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Abbreviations and Acronyms

Acronym	description
ALE	Arbitrary Lagrangian–Eulerian
AniPFM	Anisotropic Pressure Fluctuation Model
CI	Credible Interval
DOF	Degree(s) of freedom
FIV	Flow-Induced Vibration
FSI	Fluid-structure interaction
GO-VIKING	Gathering expertise On Vibration ImpaKt In Nuclear power Generation
GPR	Gaussian-Process Regression
LHS	Latin Hypercube Sampling
LOO	Leave-One-Out
MCMC	Markov Chain Monte Carlo
NRMSE	Normalized Root-Mean-Square Error
PCE	Polynomial chaos expansion
PDF	Probability Density Function
QoI(s)	Quantity(ies) of Interest
RBF	Radial-Basis Function
RMSE	Root-Mean-Square Error
RMS	Root-mean-square

SA	Sensitivity Analysis
SBM	Synthetic Bubble Model
SST	SST $k - \omega$ turbulence model
TIV	Turbulence-Induced Vibration
TKE	Turbulent Kinetic Energy
UDF	User-defined function
UQ	Uncertainty quantification
URANS	Unsteady Reynolds-Averaged Navier-Stokes
VOF	Volume of fluid
WP	Work package

Summary

In this report, efficient UQ is demonstrated on the two-phase cross-flow GO-VIKING WP4 case TITAN as part of Task 5.2. As described in deliverable 5.3, polynomial chaos expansion is chosen to propagate the uncertainty. An uncertain input, the flow velocity, is propagated through an FSI simulation model to an uncertain output, the vibration amplitude. This model uses a Synthetic Bubble Model as inlet boundary condition to be able to use a smaller inlet domain. This model has been further developed. The flow model was implicitly coupled to the structure with a Newton–Raphson method. The structural model considered two rigid cylinders that can only translate in the lift direction, so two degrees of freedom in total. This 2-DOF model was implemented for this project using a Fluent UDF. Parallelization was used as much as possible to make the UQ efficient, but also an ensemble averaging over similar samples was required to have a sufficiently accurate estimate of the RMS value to allow a 3rd order PCE fitted with the least-squares method.

This report also develops and applies a unified uncertainty-quantification framework—combining global sensitivity analysis, surrogate modelling, and Bayesian calibration—to assess and reduce turbulence-model uncertainty in flows relevant to turbulence-induced vibrations. Three cases are studied: turbulent channel flow, turbulent annular flow, and a cantilevered-rod flow, chosen as progressively more complex representatives of the FSI configuration. Across the first two cases, full Sobol analyses show that the SST model depends primarily on a small subset of parameters, with β^* and $\alpha_{\omega 1}$ consistently dominating. This enables a

reduced-dimensional surrogate-based Bayesian approach for the expensive rod geometry. Gaussian-process and Polynomial-Chaos surrogates are built to emulate the CFD solver and allow efficient posterior sampling. The calibrated posteriors and predictive distributions demonstrate strong cross-case consistency, confirming that the same dominant parameters govern the uncertainty behaviour across all geometries. While some model-form limitations persist—particularly for wall-normal stresses and TKE—the reduced parameter set provides robust and transferable predictive capability. The resulting framework offers an efficient, scalable UQ pipeline and delivers calibrated turbulence-model parameters ready for use in FSI simulations within GO-VIKING.

Keywords

Computational fluid dynamics, Two-phase flow, Fluid-structure interaction, Flow-induced vibrations, Tube bundle, Uncertainty quantification, Bayes' theorem, RANS model closure



1. Uncertainty Quantification of Flow-Induced Vibration in the TITAN setup

1.1 Introduction

In this deliverable, the non-intrusive polynomial chaos method described in deliverable 5.3 is applied to the TITAN case of WP4, a tube bundle subject to two-phase cross-flow. An uncertain pitch velocity following a Gaussian distribution was considered, and it was propagated into the uncertain root-mean-square (RMS) vibration amplitude of two transversally vibrating cylinders.

Two-phase flows occur in many shell-and-tube type heat exchangers such as condensers, evaporators and steam generators. The fluctuating forces caused by the two-phase cross-flow can cause damage to steam generators if too severe [22]. Unscheduled outages of pressurized water nuclear reactors are in 25% of the cases related to problems in the steam generator [28].

Many two-phase flows exhibit complicated, transient and erratic flow patterns which pose challenges to their numerical simulation. Lumping the intricate and ever changing interface into the subgrid scales results in closure models that require adequate calibration. If instead the interface is resolved, like in the Volume of Fluid (VOF) method, other difficulties arise.

One such difficulty is related to the representation of this interface at the inlet boundary in interface-resolved, Eulerian methods such as VOF. One option observed in literature is the supply of steady (gas) jets [30] or stratified flow at the inlet, neglecting transient behaviour. Another option is to start with an unresolved interface by setting an average void fraction at the inlet [18], relying on the model to develop a sharp interface further downstream. Both options require a long development length upstream of the zone of interest [24], entailing additional computational cost, or if this upstream domain is too short, the solution may be affected [30].

For a review of previous experimental and numerical work, the reader is referred to the paper of Benguigui et al. [22]. Two-phase flow patterns are of primary interest in characterizing FIV and the obtained regime depends on the geometry as well as on how the two-phase flow is generated and introduced [21]. Benguigui et al. [22] identify the need for deeper understanding of the inlet parameters.

Fluid-structure interaction (FSI) simulations, coupling a two-phase computational fluid dynamics (CFD) solver to a structural model, only took off recently as a research approach for FIV with multiphase flow, examples being the thesis of Benguigui [20] and the paper of Sadek et al. [32]. Assuming that FIV excitation is dominated by large gas structures, the VOF approach is a good choice. Its limited use so far for this type of investigations can partly be related to the difficulty in providing correct inlet conditions. De Moerloose et al. [23] contributed to the research by offering a novel inlet modelling approach: the Synthetic Bubble Model (SBM),

implemented in Python¹. In the absence of detailed inlet data, the SBM creates a reasonable, transient inlet condition, avoiding long precursor domains.

