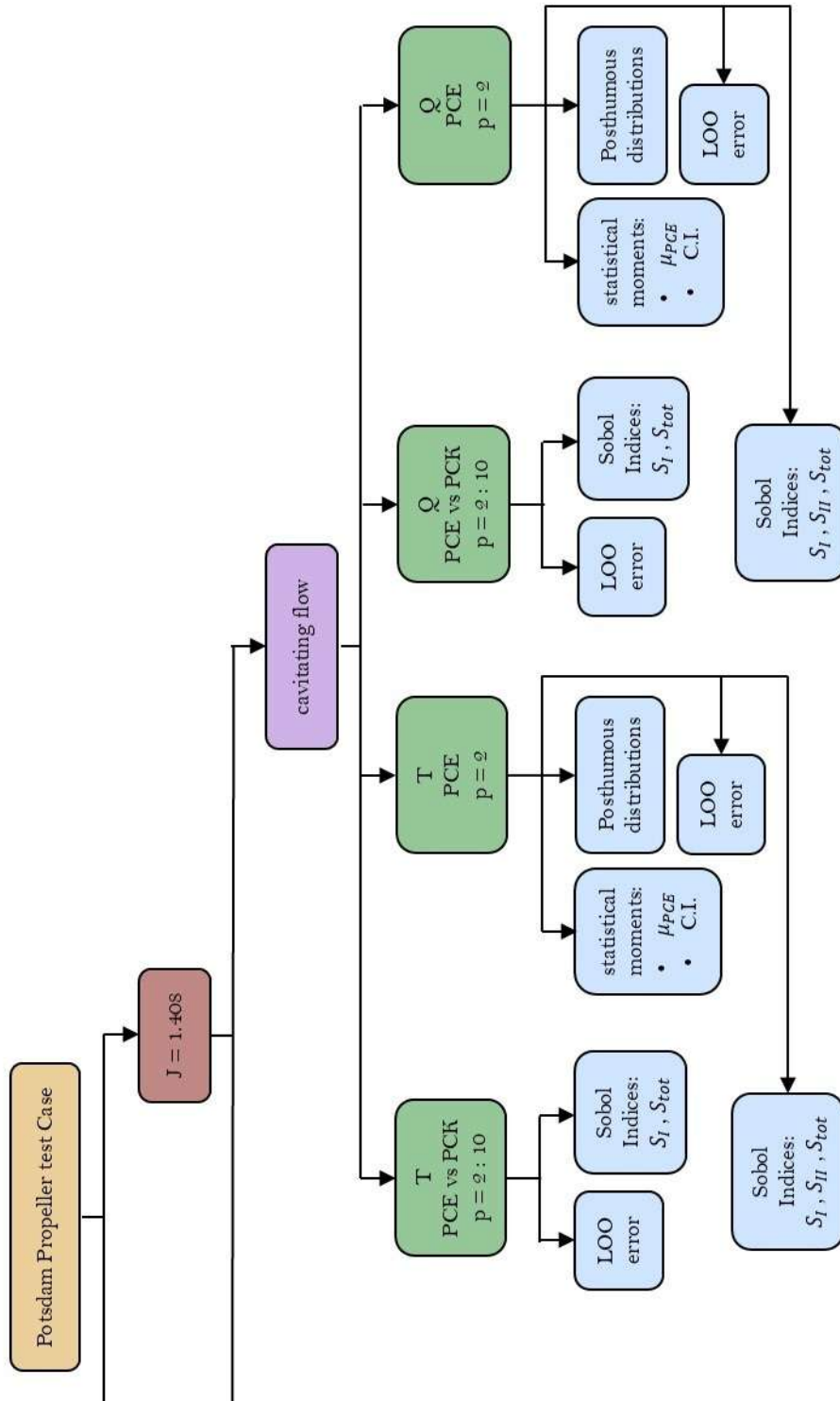


Figure 12.5: Results scheme of PPTC propeller - 5.

12.2 $J = 1.019$

12.2.1 Fully wetted flow regime

Leave-One-Out Cross-Validation error

Table 12.1 shows the Leave-One-Out Cross Validation error obtained for the thrust and torque output, respectively. The table refers to the fully wetted flow case.

Table 12.1: Leave-One-Out Cross-Validation error of thrust and torque for the fully wetted flow regime - PPTC - $J = 1.019$.

Response	ε_{LOO}	PCE order
T	0.542	II
Q	0.168	II

Statistical moments

In Table 12.2 are shown mean values and confidence intervals at the 95 % margine of error for the thrust and torque in a fully wetted flow regime.

Table 12.2: Mean values and confidence intervals of thrust and torque for a fully wetted flow regime - PPTC - $J = 1.019$.

Response	μ_{PCE}	$CI _{\text{down bound}}$	$CI _{\text{upper bound}}$	PCE order
T	-180.077	-180.457	-179.697	II
Q	11.771	11.722	11.820	II

Posterior probability distributions

In the following paragraph, the posterior probability distributions of thrust in Figure 12.6 and posthomous probability distributions of torque in Figure 12.7 for the fully wetted flow regime are represented.

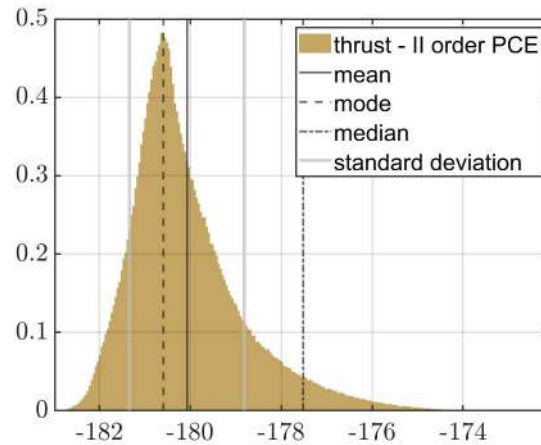


Figure 12.6: Posterior probability distribution of thrust for the fully wetted flow - PPTC - $J = 1.019$.

Those probability distributions have been generated by applying the same strategy used for the NACA66(MOD) hydrofoil and as further information, mean values, standard deviations, modes and medians for the two responses are tabulated in Table 12.3.

Table 12.3: Data of posterior distribution functions of fully wetted flow regime - PPTC - $J = 1.019$.

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
T	II	- 180.077	1.257	-180.597	-177.517
Q	II	11.771	0.163	11.788	11.587

Considering the thrust response, the probability distribution shows a skewed behaviour where most of the numerical values are switched on the left of the distribution function, showing an over-estimated tendency in of numerical solutions of simulations. this characteristic is in contrast to the probability distributions of lift coefficient of NACA66(MOD) hydrofoil which show an underestimation of numerical values. In conclusion, this distribution has a pronounced peak (kurtosis) due to the low standard deviation of the output. Similarly, the probability distribution of torque have a pointed shape as the probability distribution of thrust due to an high kurtosis and that distribution shows a set of underestimated numerical values. This behaviour is opposite to probability distributions of drag of the hydrofoil (which preserve some overestimated value).

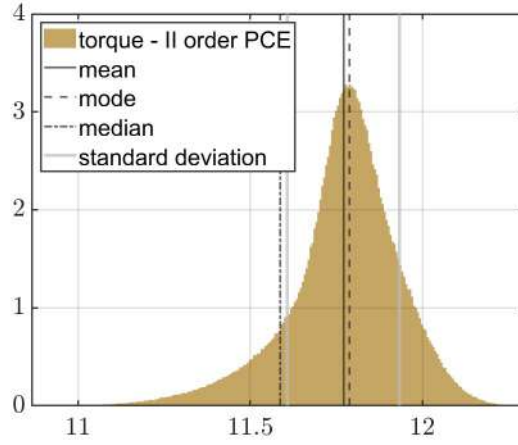


Figure 12.7: Posterior probability distribution of torque for the fully wetted flow - PPTC - $J = 1.019$.

Sobol indices

In the current section, we present the Sobol indices of thrust and torque of PPTC for the fully wetted flow regime by applying the PCE of the second order. Specifically, Figures 12.8 and 12.9 represent the Sobol indices of thrust while Figures 12.10 and 12.11 represent the Sobol indices of torque. Taking into account the Thrust response, we note that the coefficient σ_ε is the most important calibration constant when only main Sobol indices are considered but the coefficients C_{ε_1} and C_{ε_2} seem to be the most influential parameter when total Sobol indices are analyzed. This means that the non-linear effects among the calibration constants have an high impact on solutions; as a matter of fact, the thrust is mainly influenced by the variation of the pair-interaction of $C_{\varepsilon_1} - C_{\varepsilon_2}$ and the magnitude of its Sobol indices is proportional to the magnitude of main Sobol indices of C_{ε_1} and C_{ε_2} . On the other hand, the torque seems to be most influenced by C_{ε_2} and $C_{\varepsilon_1} - C_{\varepsilon_2}$.

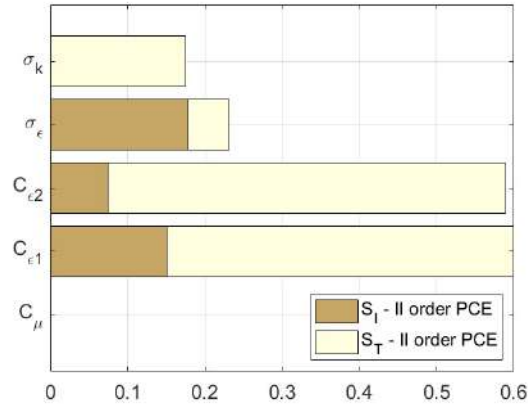


Figure 12.8: First and total order Sobol indices of thrust for the fully wetted flow regime - PPTC - $J = 1.019$.

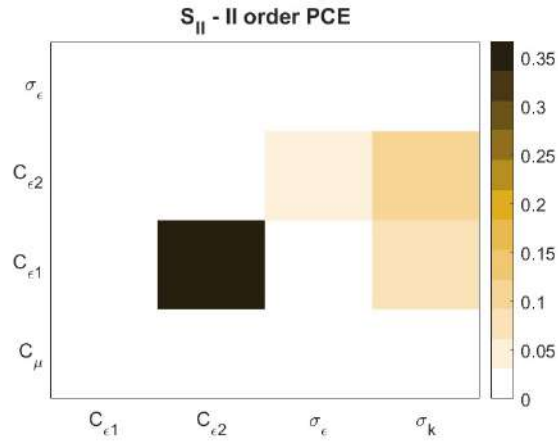


Figure 12.9: Second order Sobol indices of thrust for the fully wetted flow regime - PPTC - $J = 1.019$.

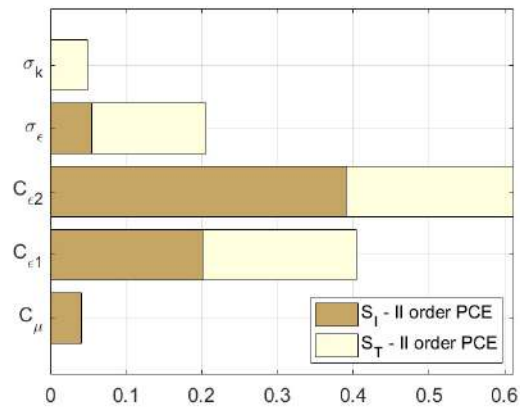


Figure 12.10: First and total order Sobol indices of torque for the fully wetted flow regime - PPTC - $J = 1.019$.

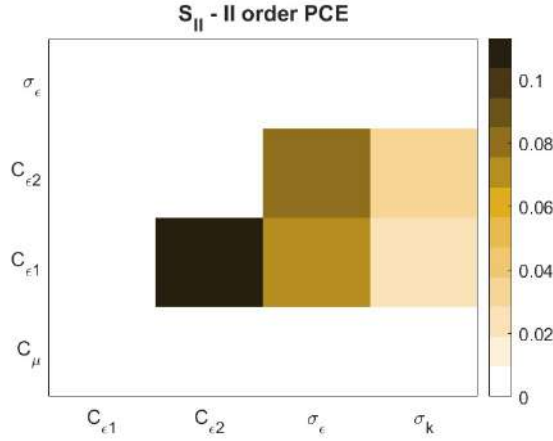


Figure 12.11: Second order Sobol indices of torque for the fully wetted flow regime - PPTC - J = 1.019.

Reduced model order analysis of PPTC

- **Motivation:** as known, the applied study has been focused on the Forward Propagation of uncertainty and the Global Sensitivity Analysis of the Standard $k - \varepsilon$ turbulence model coefficients for the prediction of some quantity of interest of objects of naval interest when fully wetted and cavitating turbulent flows are employed. The study has firstly been validated for a bi-dimensional case, i.e. the NACA66(MOD) hydrofoil where the outputs have been the drag coefficient and the lift coefficient and subsequently, the analysis has been extended to the three-dimensional test case of Potsdam Propeller Test Case where responses have been the thrust and the torque. The work has been carried out by involving the Sparse Polynomial Chaos Expansion and Sobol indices which results have been shown that the coefficients C_{μ} and σ_k are the lowest important coefficients for the outputs evaluations for both the test case investigated. At this point, a reduced model based on $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ and σ_{ε} has been generated in order to understand if it could be possible to employ only these free parameters for the Uncertainty Quantification analysis of these type of flows.
- **Leave – One – Out Cross – Validation error:** In Table 12.4 are respectively shown the Leave-One-Out Cross Validation error for the thrust and torque values for a fully wetted flow by applying the reduced order model.

Table 12.4: Leave-One-Out Cross-Validation error of thrust and torque for the fully wetted flow regime considering the reduced order model - PPTC - J = 1.019.

Response	ε_{LOO}	PCE order
T	0.0655	III
Q	0.0109	III

- **Posterior probability distributions:** In Figures 12.12 and 12.13 the posterior probability distributions of propeller outputs for the reduced order model are shown. For both the investigated responses, the probability distributions show an irregular profile with a pronounced peak at the mode value.

As further information, in Table 12.5, mean values, standard deviations, modes and medians of outputs are reported and in Figures 12.14 and 12.15, the posterior probability distributions of thrust and torque for a Polynomial Chaos of the second order and the reduced Polynomial Chaos of the third degree are compared.

Taking into account Figure 12.14, the distribution of the reduced order model has a slimmer profile than the distribution of the Polynomial Chaos of the second order; suggesting a reduction of uncertainty associated with the thrust. In this case, the application of a reduced model seems to be favorable so that fewer can be employed for this type of analysis.

A similar behaviour can be observed for the probability distributions of torque given by Figure 12.14. In this context, the flattening of the curve is more modest than the other output (thrust) but considering that fewer points and a higher polynomial degree is applied, the strategy of using a reduced order model seems to be profitable.

Table 12.5: Data of posterior distribution functions of fully wetted flow regime of reduced order model - PPTC - $J = 1.019$.

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
T	II	-180.298	0.905	-180.566	-178.898
Q	II	11.770	0.147	11.734	11.604

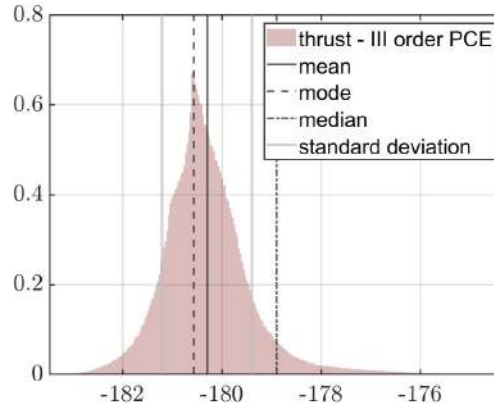


Figure 12.12: Posterior probability distribution of thrust for the fully wetted flow regime considering the reduced order model - PPTC - $J = 1.019$.

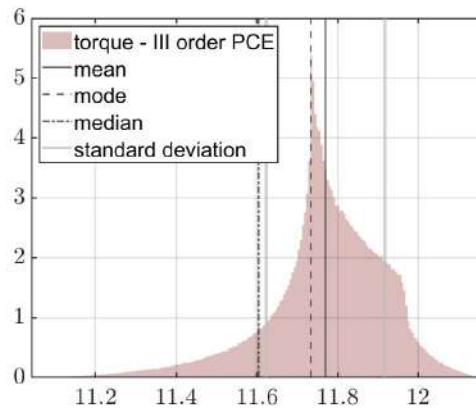


Figure 12.13: Posterior probability distribution of torque for the fully wetted flow regime considering the reduced order model - PPTC - $J = 1.019$.

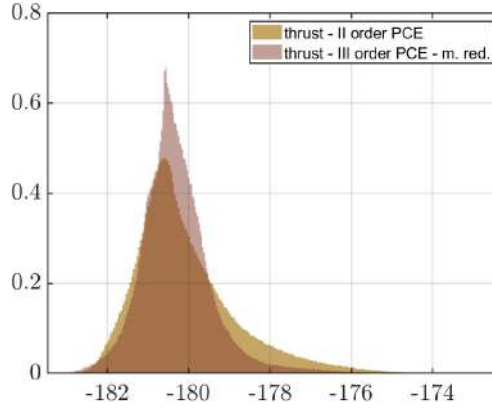


Figure 12.14: Comparison of posterior probability distributions of thrust for the fully wetted flow regime considering a PCE of II order and a reduced PCE of III order - PPTC - $J = 1.019$

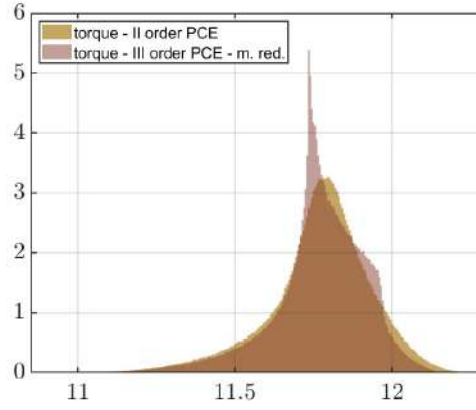


Figure 12.15: Comparison of posterior probability distributions of torque for the fully wetted flow regime considering a PCE of II order and a reduced PCE of III order - PPTC - $J = 1.019$

- **Sobol indices:** in the following section, the Sobol indices calculated by applying the reduced model analysis are shown. Considering the Sobol indices of thrust, (Figures 12.16, 12.17 and 12.18) the coefficient of the reducer order model which most influences the determination of that output is the parameter σ_ε while the most important "couple" of coefficients is $C_{\varepsilon_1} - C_{\varepsilon_2}$. It is interesting to note how, also in this case, interactions between two-coefficients weigh on the output evaluation so that they must be kept into account into the Sensitivity Analysis, in fact, paying attention on the total Sobol Indices the total weigh of all coefficients is equicomparable. On the other hand, the interaction between the three initial parameters does not have a great role in the Sobol analysis.

Observing Figures 12.19, 12.20 and 12.21, the torque is most sensitive to the variation of C_{ε_2} whose contribution is almost twice that of the others. Torque is particularly sensitive to the pairs $C_{\varepsilon_1} - C_{\varepsilon_2}$ and $C_{\varepsilon_2} - \sigma_\varepsilon$ even if the first one has a bit more influence on this output calculation. In conclusion, also in this case, the triplet weigh can be neglected from the study.

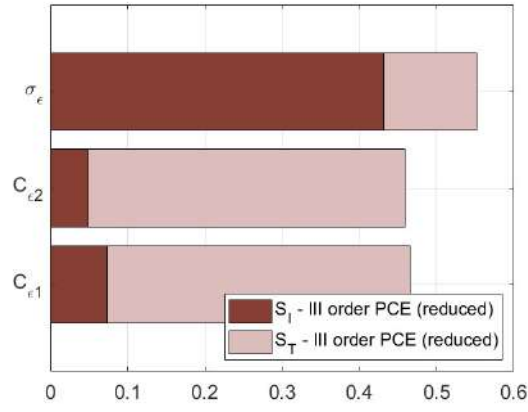


Figure 12.16: First and total order Sobol indices of thrust for the fully wetted flow regime by considering the reduced order model - PPTC - $J = 1.019$.

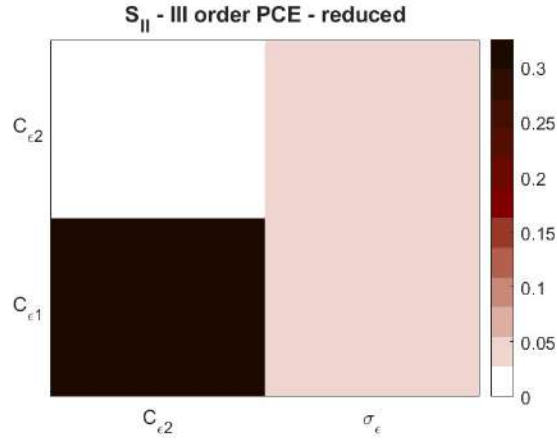


Figure 12.17: Second order Sobol indices of thrust for the fully wetted flow regime by considering the reduced order model - PPTC - $J = 1.019$.

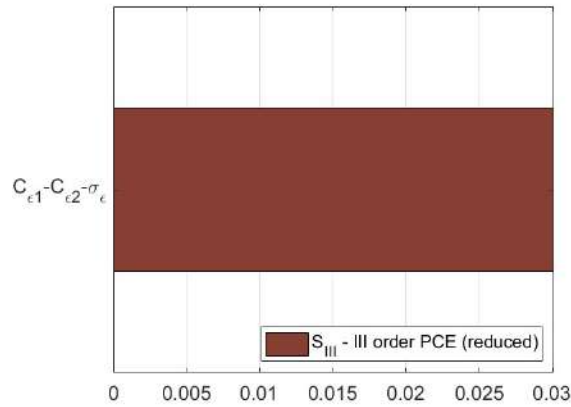


Figure 12.18: Third order Sobol indices of thrust for the fully wetted flow regime by considering the reduced order model - PPTC - $J = 1.019$.

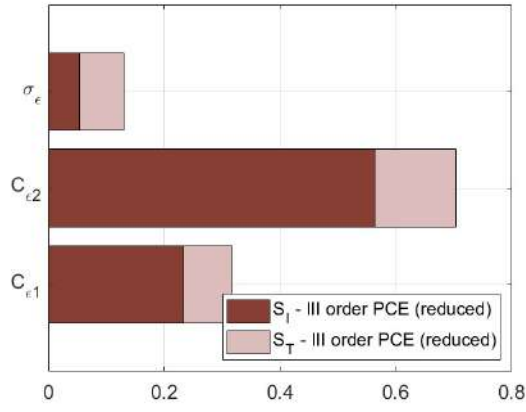


Figure 12.19: First and total order Sobol indices of torque for the fully wetted flow regime by considering the reduced order model - PPTC - $J = 1.019$.

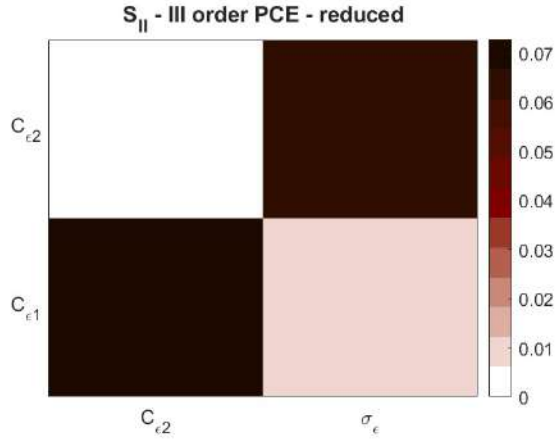


Figure 12.20: Second order Sobol indices of torque for the fully wetted flow regime by considering the reduced order model - PPTC - $J = 1.019$.

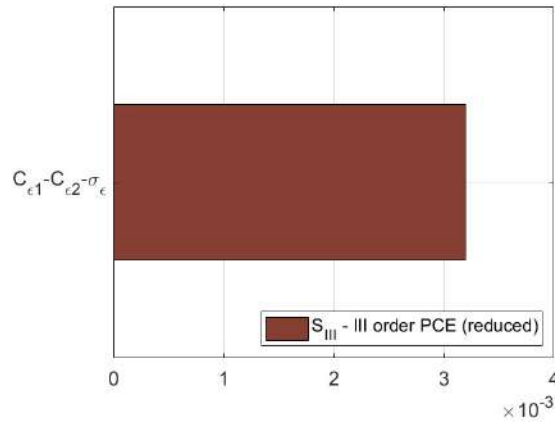


Figure 12.21: Third order Sobol indices of torque for the fully wetted flow regime by considering the reduced order model - PPTC - $J = 1.019$.

Comparison between PCE and PCK for PPTC propeller

- **Leave – One – Out Cross – Validation error:** In the current section, comparison between Polynomial Chaos Expansion and Polynomial Chaos-based Kriging has been investigated for a set of 42 collocation points for the Portsdam Propeller Test case under a fully wetted flow regime. Taking into account Figures 12.22 and 12.23, it is clear that the polynomial Chaos Kriging is more performant than the Polynomial Chaos. Furthermore, Polynomial Chaos Kriging error seems reach convergence once the seventh order is reached.

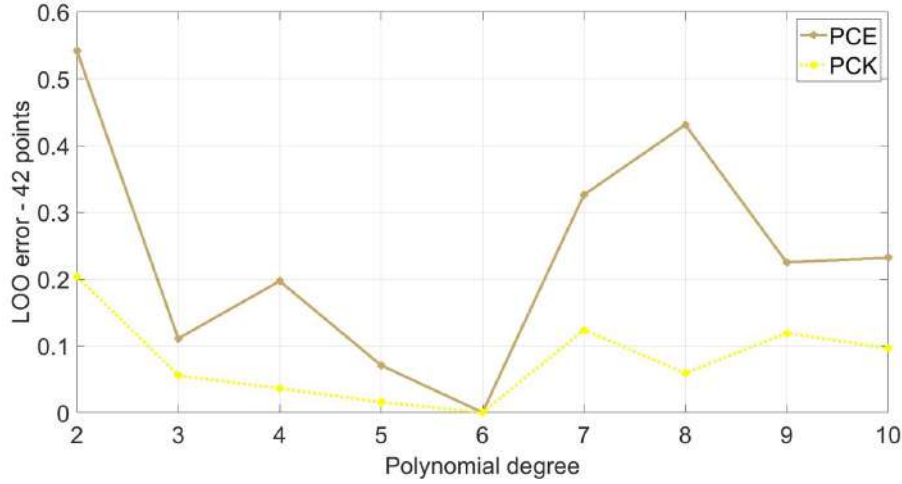


Figure 12.22: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response for 42 collocation points for a fully wetted flow - PPTC - $J = 1.019$.

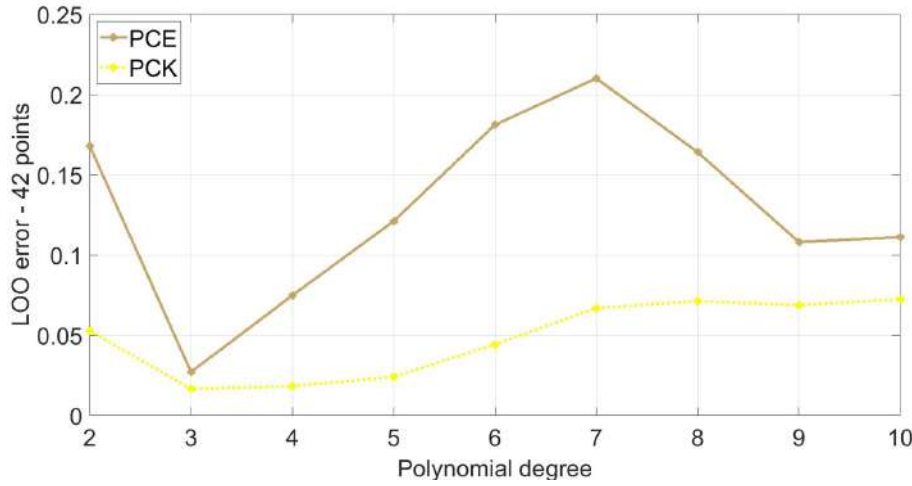


Figure 12.23: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response for 42 collocation points for a fully wetted flow - PPTC - $J = 1.019$.

- **Sobol indices:** In Figures 12.24, 12.25, 12.26 and 12.27, Sobol indices associated to the fully wetted flow regime for the PPTC propeller are shown. Considering Figures 12.24 and 12.25 where Sobol indices of thrust are given, we can note a strong irregular evolution of the indices by increasing the polynomial degree. Analyzing the importance of coefficients in main Sobol indices, we note that the most important parameter is σ_ε when the study is carried out by

the Polynomial Chaos Kriging and it is still the most important coefficient when Polynomial Chaos coefficients are employed in Sobol decomposition. From the seventh Polynomial Chaos order, main Sobol indices collapse to zero. This could be due to a too sparse set of available points to generate the response surface.

On the other hand, taking into account total Sobol indices of thrust, the most important coefficient varies when the polynomial degree varies; in fact, given a polynomial expansion, the thrust is mainly sensitive to variations of σ_ϵ , C_{ϵ_1} or C_{ϵ_2} . The situation could be caused by a limited capability of predicting non-linear effects among the five calibration constants of the Standard $k - \epsilon$ and more sampling points could be necessary.

Instead, the Sobol indices of torque (Figures 12.26 and 12.27) preserve a more regular trend by increasing the polynomial order. The most important calibration constant is C_{ϵ_2} .

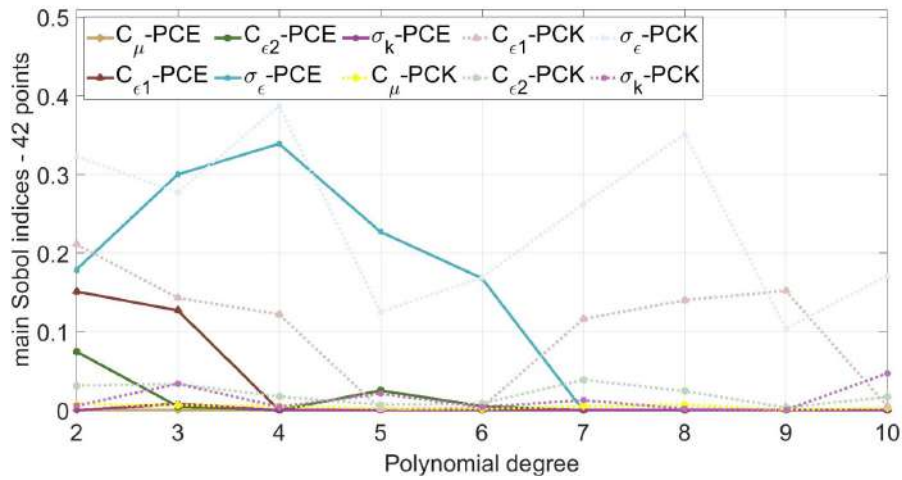


Figure 12.24: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.019$.

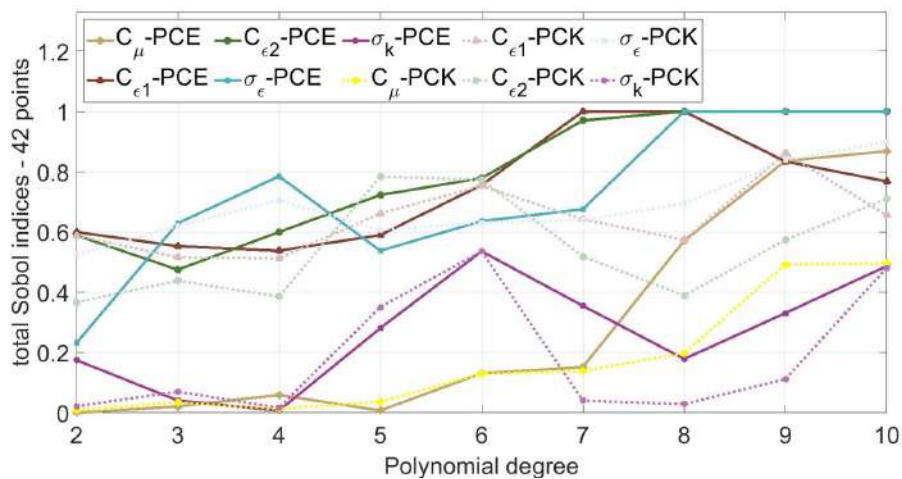


Figure 12.25: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.019$.

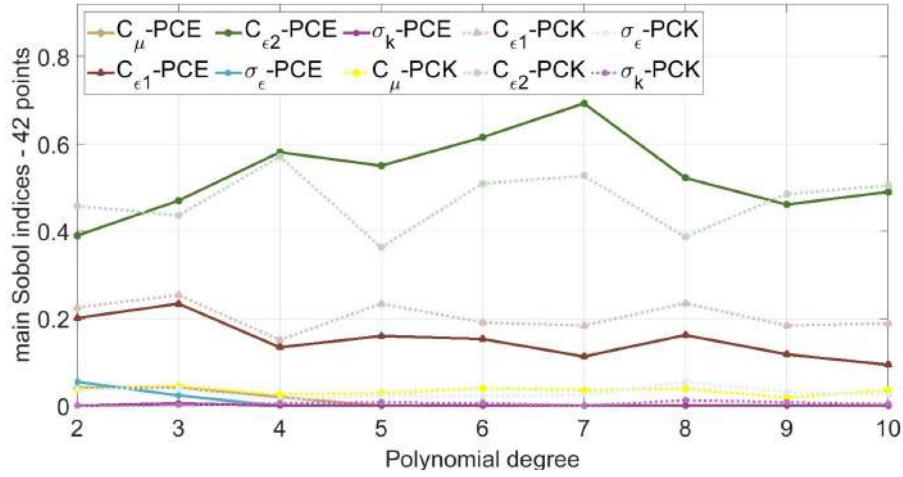


Figure 12.26: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.019$.

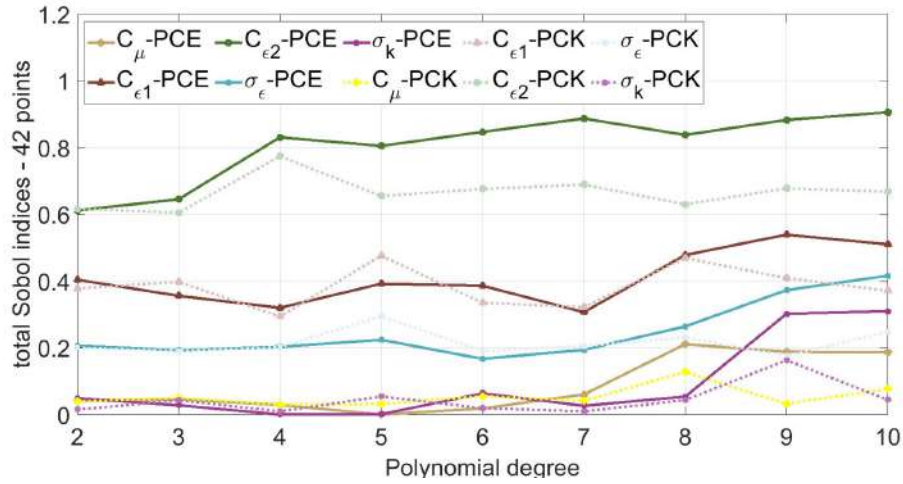


Figure 12.27: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.019$.

12.2.2 Cavitating flow regime

Leave-One-Out Cross-Validation error

In Table 12.6 are respectively shown the Leave-One-Out Cross Validation error for the thrust and torque values for a cavitating flow.

Table 12.6: Leave-One-Out Cross-Validation error of thrust and torque for the cavitating flow regime - PPTC - $J = 1.019$.

Response	ϵ_{LOO}	PCE order
T	0.427	II
Q	0.0926	II

Statistical moments

Table 12.7 shows mean values and confidence intervals at the 95% margin of error for the thrust and torque in a cavitating flow regime.

Table 12.7: Mean values and confidence intervals of thrust and torque for a cavitating flow regime - PPTC - $J = 1.019$.

Response	μ_{PCE}	$CI_{\text{down bound}}$	$CI_{\text{upper bound}}$	PCE order
T	-180.903	-181.253	-180.553	II
Q	11.819	11.770	11.868	II

Posterior probability distributions

In Figures 12.28 and 12.29 the posthumous probability distributions of propeller outputs are shown. The both distributions have a profile similar to the fully wetted flow regime case, showing a skewed behaviour of thrust and torque opposite to the lift and drag in the study of NACA66(MOD) hydrofoil.

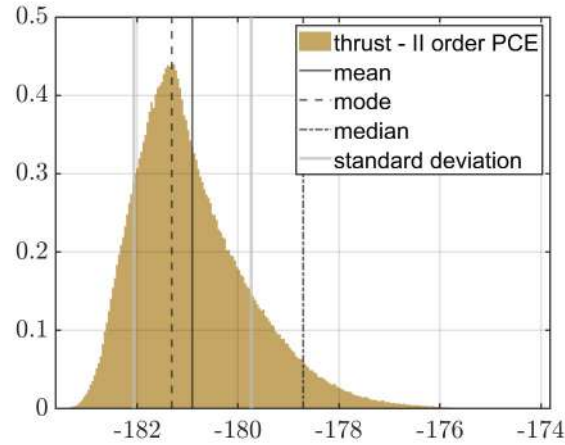


Figure 12.28: Posterior probability distribution of thrust for the cavitating flow - PPTC - $J = 1.019$.

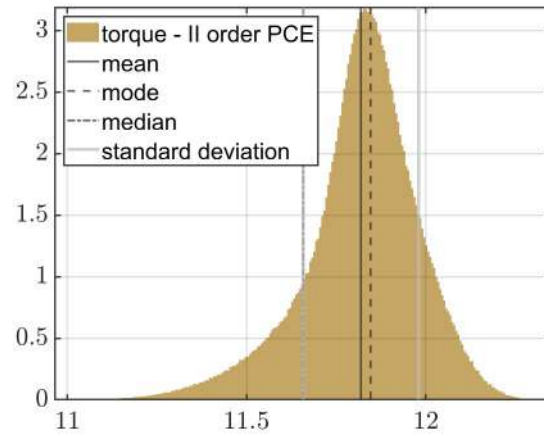


Figure 12.29: Posterior probability distribution of torque for the cavitating flow - PPTC - 1.019.

As further information, in Table 12.8, means, standard deviations, modes and medians of outputs are described.

Table 12.8: Data of posterior distribution function of cavitating flow regime - PPTC - 1.019.

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
T	II	-180.903	1.158	-181.311	-178.710
Q	II	11.819	0.161	11.845	11.658

Sobol indices

Analyzing the results of Figures 12.30, 12.31, 12.32 and 12.33, the most important coefficients for thrust and torque are the same; in fact, T and Q are mainly influenced by the variability of C_{ϵ_2} and $C_{\epsilon_1} - C_{\epsilon_2}$.

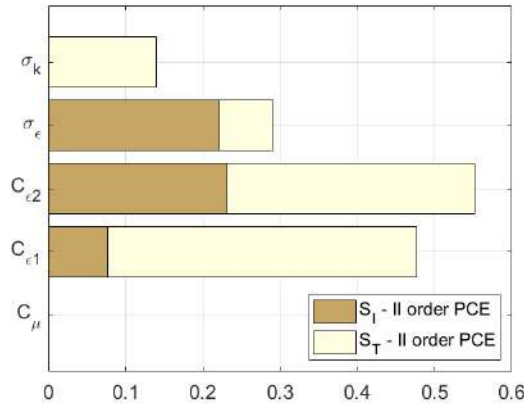


Figure 12.30: First and total order Sobol indices of thrust for the cavitating flow regime - PPTC - J = 1.019.

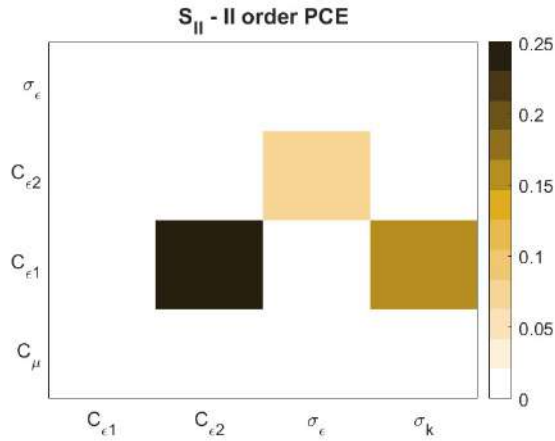


Figure 12.31: Second order Sobol indices of thrust for the cavitating flow regime - PPTC - J = 1.019.

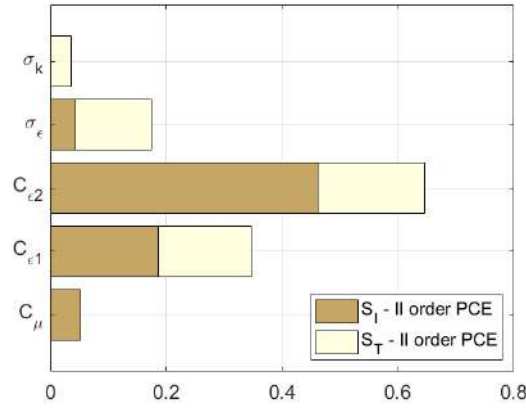


Figure 12.32: First and total order Sobol indices of torque for the cavitating flow regime - PPTC - $J = 1.019$.

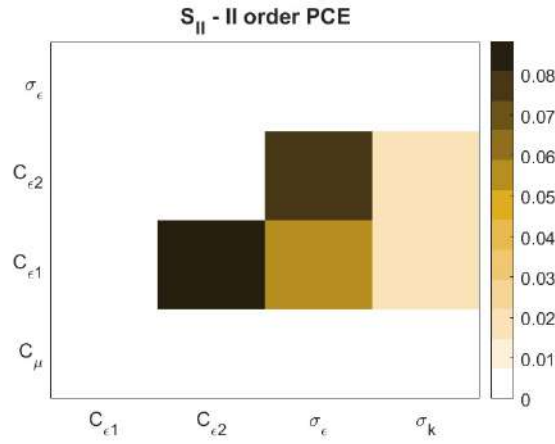


Figure 12.33: Second order Sobol indices of torque for the cavitating flow regime - PPTC - $J = 1.019$.

Reduced model order analysis of PPTC

- **Leave – One – Out Cross – Validation error:** In Table 12.9 are respectively shown the Leave-One-Our Cross Validation error for the thrust and torque values for a cavitating flow by applying the reduced third order model.

Table 12.9: Leave-One-Out Cross-Validation error of thrust and torque for the cavitating flow regime considering the reduced order model - PPTC - $J = 1.019$.

Response	ϵ_{LOO}	PCE order
T	0.258	III
Q	0.0767	III

- **Statistical moments:** In Table 12.10 are shown mean values and confidence intervals at the 95% margine of error for the thrust and torque in a cavitating flow regime.

Table 12.10: Mean values and confidence intervals of thrust and torque for a cavitating flow regime considering the reduced order model - PPTC - $J = 1.019$.

Response	μ_{PCE}	$CI_{down\ bound}$	$CI_{upper\ bound}$	PCE order
T	-180.887	-181.195	-180.579	III
Q	11.770	11.724	11.816	III

- **Posterior probability distribution:** In Figures 12.34 and 12.35 the posterior probability distributions of propeller outputs for the reduced order model are shown. The studied outputs show an asymmetric behaviour with a softer profile with respect to the fully wetted case. in Table 12.11, mean values, standard deviations, modes and medians of outputs are described and in Figures 12.36 and 12.37 are compared the posterior probability distributions of thrust and torque for a Polynomial Chaos of the second order and the reduced Polynomial Chaos of the third degree. Taking into account the thrust output, the posterior probability distribution determined by applying a reduced PCE of the third order shows a lower uncertainty due to its slimmer profile than the probability distribution of the PCE of the second order while pre probability distributions in 12.37 are almost identical.

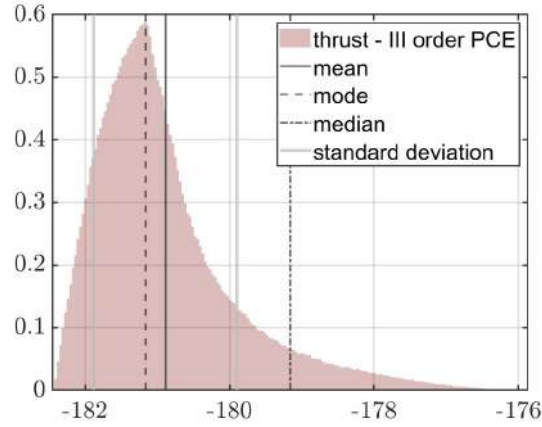


Figure 12.34: Posterior probability distribution of thrust for the fully wetted flow regime considering the reduced order model - PPTC - $J = 1.019$.

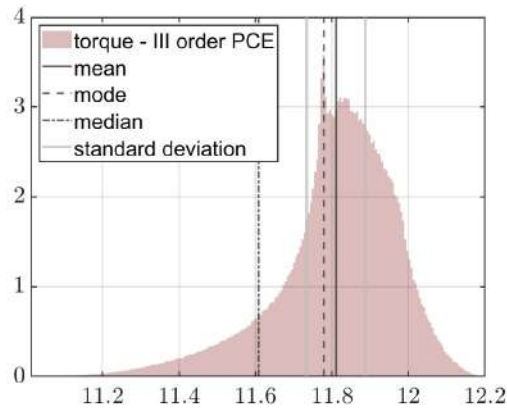


Figure 12.35: Posterior probability distribution of torque for the fully wetted flow regime considering the reduced order model - PPTC - $J = 1.019$.

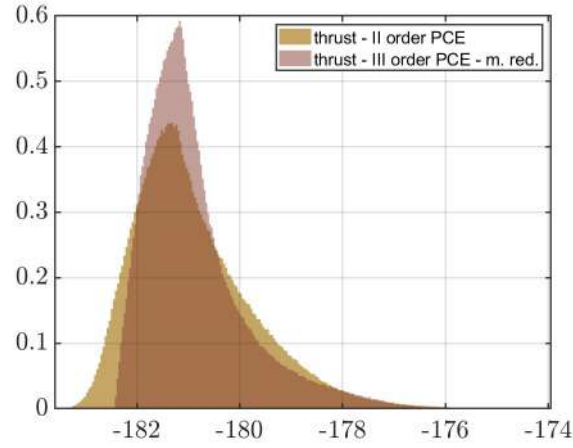


Figure 12.36: Comparison of posterior probability distributions of thrust for the cavitating flow regime considering a PCE of II order and a reduced PCE of III order - PPTC - $J = 1.019$

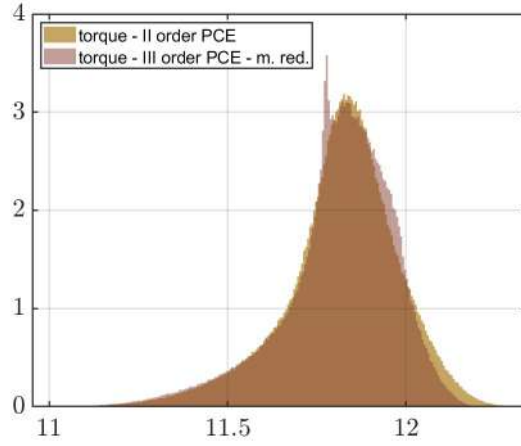


Figure 12.37: Comparison of posterior probability distributions of torque for the cavitating flow regime considering a PCE of II order and a reduced PCE of III order - PPTC - $J = 1.019$

Table 12.11: Data of posterior distribution functions of cavitating flow regime of reduced order model - PPTC - $J = 1.019$.

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
T	III	-180.887	0.994	-181.166	-179.162
Q	III	11.811	0.158	11.778	11.608

- **Sobol indices:** In Figures 12.38, 12.39, 12.40, 12.41 12.42 and 12.43 there are respectively shown the Sobol indices of thrust and torque outputs of the reduced Polynomial Chaos metamodel for a cavitating flow regime. Paying attention to 12.38 and 12.39, the thrust seems to be most influenced by the calibration constants C_{ε_2} and $C_{\varepsilon_1} - C_{\varepsilon_2}$ which is in line with the results obtained for the complete Polynomial Chaos. On the other hand, also for the torque response, the most important turbulence parameters are C_{ε_2} and $C_{\varepsilon_1} - C_{\varepsilon_2}$ and this confirms the coherence about the results of the Polynomial Chaos Expansion of the second order.

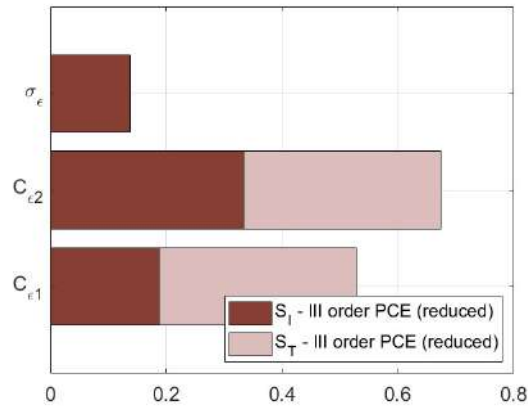


Figure 12.38: First and total order Sobol indices of thrust for the cavitating flow regime by considering the reduced order model - PPTC - $J = 1.019$.

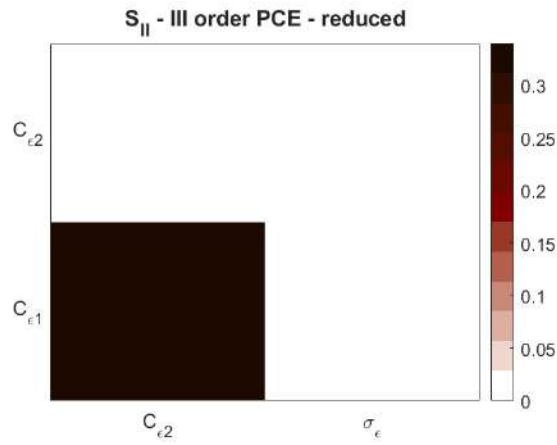


Figure 12.39: Second order Sobol indices of thrust for the cavitating flow regime by considering the reduced order model - PPTC - $J = 1.019$.

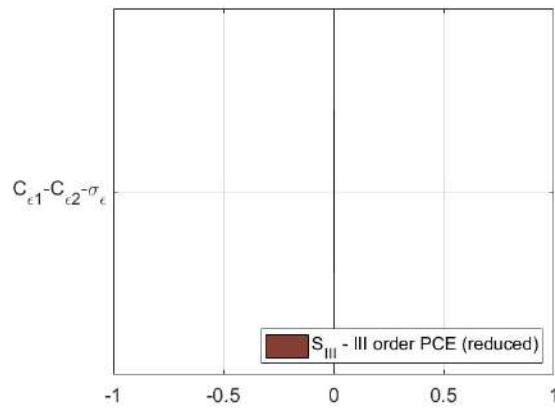


Figure 12.40: Third order Sobol indices of thrust for the cavitating flow regime by considering the reduced order model - PPTC - $J = 1.019$.

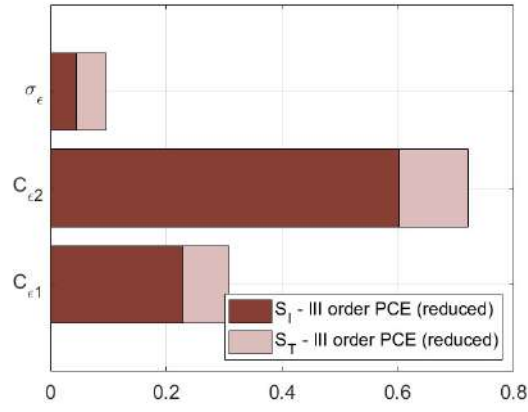


Figure 12.41: First and total order Sobol indices of torque for the cavitating flow regime by considering the reduced order model - PPTC - $J = 1.019$.

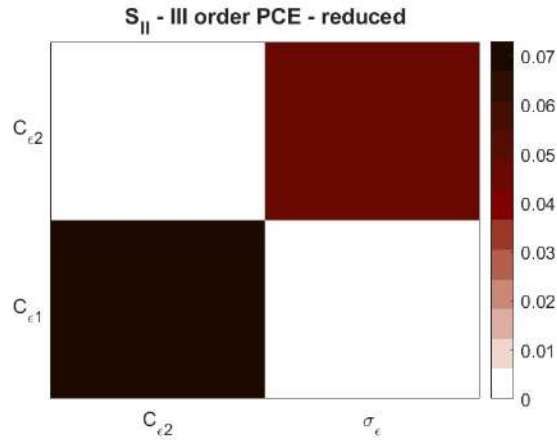


Figure 12.42: Second order Sobol indices of torque for the cavitating flow regime by considering the reduced order model - PPTC - $J = 1.019$.

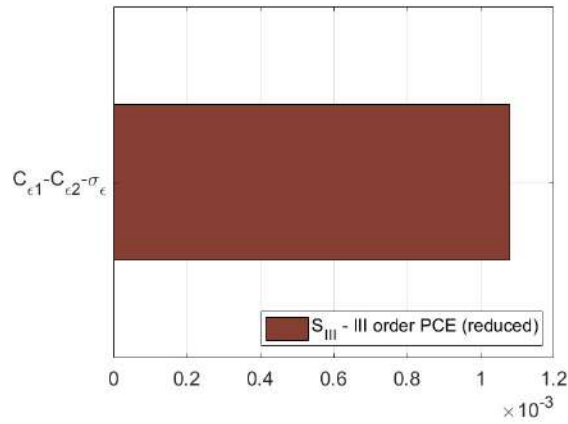


Figure 12.43: Third order Sobol indices of torque for the cavitating flow regime by considering the reduced order model - PPTC - $J = 1.019$.

Comparison between PCE and PCK for PPTC propeller

- **Leave – One – Out Cross – Validation error:** Analyzing the Leave-One-Out Cross- Validation error for the cavitating flow, we have that the Polynomial Chaos-based Kriging is more performant than the Polynomial Chaos Expansion for both thrust and torque responses. Furthermore, the Polynomial Chaos Kriging seems to converge from the seventh polynomial degree.

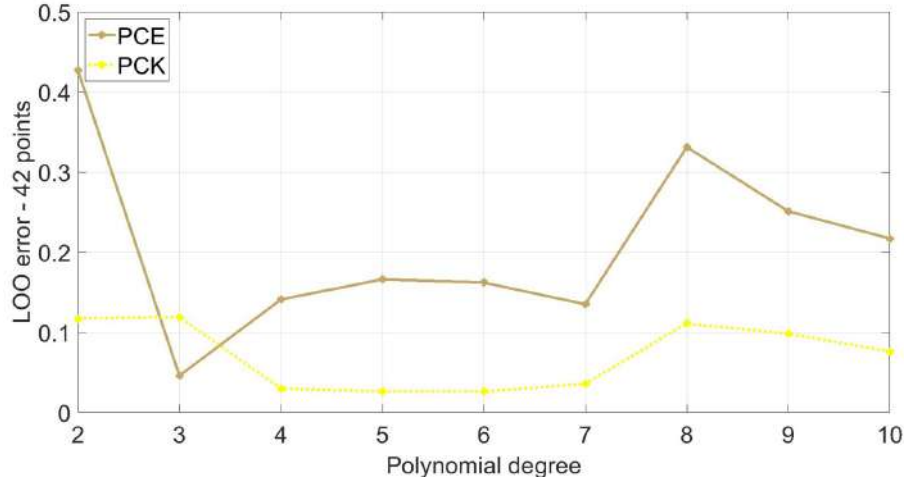


Figure 12.44: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response for 42 collocation points for a cavitating flow - PPTC - $J = 1.019$.

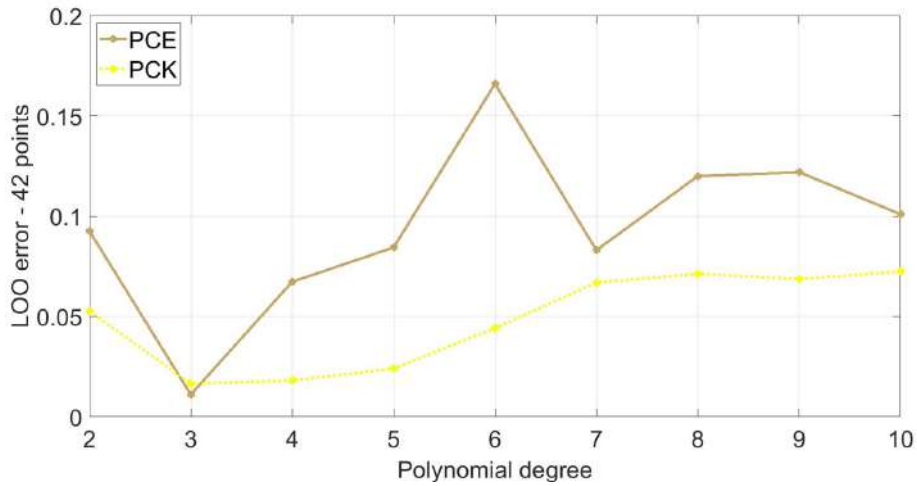


Figure 12.45: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response for 42 collocation points for a cavitating flow - PPTC - $J = 1.019$.

- **Sobol indices:** The Sobol indices for the cavitating flow regime are shown below. Specifically, in Figures 12.46 and 12.47, the results for thrust are presented and in Figures 12.48 and 12.49, the results for torque are given. Behaviour of Sobol indices are similar to the results obtained for the fully wetted flow.

Sobol indices of thrust have a chaotic behaviour; basically, the coefficient σ_ε seems to be

the most influential parameter for this output calculation when Polynomial Chaos Expansion is employed. This characteristic is also kept for the Polynomial Chaos kriging but the coefficient C_{ε_2} becomes the most important from the seventh polynomial order expansion. Considering the total Sobol indices, C_{ε_2} and C_{ε_1} seem to be the most important constants for the thrust evaluation. Sobol indices of torque preserve a more regular development along the polynomial order variation and the parameter C_{ε_2} is the most influential coefficient of the turbulence model.

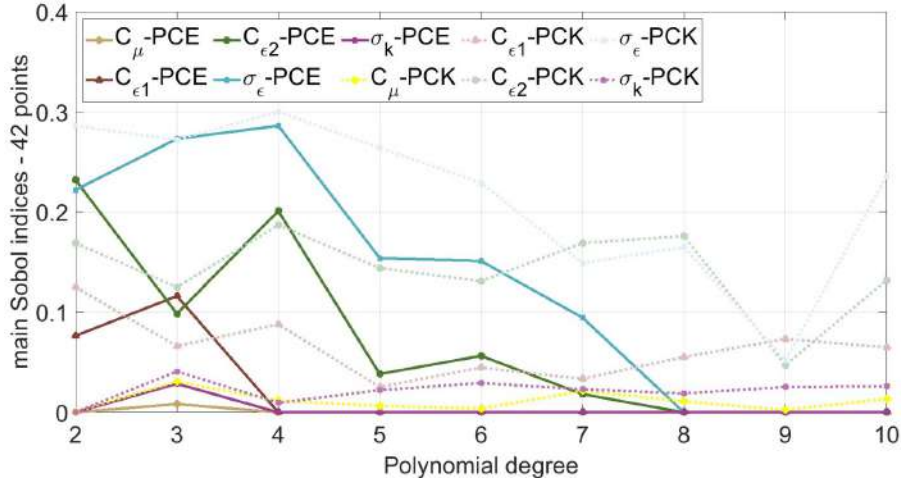


Figure 12.46: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.019$.

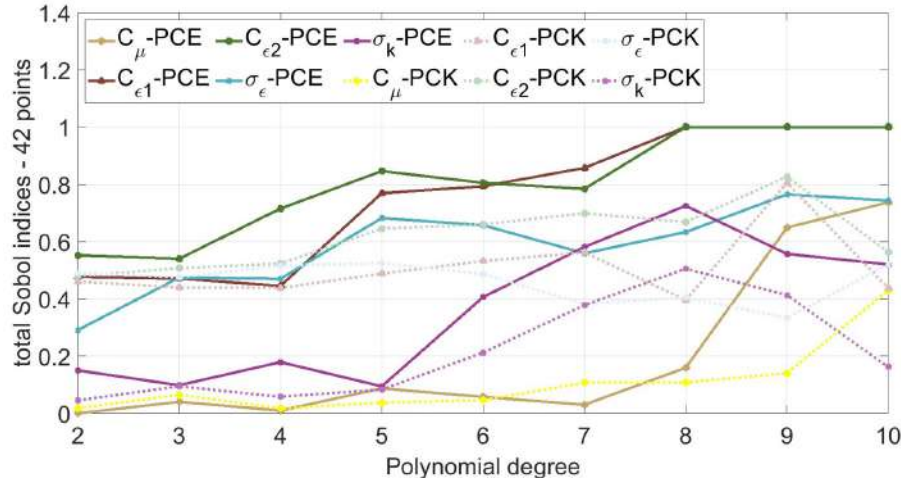


Figure 12.47: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.019$.

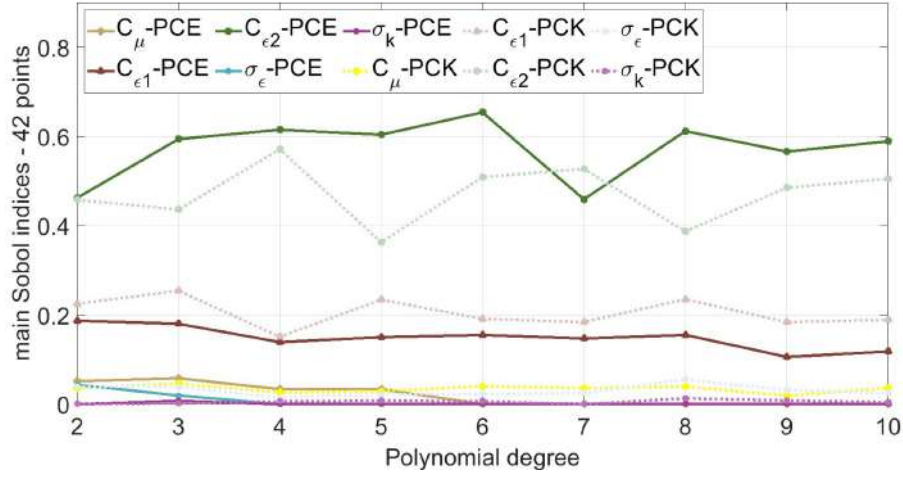


Figure 12.48: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.019$.

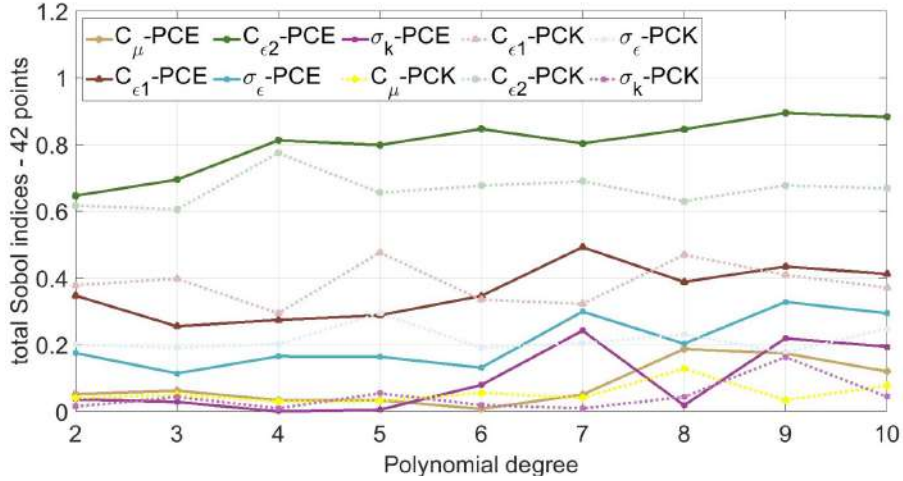


Figure 12.49: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.019$.

12.3 $J = 1.408$

12.3.1 Fully wetted flow regime

Leave-One-Out Cross-Validation error

In Table 12.12 are respectively shown the Leave-One-Out Cross-Validation error for the thrust and torque for the fully wetted flow. If we compare the results obtained for $J = 1.019$, we observe an increase in the prediction error for both outputs.

Table 12.12: Leave-One-Out Cross-Validation error of thrust and torque for the fully wetted flow regime - PPTC - $J = 1.408$.