The first contribution of the current work is making the SBM compatible with Ansys Fluent, besides OpenFOAM. The modified SBM is applied on a larger bundle than has been used in the original validation [23], namely the TITAN experiment [31], a smaller scale abstraction of a steam generator. Moreover, it is the first use of the SBM with a two-way coupled FSI simulation.

1.2 Case description

1.2.1 TITAN

The TITAN test section contains a rotated triangular tube array subject to an upward air/water flow. Due to an upstream air/water mixer, the air bubbles are assumed to be homogeneously distributed.

The tubes have a diameter D of 30 mm and a length L of 300 mm, which is also the channel depth. The channel width is 224.5 mm. The shortest distance between two tube centers, called the pitch P is equal to 43.2 mm, resulting in a pitch-to-diameter ratio P/D of 1.44.

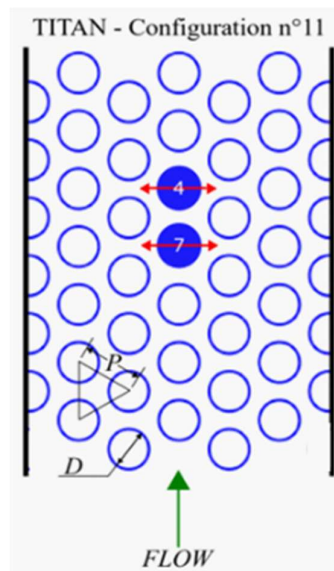


Figure 1: The considered configuration of TITAN, with two flexible cylinders [31].

Up to 15 tubes can be made flexible by mounting them on a flexible stainless steel blade, with a density of 7800 kg/m^3 , elasticity modulus of 210 GPa, Poisson ratio of 0.3 and dimension $100 \times 25 \times 4 \text{ mm}$. As the blade is much stiffer in one direction than in the perpendicular direction, it is essentially a 1-dimensional vibration. The first mode natural frequency f_n is 14.18 Hz and the damping ratio ζ is 0.045 %. In this case, configuration n°11 is considered, containing two cylinders, being cylinder 7 and cylinder 4, vibrating in the horizontal direction

¹ <https://github.com/pyfsi/SBM>

as shown in Figure 1. As will be explained in Section 1.3.3, they were modelled as 1 degree-of-freedom oscillators, coupled only by the two-phase flow.

1.2.2 Uncertainty

An uncertain pitch velocity U_p was considered. This velocity is defined as

$$U_p = U \cdot \frac{P}{P-D}$$

with U the homogeneous velocity:

$$U = \frac{Q_{air}}{S} + \frac{Q_{water}}{S}.$$

In this equation, S is the channel area upstream of the cylinders, equal to $0.0673m^2$. The homogeneous void fraction $\alpha_{air} = Q_{air}/(Q_{air} + Q_{water})$ was kept constant to a value of 0.346.

For the pitch velocity a Gaussian distribution was assumed, with a mean value of $1.2259 m/s$ and a standard deviation of $0.052 m/s$ (coefficient of variation 4.27 %):

$$U_p \sim \mathcal{N}(1.2259 m/s; 2.74 \times 10^{-3} m^2/s^2),$$

with $\mathcal{N}(\mu; \sigma^2)$ a normal distribution with mean μ and variance σ^2 .

The output quantities of interest are the root-mean-square (RMS) vibration displacement amplitudes of cylinder 4 and cylinder 7 (see Figure 1), defined as:

$$RMS(x) = \sqrt{\frac{1}{N} \sum_{i=1}^N x_i^2},$$

with x_i the displacement of the cylinder's tip at time step i and N the total number of time steps included in the calculation of the RMS.

1.3 Methodology

1.3.1 The Synthetic Bubble Model

The main idea of the SBM is to create a virtual (i.e. without flow calculation) pre-domain which extends the faces of the inlet plane perpendicularly with a user-defined number of layers, equal to the foreseen number of time steps. The SBM sets the value of the volume fraction of the phases for each cell of the pre-domain. At each time-step a new layer of this pre-domain is fed to the inlet plane, serving as the inlet profile for the void fraction.