Response	ε_{LOO}	PCE order
T	0.782	II
Q	0.246	II

Statistical moments

In Table 12.13 are shown mean values and confidence intervals at the 95 % margine of error for the thrust and torque in a fully wetted flow regime.

Table 12.13: Mean values and confidence intervals of thrust and torque for a fully wetted flow regime - PPTC - $j = 1.408$.

Response	μ_{PCE}	$CI _{\text{down bound}}$	$CI _{\text{upper bound}}$	PCE order
T	-80.574	-81.043	-80.105	II
Q	6.873	6.804	6.942	II

Posterior probability distributions

The probability distributions of thrust and torque for an advance ratio of $J = 1.408$ are shown in Figures 12.50 and 12.51 and mean values, modes, medians and standard deviations of the two responses are shown in Table 12.14. As for $J = 1.019$ in a fully wetted flow regime, we have obtained two asymmetric distributions. Specifically, the thrust preserves a left-side skewness while the torque have a right-side skewness. From a general point of view, the thrust distribution for $J = 1.019$ is more "sharp-pointed" than the thrust distribution for $J = 1.408$, suggesting a higher uncertainty associated to the second propeller operating point. In fact, this can be numerically observed by analyzing the increased standard deviations given in Table 12.14 with respect to the standard deviations given in Table 12.3. Physically, the higher amount of uncertainty seems to be justified by the more chaotic evolution of the studied turbulent flow (as justified for the Leave-One-Out Cross-Validation error). Similar conclusions can be made for the torque response.

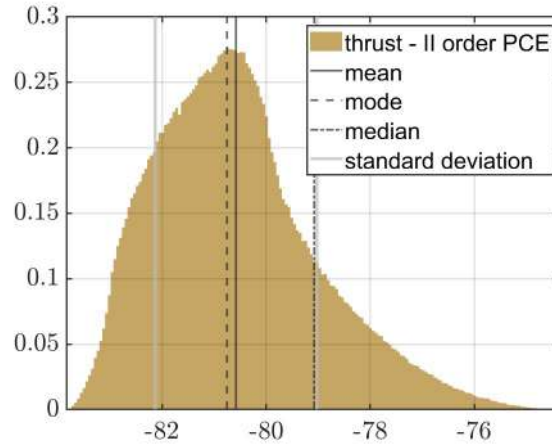


Figure 12.50: Posterior probability distribution of thrust for the fully wetted flow - PPTC - $J = 1.408$.

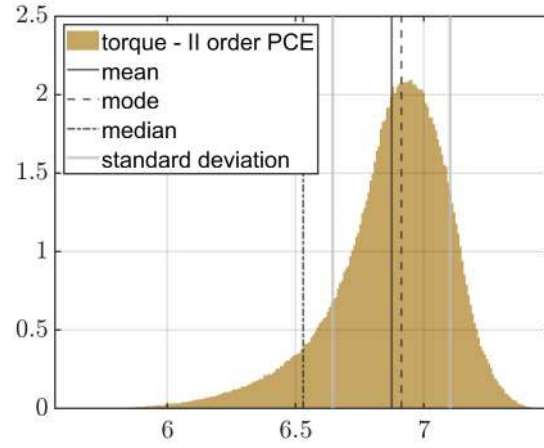


Figure 12.51: Posterior probability distribution of torque for the fully wetted flow - PPTC - $J = 1.408$.

Table 12.14: Data of posterior distribution functions of fully wetted flow regime - PPTC - $J = 1.408$.

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
T	II	- 89.574	1.552	-80.748	-79.077
Q	II	6.873	0.229	6.911	6.529

Sobol indices

Taking into account Figures 12.52, 12.53, 12.54 and 12.55, Sobol indices of outputs for the fully wetted flow are shown. If we observe these diagrams together with the diagrams shown in 12.8, 12.9, 12.10 and 12.11, we have the same ranking of importance of coefficients. In this case, the variation of advance ratio does not influence the ranking of importance of the five turbulent constants. In fact, the coefficient σ_ε is the most important parameter for the thrust when only the first order Sobol indices are analyzed while the coefficient C_{ε_1} becomes the most important when the total indices are considered. Furthermore, the interaction $C_{\varepsilon_1} - C_{\varepsilon_2}$ is the most influential non linear effect between calibration constants on the thrust calculation. Finally, the torque is mostly sensitive to the variations of C_{ε_2} and $C_{\varepsilon_1} - C_{\varepsilon_2}$ as observed for $J = 1.019$.

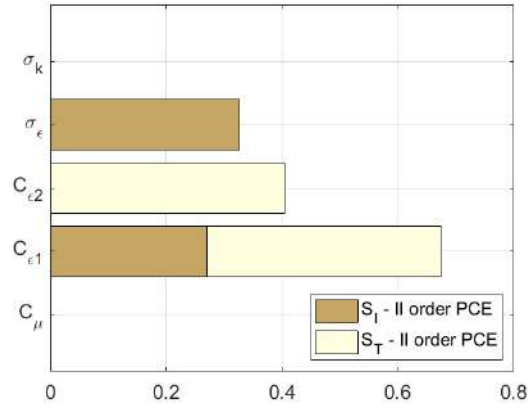


Figure 12.52: First and total order Sobol indices of thrust for the fully wetted flow regime - PPTC - $J = 1.408$.

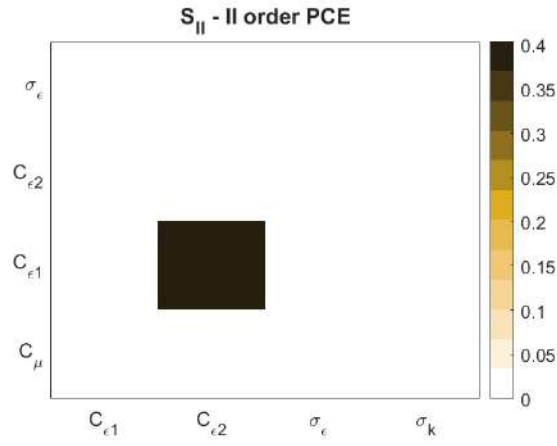


Figure 12.53: Second order Sobol indices of thrust for the fully wetted flow regime - PPTC - $J = 1.408$.

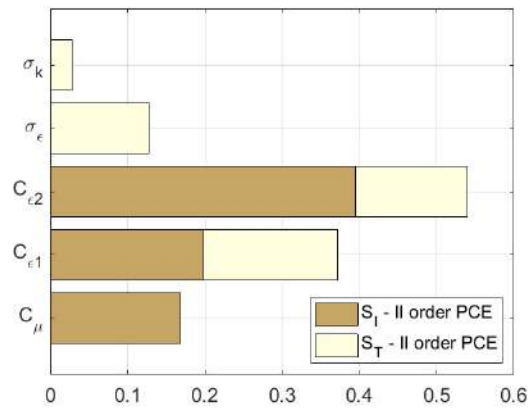


Figure 12.54: First and total order Sobol indices of torque for the fully wetted flow regime - PPTC - $J = 1.408$.

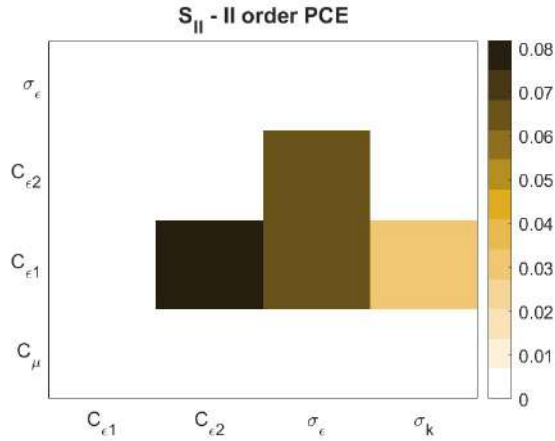


Figure 12.55: Second order Sobol indices of torque for the fully wetted flow regime - PPTC - J = 1.408.

Comparison between PCE and PCK for PPTC propeller

- **Leave – One – Out Cross – Validation error:** In Figures 12.56 and 12.57., Leave-One-Out Cross-Validation errors of thrust and torque for the two metamodels are given. Observing the Figure (12.56), Polynomial Chaos Expansion and Polynomial Chaos Kriging have an analogous Behaviour. Basically, The Polynomial Chaos-based Kriging present a lower prediction error than the Polynomial Chaos Expansion.

Analyzing the torque output, the Polynomial Chaos Kriging for torque is more performant than the Polynomial Chaos Expansion in terms of predictability.

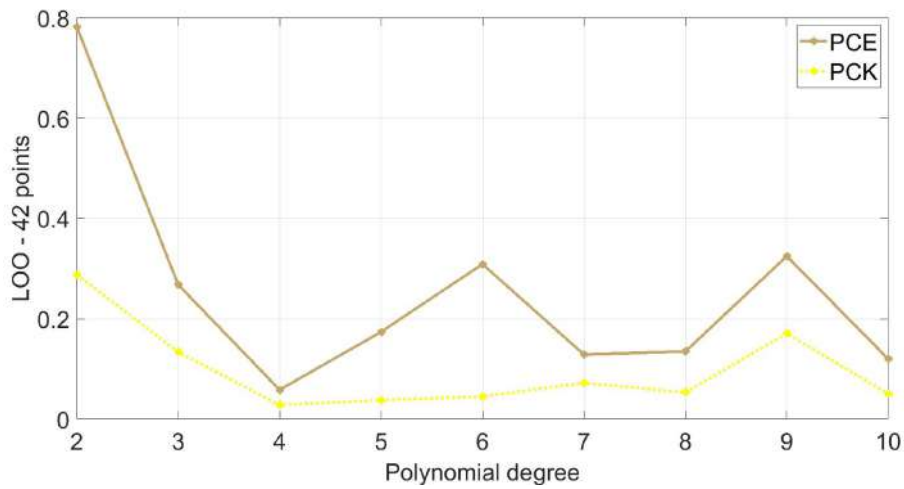


Figure 12.56: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response for 42 collocation points for a fully wetted flow - PPTC - J = 1.408.

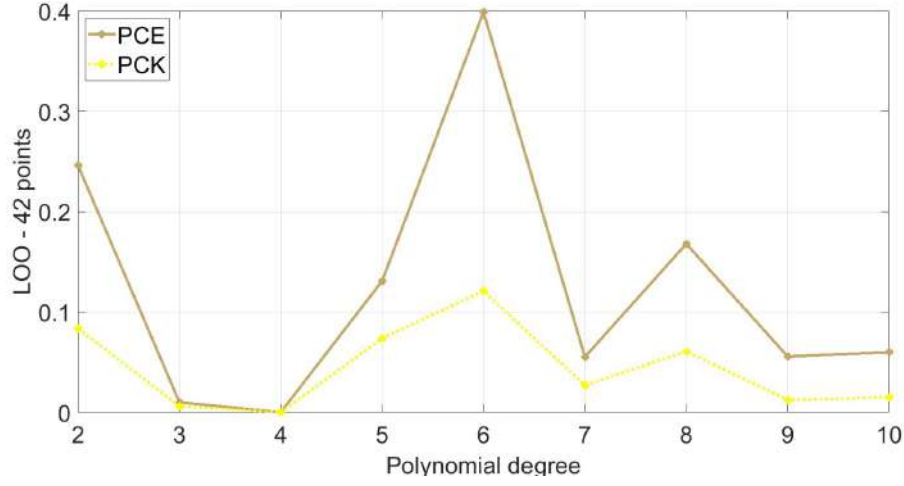


Figure 12.57: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response for 42 collocation points for a fully wetted flow - PPTC - $J = 1.408$.

- **Sobol indices:** In Figures 12.58 and 12.59, Sobol indices of thrust are represented. Considering the main Sobol indices, we observe that the turbulent coefficients σ_ε and C_{ε_1} are the most important coefficients for this problem for both the applied metamodels. Paying attention to the Sobol indices associated with the Polynomial Chaos Kriging, the most important parameter changes from σ_ε to C_{ε_1} for some polynomial order. This situation can be also observed for both Polynomial Chaos Expansion and Polynomial Chaos-based Kriging when total Sobol indices are analyzed.

Analyzing the Sobol indices of torque (given in 12.60 and 12.61), the evolution of Sobol indices for the different polynomial orders is more regular than the thrust case. For the torque output, the most important coefficient is the parameter C_{ε_2} for both the applied surrogate models.

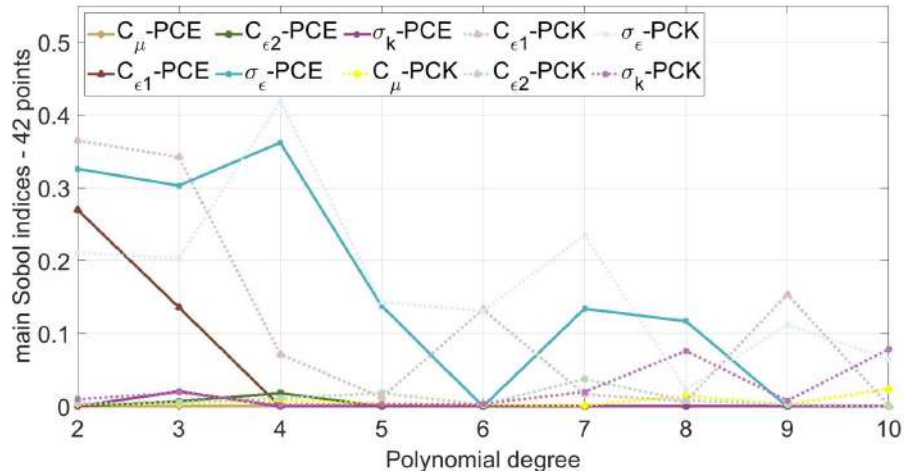


Figure 12.58: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.408$.

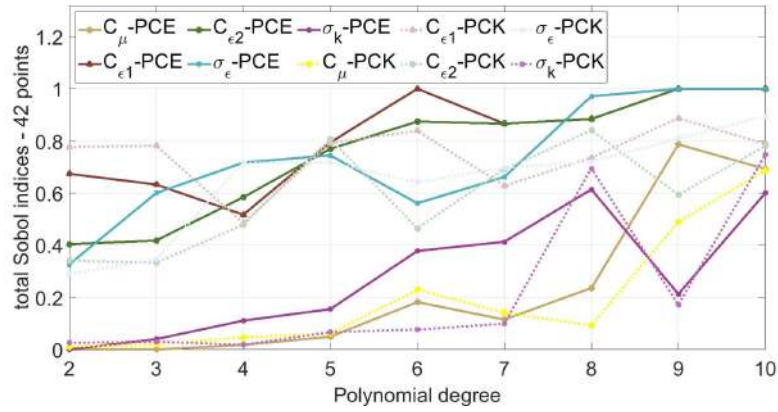


Figure 12.59: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.408$.

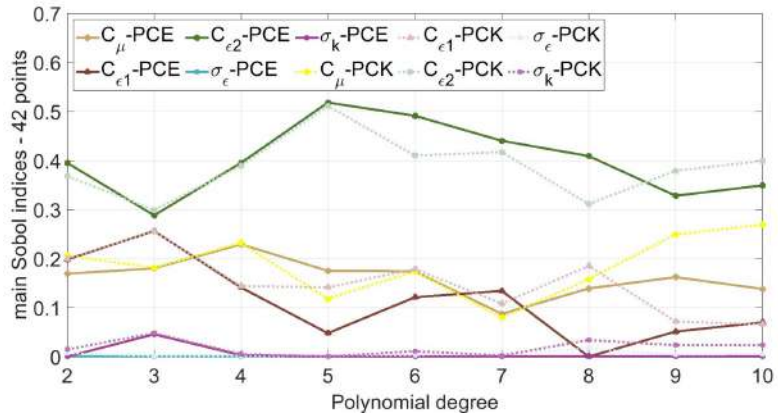


Figure 12.60: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.408$.

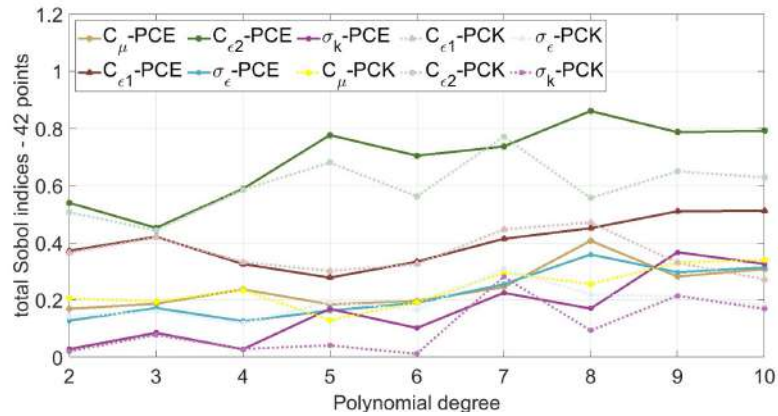


Figure 12.61: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a fully wetted flow condition - PPTC - $J = 1.408$.

12.3.2 Cavitating flow regime

Leave-One-Out Cross-Validation error

In Table 12.15 are respectively shown the Leave-One-Out Cross-Validation error for the thrust and torque for the cavitating flow. If we compare the results obtained for $J = 1.019$, also in this case we observe an increase of the prediction error for both the calculated outputs.

Table 12.15: Leave-One-Out Cross-Validation error of thrust and torque for the cavitating flow regime - PPTC - $J = 1.408$.

Response	ϵ_{LOO}	PCE order
T	0.542	II
Q	0.153	II

Statistical moments

In Table 12.16 are shown mean values and confidence intervals at the 95 % margine of error for the thrust and torque in a cavitating flow regime.

Table 12.16: Mean values and confidence intervals of thrust and torque for a cavitating flow regime - PPTC - $j = 1.408$.

Response	μ_{PCE}	$CI _{\text{down bound}}$	$CI _{\text{upper bound}}$	PCE order
T	-70.997	-71.637	-70.357	II
Q	6.489	6.401	6.577	II

Posterior probability distributions

In Figures and there are shown the Posterior probability distributions for the cavitating flow regime. Comparing the distributions of $J = 1.019$ and $J = 1.408$, distributions of thrust seem to have a similar profile while distributions of torque change the form. Distribution of torque for $J = 1.408$ sees to show a lower kurtosis and a more blunt profile. This may be justified by a higher uncertainty than the $J = 1.019$ operating case. In conclusion, means, modes, medians and standard deviations are represented in Table 12.17

Table 12.17: Data of posterior distribution functions of cavitating flow regime - PPTC - $J = 1.408$.

Response	PCE order	μ_{PCE}	σ_{PCE}	Mode	Median
T	II	-70.997	2.177	-71.940	-68.147
Q	II	6.489	0.291	6.558	6.240

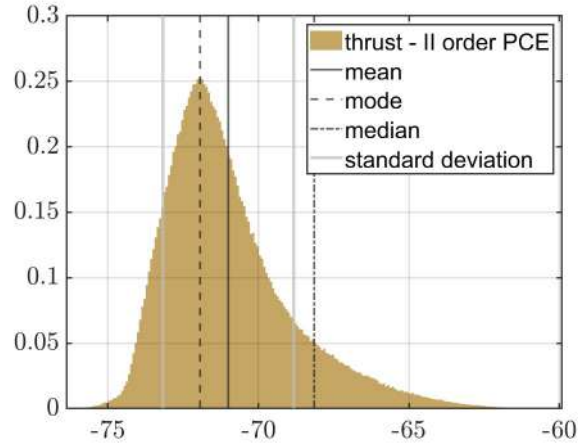


Figure 12.62: Posterior probability distribution of thrust for the cavitating flow - PPTC - $J = 1.408$.

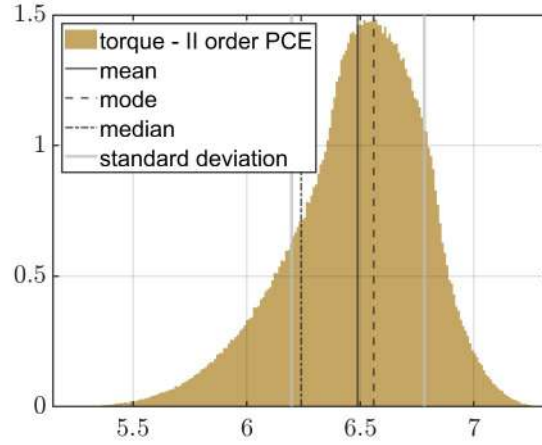


Figure 12.63: Posterior probability distribution of torque for the cavitating flow - PPTC - $J = 1.408$.

Sobol indices

Sobol indices of thrust and torque for a cavitating flow regime in the operation condition of $J = 1.408$ are represented in Figures 12.64, 12.65, 12.66 and 12.67. Considering the thrust, the most amount of uncertainty is associated with the coefficient C_{ε_2} while the most important couple seems to be $C_{\varepsilon_1} - C_{\varepsilon_2}$. Comparing those results with the fully wetted flow regime, we note that the ranking is not preserved for the main and total effects (main and total Sobol indices) but it is the same for the second order effects (second order Sobol indices).

Considering instead the torque response, we have that the coefficient C_{ε_2} is the most important parameter for the calculation of this output while the interaction between pair that most influences the determination of the torque is $C_{\varepsilon_2} - \sigma_{\varepsilon}$. Observing the results of the fully wetted flow, C_{ε_2} is the most important coefficient for both the flow regime while, analyzing the Sobol indices of second order, the ranking of importance of the second order effects of the calibration constants is not the same when the flow regime is modified.

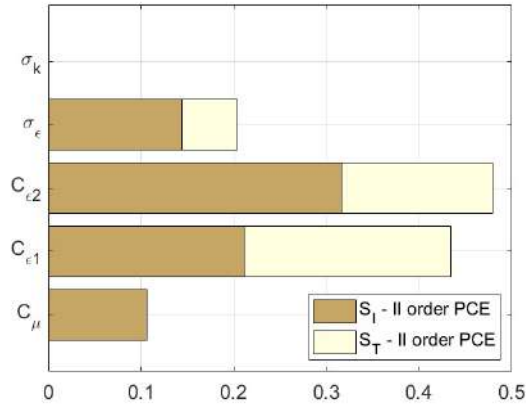


Figure 12.64: First and total order Sobol indices of thrust for the cavitating flow regime - PPTC - $J = 1.408$.

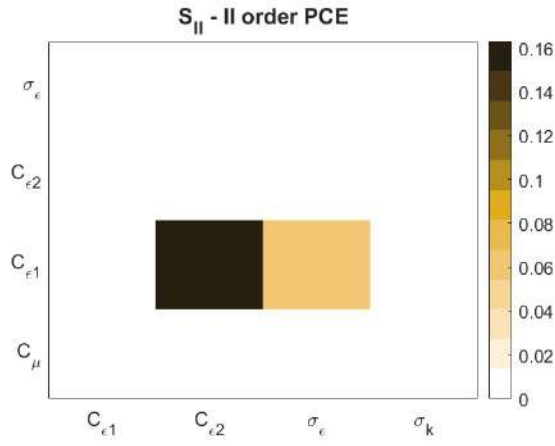


Figure 12.65: Second order Sobol indices of thrust for the cavitating flow regime - PPTC - $J = 1.408$.

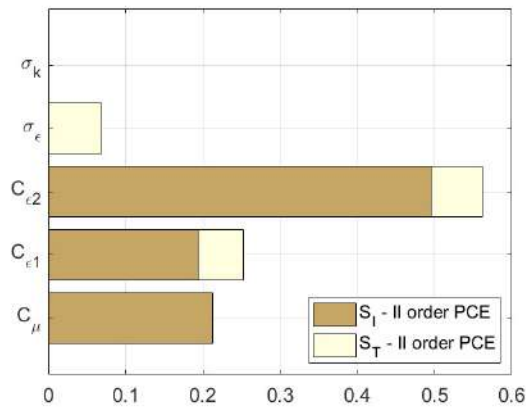


Figure 12.66: First and total order Sobol indices of torque for the cavitating flow regime - PPTC - $J = 1.408$.

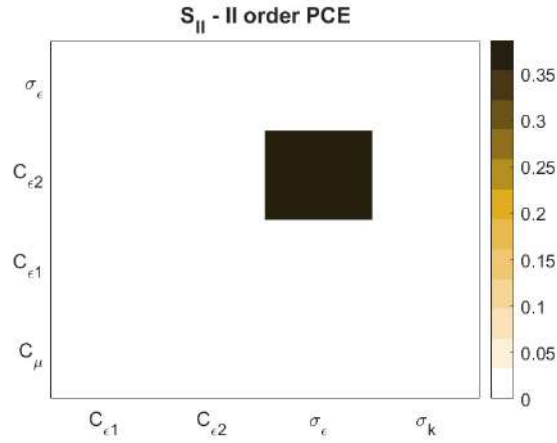


Figure 12.67: Second order Sobol indices of torque for the cavitating flow regime - PPTC - J = 1.408.

Comparison between PCE and PCK for PPTC propeller

- **Leave – One – Out Cross – Validation error:** In Figures 12.68 and 12.69, Leave-One-Out Cross-Validation errors of thrust and torque for the two metamodels are shown. Also for the cavitating flow regime, The Polynomial Chaos Kriging is more performant than the Polynomial Chaos Expansion for both the propeller responses.

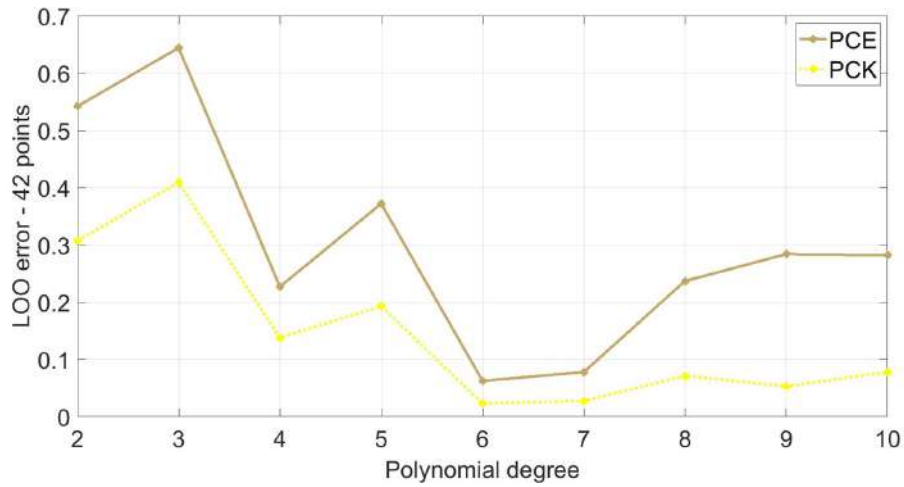


Figure 12.68: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response for 42 collocation points for a cavitating flow - PPTC - J = 1.408.

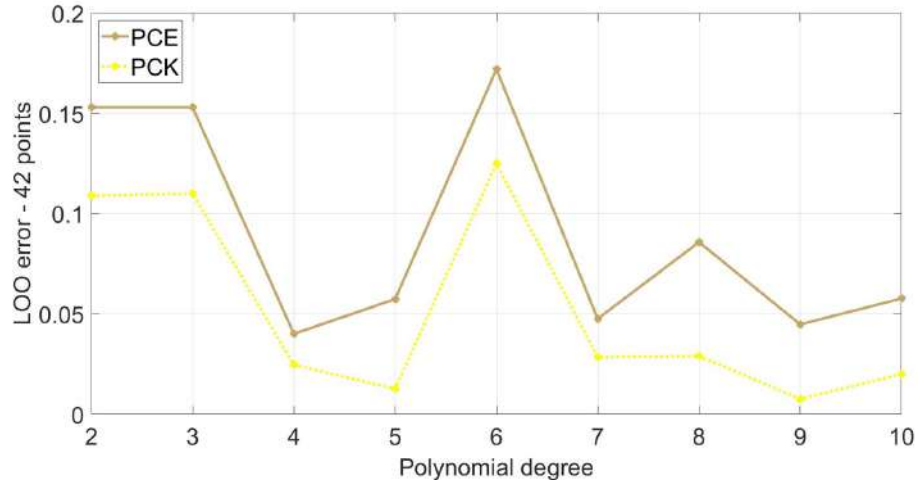


Figure 12.69: Comparison between the Leave-One-Out Cross-Validation Error trends of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response for 42 collocation points for a cavitating flow - PPTC - $J = 1.408$.

- **Sobol indices:** Considering Figures 12.70, 12.71, 12.72 and 12.73, we have the calculated Sobol indices for the Polynomial Chaos and the Polynomial Chaos Kriging. Analyzing the ranking of coefficients, we have that the most important coefficient for the evaluation of thrust and torque is the variable C_{ϵ_2} for Sobol indices calculated by Polynomial Chaos coefficients.

For Sobol indices based on Monte Carlo approaches, the most important coefficient for the thrust changes by increasing the polynomial order; specifically, when Polynomial Chaos Kriging is employed, the dominate contribution of uncertainty is associated to C_{ϵ_1} or C_{ϵ_2} .

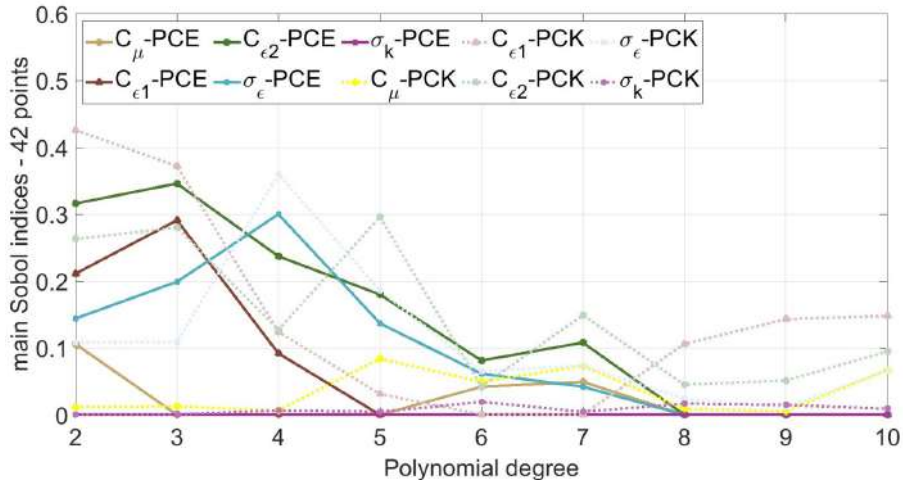


Figure 12.70: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.408$.

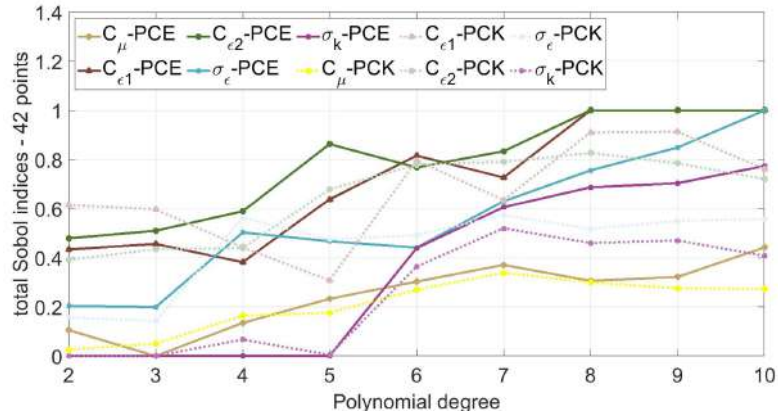


Figure 12.71: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the thrust response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.408$.

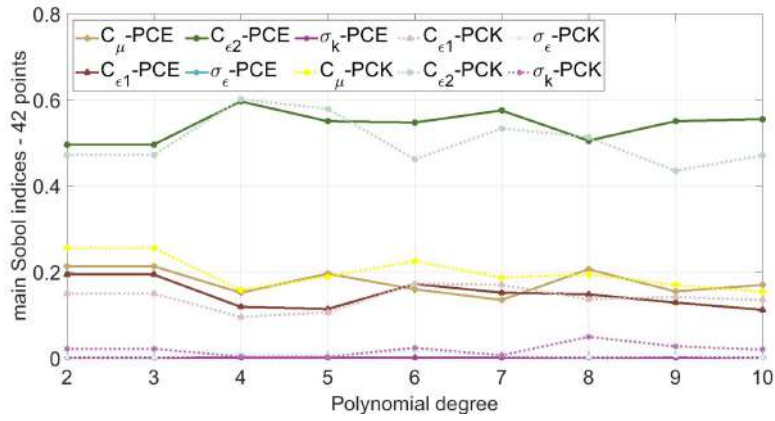


Figure 12.72: Main Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.408$.