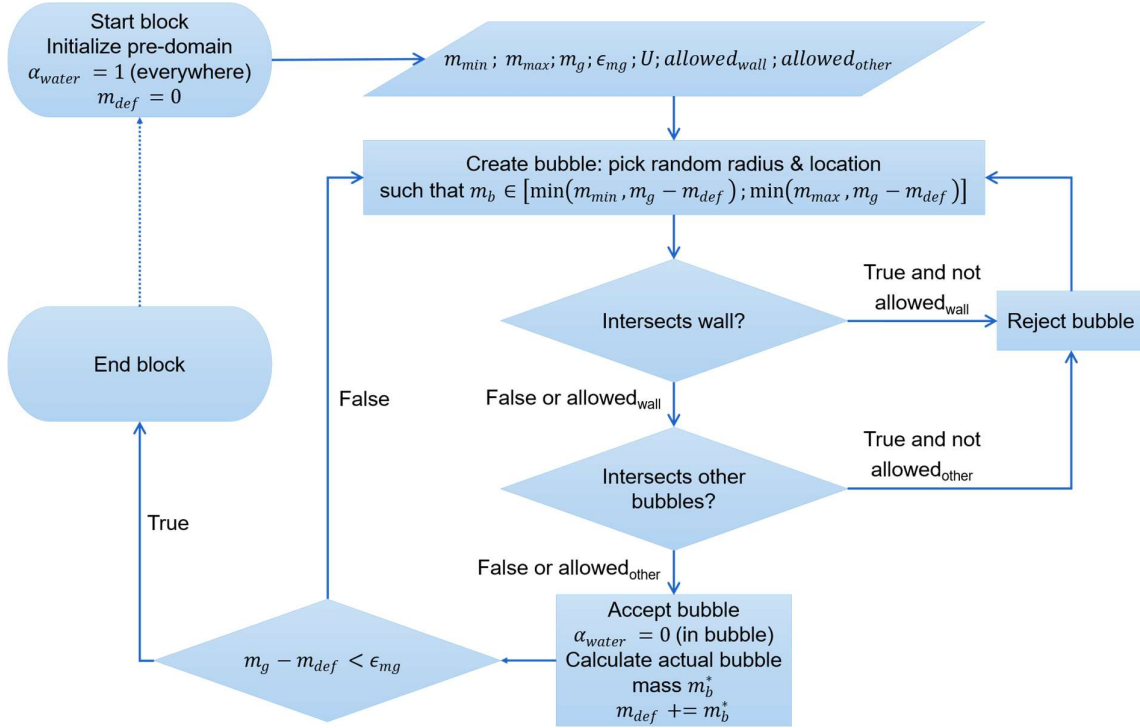


Figure 2: Simplified flowchart of the Synthetic Bubble Model. Not included are details on the initialization of the pre-domain, detection of intersections and the calculation of m_b^* .

The flowchart in Figure 2 visually explains how the SBM prepares the virtual pre-domain. In the following explanation water and air will be used as example for the phases. The algorithm starts with creating a pre-domain with the number of layers equal to the number time steps set by the user and initializing it to pure water ($\alpha_{water} = 1$). A variable m_{def} keeps track of the mass of the gas bubbles that has been defined and is initially put on 0. Following parameters related to the bubbles are specified by the user: m_{min} and m_{max} the mass of the smallest and largest possible bubble respectively, m_g the total mass of gas bubbles that needs to be defined, U , the homogeneous velocity at the inlet and $allowed_{wall}$ and $allowed_{other}$, two Boolean parameters defining whether the bubbles are allowed to intersect the walls of the domain and each other respectively.

After initialization, a loop is started which adds gas to the domain, one bubble at a time. A bubble is created at a random location, and also the estimated size (mass m_b) is in principle random, but constrained by m_{min} and m_{max} . Uniform distributions are used for the random bubble sizes by default, but other ones can also be used, if known from experiments for example, or a fixed value can be used ($m_b = m_{min} = m_{max}$). The random number generator (RNG) from the random.py library is used, with the Mersenne Twister as core generator and the system time as seed. It produces 53-bit precision floats and has a period of $2^{19937} - 1$. When the remaining amount of gas to be injected $m_g - m_{def}$ becomes less than first m_{max} and then m_{min} , it becomes the respective constraint instead. Next, it is checked whether the bubble intersects with the wall or previously defined bubbles. The bubble is then rejected or accepted according to the user's specifications. If it is accepted, the cells of the virtual pre-domain are updated to have $\alpha_{water} = 0$ and the actual mass of the bubble m_b^* is computed to update m_{def} . This loop is repeated until the difference between the mass of the bubbles

that have been defined m_{def} and the desired mass is below the tolerance ϵ_{mg} . In the course of this work, this loop was implemented more efficiently, realizing a speed-up of the generation of the virtual pre-domain by a factor of 20 compared to the original implementation, for the case of interest.

This procedure can be repeated for a new pre-domain if more data is needed, as in De Moerloose et al. [23], but it is recommended to generate all data required for the simulation at once, because otherwise the introduction of bubbles is briefly interrupted, introducing spurious periodicity and statistically non-uniform void fractions in time. The speed-up realized in this work allows to prepare long pre-domains in a reasonable amount of time. For the cases considered in this work this was between 70 minutes and 155 minutes on a single Intel Xeon Gold 6242R core to generate bubbles for 20 000 time steps.

Besides introducing bubbles in a random fashion, the SBM could easily be extended to include data, for instance from a wire mesh sensor, thanks to its ability to apply a time-dependent inlet profile in Fluent and OpenFOAM. It is worth noting that the SBM allows the user to specify the bubble size distribution in any case, but that this choice may affect the results [21, 22]. Depending on the mesh, time step and U , some bubble diameters distribution or inlet void fractions may be infeasible for the SBM to generate a pre-domain. In this work, constant bubble diameters were used per case, between 20 mm and 30 mm . For example, when 25 mm was used, $m_b = 9.69\ mg$.

1.3.2 Flow model

A depiction of the block-structured flow mesh can be seen in Figure 3. The unit blocks of which the tube bundle region consists (highlighted in red) have 5×5 or 5×6 divisions. The maximal aspect ratio in this region is 2.18 and only in the last block before the outlet (gray) the cells gradually become longer in the flow direction to an aspect ratio of 5 to smoothen the fields towards the outlet for numerical stability. The minimal orthogonal quality is 87 %. The depth of the domain was reduced from 300 mm to 100 mm to save computational cost, and the front wall and back wall were set to free slip walls. The inlet and outlet plane have 90×41 faces and the entire mesh totals 1373910 cells.

The flow is solved with Ansys Fluent 2023R1, using the unsteady Reynolds-averaged Navier–Stokes equations with the $k-\omega$ SST turbulence model. The velocity inlet was augmented with the SBM for the void fraction, providing homogeneously distributed bubbles. Inlet data was generated for 20 000 time steps of 0.0005 s . Both intersection between the bubbles and with the walls were allowed. Both phases were introduced with a uniform velocity, thus neglecting slip. Buoyancy and surface tension forces are assumed to further develop the flow while traveling through the rigid bundle, before it reaches the zone of interest with the moving rods. The flow leaves the domain through a pressure outlet.

For air the density ρ_{air} was taken 1.184 kg/m^3 and its dynamic viscosity $\mu_{air} = 1.7894 \times 10^{-5}\ Pa \cdot s$, while for water $\rho_{water} = 997.05\ kg/m^3$ and $\mu_{water} = 1.003 \times 10^{-3}\ Pa \cdot s$ was used. A surface tension of 0.07275 N/m was specified.

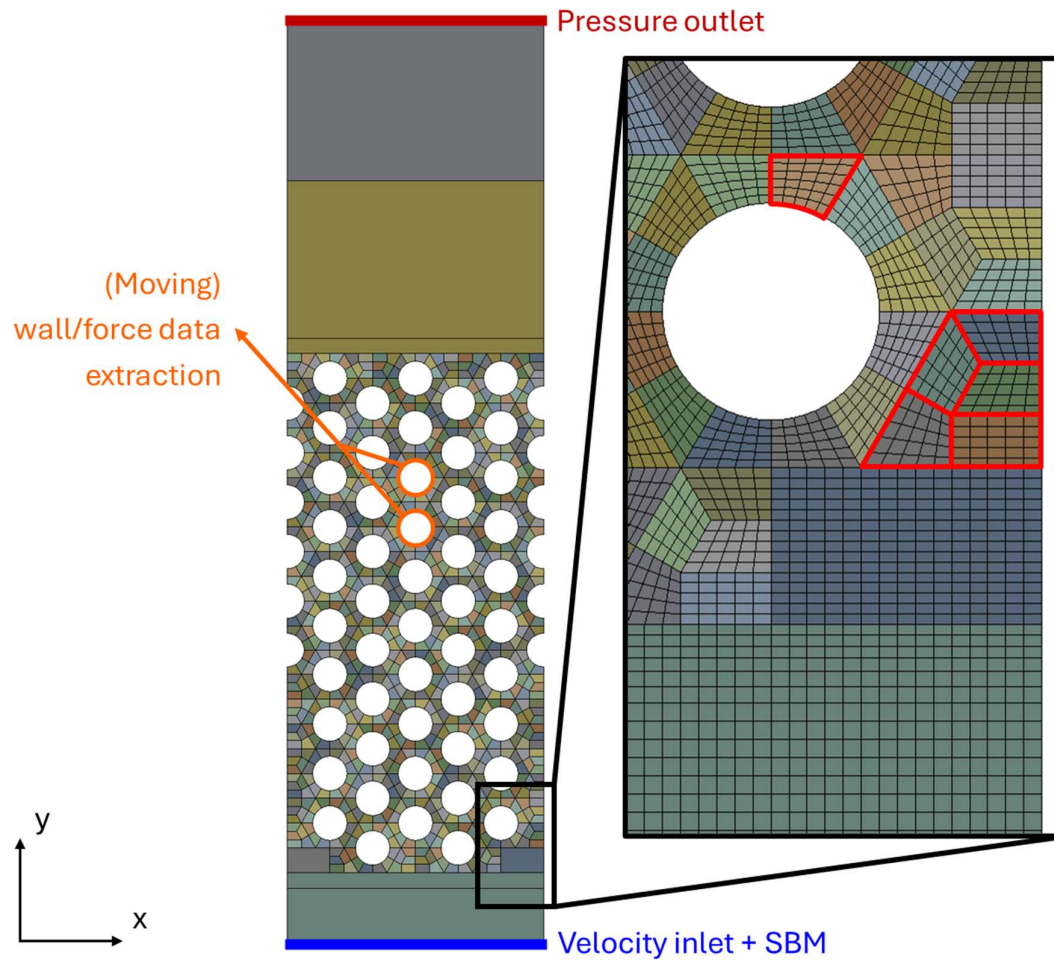


Figure 3: Flow domain, boundary conditions and mesh.

For the Volume of Fluid method both an implicit and explicit formulation exist [19]. For the latter, the cell value of the volume fraction of the current time step is directly calculated based on the known fluxes at the previous time step. Both methods were tested in this work, combined with both 1st order and 2nd order (bounded) implicit time stepping for all other flow variables. Note that for explicit VOF, only 1st order time discretization is allowed in Fluent. In order to stabilize convergence in all time steps, a velocity limiter was employed in the explicit case. It was found that the implicit VOF formulation with a 1st order time scheme was the only one that offered sufficiently reliable convergence to be used for the FSI simulations in the UQ study.

The lift forces on the moving cylinders, indicated in orange on Figure 3, were communicated to a rigid body solver in a two-way FSI loop, as described in the next section.

1.3.3 Rigid body solver

The rigid body motion coupled with the flow is solved using a Fluent UDF in an iterative FSI procedure, as demonstrated by Vierendeels et al. [34]. For this work, the procedure was extended to include two vibrating tubes as is outlined below.

The two flexibly mounted cylinders are assumed to behave as a 2 degree-of-freedom mass-spring-damper system, of which the x-direction motion is described by

$$\begin{pmatrix} F_1 \\ F_2 \end{pmatrix} = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \cdot \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix} + \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix} \cdot \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} + \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

m_1 and m_2 being the masses of the respective cylinders, c_1 and c_2 their damping constants, k_1 and k_2 their stiffnesses and F_1 and F_2 the force obtained from the flow simulation. As can be observed from this equation, the cylinders are only coupled through the two-phase flow. Writing this in an implicitly coupled FSI loop gives

$$\begin{pmatrix} F_1 \\ F_2 \end{pmatrix}^{n+1,k+1} = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \cdot \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,k+1} + \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix} \cdot \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix}^{n+1,k+1} + \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^{n+1,k+1}.$$

In this formulation, n represents the time step and k the coupling iteration. Derivative information of the forces can be used to compute a better approximation of the forces at the cylinders' new positions:

$$\begin{aligned} \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}^{n+1,k} + \begin{pmatrix} \frac{\partial F_1}{\partial \ddot{x}_1} & \frac{\partial F_1}{\partial \ddot{x}_2} \\ \frac{\partial F_2}{\partial \ddot{x}_1} & \frac{\partial F_2}{\partial \ddot{x}_2} \end{pmatrix} \cdot \begin{bmatrix} \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,k+1} - \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,k} \end{bmatrix} \\ = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \cdot \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,k+1} + \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix} \cdot \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix}^{n+1,k+1} + \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^{n+1,k+1}. \end{aligned}$$