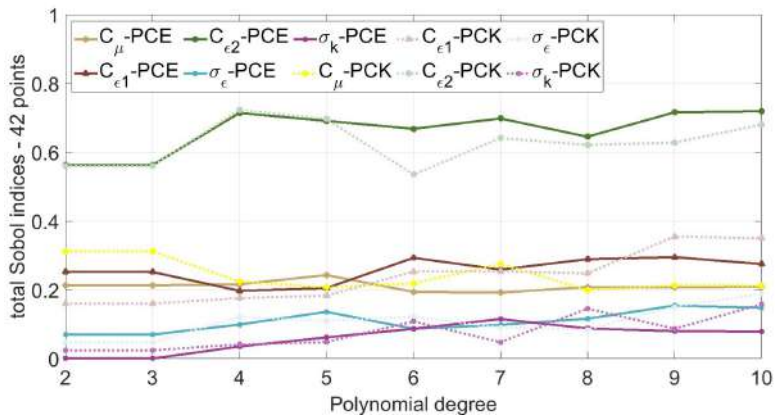


Figure 12.73: Total Sobol indices of Polynomial Chaos Expansion and Polynomial Chaos Kriging for the torque response by involving 42 collocation points in a cavitating flow condition - PPTC - $J = 1.408$.

Chapter 13

Conclusion

The work of the thesis has been focused on the Uncertainty Quantification and Sensitivity Analysis of the $k - \varepsilon$ Turbulence model coefficients aimed to predict cavitating and non-cavitating flows around object of naval interest.

Specifically, the Uncertainty Quantification has been studied in terms of a Forward Approach by employing Polynomial Chaos Expansion and Polynomial Chaos-based Kriging surrogate models and the Sensitivity Analysis has been investigated by considering a Global approach focused on the Variance-based method of Sobol decomposition.

The analysis has been applied for a two-dimensional test case, i.e. the NACA66(MOD) hydrofoil and it has been focused on global quantities, with the outputs of interest being the lift and drag coefficients. An additional analysis focused instead on local quantities. Here, the output of interest have been the pressure and friction coefficients on the airfoil surface. Subsequently, the study has been extended for a three-dimensional test case, i.e. the Potsdam Propeller Test Case (PPTC). The propeller responses have been the propeller thrust and the propeller torque. The PPTC propeller has been analyzed for the advance ratio of $J = 1.019$ and $J = 1.408$. In this manner, it has analyzed the cavitation on the back of the blade and the blade face.

In the following tables, the obtained results for the conducted analysis are summarized: in Table 13.1, the results of NACA66(MOD) hydrofoil for the fully wetted flow by applying a Polynomial Chaos Expansion from a second to a fifth polynomial order are shown; in that case the analysis has been applied for the evaluation of lift and drag coefficients. Subsequently, in Table 13.2, results about the comparison between the Polynomial Chaos Expansion and Polynomial Chaos Kriging for the determination of lift and drag in a fully wetted flow regime are shown. In Tables 13.3 and 13.4 cavitating flow regime results of NACA66(MOD) are given. Particularly, in Table 13.3 we have the results of lift and drag for a Polynomial Chaos Expansion from the second to the fifth order and in Table 13.4 there is shown the comparison of Polynomial Chaos and Polynomial Chaos-based Kriging with respect to these two hydrodynamics coefficients. In conclusion, the study of NACA66(MOD) hydrofoil has been finalized with a local analysis; in Table 13.5 there are discusses the obtained results for the pressure and friction coefficients by employing a Polynomial Chaos Expansion of the second order and a fully wetted flow.

Taking into consideration the PPTC propeller, In Table 13.6, we have the results of thrust and torque for a fully wetted flow in $J = 1.019$ by applying a Polynomial Chaos of the second and third reduced order while in Table 13.7 we have the Comparison of Polynomial Chaos Expansion and Polynomial Chaos Kriging at the same flow regime and advance ratio. Subsequently, in Tables 13.8 and 13.9 there are respectively the results about thrust and torque of the PPTC propeller at the operating point of $J = 1.019$ and the comparison between PCE and PCK for a cavitating flow regime. Considering instead the configuration $J = 1.408$, in Table 13.10 the results inherent to a Polynomial Chaos of the second order are shown and in Table 13.11 the results of thrust and torque obtained by the comparison between Polynomial Chaos Expansion and Polynomial Chaos

Kriging in a fully wetted flow condition are given. Finally, the results associated to the PPTC for $J = 1.408$ and for a cavitating flow regime are shown in Tables 13.12 and 13.13.

In conclusion, for each response and for each flow regime, the coefficients C_μ and σ_k have a negligible contribution for the evaluation of outputs. Furthermore, the magnitude of the standard deviations of the outputs obtained through Polynomial Chaos Expansion indicates a low level of uncertainty associated with the five calibration constants of the $k - \varepsilon$ turbulence model in determining the outputs of this study.

Table 13.1: Summary of results about the Global Analysis of NACA66(MOD) hydrofoil for the fully wetted flow regime by applying the Polynomial Chaos Expansion

Regime	Res.	Model	S_I	S_{II}	S_{III}	S_{IV}	S_{tot}
wetted	C_d	PCE - 2 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	/	/	σ_ε
wetted	C_d	PCE - 3 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	$C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$	/	σ_ε
wetted	C_d	PCE - 4 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	$C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$	σ_ε
wetted	C_d	PCE - 5 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	$C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$	σ_ε
wetted	C_l	PCE - 2 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	/	/	C_{ε_2}
wetted	C_l	PCE - 3 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	/	/	C_{ε_2}
wetted	C_l	PCE - 4 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_k$	/	C_{ε_2}
wetted	C_l	PCE - 5 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_k$	$C_\mu - C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon$	C_{ε_2}

Table 13.2: Summary of results about the Global Analysis of NACA66(MOD) hydrofoil for the fully wetted flow regime by applying the Polynomial Chaos Expansion vs Polynomial Chaos Kriging

Regime	Res.	Model	number of samplings	S_I	S_{tot}
wetted	C_d	PCE - 2:10 ord	42	σ_ε	σ_ε
wetted	C_d	PCK - 2:10 ord	42	σ_ε	σ_ε
wetted	C_l	PCE - 2:10 ord	42	$C_{\varepsilon_2}/\sigma_\varepsilon$	C_{ε_2}
wetted	C_l	PCK - 2:10 ord	42	C_{ε_2}	C_{ε_2}
wetted	C_d	PCE - 2:10 ord	504	σ_ε	σ_ε
wetted	C_d	PCK - 2:10 ord	504	σ_ε	σ_ε
wetted	C_l	PCE - 2:10 ord	504	C_{ε_2}	C_{ε_2}
wetted	C_l	PCK - 2:10 ord	504	C_{ε_2}	C_{ε_2}

Table 13.3: Summary of results about the Global Analysis of NACA66(MOD) hydrofoil for the cavitating flow regime by applying the Polynomial Chaos Expansion

Regime	Res.	Model	S_I	S_{II}	S_{III}	S_{IV}	S_{tot}
cav.	C_d	PCE - 2 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	/	/	σ_ε
cav.	C_d	PCE - 3 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	$C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$	/	σ_ε
cav.	C_d	PCE - 4 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	$C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$	σ_ε
cav.	C_d	PCE - 5 ord	σ_ε	$C_{\varepsilon_1} - \sigma_\varepsilon$	$C_{\varepsilon_1} - \sigma_\varepsilon - \sigma_k$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon - \sigma_k$	σ_ε
cav.	C_l	PCE - 2 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	/	/	C_{ε_2}
cav.	C_l	PCE - 3 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	/	/	C_{ε_2}
cav.	C_l	PCE - 4 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_k$	$C_\mu - C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon$	C_{ε_2}
cav.	C_l	PCE - 4 ord	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	$C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_k$	$C_\mu - C_{\varepsilon_1} - C_{\varepsilon_2} - \sigma_\varepsilon$	C_{ε_2}

Table 13.4: Summary of results about the Global Analysis of NACA66(MOD) hydrofoil for the cavitating flow regime by applying the Polynomial Chaos Expansion vs Polynomial Chaos Kriging

Regime	Res.	Model	number of samplings	S_I	S_{tot}
cav.	C_d	PCE - 2:10 ord	42	σ_ε	σ_ε
cav.	C_d	PCK - 2:10 ord	42	σ_ε	σ_ε
cav.	C_l	PCE - 2:10 ord	42	C_{ε_2}	C_{ε_2}
cav.	C_l	PCK - 2:10 ord	42	C_{ε_2}	C_{ε_2}
cav.	C_d	PCE - 2:10 ord	504	σ_ε	σ_ε
cav.	C_d	PCK - 2:10 ord	504	σ_ε	σ_ε
cav.	C_l	PCE - 2:10 ord	504	C_{ε_2}	C_{ε_2}
cav.	C_l	PCK - 2:10 ord	504	C_{ε_2}	C_{ε_2}

Table 13.5: Summary of results about the Local Analysis of NACA66(MOD) hydrofoil for the fully wetted flow regime by applying the Polynomial Chaos Expansion

Regime	Res.	Model	S_I	S_{II}	S_{tot}
wetted	C_p	PCE - 2 ord	$\sigma_\varepsilon/C_{\varepsilon_2}$	$C_{\varepsilon_1} - C_{\varepsilon_2}$	$\sigma_\varepsilon/C_{\varepsilon_2}$
wetted	C_f	PCE - 2 ord	$\sigma_\varepsilon/C_{\varepsilon_2}$	$C_{\varepsilon_1} - C_{\varepsilon_2}$	$\sigma_\varepsilon/C_{\varepsilon_2}$

Table 13.6: Summary of results about the PPTC propeller at $J = 1.019$ for the fully wetted flow by applying the Polynomial Chaos Expansion

Regime	Res.	Model	J	S_I	S_{II}	S_{tot}
wetted	T	PCE - 2 ord	1.019	σ_ε	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_1}
wetted	Q	PCE - 2 ord	1.019	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}
wetted	T	PCE - 3 ord reduced	1.019	σ_ε	$C_{\varepsilon_1} - C_{\varepsilon_2}$	σ_ε
wetted	Q	PCE - 3 ord reduced	1.019	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}

Table 13.7: Summary of results about the PPTC propeller at $J = 1.019$ for the fully wetted flow by applying the Polynomial Chaos Expansion vs Polynomial Chaos Kriging

Regime	Res.	Model	set of points	J	S_I	S_{tot}
wetted	T	PCE - 2:10 ord	42	1.019	σ_ε	$C_{\varepsilon_1}/C_{\varepsilon_2}/\sigma_\varepsilon$
wetted	T	PCK - 2:10 ord	42	1.019	σ_ε	$C_{\varepsilon_1}/C_{\varepsilon_2}/\sigma_\varepsilon$
wetted	Q	PCE - 2:10 ord	42	1.019	C_{ε_2}	C_{ε_2}
wetted	Q	PCK - 2:10 ord	42	1.019	C_{ε_2}	C_{ε_2}

Table 13.8: Summary of results about the PPTC propeller at $J = 1.019$ for the cavitating flow by applying the Polynomial Chaos Expansion

Regime	Res.	Model	J	S_I	S_{II}	S_{tot}
cav.	T	PCE - 2 ord	1.019	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}
cav.	Q	PCE - 2 ord	1.019	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}
cav.	T	PCE - 3 ord reduced	1.019	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}
cav.	Q	PCE - 3 ord reduced	1.019	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}

Table 13.9: Summary of results about the PPTC propeller at $J = 1.019$ for the cavitating flow by applying the Polynomial Chaos Expansion vs Polynomial Chaos Kriging

Regime	Res.	Model	set of points	J	S_I	S_{tot}
cav.	T	PCE - 2:10 ord	42	1.019	σ_ε	$C_{\varepsilon_1}/C_{\varepsilon_2}$
cav.	T	PCK - 2:10 ord	42	1.019	$C_{\varepsilon_2}/\sigma_\varepsilon$	C_{ε_2}
cav.	Q	PCE - 2:10 ord	42	1.019	C_{ε_2}	C_{ε_2}
cav.	Q	PCK - 2:10 ord	42	1.019	C_{ε_2}	C_{ε_2}

Table 13.10: Summary of results about the PPTC propeller at $J = 1.408$ for the fully wetted flow by applying the Polynomial Chaos Expansion

Regime	Res.	Model	J	S_I	S_{II}	S_{tot}
wetted	T	PCE - 2 ord	1.408	σ_ε	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_1}
wetted	Q	PCE - 2 ord	1408	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}

Table 13.11: Summary of results about the PPTC propeller at $J = 1.408$ for the fully wetted flow by applying the Polynomial Chaos Expansion vs Polynomial Chaos Kriging

Regime	Res.	Model	set of points	J	S_I	S_{tot}
wetted	T	PCE - 2:10 ord	42	1.408	σ_ε	$C_{\varepsilon_1}/C_{\varepsilon_2}/\sigma_\varepsilon$
wetted	T	PCK - 2:10 ord	42	1.408	$C_{\varepsilon_1}/\sigma_\varepsilon$	$C_{\varepsilon_1}/C_{\varepsilon_2}/\sigma_\varepsilon$
wetted	Q	PCE - 2:10 ord	42	1.408	C_{ε_2}	C_{ε_2}
wetted	Q	PCK - 2:10 ord	42	1.408	C_{ε_2}	C_{ε_2}

Table 13.12: Summary of results about the PPTC propeller at $J = 1.408$ for the cavitating flow by applying the Polynomial Chaos Expansion

Regime	Res.	Model	J	S_I	S_{II}	S_{tot}
cav.	T	PCE - 2 ord	1.408	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}
cav.	Q	PCE - 2 ord	1.408	C_{ε_2}	$C_{\varepsilon_1} - C_{\varepsilon_2}$	C_{ε_2}

Table 13.13: Summary of results about the PPTC propeller at $J = 1.408$ for the cavitating flow by applying the Polynomial Chaos Expansion vs Polynomial Chaos Kriging

Regime	Res.	Model	set of points	J	S_I	S_{tot}
cav.	T	PCE - 2:10 ord	42	1.408	$C_{\varepsilon_2}/\sigma_\varepsilon$	$C_{\varepsilon_1}/C_{\varepsilon_2}$
cav.	T	PCK - 2:10 ord	42	1.408	$C_{\varepsilon_1}/C_{\varepsilon_2}/\sigma_\varepsilon$	$C_{\varepsilon_1}/C_{\varepsilon_2}/\sigma_\varepsilon$
cav.	Q	PCE - 2:10 ord	42	1.408	C_{ε_2}	C_{ε_2}
cav.	Q	PCK - 2:10 ord	42	1.408	C_{ε_2}	C_{ε_2}

Appendix A

Polynomial Chaos Expansion and Sobol decomposition developments

A.1 Introduction

In the following section, there are shown the extended forms of linear systems of Non-Intrusive Polynomial Chaos Expansions and Sobol decompositions of second, third, fourth, fifth and reduced third order which have been employed in the thesis work. as reminder, there have been employed 5 initial variables and an oversampling ratio of two.

A.2 Polynomial Chaos Expansions

A.2.1 Polynomial Chaos Expansion of the second order

$$\begin{aligned} & \left\{ \begin{array}{c} Y(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(1)} \\ \vdots \\ Y(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(42)} \end{array} \right\} = \\ & = \begin{bmatrix} P_0(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(1)} & \cdots & P_{20}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(1)} \\ \vdots & \ddots & \vdots \\ P_0(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(42)} & \cdots & P_{20}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(42)} \end{bmatrix} \begin{Bmatrix} \alpha_0 \\ \vdots \\ \alpha_{20} \end{Bmatrix}. \end{aligned} \quad (\text{A.1})$$

$$\begin{aligned} Y(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k) = & \mathcal{M}_0 + \mathcal{M}_{C_\mu}(C_\mu) + \mathcal{M}_{C_{\varepsilon_1}}(C_{\varepsilon_1}) + \mathcal{M}_{C_{\varepsilon_2}}(C_{\varepsilon_2}) + \mathcal{M}_{\sigma_\varepsilon}(\sigma_\varepsilon) + \mathcal{M}_{\sigma_k}(\sigma_k) + \\ & + \mathcal{M}_{C_\mu, C_{\varepsilon_1}}(C_\mu, C_{\varepsilon_1}) + \mathcal{M}_{C_\mu, C_{\varepsilon_2}}(C_\mu, C_{\varepsilon_2}) + \mathcal{M}_{C_\mu, \sigma_\varepsilon}(C_\mu, \sigma_\varepsilon) + \\ & + \mathcal{M}_{C_\mu, \sigma_k}(C_\mu, \sigma_k) + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}}(C_{\varepsilon_1}, C_{\varepsilon_2}) + \mathcal{M}_{C_{\varepsilon_1}, \sigma_\varepsilon}(C_{\varepsilon_1}, \sigma_\varepsilon) + \\ & + \mathcal{M}_{C_{\varepsilon_1}, \sigma_k}(C_{\varepsilon_1}, \sigma_k) + \mathcal{M}_{C_{\varepsilon_2}, \sigma_\varepsilon}(C_{\varepsilon_2}, \sigma_\varepsilon) + \mathcal{M}_{C_{\varepsilon_2}, \sigma_k}(C_{\varepsilon_2}, \sigma_k) + \\ & + \mathcal{M}_{\sigma_\varepsilon, \sigma_k}(\sigma_\varepsilon, \sigma_k) \end{aligned} \quad (\text{A.2})$$

A.2.4 Polynomial Chaos Expansion of the fifth order

$$\begin{aligned} & \left\{ \begin{array}{c} Y(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(1)} \\ \vdots \\ Y(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(504)} \end{array} \right\} = \\ & = \begin{bmatrix} P_0(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(1)} & \cdots & P_{251}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(1)} \\ \vdots & \ddots & \vdots \\ P_0(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(504)} & \cdots & P_{251}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k)^{(504)} \end{bmatrix} \begin{Bmatrix} \alpha_0 \\ \vdots \\ \alpha_{251} \end{Bmatrix}. \end{aligned} \quad (\text{A.7})$$

$$\begin{aligned} Y(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k) = & \mathcal{M}_0 + \mathcal{M}_{C_\mu}(C_\mu) + \mathcal{M}_{C_{\varepsilon_1}}(C_{\varepsilon_1}) + \mathcal{M}_{C_{\varepsilon_2}}(C_{\varepsilon_2}) + \mathcal{M}_{\sigma_\varepsilon}(\sigma_\varepsilon) + \mathcal{M}_{\sigma_k}(\sigma_k) + \\ & + \mathcal{M}_{C_\mu, C_{\varepsilon_1}}(C_\mu, C_{\varepsilon_1}) + \mathcal{M}_{C_\mu, C_{\varepsilon_2}}(C_\mu, C_{\varepsilon_2}) + \mathcal{M}_{C_\mu, \sigma_\varepsilon}(C_\mu, \sigma_\varepsilon) + \\ & + \mathcal{M}_{C_\mu, \sigma_k}(C_\mu, \sigma_k) + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}}(C_{\varepsilon_1}, C_{\varepsilon_2}) + \mathcal{M}_{C_{\varepsilon_1}, \sigma_\varepsilon}(C_{\varepsilon_1}, \sigma_\varepsilon) + \\ & + \mathcal{M}_{C_{\varepsilon_1}, \sigma_k}(C_{\varepsilon_1}, \sigma_k) + \mathcal{M}_{C_{\varepsilon_2}, \sigma_\varepsilon}(C_{\varepsilon_2}, \sigma_\varepsilon) + \mathcal{M}_{C_{\varepsilon_2}, \sigma_k}(C_{\varepsilon_2}, \sigma_k) + \\ & + \mathcal{M}_{\sigma_\varepsilon, \sigma_k}(\sigma_\varepsilon, \sigma_k) + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}) + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon}(C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon) + \\ & + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, \sigma_k}(C_\mu, C_{\varepsilon_1}, \sigma_k) + \mathcal{M}_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon}(C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon) + \\ & + \mathcal{M}_{C_\mu, C_{\varepsilon_2}, \sigma_k}(C_\mu, C_{\varepsilon_2}, \sigma_k) + \mathcal{M}_{C_\mu, \sigma_\varepsilon, \sigma_k}(C_\mu, \sigma_\varepsilon, \sigma_k) + \\ & + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon) + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k}(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k) + \\ & + \mathcal{M}_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k}(C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k) + \mathcal{M}_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}(C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k) + \\ & + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon) + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k) + \\ & + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k}(C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k) + \mathcal{M}_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}(C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k) + \\ & + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k) + \mathcal{M}_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}(C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k). \end{aligned} \quad (\text{A.8})$$

A.2.5 Polynomial Chaos Expansion of the third reduced order

$$\left\{ \begin{array}{c} Y(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)^{(1)} \\ \vdots \\ Y(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)^{(40)} \end{array} \right\} = \begin{bmatrix} P_0(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)^{(1)} & \cdots & P_{19}(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)^{(1)} \\ \vdots & \ddots & \vdots \\ P_0(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)^{(40)} & \cdots & P_{19}(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)^{(40)} \end{bmatrix} \begin{Bmatrix} \alpha_0 \\ \vdots \\ \alpha_{19} \end{Bmatrix}. \quad (\text{A.9})$$

$$\begin{aligned} Y(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon) = & \mathcal{M}_0 + \mathcal{M}_{C_{\varepsilon_1}}(C_{\varepsilon_1}) + \mathcal{M}_{C_{\varepsilon_2}}(C_{\varepsilon_2}) + \mathcal{M}_{\sigma_\varepsilon}(\sigma_\varepsilon) + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}}(C_{\varepsilon_1}, C_{\varepsilon_2}) + \\ & + \mathcal{M}_{C_{\varepsilon_1}, \sigma_\varepsilon}(C_{\varepsilon_1}, \sigma_\varepsilon) + \mathcal{M}_{C_{\varepsilon_2}, \sigma_\varepsilon}(C_{\varepsilon_2}, \sigma_\varepsilon) + \mathcal{M}_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon) \end{aligned} \quad (\text{A.10})$$

A.3 Sobol decomposition

A.3.1 Sobol decomposition of the second order

$$\begin{aligned} D = & D_{C_\mu} + D_{C_{\varepsilon_1}} + D_{C_{\varepsilon_2}} + D_{\sigma_\varepsilon} + D_{\sigma_k} + D_{C_\mu, C_{\varepsilon_1}} + D_{C_\mu, C_{\varepsilon_2}} + D_{C_\mu, \sigma_\varepsilon} + D_{C_\mu, \sigma_k} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}} + \\ & + D_{C_{\varepsilon_1}, \sigma_\varepsilon} + D_{C_{\varepsilon_1}, \sigma_k} + D_{C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_{\varepsilon_2}, \sigma_k} + D_{\sigma_\varepsilon, \sigma_k} \Rightarrow S_{C_\mu}, S_{C_{\varepsilon_1}}, S_{C_{\varepsilon_2}}, S_{\sigma_\varepsilon}, S_{\sigma_k}, S_{C_\mu, C_{\varepsilon_1}}, \\ & S_{C_\mu, C_{\varepsilon_2}}, S_{C_\mu, \sigma_\varepsilon}, S_{C_\mu, \sigma_k}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_{\varepsilon_1}, \sigma_\varepsilon}, S_{C_{\varepsilon_1}, \sigma_k}, S_{C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_{\varepsilon_2}, \sigma_k}, S_{\sigma_\varepsilon, \sigma_k}. \end{aligned} \quad (\text{A.11})$$

$$\begin{cases} S_{T_{C_\mu}} = S_{C_\mu} + S_{C_\mu, C_{\varepsilon_1}} + S_{C_\mu, C_{\varepsilon_2}} + S_{C_\mu, \sigma_\varepsilon} + S_{C_\mu, \sigma_k} \\ S_{T_{C_{\varepsilon_1}}} = S_{C_{\varepsilon_1}} + S_{C_\mu, C_{\varepsilon_1}} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, \sigma_k} \\ S_{T_{C_{\varepsilon_2}}} = S_{C_{\varepsilon_2}} + S_{C_\mu, C_{\varepsilon_2}} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_2}, \sigma_k} \\ S_{T_{\sigma_\varepsilon}} = S_{\sigma_\varepsilon} + S_{C_\mu, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_{\varepsilon_2}, \sigma_\varepsilon} + S_{\sigma_\varepsilon, \sigma_k} \\ S_{T_{\sigma_k}} = S_{\sigma_k} + S_{C_\mu, \sigma_k} + S_{C_{\varepsilon_1}, \sigma_k} + S_{C_{\varepsilon_2}, \sigma_k} + S_{\sigma_\varepsilon, \sigma_k} \end{cases} \quad (\text{A.12})$$

A.3.2 Sobol decomposition of the third order

$$\begin{aligned}
D = & D_{C_\mu} + D_{C_{\varepsilon_1}} + D_{C_{\varepsilon_2}} + D_{\sigma_\varepsilon} + D_{\sigma_k} + D_{C_\mu, C_{\varepsilon_1}} + D_{C_\mu, C_{\varepsilon_2}} + D_{C_\mu, \sigma_\varepsilon} + D_{C_\mu, \sigma_k} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}} + \\
& + D_{C_{\varepsilon_1}, \sigma_\varepsilon} + D_{C_{\varepsilon_1}, \sigma_k} + D_{C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_{\varepsilon_2}, \sigma_k} + D_{\sigma_\varepsilon, \sigma_k} + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}} + D_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon} + D_{C_\mu, C_{\varepsilon_1}, \sigma_k} + \\
& + D_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_\mu, C_{\varepsilon_2}, \sigma_k} + D_{C_\mu, \sigma_\varepsilon, \sigma_k} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k} + D_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k} + D_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} \Rightarrow \\
\Rightarrow & S_{C_\mu}, S_{C_{\varepsilon_1}}, S_{C_{\varepsilon_2}}, S_{\sigma_\varepsilon}, S_{\sigma_k}, S_{C_\mu, C_{\varepsilon_1}}, S_{C_\mu, C_{\varepsilon_2}}, S_{C_\mu, \sigma_\varepsilon}, S_{C_\mu, \sigma_k}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_{\varepsilon_1}, \sigma_\varepsilon}, S_{C_{\varepsilon_1}, \sigma_k}, \\
& S_{C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_{\varepsilon_2}, \sigma_k}, S_{\sigma_\varepsilon, \sigma_k}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon}, S_{C_\mu, C_{\varepsilon_1}, \sigma_k}, S_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_\mu, C_{\varepsilon_2}, \sigma_k}, S_{C_\mu, \sigma_\varepsilon, \sigma_k}, \\
& S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k}, S_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k}, S_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}.
\end{aligned} \tag{A.13}$$

$$\left\{ \begin{aligned} S_{T_{C_\mu}} &= S_{C_\mu} + S_{C_\mu, C_{\varepsilon_1}} + S_{C_\mu, C_{\varepsilon_2}} + S_{C_\mu, \sigma_\varepsilon} + S_{C_\mu, \sigma_k} + S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_\mu, C_{\varepsilon_1}, \sigma_k} + \\ &\quad + S_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_\mu, C_{\varepsilon_2}, \sigma_k} + S_{C_\mu, \sigma_\varepsilon, \sigma_k} \\ S_{T_{C_{\varepsilon_1}}} &= S_{C_{\varepsilon_1}} + S_{C_\mu, C_{\varepsilon_1}} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, \sigma_k} + S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_\mu, C_{\varepsilon_1}, \sigma_k} + \\ &\quad + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k} + S_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k} \\ S_{T_{C_{\varepsilon_2}}} &= S_{C_{\varepsilon_2}} + S_{C_\mu, C_{\varepsilon_2}} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_2}, \sigma_k} + S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_\mu, C_{\varepsilon_2}, \sigma_k} + \\ &\quad + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k} + S_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} \\ S_{T_{\sigma_\varepsilon}} &= S_{\sigma_\varepsilon} + S_{C_\mu, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_{\varepsilon_2}, \sigma_\varepsilon} + S_{\sigma_\varepsilon, \sigma_k} + S_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_\mu, \sigma_\varepsilon, \sigma_k} + \\ &\quad + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k} + S_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} \\ S_{T_{\sigma_k}} &= S_{\sigma_k} + S_{C_\mu, \sigma_k} + S_{C_{\varepsilon_1}, \sigma_k} + S_{C_{\varepsilon_2}, \sigma_k} + S_{\sigma_\varepsilon, \sigma_k} + S_{C_\mu, C_{\varepsilon_1}, \sigma_k} + S_{C_\mu, C_{\varepsilon_2}, \sigma_k} + S_{C_\mu, \sigma_\varepsilon, \sigma_k} + \\ &\quad + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k} + S_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k} + S_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} \end{aligned} \right. \quad (\text{A.14})$$

A.3.3 Sobol decomposition of the fourth order

$$\begin{aligned}
D = & D_{C_\mu} + D_{C_{\varepsilon_1}} + D_{C_{\varepsilon_2}} + D_{S_\varepsilon} + D_{S_\sigma} + D_{C_\mu, C_{\varepsilon_1}} + D_{C_\mu, C_{\varepsilon_2}} + D_{C_\mu, S_\varepsilon} + D_{C_\mu, S_\sigma} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}} + \\
& + D_{C_{\varepsilon_1}, S_\varepsilon} + D_{C_{\varepsilon_1}, S_\sigma} + D_{C_{\varepsilon_2}, S_\varepsilon} + D_{C_{\varepsilon_2}, S_\sigma} + D_{S_\varepsilon, S_\sigma} + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}} + D_{C_\mu, C_{\varepsilon_1}, S_\varepsilon} + D_{C_\mu, C_{\varepsilon_1}, S_\sigma} + \\
& + D_{C_\mu, C_{\varepsilon_2}, S_\varepsilon} + D_{C_\mu, C_{\varepsilon_2}, S_\sigma} + D_{C_\mu, S_\varepsilon, S_\sigma} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, S_\varepsilon} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, S_\sigma} + D_{C_{\varepsilon_1}, S_\varepsilon, S_\sigma} + D_{C_{\varepsilon_2}, S_\varepsilon, S_\sigma} + \\
& + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, S_\varepsilon} + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, S_\sigma} + D_{C_\mu, C_{\varepsilon_1}, S_\varepsilon, S_\sigma} + D_{C_\mu, C_{\varepsilon_2}, S_\varepsilon, S_\sigma} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, S_\varepsilon, S_\sigma} \Rightarrow S_{C_\mu}, \\
& S_{C_{\varepsilon_1}}, S_{C_{\varepsilon_2}}, S_{S_\varepsilon}, S_{S_\sigma}, S_{C_\mu, C_{\varepsilon_1}}, S_{C_\mu, C_{\varepsilon_2}}, S_{C_\mu, S_\varepsilon}, S_{C_\mu, S_\sigma}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_{\varepsilon_1}, S_\varepsilon}, S_{C_{\varepsilon_1}, S_\sigma}, S_{C_{\varepsilon_2}, S_\varepsilon}, \\
& S_{C_{\varepsilon_2}, S_\sigma}, S_{S_\varepsilon, S_\sigma}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_\mu, C_{\varepsilon_1}, S_\varepsilon}, S_{C_\mu, C_{\varepsilon_1}, S_\sigma}, S_{C_\mu, C_{\varepsilon_2}, S_\varepsilon}, S_{C_\mu, C_{\varepsilon_2}, S_\sigma}, S_{C_\mu, S_\varepsilon, S_\sigma}, \\
& S_{C_{\varepsilon_1}, C_{\varepsilon_2}, S_\varepsilon}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, S_\sigma}, S_{C_{\varepsilon_1}, S_\varepsilon, S_\sigma}, S_{C_{\varepsilon_2}, S_\varepsilon, S_\sigma}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, S_\varepsilon}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, S_\sigma}, S_{C_\mu, C_{\varepsilon_1}, S_\varepsilon, S_\sigma}, \\
& S_{C_\mu, C_{\varepsilon_2}, S_\varepsilon, S_\sigma}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, S_\varepsilon, S_\sigma}.
\end{aligned} \tag{A.15}$$

[illegible]

A.3.4 Sobol decomposition of the fifth order

$$\begin{aligned}
D = & D_{C_\mu} + D_{C_{\varepsilon_1}} + D_{C_{\varepsilon_2}} + D_{\sigma_\varepsilon} + D_{\sigma_k} + D_{C_\mu, C_{\varepsilon_1}} + D_{C_\mu, C_{\varepsilon_2}} + D_{C_\mu, \sigma_\varepsilon} + D_{C_\mu, \sigma_k} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}} + \\
& + D_{C_{\varepsilon_1}, \sigma_\varepsilon} + D_{C_{\varepsilon_1}, \sigma_k} + D_{C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_{\varepsilon_2}, \sigma_k} + D_{\sigma_\varepsilon, \sigma_k} + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}} + D_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon} + D_{C_\mu, C_{\varepsilon_1}, \sigma_k} + \\
& + D_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_\mu, C_{\varepsilon_2}, \sigma_k} + D_{C_\mu, \sigma_\varepsilon, \sigma_k} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k} + D_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k} + D_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} + \\
& + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k} + D_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k} + D_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} + \\
& + D_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k} \Rightarrow S_{C_\mu}, S_{C_{\varepsilon_1}}, S_{C_{\varepsilon_2}}, S_{\sigma_\varepsilon}, S_{\sigma_k}, S_{C_\mu, C_{\varepsilon_1}}, S_{C_\mu, C_{\varepsilon_2}}, S_{C_\mu, \sigma_\varepsilon}, S_{C_\mu, \sigma_k}, \\
& S_{C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_{\varepsilon_1}, \sigma_\varepsilon}, S_{C_{\varepsilon_1}, \sigma_k}, S_{C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_{\varepsilon_2}, \sigma_k}, S_{\sigma_\varepsilon, \sigma_k}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon}, S_{C_\mu, C_{\varepsilon_1}, \sigma_k}, \\
& S_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_\mu, C_{\varepsilon_2}, \sigma_k}, S_{C_\mu, \sigma_\varepsilon, \sigma_k}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k}, S_{C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k}, S_{C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}, \\
& S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k}, S_{C_\mu, C_{\varepsilon_1}, \sigma_\varepsilon, \sigma_k}, S_{C_\mu, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}, S_{C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon, \sigma_k}.
\end{aligned} \tag{A.17}$$

[illegible]

A.3.5 Sobol decomposition of the third reduced order

$$\begin{aligned}
D &= D_{C_{\varepsilon_1}} + D_{C_{\varepsilon_2}} + D_{\sigma_\varepsilon} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}} + D_{C_{\varepsilon_1}, \sigma_\varepsilon} + D_{C_{\varepsilon_2}, \sigma_\varepsilon} + D_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} \Rightarrow S_{C_{\varepsilon_1}}, S_{C_{\varepsilon_2}}, S_{\sigma_\varepsilon}, \\
&S_{C_{\varepsilon_1}, C_{\varepsilon_2}}, S_{C_{\varepsilon_1}, \sigma_\varepsilon}, S_{C_{\varepsilon_2}, \sigma_\varepsilon}, S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}.
\end{aligned} \tag{A.19}$$

$$\begin{cases}
S_{T_{C_{\varepsilon_1}}} = S_{C_{\varepsilon_1}} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} \\
S_{T_{C_{\varepsilon_2}}} = S_{C_{\varepsilon_2}} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}} + S_{C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon} \\
S_{T_{\sigma_\varepsilon}} = S_{\sigma_\varepsilon} + S_{C_{\varepsilon_1}, \sigma_\varepsilon} + S_{C_{\varepsilon_2}, \sigma_\varepsilon} + S_{C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon}
\end{cases} . \tag{A.20}$$

Appendix B

Uncertainty Quantification methods

B.1 Introduction

In the current chapter there are described more in detail, the developed methods for studying the Uncertainty Quantification theory which have been cited in the chapter of "Uncertainty Quantification theory".