Or, for ease of notation:

$$\mathbf{F}^{n+1,k} + \mathbf{J} \cdot (\ddot{\mathbf{X}}^{n+1,k+1} - \ddot{\mathbf{X}}^{n+1,k}) = \mathbf{M} \cdot \ddot{\mathbf{X}}^{n+1,k+1} + \mathbf{C} \cdot \dot{\mathbf{X}}^{n+1,k+1} + \mathbf{K} \cdot \mathbf{X}^{n+1,k+1}$$

$$\Leftrightarrow (\mathbf{J} - \mathbf{M}) \cdot \ddot{\mathbf{X}}^{n+1,k+1} = -\mathbf{F}^{n+1,k} + \mathbf{J} \cdot \ddot{\mathbf{X}}^{n+1,k} + \mathbf{C} \cdot \dot{\mathbf{X}}^{n+1,k+1} + \mathbf{K} \cdot \mathbf{X}^{n+1,k+1}.$$

In this notation, $\mathbf{J}$ represents the Jacobian matrix, $\mathbf{M}$ the mass matrix, $\mathbf{C}$ the damping matrix, $\mathbf{K}$ the stiffness matrix, $\mathbf{F}$ the force vector and $\mathbf{X}$ the displacement vector. The following Newmark time integration scheme allows further substitutions:

$$\dot{\mathbf{X}}^{n+1,k+1} = \dot{\mathbf{X}}^n + (1 - \beta)\Delta t \ddot{\mathbf{X}}^n + \beta\Delta t \ddot{\mathbf{X}}^{n+1,k+1}$$

$$\mathbf{X}^{n+1,k+1} = \mathbf{X}^n + \Delta t \dot{\mathbf{X}}^n + \gamma\Delta t^2 \ddot{\mathbf{X}}^n + \alpha\Delta t^2 \ddot{\mathbf{X}}^{n+1,k+1}.$$

This finally results in

$$\begin{aligned} (\mathbf{J} - \mathbf{M} - \mathbf{C}\beta\Delta t - \mathbf{K}\alpha\Delta t^2) \ddot{\mathbf{X}}^{n+1,k+1} \\ = -\mathbf{F}^{n+1,k} + \mathbf{J} \cdot \ddot{\mathbf{X}}^{n+1,k} + \mathbf{C}(\dot{\mathbf{X}}^n + (1 - \beta)\Delta t \ddot{\mathbf{X}}^n) + \mathbf{K}(\mathbf{X}^n + \Delta t \dot{\mathbf{X}}^n + \gamma\Delta t^2 \ddot{\mathbf{X}}^n) \\ \Leftrightarrow \ddot{\mathbf{X}}^{n+1,k+1} = (\mathbf{J} - \mathbf{M} - \mathbf{C}\beta\Delta t - \mathbf{K}\alpha\Delta t^2)^{-1} \left(-\mathbf{F}^{n+1,k} + \mathbf{J} \cdot \ddot{\mathbf{X}}^{n+1,k} + \mathbf{C}(\dot{\mathbf{X}}^n + (1 - \beta)\Delta t \ddot{\mathbf{X}}^n) \right. \\ \left. + \mathbf{K}(\mathbf{X}^n + \Delta t \dot{\mathbf{X}}^n + \gamma\Delta t^2 \ddot{\mathbf{X}}^n) \right) \end{aligned}$$

The forces on the moving cylinders, $\mathbf{F}^{n+1,k}$, are calculated by the flow solver at every coupling iteration k , leading to a new prediction of the displacements through the acceleration $\ddot{\mathbf{x}}^{n+1,k+1}$. This displacement is imposed onto the flow simulation by deforming the mesh in the arbitrary Lagrangian–Eulerian (ALE) mesh motion framework. The iteration loop is repeated until the residual, $((F_1 - m_1 \cdot \ddot{x}_1 - c_1 \cdot \dot{x}_1 - k_1 \cdot x_1)^2 + (F_2 - m_2 \cdot \ddot{x}_2 - c_2 \cdot \dot{x}_2 - k_2 \cdot x_2)^2)^{1/2}$ has decreased 3 orders of magnitude at least.

Solving the FSI-loop requires knowledge of the derivatives in $\mathbf{J}$, which are not generally available. Therefore, they are estimated in the first two coupling iterations of each time step using a perturbation δ of the acceleration:

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,0} = \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^n,$$

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,1} = \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^n + \begin{pmatrix} \delta \\ 0 \end{pmatrix},$$

and

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^{n+1,2} = \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix}^n + \begin{pmatrix} 0 \\ \delta \end{pmatrix}.$$

At $k = 1$, the first column of $\mathbf{J}$ can be estimated:

$$\frac{\partial F_1}{\partial \ddot{x}_1} = \frac{F_1^{n+1,1} - F_1^{n+1,0}}{\ddot{x}_1^{n+1,1} - \ddot{x}_1^{n+1,0}} = \frac{F_1^{n+1,1} - F_1^{n+1,0}}{\delta} \text{ and}$$

$$\frac{\partial F_2}{\partial \ddot{x}_1} = \frac{F_2^{n+1,1} - F_2^{n+1,0}}{\ddot{x}_1^{n+1,1} - \ddot{x}_1^{n+1,0}} = \frac{F_2^{n+1,1} - F_2^{n+1,0}}{\delta}.$$

At $k = 2$, the second column of $\mathbf{J}$ can be estimated:

$$\frac{\partial F_1}{\partial \ddot{x}_2} = \frac{F_1^{n+1,2} - F_1^{n+1,0}}{\ddot{x}_2^{n+1,2} - \ddot{x}_2^{n+1,0}} = \frac{F_1^{n+1,2} - F_1^{n+1,0}}{\delta} \text{ and}$$

$$\frac{\partial F_2}{\partial \ddot{x}_2} = \frac{F_2^{n+1,2} - F_2^{n+1,0}}{\ddot{x}_2^{n+1,2} - \ddot{x}_2^{n+1,0}} = \frac{F_2^{n+1,2} - F_2^{n+1,0}}{\delta}.$$

The forces result from the CFD simulation given a certain acceleration. A value of $\delta = 0.1 \text{ m/s}^2$ was found to work well for this simulation. For the Newmark scheme, $\alpha = 1.0$, $\beta = 1.0$ and $\gamma = 0.0$ were used, which is in fact a backward Euler scheme.