B.2 Monte Carlo methods

Monte Carlo methods are a wide class of computational algorithms that rely on repeated random sampling to obtain numerical results. The problem inherent in the curse of dimensionality can be circumvented by resorting to random sampling of the integration domain and their implementation find application in optimization and numerical integration problems. Monte Carlo methods are an application of LLN (Law of Large Numbers) and are classified in **Vanilla Monte Carlo methods**, **Markov Chain Monte Carlo methods** and **Multi Level Monte Carlo methods**.

B.2.1 Vanilla Monte Carlo

Vanilla Monte Carlo is the simplest formulation of Monte Carlo methods where given the output $Y(\boldsymbol{\xi})$ as function of the initial variables vector $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}^T$ with respect the model $\mathcal{M}(\boldsymbol{\xi})$ such that $Y(\boldsymbol{\xi}) = \mathcal{M}(\boldsymbol{\xi})$. the expected value of the response $\mathbb{E}[Y(\boldsymbol{\xi})]$ (i.e. the mean value μ_{VMC}) is the arithmetic mean of the sampled values K while the variance σ_{VMC}^2 is the expected value of the squared deviation from the mean of the sampled points:

$$\mu_{\text{VMC}} = \mathbb{E}[\mathcal{M}(\boldsymbol{\xi})] = \frac{1}{K} \sum_{i=1}^K \mathcal{M}_i(\boldsymbol{\xi}) = \frac{1}{K} \sum_{i=1}^K Y_i(\boldsymbol{\xi}) \quad (\text{B.1})$$

$$\sigma_{\text{VMC}}^2 = \sum_{i=1}^K \frac{(Y_i(\boldsymbol{\xi}) - \mu_{\text{VMC}})^2}{K - 1}. \quad (\text{B.2})$$

B.2.2 Markov Chain Monte Carlo

Markov Chain Monte Carlo is a Monte Carlo method that applies a sampling strategy from a probability distribution of reference by using a Markov Chain. The algorithm converges when the convergence of the given probability distribution is reached.

B.2.3 Multi Level Monte Carlo

Multi Level Monte Carlo methods are associated with the resolution of ordinary differential equations or partial differential equations where the accuracy of the solution Y is given by the choice of time step and mesh refinement. If we have a set of approximations $[\mathcal{M}_0(\boldsymbol{\xi}), \dots, \mathcal{M}_{\bar{K}}(\boldsymbol{\xi})]$ of $Y(\boldsymbol{\xi})$, the expected value is calculated as:

$$\begin{aligned} \mu_{\text{MLMC}} = \mathbb{E}[\mathcal{M}(\boldsymbol{\xi})] &= \mathbb{E}[\mathcal{M}_0(\boldsymbol{\xi})] + \sum_{j=1}^{\bar{K}} \mathbb{E}[\mathcal{M}_j(\boldsymbol{\xi}) - \mathcal{M}_{j-1}(\boldsymbol{\xi})] = \frac{1}{\bar{K}} \sum_{k=1}^{\bar{K}} \mathcal{M}_0(\boldsymbol{\xi}^{(k)}) + \\ &+ \sum_{j=1}^{\bar{K}} \left\{ \frac{1}{K} \sum_{i=1}^K [\mathcal{M}_j(\boldsymbol{\xi}^{(i)}) - \mathcal{M}_{j-1}(\boldsymbol{\xi}^{(i)})] \right\}, \end{aligned} \quad (\text{B.3})$$

where $\boldsymbol{\xi}^{(i)}$ is the i -mode of $\boldsymbol{\xi}$.

B.3 Quasi Monte Carlo methods

Quasi Monte Carlo methods use low-discrepancy sequences to achieve variance reduction. In contrast, classical Monte Carlo approaches use sequences based on pseudorandom values, this is the main difference between the two methodologies. Two important Quasi Monte Carlo methods are **Van Der Corput sequences**, **Halton sequence** and **Sobol sequence**.

B.3.1 Van Der Corput sequence

Van Der Corput sequence is used to generate a sequence of samplings which covers the sampling domain more uniformly than the pseudorandom points method. The sequence is generated in $]0,1[$ with base $b \in \mathbb{N}, b > 1$ and the samples are generated as:

$$\xi_n^{(b)} = \sum_{i=0}^K d_i(n) b^{-i-1} \quad \text{for } 0 \leq d_i(n) < b. \quad (\text{B.4})$$

where:

$$n = \sum_{i=0}^K d_i(n) b^i \quad (\text{B.5})$$

B.3.2 Halton sequence

Halton sequences are expressed in terms of Van Der Corput sequences in the multi-dimensional interval $]0,1[^d$ with bases $(b_1, \dots, b_n) \in \mathbb{N} > 1$ such that the sampling set is defined as:

$$\xi_n = \left(\xi_n^{(b_1)}, \dots, \xi_n^{(b_d)} \right). \quad (\text{B.6})$$

B.3.3 Sobol sequence

Sobol sequences belong to the family of quasi-random sampling methods. The objective is to create a sampling set as uniformly as possible taking into account the previous samples. The quality of Sobol sequences is described by the discrepancy metric in the exploration of the multi-dimensional parameter space, defined as the maximum deviation between the theoretical given by $\frac{1}{K}$ and the point density. The scope of Sobol sequence is to create sampling with low discrepancy. The number of samples generated is:

$$K = 2^i \quad \text{for } i \in \mathbb{N}^+. \quad (\text{B.7})$$

B.4 Pseudo Monte Carlo methods

Pseudo Monte Carlo methods are based on deterministic samplings which can be interpreted as random from a particular point of view. The most common methods of this class is the **Latin Hypercube Sampling method**.

B.4.1 Latin Hypercube Sampling methods

Latin Hypercube Sampling is a stratified sampling method which divides each dimension d of the subspace D_{ξ_i} of the domain D_{ξ} into N non-overlapping subsets $\{D_{\xi_{ij}}\}_{j \in \{1, \dots, N\}}$ with the stratum probability $\frac{1}{N}$. In this manner, the sampling space (domain) is covered more uniformly and it is reconstructed as:

$$D_{\xi_i} = \bigcup_{j \in \{1, \dots, N\}} D_{\xi_{ij}} \quad \forall i \in \{1, \dots, d\} \quad (\text{B.8})$$

and:

$$D_{\xi_{ij}} \cap D_{\xi_{ik}} = \emptyset \quad \text{for } j \neq k \in \{1, \dots, N\}. \quad (\text{B.9})$$

B.5 Wavelet Expansion

Wavelet Expansions are composed by Wavelet basis, defined in the $L^2(\mathbb{R}^n)$ or $L^2\left(\frac{\mathbb{R}^n}{2^n}\right)$. These basis are orthonormal basis consisting of appropriately scaled and shifted copies of a single basic element that has some self-similarity; a model $\mathcal{M}$ is associated to a scale and shifted version $\mathcal{M}_{ij}$ as in the following expression:

$$\mathcal{M}_{ij}(\xi) = \mathcal{M}(2^i \xi - j) \quad (\text{B.10})$$

Considering a rate of decay, Wavelets are used to create a function space (Besov space) which satisfy the nesting, density, zero intersection, scaling intersection, kernel and Riesz basis function properties. The first function of the family is a scaling function named "father wavelet" $\phi(\xi)$ which is associated with a "mother wavelet" $\varphi(\xi)$ through a shifting and scaling process as below:

$$\phi(\xi) = \sum_{i \in \mathbb{Z}} \alpha_{\text{WE}_i} \phi(2\xi - i) \Rightarrow \varphi(\xi) = \sum_{i \in \mathbb{Z}} (-1)^i \alpha_{\text{WE}_{i+1}} \phi(2\xi + 1), \quad (\text{B.11})$$

where α_{WE} are wavelet coefficients. Two typical Wavelet Expansions are **Haar Wavelet** and **B – spine Wavelet**.

B.5.1 Haar Wavelet

In Haar Wavelet the father function is defined as:

$$\phi(\xi) = \mathbb{I}_{[0,1[} \quad (\text{B.12})$$

where its mother counterpart is given by:

$$\varphi(\xi) = \phi(2\xi) - \phi(2\xi - 1) = \begin{cases} 1 & \text{for } 0 \leq \xi < \frac{1}{2} \\ -1 & \text{for } \frac{1}{2} \leq \xi < 1 \\ 0 & \text{otherwise} \end{cases} \quad (\text{B.13})$$

B.5.2 B-spline Wavelet

The B-spline Wavelet is defined as a piecewise polynomial of degree equal to p where its father Wavelet is expressed as:

$$\phi_p = \begin{cases} \mathbb{I}_{[0,1[} & \text{for } p = 0 \\ \phi_{p-1} \star \phi_0 & \text{otherwise} \end{cases}, \quad (\text{B.14})$$

and

$$(\phi_{p-1} \star \phi_0)(\xi) = \int_{\mathbb{R}} \phi_{p-1}(\zeta) \phi_0(\xi - \zeta) d\zeta \quad (\text{B.15})$$

B.6 Karhunen-Loeve Expansion

Karhunen-Loeve Expansion is a decomposition (series expansion) of a square-integrable stochastic process with continuous covariance matrix by using orthogonal deterministic basis functions and uncorrelated random coefficients that represent the random variables of the problem. If $\varphi = \{\varphi_1, \dots, \varphi_M\}^T$ are orthonormal eigenfunctions representing the basis functions of the expansion and $\alpha_{\text{KLE}} = \{\alpha_{\text{KLE}_1}, \dots, \alpha_{\text{KLE}_M}\}^T$ are the associated coefficients, the stochastic process is expressed in the below series within the L^2 space:

$$Y(\xi) = \sum_{i=1}^M \alpha_{\text{KLE}_i} \varphi_i(\xi). \quad (\text{B.16})$$

Considering the set of eigenvalues $\lambda = \{\lambda_1, \dots, \lambda_M\}$ of the eigenfunctions, the covariance value of the stochastic process is calculated as:

$$\text{Cov}\{\xi, \zeta\} = \sum_{i=1}^M \lambda_i \varphi_i(\xi) \varphi_i(\zeta) \quad \forall \xi \in D_\xi \text{ and } \forall \zeta \in D_\zeta. \quad (\text{B.17})$$

As introduced, Karhunen-Loeve coefficients are random variable which can be determined as:

$$\alpha_{\text{KLE}_i} = \int_{D_\xi} Y(\xi) \varphi_i(\xi) d\xi \quad (\text{B.18})$$

with the respective expected value:

$$\mathbb{E}[\alpha_{\text{KLE}_i}] = \mathbb{E}\left[\int_{D_\xi} Y(\xi) \varphi_i(\xi) d\xi\right] = \int_{D_\xi} \mathbb{E}[Y(\xi)] \varphi_i(\xi) d\xi = 0 \quad (\text{B.19})$$

$$\begin{aligned} \mathbb{E}[\alpha_{\text{KLE}_j} \alpha_{\text{KLE}_i}] &= \mathbb{E}\left[\int_{D_\xi} Y(\xi) \varphi_j(\xi) d\xi \int_{D_\xi} Y(\xi) \varphi_i(\xi) d\xi\right] = \\ &= \int_{D_\xi} \varphi_j(\xi) [\text{Cov}\{\xi, \zeta\} \varphi_i(\zeta) d\zeta] d\xi = \int_{D_\xi} \varphi_j(\xi) \lambda_i \varphi_i(\xi) d\xi = \lambda_i \delta_{ij} \end{aligned} \quad (\text{B.20})$$

where δ_{ij} is the Kronecker delta. Karhunen-Loeve Expansion has the advantage that the mean-square error is minimal but it can be applied only if covariance is known a priori, in fact, if covariances are known, stochastic processes can be represented in "covariance structure" providing a simple method for sampling Gaussian measures on Hilbert spaces.

B.7 Neumann Expansion

Neumann Expansion are used to obtain approximated numerical solutions of linear systems by summing k -times the application of an operator $\mathbf{P}$. Given a known response vector $\mathbf{Y}(\xi)$, a known system matrix $\mathbf{\Psi}(\xi)$ and an unknown vector of coefficients α_{NE} such that:

$$\mathbf{Y}(\boldsymbol{\xi}) = \boldsymbol{\Psi}(\boldsymbol{\xi})\boldsymbol{\alpha}_{\text{NE}}. \quad (\text{B.21})$$

The Neumann series is employed to iteratively calculate the vector of coefficients; the system matrix is decomposed as:

$$\boldsymbol{\Psi}(\boldsymbol{\xi}) = \boldsymbol{\Psi}_0(\boldsymbol{\xi}) + \Delta\boldsymbol{\Psi}(\boldsymbol{\xi}) = \boldsymbol{\Psi}(\boldsymbol{\xi}) (\mathbb{I} - \mathbf{P}) \quad (\text{B.22})$$

where:

$$\boldsymbol{\Psi}_0(\boldsymbol{\xi}) : \text{matrix of initial conditions} \quad (\text{B.23})$$

$$(\mathbb{I} - \mathbf{P})^{-1} \approx \sum_{i=0}^M \mathbf{P}_i \quad (\text{B.24})$$

and the coefficients are calculated as:

$$\boldsymbol{\alpha}_{\text{NE}} = (\mathbb{I} - \mathbf{P})^{-1} \boldsymbol{\alpha}_{\text{NE}_0} \quad (\text{B.25})$$

where the initialization is imposed as:

$$\boldsymbol{\alpha}_{\text{NE}_0} = \boldsymbol{\Psi}_0^{-1}(\boldsymbol{\xi})\mathbf{Y}(\boldsymbol{\xi}). \quad (\text{B.26})$$

B.8 Taylor Series Expansion

Taylor expansion represents outputs of systems in Taylor series where each initial variable ξ_i is associated with the own mean value μ_{TS_i} :

$$Y = \mathcal{M}(\boldsymbol{\mu}_{\text{TS}}) + \sum_{i=1}^n \left. \frac{\partial \mathcal{M}}{\partial \xi_i} \right|_{\boldsymbol{\mu}_{\text{TS}}} (\xi_i - \mu_{\text{TS}_i}) + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \left. \frac{\partial^2 \mathcal{M}}{\partial \xi_i \partial \xi_j} \right|_{\boldsymbol{\mu}_{\text{TS}}} \times (\xi_i - \mu_{\text{TS}_i}) (\xi_j - \mu_{\text{TS}_j}) + \dots \quad (\text{B.27})$$

The quantities $\frac{\partial \mathcal{M}}{\partial \xi_i}$, $\frac{\partial^2 \mathcal{M}}{\partial \xi_i \partial \xi_j}$... represent the sensitivity terms of the series which quantify the importance of the single variables and interactions between variables on the output evaluation. They are calculated by using sensitivity estimators such as **first – order forward finite difference method**, **central difference method** and **modified forward finite difference methods** and the mean value and variance can be determined in the same way as in Vanilla Monte Carlo for K available samplings.

B.9 Perturbation method

The current method is based on determining an approximate solution of $Y(\boldsymbol{\xi})$ starting from an exact solution $Y_0(\boldsymbol{\xi})$ by introducing a power series in a small parameter ϵ :

$$Y(\boldsymbol{\xi}) = Y_0(\boldsymbol{\xi}) + \epsilon^1 Y_1(\boldsymbol{\xi}) + \dots + \epsilon^n Y_n(\boldsymbol{\xi}) + \dots \quad (\text{B.28})$$

The first order term of the series is the known solution to the solvable problem while the higher order terms are unknown and generally become smaller and smaller by increasing the series order. The approximate solutions are obtained by truncating the expansion. If the series converges in ϵ with a nonzero radius of convergence, the problem is called "regular" and the approximate solutions converge asymptotically to the true solution. Otherwise, if the series does not converges, a good approximation can be yet achieved if the truncation is applied at a point where its elements are minimized.

B.10 First-order Reliability methods

The aim is to determine the probability of failure P_f of a probability phenomenon. Let $\mathcal{M}(\boldsymbol{\xi})$ be the limit state function, the probability of failure is determined as:

$$P_f = \mathbb{P}[\mathcal{M}(\boldsymbol{\xi}) \leq 0] = \int_{D_{\boldsymbol{\xi}}} \mathbb{1}[\mathcal{M}(\boldsymbol{\xi}) \leq 0] \mathcal{M}(\boldsymbol{\xi}) d\boldsymbol{\xi} \quad (\text{B.29})$$

Often, the probability of failure is transformed to work into the standard Gaussian variable space and the original random vector is mutated into a standard Gaussian random vector. To execute the modification, an isoprobabilistic transformation $Z = T(\boldsymbol{\xi})$ with a suitable invertible operator $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is introduced. Let $\tilde{\mathcal{M}}(\boldsymbol{\zeta}) = \mathcal{M}[T^{-1}(\boldsymbol{\zeta})]$ be the transformed limit state function, the probability of failure is modified as:

$$P_f = \int_{\mathbb{R}^n} \mathbb{1}[\tilde{\mathcal{M}}(\boldsymbol{\zeta}) \leq 0] f_n(\boldsymbol{\zeta}) d\boldsymbol{\zeta} \quad (\text{B.30})$$

where f_n is the standard normal density function in $\mathbb{R}^n$. First-order Reliability methods express $\mathcal{M}(\boldsymbol{\xi})$ of the probability of failure through linearized approximations (generally Taylor series expansions). If $\boldsymbol{\xi}^*$ is a suitable point of the system, $\mathcal{M}(\boldsymbol{\xi})$ is approximated as:

$$\mathcal{M}(\boldsymbol{\xi}) \approx \underbrace{\mathcal{M}(\boldsymbol{\xi}^*)}_{\text{zero-order term}} + \underbrace{\langle \boldsymbol{\xi} - \boldsymbol{\xi}^*, \nabla \mathcal{M}(\boldsymbol{\xi}^*) \rangle}_{\text{first-order term}} \quad \forall \boldsymbol{\xi} \in D_{\boldsymbol{\xi}}. \quad (\text{B.31})$$

One common application of First-order Reliability methods is the **mean value first – order second – moment method**.

B.10.1 Mean value first-order second-moment method

the main characteristic of this method is the use of a first-order Taylor series expansion of $\mathcal{M}(\boldsymbol{\xi})$ about the mean point of the input random vector of interest:

$$\mathbb{E}[\boldsymbol{\xi}] \rightarrow \boldsymbol{\xi}^* \quad (\text{B.32})$$

and then:

$$\mathcal{M}(\boldsymbol{\xi}) \approx \mathcal{M}(\mathbb{E}[\boldsymbol{\xi}]) + \langle \boldsymbol{\xi} - \mathbb{E}[\boldsymbol{\xi}], \nabla \mathcal{M}(\mathbb{E}[\boldsymbol{\xi}]) \rangle. \quad (\text{B.33})$$

If $\mathcal{M}(\boldsymbol{\xi})$ is normally distributed, it can be approximated by the Cornell reliability index. The main disadvantage of this method is the failure to be invariant to distinct formulations of mathematically equivalent problems and to be performant only for linear and Gaussian distributions but an advantage is to impose a probability preserving transformation in the standard Gaussian space.

B.11 Second-order Reliability methods

Second-order reliability methods are the mainly common used most-probable point based methods. They are applied when $\mathcal{M}(\boldsymbol{\xi})$ is far from linearity. Considering the transformed standard Gaussian space, and the modified probability of failure, we have:

$$\tilde{\mathcal{M}}(\boldsymbol{\zeta}) \approx \tilde{\mathcal{M}}(\boldsymbol{\zeta}^*) + \langle \boldsymbol{\zeta} - \boldsymbol{\zeta}^*, \nabla \tilde{\mathcal{M}}(\boldsymbol{\zeta}^*) \rangle + \frac{1}{2} \langle \boldsymbol{\zeta} - \boldsymbol{\zeta}^*, \text{Hess} \{ \tilde{\mathcal{M}}(\boldsymbol{\zeta}^*) \} (\boldsymbol{\zeta} - \boldsymbol{\zeta}^*) \rangle. \quad (\text{B.34})$$

The probability of failure can be calculated by applying a sampling procedure between the linear and quadrature approximations of the limit state surface and applying the first order theory to cover the probability domain or through an asymptotic approach to determine the curvature of the limit state surface at the most probable point.

B.12 Full Factorial Numerical Integration method

The following method provides an estimate of output distribution moments via direct numerical integration where the uncertain parameters are discretized into K number of nodes (samplings). Let W_{j_n} be the numerical integration weights, ξ_{j_n} be the uncertain variables and $Y(\boldsymbol{\xi}) = \mathcal{M}(\boldsymbol{\xi})$ be the system response, the k -th statistical moment $\mathbb{E}(Y_k)$ is estimated as shown below:

$$\mathbb{E}[Y_k(\boldsymbol{\xi})] = \sum_{j_1=1}^K W_{j_1} \cdots \sum_{j_n=1}^K W_{j_n} \times [\mathcal{M}(\xi_{j_1}, \dots, \xi_{j_n})]_k. \quad (\text{B.35})$$

Using appropriate quadrature formulas, the full factorial numerical integration method calculate all possible combinations of ξ_{j_n} to determine $\mathcal{M}(\boldsymbol{\xi})$. If the number variables (interval parameters) is n , the numerical iterations of $\mathcal{M}(\boldsymbol{\xi})$ is K^n .

B.13 Dimension Reduction method

The Dimension Reduction method is similar to the full factorial numerical integration method, in fact, the both methodology use (B.35). As difference, the current method approximates the multivariate function output as an addition of a set of univariate functions which are priorly calculated than the statistical moments. The approximation function is given by:

$$\mathcal{M}(\boldsymbol{\xi}) \approx \hat{\mathcal{M}}(\boldsymbol{\xi}) = \sum_{i=1}^K \mathcal{M}_i(\boldsymbol{\xi}^{(i)}) - (K-1)\mathcal{M}(\mu_{\text{DR}}) \quad (\text{B.36})$$

where μ_{DR} is the system mean value. $\mathcal{M}_i(\boldsymbol{\xi}^{(i)})$ are calculated by using the value of one variable from the sampling pool of the $K \times n$ dimensional $\boldsymbol{\xi}$ while keeping the rest of the variables at their mean value μ_{DR} :

$$\mathcal{M}_i(\boldsymbol{\xi}^{(i)}) = \mathcal{M}(\boldsymbol{\xi}^{(i)}, \boldsymbol{\xi}^{(i')} = \mu_{\text{DR}}^{(i')}) \quad \forall i, i' \in \{1, \dots, K\} \text{ and } i \neq i'. \quad (\text{B.37})$$

In this method the needed number of function evaluations is $Kn + 1$.

B.14 Kriging

Kriging is a realization of a Gaussian random process whose parameters are estimated from the available computer runs that are input vectors and response variance. given a set of $\boldsymbol{\theta} = \{\theta_1, \dots, \theta_n\}^T$ hyperparameters, a response $Y(\boldsymbol{\theta}, \boldsymbol{\xi})$ is expressed as the sum of a trend behaviour $\boldsymbol{\beta}^T(\boldsymbol{\theta})\mathbf{f}(\boldsymbol{\theta})$ and a perturbation process: $\sigma_K^2 Z(\boldsymbol{\xi}, \boldsymbol{\theta})$:

$$Y(\boldsymbol{\theta}, \boldsymbol{\xi}) = \mathcal{M}(\boldsymbol{\theta}, \boldsymbol{\xi}) = \boldsymbol{\beta}^T(\boldsymbol{\theta})\mathbf{f}(\boldsymbol{\xi}) + \sigma_K^2 Z(\boldsymbol{\xi}, \boldsymbol{\theta}), \quad (\text{B.38})$$

where $\boldsymbol{\beta}(\boldsymbol{\theta}) = \{\beta_0(\boldsymbol{\theta}), \dots, \beta_M(\boldsymbol{\theta})\}^T$ are regression parameters, $\mathbf{f}(\boldsymbol{\xi}) = \{f_0(\boldsymbol{\xi}), \dots, f_M(\boldsymbol{\xi})\}^T$ are regression functions, $Z(\boldsymbol{\xi}, \boldsymbol{\theta})$ is a stationary gaussian process and σ_K^2 is the process variance of Kriging. The stationary gaussian process is characterized by a zero mean and unit variance, while its covariance is defined by the correlation function between the points of the model $R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta})$:

$$\text{Cov}\{Z(\boldsymbol{\xi}, \boldsymbol{\theta})\} = R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}). \quad (\text{B.39})$$

Correlation functions are also named kernels and describe similarity between observation data and new points. In accordance with trends, Kiging can be a **Simple Kriging**, **Ordinary Kriging** or **Universal Kriging**:

- **Simple Kriging**: in Simple Kriging, regression functions are arbitray and known while regression parameters are posed equal to 1:

$$\boldsymbol{\beta}^T(\boldsymbol{\theta})\mathbf{f}(\boldsymbol{\theta}) = \sum_{i=0}^M f_i(\boldsymbol{\xi}). \quad (\text{B.40})$$

- **Ordinary Kriging:** Ordinary Kriging is defined by one only regression parameter and regression function. Generally, the regression function is imposed to be unitary:

$$\beta^T(\boldsymbol{\theta})\mathbf{f}(\boldsymbol{\xi}) = \beta_0(\boldsymbol{\theta})f_0(\boldsymbol{\xi}) \quad \underbrace{=}_{\substack{\text{for convention} \\ f_0(\boldsymbol{\xi})=1}} \quad \beta_0(\boldsymbol{\theta}). \quad (\text{B.41})$$

- **Universal Kriging:** Universal Kriging is the most common used Kriging where the trend is constructed by a general polynomial expansion:

$$\beta^T(\boldsymbol{\theta})\mathbf{f}(\boldsymbol{\xi}) = \sum_{i=1}^M \beta_i(\boldsymbol{\theta})f_i(\boldsymbol{\xi}). \quad (\text{B.42})$$

Beyond its trend, Kriging is also shaped by the typology of adopted correlation function. Specifically there are defined linear correlation functions:

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}) = \max \left\{ 0, 1 - \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}'|}{\boldsymbol{\theta}} \right\}, \quad (\text{B.43})$$

exponential correlation functions:

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}) = e^{-\frac{|\boldsymbol{\xi} - \boldsymbol{\xi}'|}{\boldsymbol{\theta}}} \quad (\text{B.44})$$

and Matérn correlation functions:

$$R(|\boldsymbol{\xi} - \boldsymbol{\xi}'|, \boldsymbol{\theta}, \hat{v}) = \frac{1}{2^{\hat{v}-1}\Gamma(\hat{v})} \left(2\sqrt{\hat{v}} \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}'|}{\boldsymbol{\theta}} \right)^{\hat{v}} \mathcal{K}_{\hat{v}} \left(2\sqrt{\hat{v}} \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}'|}{\boldsymbol{\theta}} \right), \quad (\text{B.45})$$

where $\hat{v} \geq \frac{1}{2}$ is a shape parameter, Γ is the Euler gamma function and $\mathcal{K}_{\hat{v}}$ is the modified Bessel function of II kind. In accordance with specific values of shape parameters, Matérn correlation functions can be Gaussian, 3/2 or 5/2. Furthermore, kriging is homoscedastic or heteroscedastic. Homoscedasticity is the property of initial random variables to have the same finite variance, named also "homogeneity of variance". In terms of regression modelling this means that the residuals of a numerical model are constant across all levels of the independent variables of the problem. In conclusion, heteroscedasticity is characterized by different finite variances of all variables.