The system constants of the tubes were computed from the stiffness, frequency and damping ratio and are actually equal for both tubes. The stiffness was calculated by applying beam theory to the flexible blade and considering the cylinder to which it is connected as perfectly rigid, using the dimensions and material properties in Section 1.2. The ratio between a force applied in the cylinder's middle and its displacement at the same location yields a stiffness of $k_1 = k_2 = 6857.14 \text{ N/m}$. The displacements that are obtained from the FSI simulations also consider the middle of the tube, by using this stiffness factor. They are scaled with a factor of 1.73 to obtain the displacement at the end of the cantilevered cylinder, which was derived

using beam theory as the ratio between the displacement at the tube endpoint and the tube midpoint.

From the stiffness and the natural frequency (14.18 Hz), the masses were derived as $m_1 = m_2 = 863.835 \times 10^{-3} \text{ kg}$. Using the damping ratio of 0.045 % the damping constants $c_1 = c_2 = 69.2675 \times 10^{-3} \text{ Ns/m}$ were obtained.

1.3.4 Uncertainty quantification

To propagate the uncertain pitch velocity U_p , the non-intrusive polynomial chaos method [27, 35] proposed in GO-VIKING Deliverable 5.3 is used.

For expansion of a generic stochastic outcome $s(\vec{x}, t, \vec{\xi})$ in polynomials Ψ_k of the random vector $\vec{\xi} = (\xi_1, \xi_2, \dots, \xi_d)$ (the components of $\vec{\xi}$ assumed mutually independent for the purpose of this work), one can write [35]:

$$s(\vec{x}, t, \vec{\xi}) = \sum_{k=0}^{\infty} s_k(\vec{x}, t) \Psi_k(\vec{\xi}) \approx \sum_{k=0}^P s_k(\vec{x}, t) \Psi_k(\vec{\xi}).$$

Applied to this work, $\vec{\xi}$ would only have one component being the uncertain pitch velocity U_p , and $s(\vec{x}, t, \vec{\xi})$ is a scalar outcome, being the RMS vibration amplitude. The expansion can be seen to have a deterministic part and a stochastic part. The first one is defined by the coefficients $s_k(\vec{x}, t)$, also called the stochastic modes of the expansion, with $\vec{x}$ representing a spatial coordinate and t representing time. The second part is one of the polynomials $\Psi_k(\vec{\xi})$. The number of terms $P + 1$ is related to the expansion order, i.e. the largest polynomial order o present in the sum, as follows [26]:

$$P + 1 = \binom{o + d}{o} = \frac{(o+d)!}{o!d!},$$

with d the number of dimensions of the stochastic vector $\vec{\xi}$, in this case 1.

The coefficients/modes $s_k(\vec{x}, t)$ are multiplied by the polynomials Ψ_k of the random variable $\vec{\xi}$, which are orthogonal according to the following inner product:

$$\langle \Psi_i(\vec{\xi}), \Psi_j(\vec{\xi}) \rangle = \int_{\Xi} \Psi_i(\vec{\xi}) \Psi_j(\vec{\xi}) f_p(\vec{\xi}) d\vec{\xi} = \delta_{ij},$$

with Ξ the support (which can be infinite) of weight function $f_p(\vec{\xi})$.

$s(\vec{x}, t, \vec{\xi})$ is approximated by its spectral decomposition, much akin to Fourier decomposition. The set of polynomials is directly related to the weight function $f_p(\vec{\xi})$, due to the orthogonality property. For example, the standard normal distribution corresponds to Hermite polynomials. A PCE approach where the weight function is matched to the probability density is referred to as the generalized Polynomial Chaos (gPC) method as described in reference [35].

Different non-intrusive approaches exist, but they all determine the coefficients based on a sampling of the stochastic output, thus the model is run in a deterministic way for different

realizations of the stochastic input. In this work, the PCE coefficients are determined using a least-squares regression method [27]. This means that the sample size should be at least $P + 1$.

Simulations were run for 5 different values of U_p , given in Table 1, allowing a polynomial chaos expansion up to the 4th order.

Table 1: The different values of U_p used for which the simulation model was evaluated to propagate the uncertainty.

U_p (m/s)	1.0764	1.1549	1.2259	1.2968	1.3753
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A general advantage of non-intrusive methods is that the different deterministic evaluations can be run in parallel, with optimal efficiency as they are completely separate computations. This property has extensively been exploited to execute the sample evaluations for this work in a reasonable amount of time. The non-intrusive PCE method is implemented in the open-source Python software package Chaospy² [25].

The FSI simulations were run for 15 200 time steps, which corresponds to 7.6 s of flow time. The first 1 s of flow time was not included in the computation of the RMS displacements, to omit the initial transient. This initial transient comprises the start-up of the simulation from initial conditions, as well as the time it takes for the bubbles to travel from the inlet and reach cylinders 4 and 7.

As the RMS-value of the tip displacement converges rather slowly in time, each sample point was evaluated in 5 parallel simulations, to leverage the parallelization possibility. By assuming that the vibration signal in stationary regime is an ergodic stochastic process, the RMS was computed as the ensemble average of these 5 parallel simulations, to improve the estimate. It is noteworthy that the 5 parallel simulations for each value of U_p did use a different value of the bubble diameter, ranging from 20 mm to 30 mm, to allow to study its effect simultaneously, although no significant influence of the diameter in this range was found.

The computational cost of a typical simulation after reaching the stationary FSI regime was around 10 000 core hours per second of flow time, using 256 AMD EPYC 7763 cores for each simulation. With 15 200 time steps, or 7.6 seconds of flow time simulated, for $5 \times 5 = 25$ simulations, this yields an estimate of 1.875×10^6 core hours used in total.

1.4 Results

1.4.1 FSI simulation

Figure 4 shows the FSI result in the frequency domain using the power spectral density of the displacement of the cylinders. It can be seen that there is a low-frequency plateau, related to the presence of the bubbles in the flow, which is present until the first resonance peak at about 12.6 Hz. This frequency is close to the natural frequency of 14.18 Hz, but slightly

² <https://chaospy.readthedocs.io>

reduced due to the added-mass effect, as the inertia of the fluid surrounding the cylinders virtually increases their mass.

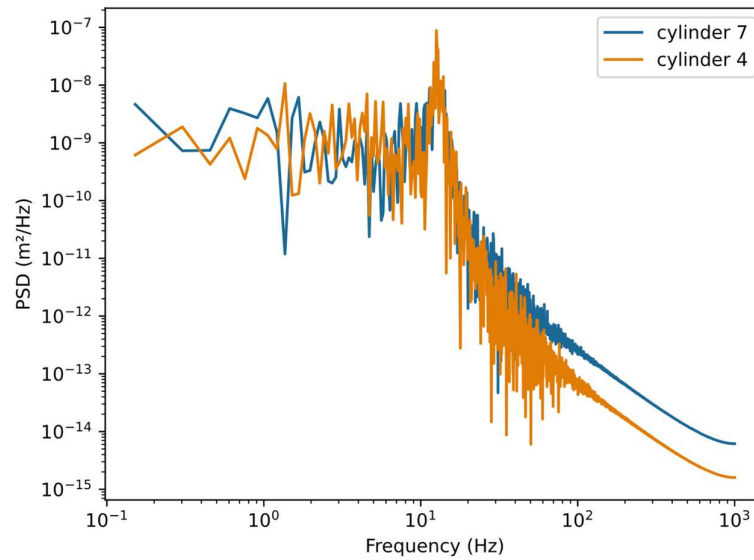
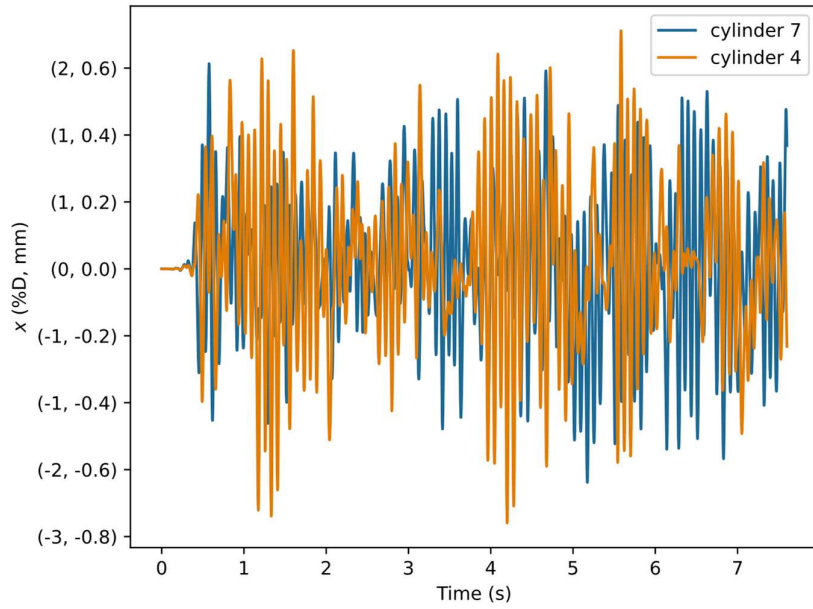
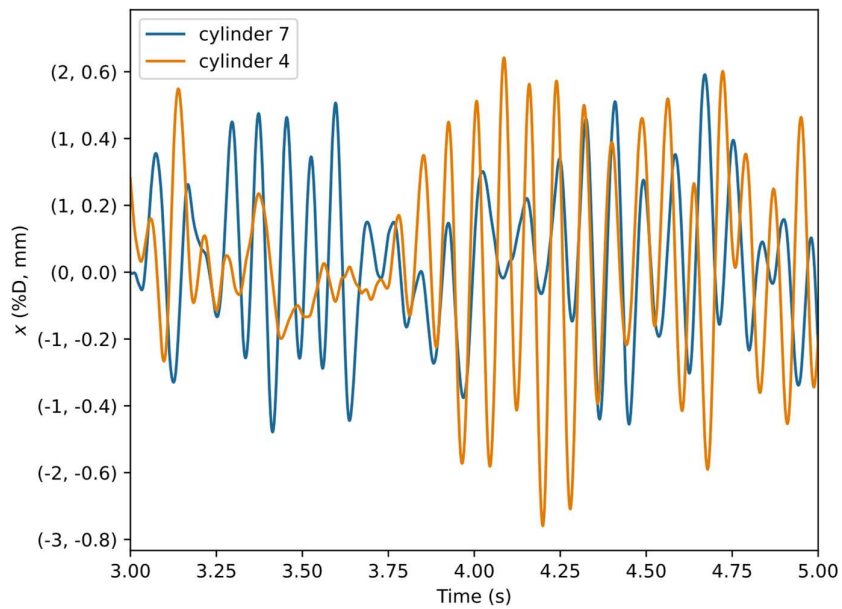


Figure 4: The power spectral density of the displacement signal for $U_p = 1.2259 \text{ m/s}$.