B.15 Qualitative Possibility theory

The main idea behind qualitative theory is that the state of the world is always believed to be as normal as possible, neglecting less normal states. Let A and B be two distinct events, the quantity $A \geq_{\Pi} B$ means that there exists a normal state where A holds that is at least as normal as any normal state where B holds, in words this means: "A is at least as certain as B". The temporal events are true in all the most plausible states such that $A >_N \emptyset$. For large S and generated by propositional languages, qualitative possibility distributions are encoded in possibilistic logic. A possibilistic logic base K is a pair $(\phi, \tilde{\alpha})$ where ϕ is a Boolean operator and $\tilde{\alpha}$ is an element of a totally ordered set L . The main constraint is:

$$N(\phi) \geq \tilde{\alpha} \quad (\text{B.46})$$

where $N(\phi)$ is the degree of necessity of the set of models of ϕ . In the argument of dependency and independency, the conditional possibility is expressed as:

$$\Pi(B|A) = \begin{cases} 1 & \text{for } \Pi(B \cap A) = \Pi(A) \\ \Pi(B \cap A) & \text{otherwise} \end{cases} \quad (\text{B.47})$$

B.16 Quantitative Possibility theory

The quantitative possibility theory is applied for unitary possibility ranges. If $\pi(s) \in [0, 1]$ is a possibility distribution and $\mathbf{P}(\pi)$ is a probability measure such that $\mathbb{P} \leq \Pi$, $\forall A \subseteq S$ we have $\mathbb{P}(A) \leq \Pi(A)$ and the possibility measure Π coincides with the upper probability function $\mathbb{P}^*$ such that:

$$\mathbb{P}^*(A) = \sup \{ \mathbb{P}(A) \mid \mathbb{P} \in \mathbf{P}(\pi) \}. \quad (\text{B.48})$$

The necessity measure N is calculated as the lower of the probability function $\mathbb{P}_*$:

$$\mathbb{P}_*(A) = \inf \{ \mathbb{P}(A), \mathbb{P} \in \mathbf{P}(\pi) \}. \quad (\text{B.49})$$

$\mathbb{P}$ and π are consistent $\Leftrightarrow \mathbb{P} \in \mathbf{P}(\pi)$. The relationship between possibility measures and imprecise probabilistic reasoning are described by the representation of non-parametric families of probability functions. Furthermore, possibility measures can be computed by involving nested confidence subsets $\{A_1, \dots, A_m\}$ where $A_i \subset A_{i+1}$ for $i = 1, \dots, m-1$ each A_i has a positive confidence level λ_i which can be interpreted as a lower bound of $\mathbb{P}(A_i)$ and its possibility distribution is given by:

$$\pi(s) = \min_{i=1, \dots, m} \{ \pi_i(s) \} = \begin{cases} 1 & \text{for } j \in A_1 \\ 1 - \lambda_{j-1} & \text{for } j = \max \{ i : s \notin A_i \} > 1 \end{cases} \quad (\text{B.50})$$

B.17 Bayesian Inference

Bayesian inference is a method for summarizing uncertainty and making estimates and predictions using probability statements conditional on observed data and an assumed model. Firstly, let $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}^T$ be a sampling vector and f_θ be a density function with an unknown hyperparameter $\theta \in \Theta$; in this manner, it is possible to define the likelihood function as:

$$\ell(\theta|\boldsymbol{\xi}) = \prod_{i=1}^n f_\theta(\xi_i) \quad (\text{B.51})$$

which gives information about θ due to $\boldsymbol{\xi}$. From (B.51) it is possible to define a posterior distribution function π on θ which is the main pillar of the Bayesian inference:

$$\pi(\theta|\boldsymbol{\xi}) = \frac{\ell(\theta|\boldsymbol{\xi})\pi(\theta)}{\int \ell(\theta|\boldsymbol{\xi})\pi(\theta)d\theta} \quad (\text{B.52})$$

where $\pi(\theta)$ is the prior distribution function which is chosen by experimental or computational groups. The uncertainty behind the parameter θ is often modeled as a random quantity, this leads to interpret f_θ as the conditional density function of ξ_i given θ . The quantity $\ell(\theta|\boldsymbol{\xi})\pi(\theta)$ is then the joint density function of $(\boldsymbol{\xi}, \theta)$ and $\int \ell(\theta|\boldsymbol{\xi})\pi(\theta)d\theta$ is the marginal likelihood $m(\boldsymbol{\xi})$. It is pointed out that when a probability measure on the parameter space Θ is imposed, it is possible to study the probability of θ to belong to a specific probability region with a proper meaning. The practical aspect of the Bayesian analysis in the determination of the inferential assessment conditional on the realized value of $\boldsymbol{\xi}$, giving a probabilistic meaning to the conditioning by allocating to θ a probability prior distribution π . For instance, let $\hat{\theta}$ and θ be two estimations which are evaluated by the quadratic loss function:

$$L(\theta, \hat{\theta}) = \|\theta - \hat{\theta}\|^2. \quad (\text{B.53})$$

The corresponding Bayes procedure is the expected value of θ under the posterior distribution:

$$\hat{\theta} = \int \theta \pi(\theta|\boldsymbol{\xi}) d\theta = \frac{\int \theta \ell(\theta|\boldsymbol{\xi}) \pi(\theta) d\theta}{m(\boldsymbol{\xi})} \quad (\text{B.54})$$

when no specific loss functions are available, it is possible to express (B.54) by introducing the maximum a posteriori estimator:

$$\hat{\theta} = \operatorname{argmax}_{\theta} \{\pi(\theta|\boldsymbol{\xi})\} = \operatorname{argmax}_{\theta} \{\pi(\theta)\ell(\theta|\boldsymbol{\xi})\} \quad (\text{B.55})$$

where the maximize process is provided in closed form.

Appendix C

Sensitivity Analysis methods

C.1 Introduction

In the current chapter, the developed methods for studying the Sensitivity Analysis which have been cited in the chapter of "Sensitivity Analysis" are described more in detail.

C.2 Derivative method

The scope of this method is based on determining the partial derivatives of the output value by recalculations of the response using specified parameter values increased by a small amount $\delta\xi_i$, in other words, the aim is to calculate the exact slope provided by $\frac{\partial Y(\boldsymbol{\xi})}{\partial \xi_i}$ with $i = 1, \dots, n$ of the model response $Y(\boldsymbol{\xi}) = \mathcal{M}(\boldsymbol{\xi})$ with respect to the i -th model data ξ_i :

$$\frac{\partial Y(\boldsymbol{\xi})}{\partial \xi_i} = \frac{\mathcal{M}(\xi_1, \dots, \xi_i + \delta\xi_i, \dots, \xi_n) - \mathcal{M}(\boldsymbol{\xi})}{\delta\xi_i}. \quad (\text{C.1})$$

The method does not require additional model development but it is very expensive for non-linear problems. It is important to get $\delta\xi_i$ as small as possible because a large value of slope means that the local linearity is violated and then, the Local Sensitivity Analysis cannot be rigorously applied but on the contrary, values too small of $\delta\xi_i$ generate an annoying problem due to the excessive computational cost.

C.3 Direct method

This approach is based on replacing the original set of equations of the form:

$$\begin{cases} \frac{dY}{dt} = \mathcal{M}(Y, t, \boldsymbol{\xi}) \\ Y(t_0) = Y_0 \end{cases} \quad (\text{C.2})$$

with a suitable auxiliary set of equations which are solved either independently or together with the original set of equations. There are several way of using direct methods, one of the most famous is the **Decoupled Direct method**. The purpose is to use the Jacobian matrix of the original system (at a given time instant) to solve the auxiliary system (at the same fixed time step):

$$\begin{cases} \frac{d\tilde{Y}_i}{dt} = J\{Y, t, \boldsymbol{\xi}\} \tilde{Y}_i + \mathcal{M}_i(Y, t, \boldsymbol{\xi}) \\ \tilde{Y}_i(t_0) = \frac{\partial Y_0}{\partial \xi_i} \end{cases} \quad (\text{C.3})$$

Briefly the matrix determines the solution of both problems. The problem is to rewrite the mathematical equations.

C.4 Green's function method

Green's function method substitutes the decoupled direct method when the writing of auxiliary equations is too hard. The goal is to use the original mathematical structure, simplifying it by the reduction of the differential equations in terms of the number of equations and in terms of the equation order; the obtained equations are first order equations. In conclusion, the modified equations are rewritten in integral form. The integrals are evaluated in a recursive manner. In some cases, Green's function method is modified with the Magnus method. The application of the Magnus method is able to drastically reduce the computational effort required to calculate the linear sensitivity coefficients.

C.5 Adjoint method

This tool is used when the number of system parameters widely exceeds the number of responses. It needs the construction of an appropriately adjoint sensitivity system which depends on the deterministic/state variables $\mathbf{x} = \{x_1, \dots, x_m\}^T$, initial/random variables $\boldsymbol{\xi} = \{\xi_1, \dots, \xi_n\}^T$ and the time t :

$$\begin{cases} M(\mathbf{x}, \dot{\mathbf{x}}, \boldsymbol{\xi}, t) = 0 \\ \mathbf{x}(t=0) = \mathbf{x}_0 \end{cases} \quad (\text{C.4})$$

which is linear in the adjoint function:

$$M(\mathbf{x}, \boldsymbol{\xi}) = \int_0^{\text{Time}} \mathcal{M}(\mathbf{x}, \boldsymbol{\xi}, t) dt \quad (\text{C.5})$$

and is independent of any parameter variations. The adjoint function is determined by the resolution of the adjoint sensitivity equation for each response function. If state variables are defined, the equation is independent with respect to the starting model. Since the function has been discovered, sensitivities of all system parameters can be obtained through the use of quadratures. This method is usefull for a large number of sensitivity parameters and few objective functions.

C.6 McDiarmid diameters

The McDiarmid diameters measure the sensitivity of a function $\mathcal{M}$ of $\boldsymbol{\xi} = (\xi_1, \dots, \xi_n)$ variables to variations in those variables defined in L^∞ -norm. Let $\mathcal{M} : D_{\boldsymbol{\xi}} = \prod_{i=1}^K D_{\xi_i} \rightarrow \mathbb{K}$, the McDiarmid sub-diameters are defined as:

$$\mathcal{D}_i \{\mathcal{M}\} = \sup \{ |\mathcal{M}(\boldsymbol{\xi}) - \mathcal{M}(\boldsymbol{\zeta})| \mid \boldsymbol{\xi}, \boldsymbol{\zeta} \in D_{\boldsymbol{\xi}}, \boldsymbol{\xi}_j = \boldsymbol{\zeta}_j \text{ for } j \neq i \} \quad (\text{C.6})$$

and they are applied to define the global McDiarmid diameter:

$$\mathcal{D} \{\mathcal{M}\} = \sqrt{\sum_{i=1}^K \mathcal{D}_i \{\mathcal{M}\}^2}. \quad (\text{C.7})$$

McDiarmid diameters are based on the McDiarmid inequality which bounds the deviation between the samples of interest $\boldsymbol{\xi}$ and the expected values of the system given by $\mathcal{M}$:

$$\mathbb{P} [\mathcal{M}(\boldsymbol{\xi}) \geq \mathbb{E}[\mathcal{M}(\boldsymbol{\xi})] + t] \leq e^{-2\left(\frac{t}{\mathcal{D} \{\mathcal{M}\}}\right)^2} \quad \forall t \geq 0 \in \mathbb{R} \quad (\text{C.8})$$

$$\mathbb{P} [\mathcal{M}(\boldsymbol{\xi}) \leq \mathbb{E}[\mathcal{M}(\boldsymbol{\xi})] - t] \leq e^{-2\left(\frac{t}{\mathcal{D} \{\mathcal{M}\}}\right)^2} \quad \forall t \geq 0 \in \mathbb{R} \quad (\text{C.9})$$

$$\mathbb{P} [\mathcal{M}(\boldsymbol{\xi}) - \mathbb{E}[\mathcal{M}(\boldsymbol{\xi})] \geq t] \leq 2e^{-2\left(\frac{t}{\mathcal{D} \{\mathcal{M}\}}\right)^2} \quad \forall t \geq 0 \in \mathbb{R} \quad (\text{C.10})$$

The probability of exceeding that bound is less than a value equat to ϵ .

C.7 Morris method

The Morris method is a screening-based method aimed at calculating the two sensitivity measures of μ_{M_i} and σ_{M_i} . μ_{M_i} is used for assessing the overall importance of the parameter space and σ_{M_i} quantifies the interactions and the nonlinear effects among input variables. This approach is based on the perturbation of the parameter space and belongs to the Global Sensitivity Analysis family because the baseline changes for each iteration so that μ_{M_i} and σ_{M_i} are calculated by averaging at different points of the input space. The parameter space is divided into a discrete number of values named p levels in which K samplings are applied:

$$Y(\boldsymbol{\xi})|_{\xi_i} = \frac{\mathcal{M}(\xi_1, \dots, \xi_i + \Delta\xi_i, \dots, \xi_n) - \mathcal{M}(\boldsymbol{\xi})}{\Delta\xi_i} \quad \text{for } i = 1, \dots, n \quad (\text{C.11})$$

where:

$$\Delta\xi_i = \left\{ 0, \frac{1}{p-1}, \frac{2}{p-1}, \dots, 1 \right\} \quad (\text{C.12})$$

Finally, the Morris sensitivity measures are determined by introducing the elementary effects which are function of p and K :

$$\mu_{M_i} = \frac{1}{K} \sum_{i=1}^K Y(\boldsymbol{\xi}^{(i)})|_{\xi_i} \quad \text{for } i = 1, \dots, n \quad (\text{C.13})$$

$$\sigma_{M_i} = \sqrt{\frac{\sum_{i=1}^K \left[Y(\boldsymbol{\xi}^{(i)})|_{\xi_i} - \mu_{M_i} \right]^2}{K-1}} \quad \text{for } i = 1, \dots, n \quad (\text{C.14})$$

This method is useful for many input variables where the interaction effects are lesser than the independent effects but it is disadvantageous for the fact that the sampling strategy does not converge to the mean of the model output. This methodology provides qualitative measures by ranking input factors but it does not provide the effects of different factors on responses.

C.8 Cotter method

The Cotter method applies two-level fractional factorial design where all initial variables of the problem vary within a known interval, described by its own low and high levels. A set of simulations is carried out by computing the responses of the system with specific settings of the input parameters: the first simulation is applied by imposing the variables to the low values of their interval:

$$Y_0(\boldsymbol{\xi}) = \mathcal{M}(\xi_1^{\min}, \dots, \xi_n^{\min}) \quad (\text{C.15})$$

the intermediate simulations are computed by fixing a variables to an extreme (low or high):

$$Y_i(\boldsymbol{\xi}) = \mathcal{M}(\xi_1^{\min}, \dots, \xi_i^{\max}, \dots, \xi_n^{\min}) \quad \text{for } i = 1, \dots, n \quad (\text{C.16})$$

while the others variables are set to the opposite extreme value (high or low):

$$Y_i(\boldsymbol{\xi}) = \mathcal{M}(\xi_1^{\max}, \dots, \xi_i^{\min}, \dots, \xi_n^{\max}) \quad \text{for } i = n+1, \dots, 2n \quad (\text{C.17})$$

and the last simulation is performed with all variables set to the high extreme:

$$Y_{2n+1}(\boldsymbol{\xi}) = \mathcal{M}(\xi_1^{\max}, \dots, \xi_n^{\max}) \quad (\text{C.18})$$

If n is the number of the input parameters of the problem, the cycle of simulations is completed for $2(n+1)$ simulations. In conclusion, the importance of variables are measured by the coefficient $I_{\text{Cotter}}(\xi_i)$ which is determined by calculating the expectation of the importance of odd and even order effects $C_{\text{odd}}(\xi_i)$ $C_{\text{even}}(\xi_i)$ which are given by the computed combinations of simulations:

$$I_{\text{Cotter}}(\xi_i) = |C_{\text{odd}}(\xi_i)| + |C_{\text{even}}(\xi_i)| \quad (\text{C.19})$$

where:

$$C_{\text{odd}}(\xi_i) = \frac{1}{4} [Y_{2n+1}(\xi) - Y_{n+i}(\xi) + Y_i(\xi) - Y_0(\xi)] \quad (\text{C.20})$$

$$C_{\text{even}}(\xi_i) = \frac{1}{4} [Y_{2n+1}(\xi) - Y_{n+i}(\xi) - Y_i(\xi) + Y_0(\xi)]. \quad (\text{C.21})$$

This method can be employed for both dependent and independent initial variables.

C.9 Fourier Amplitude Sensitivity Test

The classical application of the Fourier Amplitude Sensitivity Test considers only the linear effects neglecting the interaction effects among variables and then only first-order sensitivity indices can be computed. Input variables are sampled over a periodic curve which cover the entire parameter space. The initial random variables $\xi = \{\xi_1, \dots, \xi_n\}^T$ are associated with integer frequencies $\omega = \{\omega_1, \dots, \omega_n\}^T$ in order to construct the Fourier transform of outputs. When the Fourier transform is determined, the first-order variance-based sensitivity indices are evaluated by using the Fourier coefficients c_ω at the given frequencies:

$$S_i^{\text{FAST}} = \frac{\sum_{j=1}^{+\infty} |c_{j\omega_i}|^2}{\sum_{\omega=1}^{+\infty} |c_\omega|^2} \quad \text{for } i = 1, \dots, n \quad (\text{C.22})$$

where:

$$s_k = \frac{2\pi k}{K} \quad \text{for } k = 1, \dots, K \quad (\text{C.23})$$

$$c_\omega = \frac{1}{\pi} \int_0^{2\pi} \mathcal{M}[\xi(s)] e^{-i\omega s} ds. \quad (\text{C.24})$$

In conclusion, it is important to choose the sequence of frequencies in order to avoid interference among higher harmonics.

C.10 Standardized Regression Coefficient method

The Standardized Regression Coefficient method is used to express an output value through a linear regression in terms of the initial variables of the problem by applying a sampling strategy of the initial variables to calculate the associated responses:

$$\frac{Y(\xi) - \bar{Y}(\xi)}{\sigma_{\text{SRC}_Y}} = \alpha_{s_1} \left(\frac{\xi_1 - \bar{\xi}_1}{\sigma_{\text{SRC}_{\xi_1}}} \right) + \dots + \alpha_{s_n} \left(\frac{\xi_n - \bar{\xi}_n}{\sigma_{\text{SRC}_{\xi_n}}} \right) = \sum_{i=1}^n \text{SRC}[Y(\xi), \xi_i] \left(\frac{\xi_i - \bar{\xi}_i}{\sigma_{\text{SRC}_{\xi_i}}} \right) \quad (\text{C.25})$$

where $\bar{Y}(\xi)$ is the average value of samples $[Y(\xi^{(1)}), \dots, Y(\xi^{(K)})]$, $\bar{\xi}_i$ is the average value of the samplings $[\xi^{(1)}, \dots, \xi^{(K)}]$, σ_{SRC_Y} is the standard deviation of response, $\sigma_{\text{SRC}_{\xi_i}}$ is the standard deviation of i -th initial variable and α_{R_i} are regression coefficients. The regression coefficients α_{R_i} of the series are computed by involving a Least-Square Estimator in order to determine the Standardized Regression Coefficient indices. The indices give a measure of importance of the initial variables for the calculation of the output and they are obtained by normalizing each regression coefficient with the standard deviation of the associated initial parameter and the total standard deviation of the system:

$$\alpha_{s_i} = \text{SRC}[Y(\xi), \xi_i] = \alpha_{R_i} \frac{\sigma_{\text{SRC}_{\xi_i}}}{\sigma_{\text{SRC}_Y}} \quad (\text{C.26})$$

This method is suitable for linear models and independent input variables.

C.11 Standardized Rank Regression Coefficient method

The Standardized Rank Regression Coefficient method is the straightforward extension of the classical Standardized Regression Coefficient method which is constructed by replacing the coefficient matrix and the response vector with their rank transformation.

C.12 Ordinary Regression Coefficient method

The application of the Ordinary Regression Coefficient method follows the same way employed for the implementation of the Standardized Regression Coefficient method except that the process of normalization by using the standard deviations of the system is not applied:

$$Y(\xi^{(j)}) = \alpha_0 + \sum_{i=1}^n \alpha_i \xi_i^{(j)} \quad \text{for } j = 1, \dots, K. \quad (\text{C.27})$$

The regression coefficients of the linear regression of outputs are interpreted as absolute sensitivity measures which quantify the absolute change $\Delta Y(\xi)$ of the response due to the local change $\Delta \xi_i$ of the i -th initial variable while all others remain constant:

$$\text{ORC}_{\xi_i} = \left. \frac{\Delta Y(\xi)}{\Delta \xi_i} \right|_{\xi_j = \text{const.}} \quad \text{for } j \neq i. \quad (\text{C.28})$$

C.13 Normalized Regression Coefficient method

The Normalized Regression Coefficient method is similar to the Standardized Regression Coefficient method where the normalization of the regression coefficients is conducted by dividing the data by their average values:

$$\frac{Y(\xi)}{\bar{Y}(\xi)} = \sum_{i=1}^n \text{NRC}[Y(\xi), \xi_i] \frac{\xi_i}{\bar{\xi}_i} \quad (\text{C.29})$$

where:

$$\text{NRC}[Y(\xi), \xi_i] = \alpha_{R_i} \left[\frac{\bar{\xi}_i}{\bar{Y}(\xi)} \right]. \quad (\text{C.30})$$

This method is based on a relative sensitivity measure of the weighted change of the response with respect to its mean due to the weighted change of a given random variable dimensionless by its mean. The following method is suitable for independent initial variables.

C.14 Stepwise method

The Stepwise regression method is based on an automatic procedure to determine a choice for the set of predictor variables. At each step, a variable is selected from the set of variables and it is added or removed by a set criterion based on an array of t or f -tests. In this manner an ultimate group of variables is generated for the prediction of the model. Stepwise regression can be developed by using a **forward selection approach**, **backward elimination approach** or **bidirectional elimination approach**.

C.14.1 Forward selection or backward elimination

The stepwise regression is initialized with an empty set or a set of all initial parameters. For all variables of the model, a t -test is involved to estimate and square the considered coefficient. That parameter is designed as a F -to-remove statistic while for each variable outside the model the t -test is applied to the variable itself which is then squared. The variable becomes the F -to-outer-statistic.

C.14.2 Bidirectional elimination

The approach calculates the variables with highest F-to-enter statistic and those parameters are identified in the model or the approach determines the variables of lowest F-to-remove statistic and remove them from the model.

C.15 Linear Correlation Coefficient method

The Linear Correlation Coefficient method is the simplest Correlation-based method. It quantifies the importance of the variable ξ_i on the response $Y(\boldsymbol{\xi})$ by analysing the Correlation Coefficient r_{Y,ξ_i} which is computed by the ratio of the covariance of $Y(\boldsymbol{\xi})$ and ξ_i to the products of the variances of Y and ξ_i :

$$r_{Y,\xi_i} = \frac{\text{Cov}\{Y(\boldsymbol{\xi}), \xi_i\}}{\sigma_{\text{LCC}_Y}^2 \sigma_{\text{LCC}_{\xi_i}}^2} = \frac{\sum_{j=1}^K (\xi_i^{(j)} - \bar{\xi}_i) [Y(\boldsymbol{\xi}^{(j)}) - \bar{Y}(\boldsymbol{\xi})]}{\sqrt{\sum_{j=1}^K (\xi_i^{(j)} - \bar{\xi}_i)^2 \sum_{j=1}^K [Y(\boldsymbol{\xi}^{(j)}) - \bar{Y}(\boldsymbol{\xi})]^2}} \quad (\text{C.31})$$

The values of Correlation Coefficients vary between -1 and +1; if the coefficient is near the extremes, the output can be expressed as a linear function of the considered initial variables. The Linear Correlation Coefficient is a relative sensitivity measure as it measures the relative variation of the response value in terms of its standard deviation if the given initial parameter changes relatively in terms of its standard deviation while the correlated sources change accordingly. The Linear Correlation Coefficient is also an uncertainty measure because it expresses the variability of a quantity with relation to its standard deviation. If the sensitivity between input variables and the output is almost linear and the correlation among input variables is weak, the Linear Correlation Coefficient Method can be approximated by the Standardized Regression Coefficient method:

$$\frac{\Delta Y(\boldsymbol{\xi})}{\sigma_{\text{LCC}_Y}} = \sum_{j=1}^n \text{SRC}[Y(\boldsymbol{\xi}), \xi_j] \frac{\Delta \xi_i}{\sigma_{\text{LCC}_{\xi_j}}} = \sum_{j=1}^n \text{SRC}[Y(\boldsymbol{\xi}), \xi_j] r_{\xi_i, \xi_j} \left(\frac{\Delta \xi_i}{\sigma_{\text{LCC}_{\xi_i}}} \right) = \text{LCC}_{\xi_i} \frac{\Delta \xi_i}{\sigma_{\text{LCC}_{\xi_i}}} \quad (\text{C.32})$$

In general, the ratio between Linear Correlation Coefficients and Standardized Correlation Coefficients is a measure of the influence of correlation on the Uncertainty of parameters; if that ratio is unitary, this influence is negligible.

C.16 Partial Correlation Coefficient method

The Partial Correlation Coefficient method takes into account the correlations among variables which are incorporated into the outputs when the Linear Correlation Coefficient method is employed. In this approach, the linear effects among input parameters are neglected and then, the sensitivity of single variables on the response is analyzed. Partial Correlation indices are the inverse values of the Linear Correlation indices and are calculated as:

$$\text{PCC}_{\xi_i} = -\frac{c_{\xi_i, Y}}{\sqrt{c_{\xi_i, \xi_i} c_{Y, Y}}} = r_{\tilde{Y}, \xi_i} \quad (\text{C.33})$$

where $c_{\xi_i, Y}$, c_{ξ_i, ξ_i} , $c_{Y, Y}$ are elements of the correlation matrix $\mathbf{C}$:

$$\mathbf{C} = \begin{bmatrix} r_{\xi_1, \xi_1} & \cdots & r_{\xi_1, \xi_n} & r_{\xi_1, Y} \\ \vdots & \ddots & \vdots & \vdots \\ r_{\xi_n, \xi_1} & \cdots & r_{\xi_n, \xi_n} & r_{\xi_n, Y} \\ r_{Y, \xi_1} & \cdots & r_{Y, \xi_n} & r_{Y, Y} \end{bmatrix}^{-1} \quad (\text{C.34})$$

whose elements are calculated by following the setting of (C.31). The Partial Correlation Coefficient is a relative sensitivity measure as it measures the relative variation of the response value in terms of its standard deviation if the given initial parameter changes relatively in terms of its standard

deviation after removing the influence of the other correlated variables from the response and the considered input parameter. It is also an uncertainty measure because it expresses the variability of a quantity with relation to its standard deviation. Since the Partial Correlation Coefficients are computed from the modification (inverse function) of the Linear Correlation Coefficients, the response and input variables inglobed in the coefficients are a sort of modified response and modified variables:

$$\frac{\Delta \tilde{Y}(\boldsymbol{\xi})}{\sigma_{\text{PCC}_{\tilde{Y}}}} = \text{PCC}_{\xi_i} \frac{\Delta \tilde{\xi}_i}{\sigma_{\text{PCC}_{\tilde{\xi}_i}}} \quad (\text{C.35})$$

C.17 Semi-Partial Correlation Coefficient method

Semi-Partial Correlation Coefficient method is a hybrid formulation between Linear Correlation Coefficient method and Partial Correlation Coefficient method where input parameters and their standard deviations are modified while the quantities associated with the response remain the same as in the Linear Correlation Coefficients:

$$\text{SPC}_{\xi_i} = r_{Y, \tilde{\xi}_i} \quad (\text{C.36})$$

$$\frac{\Delta Y(\boldsymbol{\xi})}{\sigma_{\text{SPC}_Y}} = \text{SPC}_{\xi_i} \frac{\Delta \tilde{\xi}_i}{\sigma_{\text{SPC}_{\tilde{\xi}_i}}} \quad (\text{C.37})$$

C.18 Borgonovo indices

Borgonovo indices δ_{ξ_i} quantify the expected shift of the output probability distribution function for a fixed initial variable in terms of the measure defined by the index where for lessest important variables, the expected shift is close to zero. Borgonovo indices are suitable for both dependent and independent initial variables and are defined as integral function of the probability distribution function of the response and the conditional probability distribution function of the output with respect to the considered parameter:

$$\delta_{\xi_i} = \frac{1}{2} \mathbb{E} \left[\int_{D_Y} |f_Y(y) - f_{Y|\xi_i}(y)| dy \right], \quad (\text{C.38})$$

where f_Y is the probability distribution function of Y and $f_{Y|\xi_i}$ is the probability distribution function of Y conditioned to ξ_i . Borgonovo indices can be calculated by employing **histogram –based Estimation** or **Cumulative Distribution Functions –based Estimation**.

C.18.1 Histogram-bases Estimation

In Histogram Estimations, a set of sampling points are applied to the input vector to calculate the corresponding model evaluations (output vector). The probability distribution function of the response is directly calculated from the output vector through the application of histograms while the conditional probability distribution function is similarly determined by introducing samples classes. Each class includes all samplings whose realizations lie between its extremes and for each of them, a hystogram is applied. Borgonovo indices are calculated by a series of absolute differences among the conditional and unconditional probability density functions.

C.18.2 Cumulative Distribution Functions-based Estimation

In Cumulative Distribution Functions-based Estimation, the integral function in the the Borgonovo indices is replaced with a summation of the difference of the conditional and unconditional cumulative distribution functions at the crossing points of the probability distribution function of the response and the conditional probability distribution function of the output with respect to the considered variable.

C.19 Cumulative Distribution-based Sensitivity Measures method

In this method, the sensitivity indices β_{ξ_i} are computed by taking into account the expected value of the distance or divergence h between the unconditional cumulative distribution function of the output and the conditional cumulative distribution function of the output with respect to a given initial variable:

$$\beta_{\xi_i} = \mathbb{E} [h \{f_Y, f_{Y|\xi_i}\}]. \quad (\text{C.39})$$

C.20 Multivariate Adaptive Regression Splines method

The Multivariate Adaptive Regression Splines method has been formulated to be a combination of spline regressions, stepwise model fitting and recursive partitioning. Considering an initial vector ξ , a tensor product spline $g(\xi)$ along the input vector is generated. The tensor is composed by polynomial series aimed to approximate the unknown output function by fitting a multi-dimensional curve where basis functions are added to the metamodel in a stepwise manner. The first step concerns the generation of a constant model which is modified in a linear surrogate model by adding a basis function up to a metamodel composed by M basis functions which are selected to minimize the sum of squares error. When the metamodel is constructed, basis functions are deleted in a stepwise manner for $M - 2$ terms, whose removal will result in the smallest increase of the sum of squares error. Typically, the process is applied until the remaining of a linear regression model. The process is repeated to have $2M - 2$ linear models where the best candidate is associated with the lowest generalized cross validation error. The effects of the model are expressed in the tensor terms, the constant term represents the intercept, the linear components represent the main effects, the quadratic components represent the interactions between pairs and so on... (in general only the intercept and the main effects are preserved). A side effect of that model is that the final model might not have any basis function corresponding to certain input variables and thus, the Multivariate Adaptive Regression Splines method does automatic variable selection. In conclusion, the model is employed to determine the variance-based sensitivity indices of the initial parameters.

C.21 COSSO - COmponent Selection and Shrinkage Operator method

If $\mathcal{M}$ is an unknown regression model of a multivariate non-parametric regression problem, it can be decomposed as a truncated sum of partial models by applying a smoothing spline analysis. The most common approach to solve $\mathcal{M}$ is applying a penalized least squares method as the multivariate smoothing splines where the penalty terms are sum of squares norms of the model of expansion. The COmponent Selection and Shrinkage Operator is a penalized least squares method where the penalty functional is the sum of component norms instead of the classical sum of squared norms. This method can be interpreted as a LASSO - Least Selection and Shrinkage Operator method for multivariate non-parametric models.

C.22 ACOSSO - Adaptive COmponent Selection and Smoothing Operator method

The Adaptive COmponent Selection and Smoothing Operator method builds on smoothing spline ANOVA models and can be interpreted as a weighted COmponent Selection and Shrinkage Operator method where a rescaled norm is used as the penalty for each of the functional components. This method allows more flexible estimations.

C.23 Gaussian Process

Gaussian Processes are stochastic processes where the realization of a random initial vector is defined through a multivariate normal distribution. A Gaussian Process is completely characterized by the mean value and covariance functions among the elements of the model.

C.24 Treed Gaussian Process

A Treed Gaussian Process is a particular Gaussian Process used for non-stationary modelling where the predictor space is partitioned by a treed partitioning process. Applying partitions there are smaller local covariance matrices. Trees Gaussian Processes can be employed for both regression and classification problems and for each partition, the Gaussian model is fitted. The growth of the Tree is based on decision-theoretic heuristics while it may be pruned by using cross-validation errors. In Treed Gaussian processes applied to regression problems, the leaf models are Gaussian Processes and for each partition the mean value and the standard deviation can be calculated considering the defined predictors and space of functions.

C.25 Support Vector Machine method

The Support vector Machine method is treated for the application of the Statistical Learning theory. Firstly, a set of training data are sampled in accordance with an unknown probability distribution function p and an error-measure loss function V . If ξ is the initial vector, the expected output is calculated by applying a model $\mathcal{M}$ which minimizes the expected error of the prediction problem. Since the probability distribution function is unknown a priori, some induction principle is used for inferring, from the available training examples, a function that minimizes the expected error. That function is restricted to be in a function space named "hypothesis space" and the problem arises about the closure of the empirical error. In few words the scope is aimed to minimize the expected error that can be achieved with models for the hypothesis space. From these considerations there are defined probabilistic bounds on the distance between empirical and expected errors. The more complex the hypothesis space, the larger the distance between empirical and expected errors. Generally, the main problem is how to measure the complexity of the hypothesis space so that it is possible to find the final optimal solution to the learning problem with the minimum empirical error. Then, the Support vector Machine method is introduced to solve this problem. The method finds the optimal hyperplane as the solution of the learning problem where the hypothesis space is considered a subset of system hyperplanes. Given the input data, this method selects a hyperplane which diverges from the input parameter space where this hyperplane is induced by a kernel; in this manner, the hypothesis space is defined as a set of hyperplanes in the feature space induced by the Kernel and the empirical error is minimized.

Appendix D

Turbulence models

D.1 Introduction

In the current chapter the developed turbulence models employed for closing the RANS problem which have been cited in the chapter of "Fluid Dynamics background" are described more in detail.

D.2 Prandtl mixing length model

This model was developed by Ludwig Prandtl who supposed that the Reynolds stress is produced by momentum transfer normal to the mean flow direction from regions of high momentum to regions of low momentum and a mixing length is defined to be the average distance over which a fluid element transfers momentum:

$$\mu_t = \rho \ell^2 \left| \frac{\partial \bar{v}}{\partial y} \right| \quad (\text{D.1})$$

$$k_{T_t} = \frac{c_p \rho \ell^2}{Pr_t} \left| \frac{\partial \bar{v}}{\partial y} \right|, \quad (\text{D.2})$$

where ℓ is a characteristic length.

D.3 Cebeci-Smith model

Cebeci-Smith model is a zero-algebraic model used in boundary layer problems. In this case, the turbulent viscosity μ_t is a function of the local boundary layer which is considered to be composed of an inner part and an outer part. The model is suitable for aerospace applications with high-speed flows and attached boundary layers. A 2D flow and a two-composed boundary layer are considered; the inner layer is close to the surface while the outer layer is more external. The turbulent eddy viscosity is calculated separately for each layer and the results are combined with each other:

$$\mu_t = \begin{cases} \mu_{t_{\text{inner}}} = \rho \ell \left[\left(\frac{\partial \bar{u}}{\partial y} \right)^2 + \left(\frac{\partial \bar{v}}{\partial x} \right)^2 \right]^{\frac{1}{2}} & \text{for } y \leq y_{\text{crossover}} \\ \mu_{t_{\text{outer}}} = a \rho \delta_1 F_k & \text{for } y > y_{\text{crossover}} \end{cases}, \quad (\text{D.3})$$

where δ_1 is the displacement thickness, F_k is the Klebanoff intermittency function and a is a calibration constant.

D.4 Baldwin-Lomax model

The Baldwin-Lomax model is a two-layer model where the turbulent eddy viscosity is a function of the local boundary layer velocity profile. The model is suitable for high-speed flows with thin

attached boundary layers. It is commonly used in quick design iterations where robustness is more important than capturing all details of the flow physics. It does not work well for large separated regions and significant curvature or rotation effects:

$$\mu_t = \begin{cases} \mu_{t_{\text{inner}}} = \rho \ell^2 \vec{\omega} & \text{for } y \leq y_{\text{crossover}} \\ \mu_{t_{\text{outer}}} = \rho \tilde{K} C_{cp} F_w F_k & \text{for } y > y_{\text{crossover}} \end{cases}, \quad (\text{D.4})$$

where $\vec{\omega}$ is the angular velocity, F_w is a wave function and $(\tilde{K}, C_{cp})$ are calibration constants.

D.5 Prandtl's one equation model

The current model uses an additional one transport equation for the dynamic of the turbulent kinetic energy k in order to solve the turbulent eddy viscosity:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (\text{D.5})$$

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho \vec{v} k) = \left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla^2 k + \left\{ \mu_t \left[\nabla \vec{v} + (\nabla \vec{v})^T \right] - \frac{2}{3} \rho k \mathbf{I} \right\} \nabla \vec{v} - C_\mu \frac{k^{\frac{3}{2}}}{\ell} \quad (\text{D.6})$$

where ε is the turbulent kinetic energy dissipation rate and (C_μ, σ_k) are calibration constants.

D.6 Baldwin-Barth model

The Baldwin-Barth model treats a further one equation for the turbulent Reynolds number $\mathcal{R}e_t$ which appears in the equation of the turbulent eddy viscosity. The model is mainly used for wall-bounded flows:

$$\mu_t = \mu C_\mu D_1 D_2 \mathcal{R}e_t \quad (\text{D.7})$$

$$\frac{\partial}{\partial t}(\rho \mathcal{R}e_t) + \nabla \cdot (\rho \vec{v} \mathcal{R}e_t) = (C_{\varepsilon_2} f_2 - C_{\varepsilon_1}) \sqrt{\mu \mathcal{R}e_t P_k} + \left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla^2 (\mu \mathcal{R}e_t) - \frac{1}{\sigma_\varepsilon} (\nabla \mu_t) \nabla (\mu \mathcal{R}e_t) \quad (\text{D.8})$$

where P_k is the production of turbulent kinetic energy, f_2, D_1 and D_2 are calibration functions and $(C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_\varepsilon)$ are coefficients.

D.7 Spalart-Allmaras model

The Spalart-Allmaras turbulence model is the most famous one-equation model applied in Fluid Dynamics. It introduces a transport equation for the kinematic turbulent eddy viscosity $\tilde{\nu}$ with several versions available for different applications; it has been modified to be employed for free shear flows, for near-wall regions with high Reynolds numbers or finite high Reynolds numbers, for laminar regions and trip terms. Typically it is applied for aerodynamics applications and its original form is:

$$\mu_t = \rho \tilde{\nu} f_{v_1} \quad (\text{D.9})$$

$$\begin{aligned} \frac{\partial \tilde{\nu}}{\partial t} + \nabla \cdot (\vec{v} \tilde{\nu}) &= C_{b_1} (1 - f_{t_2}) \tilde{W} \tilde{\nu} + \frac{1}{\sigma} \left\{ \nabla \cdot [(\nu \tilde{\nu}) \nabla \tilde{\nu}] + C_{b_2} |\nabla \tilde{\nu}|^2 \right\} - \\ &\quad - \left(C_{w_1} f_w - \frac{C_{b_1}}{k_{\text{VK}}^2} f_{t_2} \right) \left(\frac{\tilde{\nu}}{d} \right)^2 + f_{t_1} \Delta v^2, \end{aligned} \quad (\text{D.10})$$

where $f_{v_1}, \tilde{W}, f_{t_1}, f_{t_2}, C_{w_1}$ and f_w are functions, $(\sigma, C_{b_1}, C_{b_2})$ are calibration constants, $k_{\text{VK}} = 0.41$ is the Von Karman constant and Δv is the peak velocity difference.

D.8 Rahman-Siikonen-Agarwal model

This turbulence model is based on a fictitious eddy viscosity transport equation for $R = \frac{k^2}{\varepsilon}$ (which derivation comes from the $k - \varepsilon$ closure) coupled with a damping function to represent the kinematic blocking by the wall. The model is formulated by satisfying the Bradshaw and other empirical relations:

$$\mu_t = \rho k C_\mu f_\mu T_t \quad (\text{D.11})$$

$$\frac{\partial}{\partial t} (\rho R) + \nabla \cdot (\rho \bar{v} R) = \left(\mu + \frac{\mu_t}{\sigma} \right) \nabla^2 R + \rho C_1 \sqrt{k P_k T_t} - \rho C_2 \nabla \cdot (P_k T_t)^2, \quad (\text{D.12})$$

where C_1 and C_2 are numerical parameters, f_μ is a damping function, T_t is a calibration function.

D.9 Wray-Agarwal model

The model is based on a fictitious eddy viscosity transport of $R = \frac{k}{\omega}$ equation which derivation comes from the $k - \omega$ closure:

$$\mu_t = \rho f_\mu R \quad (\text{D.13})$$

$$\begin{aligned} \frac{\partial R}{\partial t} + \nabla \cdot (\bar{v} R) = & \nabla \cdot [(\sigma_R R + \nu) \nabla R] + C_1 R S + f_1 C_{2k\omega} \frac{R}{S} \nabla R \cdot \nabla S - \\ & - (1 - f_1) \min \left\{ C_{2k\varepsilon} R^2 \left[\frac{(\nabla S)^2}{S^2} \right], \nabla R \cdot \nabla R \right\}, \end{aligned} \quad (\text{D.14})$$

where $C_{2k\varepsilon}$, $C_{2k\omega}$ and σ_R are coefficients, f_1 is a calibration function and:

$$S = \sqrt{2 S_{ij} S_{ij}} \quad (\text{D.15})$$

$$S_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \quad (\text{D.16})$$

D.10 Shuai-Agarwal model

The Shuai-Agarwal model consists of a transport equation for the turbulent eddy viscosity. The model derives from the $k - k_L$ turbulence model and needs further investigations due to its recent development:

$$\mu_t = \rho C_\mu^{\frac{1}{4}} \frac{k L}{k^{\frac{1}{2}}} \quad (\text{D.17})$$

$$\begin{aligned} \frac{\partial \nu_t}{\partial t} + \nabla \cdot (\bar{v} \nu_t) = & a_1 \left(C_{\phi_1} - \frac{1}{2} \right) \frac{P_k}{S} + \left(\frac{1}{2} a_1 - \frac{C_{\phi_2}}{\sqrt{a_1}} \right) \nu_t S + \frac{\nu_t (1 - 6 f_\phi)}{d^2} + \frac{\sigma \nu_t}{2 S} \nabla \nu_t \cdot \nabla S + \\ & + \frac{3\sigma}{4} \nabla \nu_t \cdot \nabla \nu_t - \frac{\sigma}{4} \nabla S \cdot \nabla S \frac{\nu_t^2}{S^2} + \nabla \cdot [(\sigma \nu_t + \nu) \nabla \nu_t], \end{aligned} \quad (\text{D.18})$$

where f_ϕ is a damping function and $(a_1, C_{\phi_1}, C_{\phi_2})$ are calibration constants.

D.11 $k - \varepsilon$ turbulence models

$k - \varepsilon$ models use one equation for describing the dynamics of the turbulent kinetic energy and one equation for describing the dissipation rate of the turbulent kinetic energy in order to determine the turbulent eddy viscosity in RANS simulations. The three models of this class are the **Standard $k - \varepsilon$ Turbulence model**, **Realizable $k - \varepsilon$ Turbulence model** and **RNG $k - \varepsilon$ Turbulence model**.

D.11.1 Realizable $k - \varepsilon$ turbulence model

This model is a variation of the Standard $k - \varepsilon$ turbulence model. The main changes are inherent to dynamic turbulent dynamic viscosity and the transport equation of the dissipation rate of the turbulent kinetic energy. The method was introduced to satisfy particular mathematical constraints on the Reynolds stresses and is particularly suitable for planar and round jets and for flows involving rotation, boundary layers under strong adverse pressure gradients, separation and recirculation. The method is useful when strong streamline curvatures, vortices and rotations occur, furthermore it leads well for separated flows and flows with complex secondary flow features. On the other hand, this model produces non-physical viscosities when rotating and stationary fluid zones coexist :

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (\text{D.19})$$

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho \bar{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon \quad (\text{D.20})$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \bar{v} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \rho C_{\varepsilon_1} S \varepsilon - C_{\varepsilon_2} \rho \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}}. \quad (\text{D.21})$$

D.11.2 RNG $k - \varepsilon$ turbulence model

The following turbulence model is a revisitation of the Standard $k - \varepsilon$ model being able to account for the effects of the smallest scales of motion. It was derived by applying the renormalization group theory and the transport equation for the dissipation rate of turbulent kinetic energy is modified by adding a term to improve accuracy in rapidly strained flows. Furthermore, the effect of swirl on turbulence is included in the model such that accurate simulations for swirling flows are provided. Like the Realizable $k - \varepsilon$ turbulence model, only the ε transport equation is modified with respect to the Standard $k - \varepsilon$ turbulence model:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (\text{D.22})$$

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho \bar{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon \quad (\text{D.23})$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \nabla \cdot (\rho \bar{v} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + C_{\varepsilon_1} \frac{\varepsilon}{k} P_k - C_{\varepsilon_2}^* \rho \frac{\varepsilon^2}{k}, \quad (\text{D.24})$$

where $C_{\varepsilon_2}^*$ is a coefficient.

D.12 $k - \omega$ turbulence models

The following class of models is characterized by a transport equation for the turbulent kinetic energy and a transport equation about the rate of conversion of the turbulent kinetic energy into internal thermal energy ω . The models are the "**Classical**" **$k - \omega$ turbulence model**, **Baseline (BSL) $k - \omega$ turbulence model**, **Shear Stress Transport (SST) $k - \omega$ turbulence model**.

D.12.1 Classical $k - \omega$ turbulence model

The first $k - \omega$ model was developed by Kolmogorov and corrected by Wilcox. This method is more capable of predicting separated flows with respect to $k - \varepsilon$ models. Furthermore, it is easier to integrate and can be integrated through sub-layers without the use of damping functions. It is also suitable for flows with weak adverse pressure gradients:

$$\mu_t = \rho \frac{k}{\omega} \quad (\text{D.25})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_{k_1}} \right) \nabla k \right] + P_k - \beta^* \rho k \omega \quad (\text{D.26})$$

$$\frac{\partial}{\partial t} (\rho \omega) + \nabla \cdot (\rho \bar{v} \omega) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_{\omega_1}} \right) \nabla \omega \right] + C_{\alpha_1} \frac{\omega}{k} P_k - C_{\beta_1} \rho \omega^2, \quad (\text{D.27})$$

where $(C_{\alpha_1}, C_{\beta_1}, \beta^*, \sigma_{k_1}, \sigma_{\omega_1})$ are calibration constants.

D.12.2 Baseline (BSL) $k - \omega$ turbulence model

the BSL $k - \omega$ turbulence model is a hybrid combination of the Standard $k - \varepsilon$ turbulence model and the $k - \omega$ model. It takes the best performance of the first turbulence model for the calculation of fluids near edges of boundary layers and away from walls and takes the best performance of the second turbulence model for the prediction of fluids near wall surfaces and weak adverse pressure gradients. The generation of the BSL $k - \omega$ model is based on the transformation of the $k - \varepsilon$ model into a $k - \omega$ model through the application of a blending function:

$$\mu_t = \rho \frac{k}{\omega} \quad (\text{D.28})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\tilde{\sigma}_k} \right) \nabla k \right] + P_k - \beta^* \rho k \omega \quad (\text{D.29})$$

$$\frac{\partial}{\partial t} (\rho \omega) + \nabla \cdot (\rho \bar{v} \omega) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\tilde{\sigma}_\omega} \right) \nabla \omega \right] + \tilde{C}_\alpha \frac{\omega}{k} P_k - \tilde{C}_\beta \rho \omega^2 + 2(1 - F_1) \sigma_{\omega_2} \frac{\rho}{\omega} \nabla k \cdot \nabla \omega \quad (\text{D.30})$$

where σ_{ω_2} is a calibration constant, $(\tilde{\sigma}_k, \tilde{\sigma}_\omega, \tilde{C}_\alpha, \tilde{C}_\beta)$ are modified calibration constants and F_1 is a blending function.

D.12.3 Shear Stress Transport (SST) $k - \omega$ turbulence model

The following approach is a variation of the Baseline $k - \omega$ turbulence model to have better performance for adverse pressure gradients. Here, the Bradshaw's assumption is satisfied: the main shear stress and the turbulent kinetic energy in the boundary layer communicates through a linear relation:

$$\mu_t = \frac{\rho a_1 k}{\max \{a_1 \omega, \sqrt{2} S F_2\}} \quad (\text{D.31})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\tilde{\sigma}_k} \right) \nabla k \right] + \tilde{P}_k - \beta^* \rho k \omega \quad (\text{D.32})$$

$$\frac{\partial}{\partial t} (\rho \omega) + \nabla \cdot (\rho \bar{v} \omega) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\tilde{\sigma}_\omega} \right) \nabla \omega \right] + \tilde{C}_\alpha \frac{\omega}{k} \tilde{P}_k - \tilde{C}_\beta \rho \omega^2 + 2(1 - F_1) \sigma_{\omega_2} \frac{\rho}{\omega} \nabla k \cdot \nabla \omega, \quad (\text{D.33})$$

where $\tilde{P}_k$ is the modified production of turbulent kinetic energy.

D.13 k - τ model

The following model was developed for near-wall turbulent flows. The associated equations are transport equations for the turbulent kinetic energy and the time scale τ :

$$\mu_t = \rho C_\mu f_\mu k \tau \quad (\text{D.34})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{\mathbf{v}} k) + \tau \nabla \bar{\mathbf{v}} = -\rho \frac{k}{\tau} + \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] \quad (\text{D.35})$$

$$\begin{aligned} \frac{\partial}{\partial t} (\rho \tau) + \nabla \cdot (\rho \bar{\mathbf{v}} \tau) &= (C_{\varepsilon_1} - 1) \frac{\tau}{k} \tau \nabla \bar{\mathbf{v}} + \rho (C_{\varepsilon_2} f_2 - 1) + \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_{r_2}} \right) \nabla \tau \right] - \\ &\quad - \frac{2}{\tau} \left(\mu + \frac{\mu_t}{\sigma_{r_2}} \right) \nabla \tau \cdot \nabla \tau, \end{aligned} \quad (\text{D.36})$$

where f_2 is a function and σ_{r_2} is a calibration constant.

D.14 k - kL model

The k-kL model is a two-equation turbulence model based on Abdol-Hamid's closure and Menter's modification to Rotta's two-equation model where the transport equations describe the evolution of the turbulent kinetic energy and the macro length scale of the turbulent motion kL . An important characteristic is that this formulation leads to the inclusion of higher-order velocity derivatives in the source terms of the scale equations, useful for unsteady flows:

$$\mu_t = C_\mu^{\frac{1}{4}} \rho \frac{(kL)}{\sqrt{k}} \quad (\text{D.37})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{\mathbf{v}} k) = \nabla \cdot [(\mu + \sigma_k \mu_t) \nabla k] + P_k - C_\mu^{\frac{3}{4}} \rho \frac{k^{\frac{5}{2}}}{(kL)} - 2\mu \frac{k}{d^2} \quad (\text{D.38})$$

$$\frac{\partial}{\partial t} [\rho(kL)] + \nabla \cdot [\rho \bar{\mathbf{v}}(kL)] = \nabla \cdot [(\mu + \sigma_\phi \mu_t) \nabla(kL)] + C_{\phi_1} \frac{(kL)}{k} P_k - C_{\phi_2} \rho k^{\frac{3}{2}} - 6\mu \frac{(kL)}{d^2} f_\phi \quad (\text{D.39})$$

where σ_ϕ is a calibration constant.

D.15 k - ε - R_t model

The current turbulence model is a revision of the Standard $k - \varepsilon$ turbulence model with the additional equation for the undamped eddy viscosity R_t . The presence of the undamped eddy viscosity guarantees that no inflow turbulence decay occurs in external flows. In fact, $k - \varepsilon$ models may have the attitude to decay of external flow turbulence from its inflow level, being inconvenient for some simulations:

$$\mu_t = \rho C_\mu f_\mu \frac{k^2}{\varepsilon} \quad (\text{D.40})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{\mathbf{v}} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon \quad (\text{D.41})$$

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \cdot (\rho \bar{\mathbf{v}} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + T_t^{-1} (C_{\varepsilon_1} P_k - C_{\varepsilon_2} \rho \varepsilon) \quad (\text{D.42})$$

$$\frac{\partial}{\partial t} (\rho R_t) + \nabla \cdot (\rho \bar{\mathbf{v}} R_t) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_R} \right) \nabla R_t \right] + (2 - C_{R_1}) \frac{R_t}{k} P_k - (2 - C_{R_2}) \rho k - 2\rho \frac{C_\mu^*}{\sigma_R} \nabla R_t \cdot \nabla R_t, \quad (\text{D.43})$$

where $(C_{R_1}, C_{R_2}, C_\mu^*)$ are calibration parameters and T_t is a scaling function.

D.16 $\overline{v^2}$ - f model

The $\overline{v^2} - f$ turbulence model is a nonlinear eddy viscosity model for low Reynolds numbers which describes the evolution of a fluid by using the transport equations of the Standard $k - \varepsilon$ turbulence model, a transport equation for the velocity scale $\overline{v^2}$ and a transport equation for the elliptic relaxation function f of the Helmholtz type. The velocity scale can be interpreted as the velocity fluctuations which are normal to the streamlines. They are able to provide the right scaling for the representation of the damping of turbulent transport close to the wall. On the other hand, the anisotropic wall effects are modeled by f :

$$\mu_t = \rho C_\mu \overline{v^2} T \quad (\text{D.44})$$

$$\frac{\partial}{\partial t} (\rho \overline{v^2}) + \nabla \cdot (\rho \overline{v} \overline{v^2}) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_{\overline{v^2}}} \right) \nabla \overline{v^2} \right] + \rho k f - \rho \overline{v^2} \frac{\varepsilon}{k} \quad (\text{D.45})$$

$$L^2 \nabla^2 f - f = \frac{C_1 - 1}{T} \left(\frac{\overline{v^2}}{k} - \frac{2}{3} \right) - C_2 \frac{P_k}{\varepsilon} \quad (\text{D.46})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \overline{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon \quad (\text{D.47})$$

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \cdot (\rho \overline{v} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \frac{C_{\varepsilon_1}}{T} P_k - C_{\varepsilon_2} \rho \frac{\varepsilon}{T}, \quad (\text{D.48})$$

where T and L are functions and $\sigma_{\overline{v^2}}$ is a coefficient.

D.17 ζ - f model

The following model is a modification of the $\overline{v^2} - f$ model to improve the performance of simulation predictions. the velocity scale is substituted by the normalized wall-normal velocity scale ζ :

$$\mu_t = \rho C_\mu \zeta k T \quad (\text{D.49})$$

$$\frac{\partial}{\partial t} (\rho \zeta) + \nabla \cdot (\rho \overline{v} \zeta) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\zeta} \right) \nabla \zeta \right] + \rho f - \frac{\zeta}{k} P_k \quad (\text{D.50})$$

$$L^2 \nabla^2 f - f = \frac{1}{T} \left(C_1 - 1 + C_2' \frac{P_k}{\varepsilon} \right) \left(\zeta - \frac{2}{3} \right) \quad (\text{D.51})$$

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \overline{v} k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon \quad (\text{D.52})$$

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla \cdot (\rho \overline{v} \varepsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + \frac{C_{\varepsilon_1}}{T} P_k - C_{\varepsilon_2} \rho \frac{\varepsilon}{T}, \quad (\text{D.53})$$

where σ_ζ and C_2' are numerical parameters.

Appendix E

cavitation models

E.1 Introduction

In the current chapter, the most common cavitation models which have been cited in the chapter of "Cavitation" are described more in detail.

E.2 Zwart et Al. model - The Vapour Nuclei Adjusted Model

The Zwart et Al. model is based on the elaboration of the Rayleigh-Plesset equation. In the Zwart cavitation model, the simplified form of the Rayleigh-Plesset equation is taken into consideration. Neglecting the acceleration term, the initial gas pressure term, the surface tension term and the viscous term, the radius evolution is given by:

$$\frac{dR}{dt} = \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} \quad (\text{E.1})$$

and the rate of change of mass of a single bubble is given by:

$$\dot{m} = 4\pi \frac{dR}{dt} \rho_v \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)}. \quad (\text{E.2})$$

If n_b is the number of bubble for unit volume and V_b is the bubble volume, the vapour volume fraction can be expressed as:

$$\alpha = n_b V_b = \frac{4}{3} \pi R^3 n_b \quad (\text{E.3})$$

such that combining (E.2) and (E.3), we obtain the rate of mass transfer as:

$$\dot{m} = \begin{cases} -F_e \frac{3r_{\text{nuc}}(1-\alpha)\rho_v}{R} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} & \text{for } p < p_v \\ F_c \frac{3\alpha\rho_v}{R} \sqrt{\frac{2}{3} \left(\frac{p - p_v}{\rho_l} \right)} & \text{for } p > p_v \end{cases} \quad (\text{E.4})$$

where (F_e, F_c) are calibration constants and r_{nuc} is the nucleation radius (radius of nuclei). This model works well for condensation but not for vaporization. One reason is the basic hypothesis of non interaction among cavitation bubbles (true only at the first stage of cavitation evolution). As α increases the nucleation site density decreases. The Zwart model is the typical cavitation model implemented in Ansys Fluent.

E.3 Kunz et Al. model - The Ginzburg Landau Potential Model

Kunz et Al. formulated their cavitation model in terms of liquid fraction transport equations (8.42), (8.43) and (8.44). The model can also be employed for homogeneous mixtures with non-condensable gas fluids. The current model considers the mass transfer rate as the sum of two contributions where the positive part $\dot{m}^+$ is inherent to the passage from the vapour phase to the liquid phase while the negative part $\dot{m}^-$ is inherent to the passage from the liquid phase to the vapour phase. $\dot{m}^-$ is modeled to be proportional to γ and the amount by which the pressure is below the vapour pressure. The evaporation term $\dot{m}^-$ was developed by considering the Merkle et Al. work while the condensation term $\dot{m}^+$ was developed by taking into account the Ginzburg-Landau theory of superconductivity. For two-phase flows, Kunz model is expressed as:

$$\dot{m} = \dot{m}^- + \dot{m}^+ = \begin{cases} \dot{m}^- = \frac{C_{\text{dest}} \rho_v \gamma \min\{0, p - p_v\}}{\frac{1}{2} \rho_l U_\infty^2 t_\infty} \\ \dot{m}^+ = \frac{C_{\text{prod}} \rho_v \gamma^2 (1 - \gamma)}{t_\infty} \end{cases} \quad (\text{E.5})$$

while for three-phase flows, the equation is modified as:

$$\dot{m} = \dot{m}^- + \dot{m}^+ = \begin{cases} \dot{m}^- = \frac{C_{\text{dest}} \rho_v \gamma \min\{0, p - p_v\}}{\frac{1}{2} \rho_l U_\infty^2 t_\infty} \\ \dot{m}^+ = \frac{C_{\text{prod}} \rho_v (\gamma - \alpha_{ng})^2 (1 - \gamma - \alpha_{ng})}{t_\infty} \end{cases} \quad (\text{E.6})$$

where ($C_{\text{dest}}, C_{\text{prod}}$) are calibration constants and t_∞ is the characteristic time scale. Kunz model is the typical cavitation model implemented in OpenFOAM.

E.4 Denner et Al. model - The Polytrropic Closure Model

The following cavitation model has been developed to simulate acoustic cavitation in polytropic gas-liquid systems. The governing equations are coupled with a density equation which is a function of the pressure of the system. The model is based on the Noble-Abel stiffened-gas model to describe the repulsion and attraction among particles. The thermal equation of state can be written as:

$$p = \left(\frac{c_p}{c_v} - 1 \right) \frac{c_v T}{\frac{1}{\rho} - b} - \Pi, \quad (\text{E.7})$$

where b is the co-volume and Π is the pressure constant. In the current model, the surface tension and gravity effects have been neglected.

E.5 Ghahramani et Al. model - The Euler Lagrangian Multiscale Model

The implementation of the Ghahramani model is preceded by the re-evaluation of numerical simulations by applying other cavitation models such as the Schnerr-Sauer cavitation model. Afterward, the application of this method allows to analyze more cavitating effects as bubble-flow interaction, motion of bubbles, dynamics of bubbles, bubble-bubble collision and bubble break-up:

- **Bubble – flow interaction:** the bubble-flow interaction (effect of bubble presence) is taken into account by the presence of the volume fraction of the bubble in the mixture properties (8.43) and (8.44). As is well known, γ is the liquid fraction where $1 - \gamma$ represents the bubble fraction in the computational cell. It is possible to calculate the phase change source term from the bubble size and the distribution variation. Furthermore, the vapour volume fraction is determined from the instantaneous bubble sizes and locations but bubbles grow and occupy more than one only grid cell and then, a number of cells N_{cell} needs to be considered to evaluate their sizes. Considering a parcel i , the void fraction of the parcel in cell j is estimated as:

$$v_{ij} = \frac{1}{V_{\text{cell}_j}} \left(\frac{4}{3} \pi n_i R_i^3 \right) f \left(\frac{|\mathbf{x}_{ij}|}{R_i} \right) \quad (\text{E.8})$$

where n_i is the number of bubbles in the parcel i , $f \left(\frac{|\mathbf{x}_{ij}|}{R_i} \right)$ is the Gaussian distribution function and $|\mathbf{x}_{ij}|$ is the distance between the cell and the parcel centre. It is important to remember that the considered cells are located around the host cell of the bubble and they are partially or fully occupied by the parcel and its volume is not distributed over the unoccupied neighbouring cells. The previous equation does not guarantee that the volume of the parcel is conserved and so, it is modified. In conclusion, from the condition that a cell can be occupied by $N_b > 1$ parcels, the vapour void fraction (bubble fraction) of the cell j is given by:

$$1 - \beta_j = \sum_{i=1}^{N_b} v_{ij}^c = \sum_{i=1}^{N_b} v_{ij} \left(\frac{\frac{4}{3} \pi n_i R_i^3}{\sum_{k=1}^{N_{\text{cell}}} v_{ik} V_{\text{cell}_k}} \right). \quad (\text{E.9})$$

In regions where important pressure drops are registered, the bubble growth can increase exponentially and parcels can become larger than the hosting cells.

- **Bubbles motion:** the motion of bubbles is evaluated by applying a Lagrangian approach to the instantaneous position $\mathbf{x}_b$ and velocity $\mathbf{v}_b$ of bubbles as:

$$\frac{d\mathbf{x}_b}{dt} = \mathbf{v}_b \quad (\text{E.10})$$

$$m_b \frac{d\mathbf{v}_b}{dt} = \mathbf{F}_d + \mathbf{F}_l + \mathbf{F}_a + \mathbf{F}_p + \mathbf{F}_b + \mathbf{F}_g, \quad (\text{E.11})$$

where m_b is the bubble mass, $\mathbf{F}_d$ is a drag force, $\mathbf{F}_l$ is a lift force, $\mathbf{F}_a$ is an added mass force, $\mathbf{F}_p$ is a pressure gradient force, $\mathbf{F}_b$ is a buoyancy force and $\mathbf{F}_g$ is a gravity force.

- **Dynamics of bubbles:** the dynamics of bubbles is described by the Rayleigh-Plesset equation (8.33) where the pressure $p_\infty(t)$ is replaced by p_{2R} which represents the surface-average pressure of the mixture over a concentric sphere with radius $2R$ (local pressure around the bubble). The choice of a $2R$ distance in p_{2R} is justified by a more accurate analysis.
- **Bubble – bubble collision:** the collision phenomenon can be studied by considering two analyses; the first one concerns the incidence of collision and the second one treats the outcome of collision. The incidence of collision is determined by investigating the collision possibility among bubbles and the algorithm employed in this scope is the cell occupancy concept which calculates the possible collisions among close bubbles. When a collision occurs, a pair of bubbles may coalesce to generate a larger bubble or bounce back from each other. To understand which of the two situations occurs, relative velocity and interaction time of bubbles are observed. Physically, a liquid film is trapped between two bubbles when they collide and for a long interaction time, the film can drain to a sufficiently small thickness such that the bubbles coalesce, otherwise they bounce back from each other. From this explanation, the outcome of collision is considered a function of two time scale:

$$t_i = \frac{\pi}{4} \left(\frac{\rho D_{\text{eq}}^3}{6S} \right)^{\frac{1}{2}} : \text{interaction time} \quad (\text{E.12})$$

$$t_d = \tilde{k} \frac{\rho v_{\text{rel}} D_{\text{eq}}^2}{8S} : \text{liquid film drainage time} \quad (\text{E.13})$$

where v_{rel} is the relative velocity between two bubbles in the normal direction, $\tilde{k}$ is the correction factor and:

$$D_{\text{eq}} = \frac{4R_1R_2}{R_1 + R_2} : \text{equivalent diameter of bubbles} \quad (\text{E.14})$$

At this point, the coalescence probability P_{coal} is expressed as:

$$P_{\text{coal}} = e^{-\frac{t_d}{t_i}} \quad (\text{E.15})$$

- **Bubble break – up:** bubble break-up is due to the non uniform pressure distribution on the bubble. The most important characteristics of this phenomenon are turbulent fluctuations and collisions, viscous shear stress, shearing off process and interfacial instability. Bubble break-up has been studied from different points of view and methodologies but the most common method is the application of a critical Weber number.

E.6 Hsiao et Al. model - The Ghost Fluid Multiscale Model

The Hsiao et Al. model is based on the analysis of sheet and cloud cavitation by introducing three scales of study: a macro-scale approach, an inter-scale approach and a micro-scale approach. At the macro-scale, a two-phase continuum-based flow is solved on an Eulerian grid. In this step, gas-liquid interfaces of large bubbles, air pockets and cavities are identified and solved with a level set method. Mathematically the Navier-Stokes equations in reference of the mixture density and mixture dynamic viscosity are solved. In micro-scale approach, transport of nuclei and micro-bubbles, nucleation from solid surfaces and bubble dynamics are studied. Here, bubbles are tracked in a Lagrangian fashion and in conclusion, inter-scale approach aims to join macro and micro scale approaches to analyze bubbles growth, bubble shrink, bubble break-up... through the application of a Discrete Singularity Model (DSM) and a Level Set Method (LSM). The Level Set Method is employed to simulate the large free surface deformations which are responsible for folding and break-up of sheet cavities. It is defined a smooth function $\tilde{\varphi}(\mathbf{x}, t)$ at a signed distance $d(\mathbf{x})$ from the liquid-gas interface such that its zero level corresponds to the liquid-gas interface:

$$\tilde{\varphi}(\mathbf{x}, 0) = d(\mathbf{x}). \quad (\text{E.16})$$

$\tilde{\varphi}(\mathbf{x}, t)$ is enforced to be a material surface at each time step using:

$$\frac{d\tilde{\varphi}}{dt} = \frac{\partial \tilde{\varphi}}{\partial t} + \mathbf{v}_{\text{in}} \nabla \tilde{\varphi} = 0 \quad (\text{E.17})$$

where $\mathbf{v}_{\text{in}}$ is the interface velocity. The integration of (E.17) does not guarantee that the thickness of the interface region remains constant and then, the smooth function is conducted by solving a re-initialization equation in pseudo time iterations as:

$$\frac{\partial \tilde{\varphi}}{\partial \hat{t}} = \text{sign} \{ \varphi_0 \} (1 - |\nabla \varphi|) \quad (\text{E.18})$$

where $\hat{t}$ is the pseudo-time and φ_0 is the initial distribution. Finally, (E.17) and (E.18) are solved by a ghost fluid method. The sub-grid nuclei inside the flow are identified by using a Discrete Singularity Model. The method aims to study the inception and erosion of bubbles by applying a surface average pressure approach to average fluid quantities along bubble surfaces. This method describes the bubble dynamics by applying a modified Rayleigh-Plesset equation for an equivalent cavitating bubble:

$$\rho \left[R \frac{dR^2}{dt^2} + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 \right] = p_v - p_{\text{enc}} + p_{g0} \left(\frac{R_0}{R} \right)^{3\gamma} - \frac{2S}{R} - 4\mu \frac{dR}{dt} \frac{1}{R} + \rho \frac{l |\mathbf{v}_s|^2}{4} \quad (\text{E.19})$$

$$\mathbf{v}_s = \mathbf{v}_{\text{enc}} - \mathbf{v}_b : \text{slip velocity} \quad (\text{E.20})$$

where p_{enc} is the surface average pressure seen by the bubble, $\mathbf{v}_{\text{enc}}$ is the encountered liquid velocity and $\mathbf{v}_b$ is the bubble transition velocity.

E.7 Li and Carrica model - The Population Balance Model

The Li and Carrica model solves the two-phase homogeneous mixture transport equations in terms of the liquid fraction phase while the distribution of bubbles in the flow is described by a Boltzmann-like transport equation of the type:

$$\frac{\partial f}{\partial t} + \nabla \cdot (\bar{\mathbf{v}}f) + \frac{\partial}{\partial m} (\dot{m}f) = f + \chi + \hat{S}, \quad (\text{E.21})$$

where f is the bubble size distribution function, β is the source of bubble break-up, χ is the source of bubble coalescence and $\hat{S}$ is the source of bubble entrainment. In practice, the Boltzmann equation and the vapour fraction are discretized; in particular, the second one is considered as the sum of a set of bubble group where each group has bubbles with the same mass and density. Li and Carrica proposed a model for the quantities in the Boltzmann equation:

- **mass transfer:** the formulation of the mass transfer is based on the Rayleigh-Plesset equation. As hypothesis, thermal and viscous damping effects, surface tension and non-condensable gas are neglected. The mass transfer model is formulated by analyzing an isolated bubble which interact with others while the amount of void and liquid fractions are quantified by adding damping functions. In conclusion, the model is given by:

$$\dot{m} = \sqrt{\frac{32}{3}} \pi \rho_v R^2 \left[\frac{p_v - p}{\sqrt{\rho \max\{|p_v - p| \epsilon\}}} \right] \psi(\alpha) \quad (\text{E.22})$$

$$\psi(\alpha) = 1 - \frac{1}{2} \{1 + \tanh[a(\alpha - b)]\} \quad (\text{E.23})$$

where ϵ is a controlling number and (a, b) are constants.

- **Bubble coalescence:** the coalescence of bubbles consists in the union of two or more bubbles into a larger one but studying multiple bubble coalescence is very complex and the following model considers the coalescence of only two bubbles. The total coalescence is given by:

$$\chi = \chi^+ + \chi^- \quad (\text{E.24})$$

where:

$$\chi^+(m) = \frac{1}{2} \int_0^m Q(m - m', m') f(m - m') f(m') dm' \quad (\text{E.25})$$

represents the source of bubbles of size m due to coalescence of smaller bubbles and:

$$\chi^-(m) = f(m) \int_0^{+\infty} Q(m, m') f(m') dm' \quad (\text{E.26})$$

is the loss of bubbles of size m due to coalescence with any other bubble. In (E.25) and (E.26) we have the coalescence kernel $Q(\cdot)$.

- **Bubble break – up:** bubble break-up is mainly induced by turbulent effects and essentially its model takes into account this characteristic. it is defined as follows:

$$\beta(m) = \beta^+(m) - \beta^-(m) \quad (\text{E.27})$$

where:

$$\beta^+(m) = \int_m^{+\infty} h(m, m') b(m') f(m') dm' : \text{production term} \quad (\text{E.28})$$

$$\beta^-(m) = b(m) f(m) : \text{distruction term} \quad (\text{E.29})$$

$$b(m) : \text{break - up function} \quad (\text{E.30})$$

In conclusion, the bubble entrainment is often neglected for its complicated modelling.

E.8 Kubota et Al. model - The Bubble Cluster Model

The Kubota model is divided into two modelling of cavitation: cavitation is "observed" from a macroscopic point of view and from a microscopic point of view. The model of macroscopic cavitation is based on the classical transport equation model for homogeneous two flow mixtures where the mixture density and the dynamic viscosity density are expressed as function of the vapour fraction. The macroscopic modelling is coupled with a microscopic modelling by using a local homogeneous model. A simplified Rayleigh-Plesset equation without the surface tension and viscous damping effects are neglected where the bubbles are considered spherical. In this method, the continuous domain is discretized in finite grid points where inside the grid, interactions among individual bubbles are considered. These effects are named sub-grid scale bubble interaction. Let r be a radial distance of reference, only bubble interactions inside that distance are taken into account. The total velocity potential due to other bubbles at the origin 0 is:

$$\sum_{i=1}^n \frac{1}{r_i} \frac{dR_i}{dt} R_i^2 \quad \text{for } R_i \ll r_i \quad (\text{E.31})$$

where, for hypothesis, the position of bubbles do not change at the moment of calculus. Assuming that:

$$\nabla \left(\sum_{i=1}^n \frac{1}{r_i} \frac{dR_i}{dt} R_i^2 \right) = 0 \quad (\text{E.32})$$

$$R_i = R \quad (\text{E.33})$$

and considering the Rayleigh-Plesset equation where the number of bubbles in a sphere of radius Δr is equal to $\frac{4}{3}n\pi(\Delta r)^3$, we have:

$$\begin{aligned} 2\pi\Delta r^2 \left[nR^2 \frac{d^2 R}{dt^2} + \frac{dn}{dt} R^2 \frac{dR}{dt} + 2nR \left(\frac{dR}{dt} \right)^2 \right] + R \frac{d^2 R}{dt^2} + \frac{3}{2} \left(\frac{dR}{dt} \right)^2 &= (1 + 2\pi\Delta r^2 nR) R \frac{d^2 R}{dt^2} + \\ + \left[\frac{3}{2} 4\pi (\Delta r)^2 nR \right] \left(\frac{dR}{dt} \right)^2 + 2\pi (\Delta r)^2 \frac{dn}{dt} R^2 \frac{dR}{dt} &= \frac{p_v - p}{\rho_l} \end{aligned} \quad (\text{E.34})$$

E.9 Shi et Al. model - The Heat Balance Model

The Shi et Al. cavitation model is based on the Kubota cavitation model where the transport equation of the liquid phase is solved in a homogeneous two-phase mixture flow. The main difference between that model and the Kubota model is the presence of thermal effects in the mass transport process in the first one. Applying the Fourier's law, the heat balance across the bubble interface is expressed as:

$$4\pi\dot{q}_R R^2 = \frac{4}{3}\pi\rho_v L \frac{d}{dt} (R^3) \quad (\text{E.35})$$

where L is the latent heat. The mass transport equation is given by:

$$\dot{m} = \begin{cases} F_e \frac{3(1-\alpha)\rho_v}{R} \left[\sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} + \frac{\rho_l c_p \sqrt{a} \max\{T_c - T_\infty, 0\}}{\rho_v L \sqrt{t}} \right] & \text{for } p < p_v \\ F_c \frac{3\alpha\rho_l}{R} \left[\sqrt{\frac{2}{3} \left(\frac{p - p_v}{\rho_l} \right)} + \frac{\rho_l c_p \sqrt{a} \max\{T_\infty - T_c, 0\}}{\rho_v L \sqrt{t}} \right] & \text{for } p > p_v \end{cases} \quad (\text{E.36})$$

where T_∞ is the free-stream temperature and T_c is the local temperature.

E.10 Deshpande et Al. model - The Thermodynamic Interface Model

In the current model, the cavity is treated as a constant pressure region where particular points of the cavity surface are switched from a solid wall to a cavity region if the local pressure falls below the vapour pressure of the fluid. The cavity is modelled by ensuring non-negative thickness at each point of the cavity surface such that cavity pressure and cavity surface can be calculated. Specifically, a continuous vaporization process is implemented and the shape and size of the cavity is calculable by the two phase pressures, velocity and temperature. The cavity pressure is given by the liquid vapour pressure at the temperature of the interface region and then, the application of the method requires the resolution of the energy equation. Taking into account the liquid-vapour interface, the needed heat for the production of vapour is supplied by the surrounding liquid whose flow is determined as:

$$\dot{q}_S ds = \rho_v L dQ \quad (\text{E.37})$$

where ds is the surface element, dQ is the volume flow rate of the vapour added to the cavity through ds . Considering the Fourier's law of heat, the normal temperature gradient at the liquid surface is determined as:

$$\frac{dT}{dn} = -\frac{\rho_v}{K_T} L \frac{dQ}{ds} = -\frac{\rho_v}{\rho_l} \frac{1}{a} \frac{L}{c_p} \frac{dQ}{ds} \quad (\text{E.38})$$

where a is the thermal diffusivity. it must be used as boundary condition for the energy equation of the two-phase homogeneous flow Navier-Stokes equations.

E.11 Huang and Wang model - The Density based Convex Combination Model

The Huang and Wang cavitation model is a modified density-based method that is able to analyze unsteady cloud cavitation structures by solving (8.42). The mass transport equation is defined as:

$$\dot{m} = \begin{cases} \chi \left(\frac{\rho}{\rho_l} \right) \dot{m}_k^- + \left[1 - \chi \left(\frac{\rho}{\rho_l} \right) \right] \dot{m}_s^- & \text{for } p < p_v \\ \chi \left(\frac{\rho}{\rho_l} \right) \dot{m}_k^+ + \left[1 - \chi \left(\frac{\rho}{\rho_l} \right) \right] \dot{m}_s^+ & \text{for } p > p_v \end{cases} \quad (\text{E.39})$$

where:

$$\chi \left(\frac{\rho}{\rho_l} \right) = \frac{1}{2} + \frac{\tanh \left[\frac{C_1 (0.6 \frac{\rho}{\rho_l} - C_2)}{0.2(1-2C_2)+C_2} \right]}{2 \tanh(C_1)}. \quad (\text{E.40})$$

The two added mass transport equation models $\dot{m}_k$ and $\dot{m}_s$ are developed by assuming different cavitating characteristics. $\dot{m}_k$ analyzes the growth and collapse of bubble clusters considering the simplified Rayleigh-Plesset equation:

$$\dot{m}_k^- = -C_{\text{dest}} \frac{3\alpha}{R} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} \quad (\text{E.41})$$

$$\dot{m}_k^+ = C_{\text{prod}} \frac{3\alpha}{R} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} \quad (\text{E.42})$$

Instead, the implementation of $\dot{m}_s$ provides information about the cavity interface. Mass and normal momentum are studied at a liquid-vapour interface under the assumption of a homogeneous equilibrium flow condition so that the mass transfer is implemented as:

$$\dot{m}_s^- = \frac{\rho_l^2 \min \{p - p_v, 0\} \gamma}{\rho_v (v_{vn} - v_{in})^2 (\rho_l - \rho_v) t_\infty} \quad (\text{E.43})$$

$$\dot{m}_s^+ = \frac{\rho_l \max \{p - p_v, 0\} (1 - \gamma)}{\rho_v (v_{vn} - v_{in})^2 (\rho_l - \rho_v) t_\infty} \quad (\text{E.44})$$

where v_{vn} is the vapour face velocity and v_{in} is the interface velocity. The interface velocity is needed in (E.43) and (E.44) only for time-dependent problems. C_1 , C_2 , C_{dest} and C_{prod} are the constants of the model.

E.12 Konstantinov et Al. model - The Viscosity Oriented Model

Konstantinov model was developed by considering non-dimensional speeds depending on the Reynolds number, approximations of non-dimensional speeds depending on the Reynolds number, approximations of non-dimensional speeds of bubble growth by introducing approximating functions and dynamic components for the mass transfer rate. Under these hypothesis, bubbles growth is evaluated by the following modified Rayleigh-Plesset equation:

$$\frac{dR}{dt} = \sqrt{\frac{2}{3}} \tanh \left[1.221 \left(\frac{R_0 \sqrt{\Delta p \rho}}{4\mu} \right)^{0.353} \right] \sqrt{\frac{\Delta p}{\rho}} \quad (\text{E.45})$$

and the mass transfer expression is:

$$\dot{m} = \begin{cases} F_e \frac{3r_{\text{nuc}}(1-\alpha)\rho_v}{R_0} \tanh \left[1.22 \left(\frac{R_0 \sqrt{(p_v - p)\rho}}{4\mu} \right)^{0.35} \right] \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} & \text{for } p < p_v \\ F_c \frac{3\alpha\rho_v}{R_0} \tanh \left[1.22 \left(\frac{R_0 \sqrt{(p_v - p)\rho}}{4\mu} \right)^{0.35} \right] \sqrt{\frac{2}{3} \left(\frac{p - p_v}{\rho_l} \right)} & \text{for } p > p_v \end{cases} \quad (\text{E.46})$$

E.13 Goncalves and Charriere model - The Four Equation Model

The Goncalves and Charriere model treats cavitation as a homogeneous mixture flow in thermal and mechanical equilibrium where the governing equations are flow homogeneous mixture continuity, vapour fraction transport and energy balance equations. The model introduces an equation of state for the pressure field in order to describe the thermodynamic effects of cavitation. The barotropic law of pressure is defined as:

$$p(\rho) = p_v + \left(\frac{\rho_l - \rho_v}{2} \right) c_{\text{baro}}^2 \arcsin \left(\frac{2\rho - \rho_l - \rho_v}{\rho_l - \rho_v} \right) \quad (\text{E.47})$$

where c_{baro} is the minimal speed of sound in the mixture. The speed of sound of homogeneous mixture is calculated as:

$$c^2 = \frac{c_{\text{baro}}^2}{2\sqrt{\alpha(1-\alpha)}} \quad (\text{E.48})$$

and the effects described by the pressure equation are directly implemented into the vapour fraction equation as:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \bar{\mathbf{v}}) \left[\left(\frac{\rho_l c_l^2 - \rho_v c_v^2}{\frac{\rho_l c_l^2}{1-\alpha} + \frac{\rho_v c_v^2}{\alpha}} \right) + \alpha \right] \nabla \cdot \bar{\mathbf{v}} + \underbrace{\left(\frac{\frac{c_v^2}{\alpha} + \frac{c_l^2}{1-\alpha}}{\frac{\rho_l c_l^2}{1-\alpha} + \frac{\rho_v c_v^2}{\alpha}} \right)}_{\text{interfacial density}} \dot{m} \quad (\text{E.49})$$

$$\dot{m} = \frac{\rho_l \rho_v}{\rho_l - \rho_v} \left[1 - \left(\frac{c}{c_{\text{wall}}} \right)^2 \right] \nabla \cdot \bar{v} \quad (\text{E.50})$$

where c_v is the speed of sound of vapour phase, c_l is the sound of speed of liquid phase and c_{wall} is the propagation of acoustic waves without mass transfer. c_{wall} is derived from the weighted harmonic mean of speeds of sound of each phase. When heat and mass transfer effects are employed, c decreases to the thermodynamic equilibrium one and this limit is evaluated by considering the conditions of local thermodynamic equilibrium. In conclusion, when regions of higher pressure than p_v are analyzed, the void ratio must be destroyed to correctly simulate the cavitating phenomenon. The realization of this condition is satisfied by modifying (E.50) with a destruction term:

$$\dot{m} = \frac{\rho_l \rho_v}{\rho_l - \rho_v} \left[1 - \left(\frac{c}{c_{\text{wall}}} \right)^2 \right] \nabla \cdot \bar{v} - 2 \frac{c_{\text{des}} \alpha \rho_v \max\{0, p - p_v\}}{\rho_{\text{ref}} V_{\text{ref}}^2} \quad (\text{E.51})$$

where c_{des} is a tunable parameter.

E.14 Ventikos and Tzabiras model - The Thermodynamics Variable Model

The current method considers the cavitating flow as two distinct flows where each of them can become the other and conversely. Each phase has its own governing equations and the passage between phases is controlled by boundary conditions. Pressure and enthalpy of liquid and vapour are used to calculate the fluid properties (ρ, μ, T, K, c_p) by using existing tables.

E.15 Banerjee and Saritha model - The Lattice Boltzmann EOS Model

Banerjee and Saritha use the Lattice-Boltzmann theory to simulate the cavitation arisement. The motion of fluids is described by a set of discrete single-particle density distribution functions and the BGK collision operator is introduced to model the forces. Density distribution function is described by an evolution equation of the form:

$$f_i(x + e_i \delta t, t + \delta t) = f_i(x, t) + \frac{1}{\tau} [f_i^{\text{eq}}(x, t) - f_i(x, t)] + \Delta f_i(x, t) \quad (\text{E.52})$$

where e_i is the direction of interest, $\Delta f_i(x, t)$ is the local external force and $f_i^{\text{eq}}(x, t)$ is an equilibrium distribution function. From the previous assumptions, we can determine the density system and the velocity as:

$$\rho = \sum_{i=1}^n f_i \quad (\text{E.53})$$

$$v = \frac{1}{\rho} \sum_{i=1}^n e_i f_i \quad (\text{E.54})$$

After, the Navier-Stokes equations can be recovered through the Chapman-Enskog expansion procedure. The velocity field obtained from this procedure is not the velocity under the real external forces of the problem, therefore, the real force system is determined by applying the Kupersh-tokh and Medvedev's exact difference method. The real fluid velocity U is expressed in terms of interaction potential force F and it is given by:

$$\rho U = \rho v + \frac{\delta t}{2} F \quad (\text{E.55})$$

F and p can be calculated by involving the Shan and Chen method or the Peng-Robinson equation of state.

E.16 Shingal et Al. model - The Full Cavitation Model

For hypothesis, a homogeneous flow without presence of non condensed gases is treated. Let f_v and f_l be respectively the liquid mass fraction and the vapour mass fraction of the flow. The density of the mixture is written as:

$$\rho = \frac{\rho_v}{f_v} + \frac{\rho_l}{f_l} = \frac{\rho_v}{f_v} + \frac{\rho_l}{f_v - 1}. \quad (\text{E.56})$$

The vapour mass transport α and the liquid mass transport γ can be evaluated as:

$$\begin{cases} \alpha \equiv f_v \frac{\rho}{\rho_v} \\ \gamma \equiv f_l \frac{\rho}{\rho_l} = (f_v - 1) \frac{\rho}{\rho_l} \end{cases} \Rightarrow \rho = \alpha \rho_v + (1 - \alpha) \rho_l. \quad (\text{E.57})$$

For hypothesis, there exist a zero velocity split between the fluid and bubbles and the bubble dynamics are described by the generalized Rayleigh-Plesset equation. To obtain an expression for the net phase change rate we write a liquid phase transport equation:

$$\frac{\partial}{\partial t} (\rho_l \gamma) + \nabla \cdot (\rho_l \gamma \mathbf{v}) = -(R_e - R_c) \Rightarrow \frac{\partial}{\partial t} [\rho_l (1 - \alpha)] + \nabla \cdot [\rho_l (1 - \alpha) \mathbf{v}] = -(R_e - R_c) \quad (\text{E.58})$$

a vapour phase transport equation:

$$\frac{\partial}{\partial t} (\rho_v \alpha) + \nabla \cdot (\rho_v \alpha \mathbf{v}) = -(R_e - R_c) \quad (\text{E.59})$$

and a mixture transport equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (\text{E.60})$$

where R_e and R_c are respectively the vapour generation and condensation rate. Combining (E.58), (E.59) and (E.60) we obtain a relation between the density of the mixture and the vapour volume fraction:

$$\frac{D\rho}{Dt} = -(\rho_l - \rho_v) \frac{D\alpha}{Dt}. \quad (\text{E.61})$$

Applying (8.33) with respect to ρ_l without the initial gas pressure component, surface tension component and the viscosity component, we elaborate the lagrangian the the mixture equation and using (E.58), (E.59) and (E.61) we have:

$$R_e - R_c = (4n\pi)^{\frac{1}{3}} (3\alpha)^{\frac{2}{3}} \frac{\rho_v \rho_l}{\rho} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} - R \frac{D^2 R}{Dt^2} \right)}. \quad (\text{E.62})$$

Neglecting the diffusion term, we can write the transport equation for f_v as:

$$\frac{\partial}{\partial t} (\rho f_v) + \nabla \cdot (\rho \mathbf{v} f_v) = (4n\pi)^{\frac{1}{3}} (3\alpha)^{\frac{2}{3}} \frac{\rho_v \rho_l}{\rho} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} - R \frac{D^2 R}{Dt^2} \right)}. \quad (\text{E.63})$$

This equation is referred as the reduced bubble dynamics formulation and it is used to model R_e and R_c . In the absence of a general model for estimating of the number density, the phase change rate expression is rewritten in terms of bubble radius as:

$$R_e = \frac{3\alpha}{R} \frac{\rho_v \rho_l}{\rho} \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} \quad (\text{E.64})$$

For simplicity, R is approximated to the value at the limited condition and taking into account the following consideration: the volume phase change rates $\propto$ volume fractions of the donor phase, the relative velocity between the liquid and the vapour phase and local turbulent velocity fluctuations are of the order of 1 to 10% of the mean velocity and $\lim_{\alpha \rightarrow 0} R \rightarrow 0$. Then, the Singhal model of the mass transfer is:

$$\dot{m} = \begin{cases} -C_e \frac{\sqrt{k}}{T} \rho_l \rho_v \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} (1 - f_v) & \text{for } p < p_v \\ C_c \frac{\sqrt{k}}{T} \rho_l \rho_l \sqrt{\frac{2}{3} \left(\frac{p_v - p}{\rho_l} \right)} f_v & \text{for } p > p_v \end{cases} \quad (\text{E.65})$$

where (C_e, C_c) are calibration constants.

E.17 Senocak and Shyy model - The Interphase Mass and Normal Momentum Model

The current cavitation model has been developed by considering the liquid-vapour interface in order to express the mass conservation equation at the interface as:

$$\rho_l (v_{l,n} - v_{i,n}) = \rho_v (v_{v,n} - v_{i,n}) \quad (\text{E.66})$$

and the normal conservation momentum at the interface as:

$$p_v - p_l = S \left(\frac{1}{R_1} + \frac{1}{R_2} \right) + 2\mu_v \frac{\partial v_{v,n}}{\partial n} - 2\mu_l \frac{\partial v_{l,n}}{\partial n} + \rho_l (v_{l,n} - v_{i,n})^2 - \rho_v (v_{v,n} - v_{i,n})^2, \quad (\text{E.67})$$

where $v_{l,n}$ is the velocity of the liquid phase in the normal direction, $v_{i,n}$ is the velocity of the interface in the normal direction and $v_{v,n}$ is the velocity of the vapour phase in the normal direction. In this model, the heat transport is neglected. For hypothesis, the phase change takes place between the vapour and mixture phases such that in sharp interface limit, (8.43) represents vapour and liquid density together. Then, the liquid phase is represented by the mixture phase and (E.66) and (E.67) are re-written by neglecting the surface tension and viscous effects:

$$\rho_v (v_{v,n} - v_{i,n}) = \rho_m (v_{m,n} - v_{i,n}) \quad (\text{E.68})$$

$$p_v - p_l = \rho_m (v_{m,n} - v_{i,n})^2 - \rho_v (v_{v,n} - v_{i,n})^2. \quad (\text{E.69})$$

(E.68) and (E.69) can be put together to expreme the following condition:

$$\begin{aligned} p_v - p_l &= \rho_v (v_{v,n} - v_{i,n})^2 \left(\frac{\rho_v}{\rho_m} - 1 \right) = \rho_v (v_{v,n} - v_{i,n})^2 \left[\frac{\rho_v}{\rho_l \gamma + \rho_v (1 - \gamma)} \right] \Rightarrow \\ \Rightarrow \gamma &= \frac{\rho_l (p_l - p_v) \gamma}{\rho_v (v_{v,n} - v_{i,n})^2 (\rho_l - \rho_v)} + \frac{(p_l - p_v) (1 - \gamma)}{(v_{v,n} - v_{i,n})^2 (\rho_l - \rho_v)} \end{aligned} \quad (\text{E.70})$$

(E.70) represents the interfacial boundary condition which is implemented into the liquid transport equation as a source term. In conclusion, the liquid fraction transport equation is:

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (\gamma \bar{\mathbf{v}}) = \frac{\rho_l (p_l - p_v) \gamma}{\rho_v (v_{v,n} - v_{i,n})^2 (\rho_l - \rho_v) t_\infty} + \frac{(p_l - p_v) (1 - \gamma)}{(v_{v,n} - v_{i,n})^2 (\rho_l - \rho_v) t_\infty} \quad (\text{E.71})$$

E.18 Liu et Al. model - The Wake Closure Model

The Liu cavitation model treats attached cavitation and in particular cavitation is considered as a large cavity bubble on the wall with an interface to bulk flow. The cavity and interface surfaces are considered free surfaces and for hypothesis, the pressure inside the cavity is assumed to be equal to the local vapour pressure of fluids and the rear part of the bubble is approximated with a wake model when the pressure is no longer equal to the vapour pressure. Constructions of bubbles are characterized by three elements: location of inception, forebody profile and afterbody profile. The inception of cativation can be reached by analyzing the point of non-cavitation wall where the pressure is minimal and drops below the local vapour pressure. If cavitation arises

downstream to a sharp corner of a wall, inception often occurs at the sharp corner. Instead, the afterbody profile occurs at the point on the cavity surface where the local height is (for example) half of the maximal height of the cavity and it smoothly links the forebody profile and the local wall surface. Furthermore, the length of the closure domain and the cavity attached point are determined by a wake closure model. In this method, solutions about the cavity shape and the flow field are calculated when the pressure on the cavity surface converges to a constant value equal to the vapour pressure of fluid and the free surface boundary condition is imposed on the cavity surface. The algorithm is to enforce the pressure on the forebody on the cavity surface approach to a constant local vapour pressure by a cavity shape which is determined iteratively. The convergence is reached when the pressure on the forebody of the cavity is uniformly distributed to the local vapour pressure. From a general point of view, the cavity shape and the pressure distribution are correlated by a relationship of the type:

$$f\left(r, \frac{\partial r}{\partial s}, \dots, \frac{\partial^n r}{\partial s^n}, \dots, p, \frac{\partial p}{\partial s}, \dots, \frac{\partial^n p}{\partial s^n}, \dots\right) = 0 \quad (\text{E.72})$$

where r is the local cavity thickness, p is the local cavity pressure and s is the distance coordinate along the wall in the bulk flow direction. If i is the current direction, we write:

$$f\left(r^{(i)}, \frac{\partial r^{(i)}}{\partial s}, \dots, \frac{\partial^n r^{(i)}}{\partial s^n}, \dots, p^{(i)}, \frac{\partial p^{(i)}}{\partial s}, \dots, \frac{\partial^n p^{(i)}}{\partial s^n}, \dots\right) = 0. \quad (\text{E.73})$$

The value $p^{(i)}$ does not meet the pressure boundary condition along the cavity surface and deviates from the local pressure, then the shape needs to be modified in:

$$r^{(i+1)} = r^{(i)} + \Delta r^{(i)} \quad (\text{E.74})$$

and:

$$p^{(i+1)} = p_v. \quad (\text{E.75})$$

(E.73) is re-written as:

$$f\left(\Delta r^{(i)}, \frac{\partial \Delta r^{(i)}}{\partial s}, \dots, \frac{\partial^n \Delta r^{(i)}}{\partial s^n}, \dots, p_v - p^{(i)}, -\frac{\partial p^{(i)}}{\partial s}, \dots, -\frac{\partial^n p^{(i)}}{\partial s^n}, \dots\right) = 0. \quad (\text{E.76})$$

A polynomial approximation of (E.76) is after applied to have:

$$\hat{\alpha}_0 \Delta r^{(i)} + \hat{\alpha}_1 \frac{\partial \Delta r^{(i)}}{\partial s} + \dots + \hat{\alpha}_n \frac{\partial^n \Delta r^{(i)}}{\partial s^n} = \hat{\beta}_0 (p_v - p^{(i)}) + \hat{\beta}_1 \frac{\partial p^{(i)}}{\partial s} + \dots + \hat{\beta}_n \frac{\partial^n p^{(i)}}{\partial s^n} \quad (\text{E.77})$$

where $(\hat{\alpha}_0, \dots, \hat{\alpha}_n, \hat{\beta}_1, \dots, \hat{\beta}_n)$ are polynomial coefficients that are calculated at each iteration from the current solution by solving the following equation with respect to each grid point on the cavity surface:

$$\alpha_0 r^{(i)} + \alpha_1 \frac{\partial r^{(i)}}{\partial s} + \dots + \alpha_n \frac{\partial^n r^{(i)}}{\partial s^n} = \beta_0 p^{(i)} - \beta_1 \frac{\partial p^{(i)}}{\partial s} - \dots - \beta_n \frac{\partial^n p^{(i)}}{\partial s^n}. \quad (\text{E.78})$$

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