The displacement signals of the cylinders' tip with respect to time are shown in Figure 5, for the simulation with U_p equal to its average value of 1.2259 m/s and a bubble diameter of 25 mm . It can be seen that the vibration starts after about 0.4 s , when the bubbles start reaching cylinder 4 and 7 after their upward journey from the inlet. The signal is confirmed to be periodic, but the amplitude is variable over time. This is related to the chaotic nature of the exciting loads on the cylinders. From the zoomed-in plot (Figure 5b), it can be seen that the figures are smooth and well-resolved in time. The maximal deflection of the tip is about 0.6 mm , or 2 % of the diameter of the cylinders, for both cylinders. Cylinder 4 and 7 have an RMS amplitude of 0.2498 mm and 0.2258 mm for this simulation, respectively.



(a)



(b)

Figure 5: (a) Displacement signal of the cylinder's tip as a function of time and (b) zoomed-in version between 3 s and 5 s, for $U_p = 1.2259$ m/s.

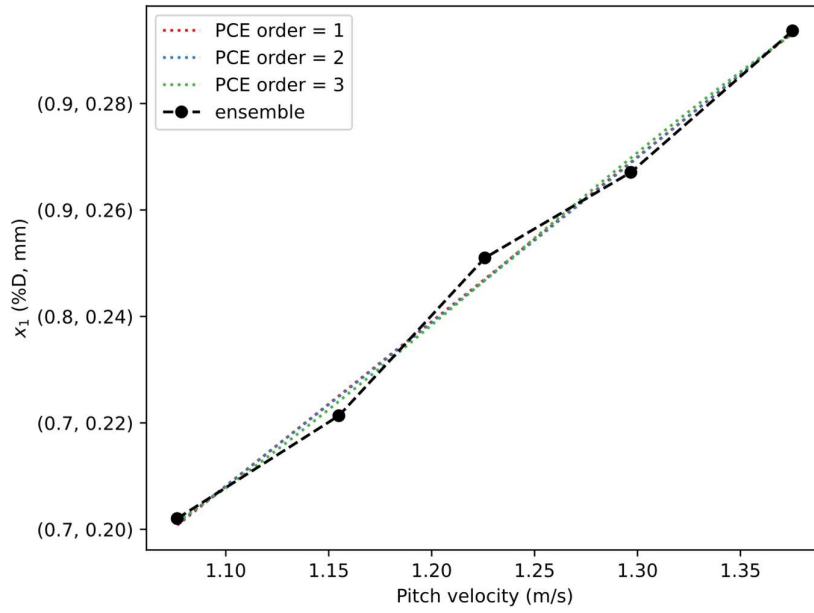
1.4.2 Uncertainty quantification

As mentioned in Section 1.3.4, the polynomial chaos expansion coefficients were determined using the least-squares method, fitting to simulation results for 5 different values of U_p . For each value, an ensemble average of the 5 simulations with different bubble diameter was taken to speed up the statistical convergence of the RMS-value of the tip displacement. The ensemble averaged results are shown as the black dashed line in Figure 6. It can be seen that the models converge quickly as a function of the polynomial order.

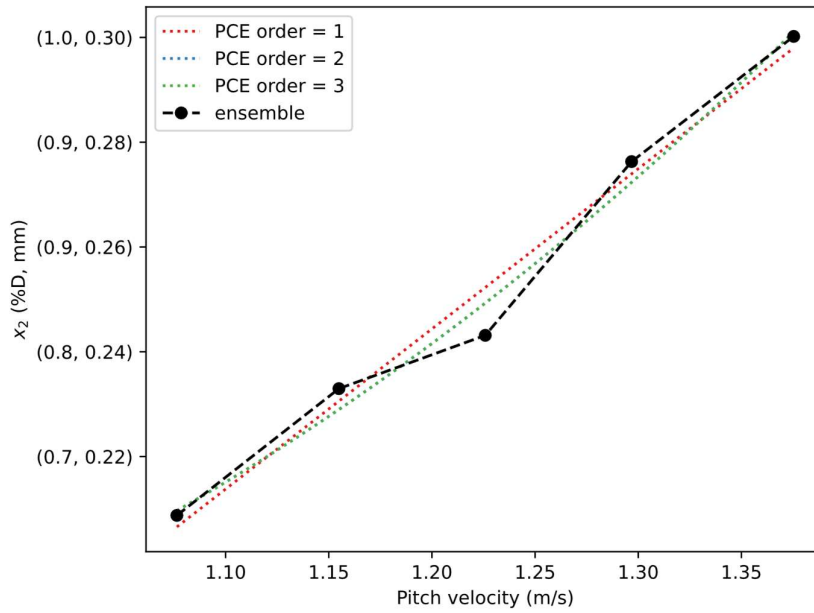
A 4th order expansion (not shown) leads to an overfitting phenomenon, strongly distorting the results. This behaviour is related to the RMS value not being completely converged, as is most apparent in the ensemble average shown in Figure 6. Its remaining error limits the polynomial chaos order that can be used.

Table 2: Descriptive statistics of the RMS vibration amplitude for cylinder 7 and cylinder 4, for the 1st, 2nd and 3rd order polynomial chaos expansion.

	Order 1	Order 2	Order 3
Cylinder 7			
Expected value RMS (mm)	0.2470	0.2469	0.2469
Standard deviation RMS (mm)	0.0162	0.0162	0.0167
Coefficient of variation RMS (%)	6.55 %	6.56 %	6.77%
Cylinder 4			
Expected value RMS (mm)	0.2523	0.2500	0.2500
Standard deviation RMS (mm)	0.0160	0.0160	0.0162
Coefficient of variation RMS (%)	6.34 %	6.41 %	6.41 %



(a)



(b)

Figure 6: Comparison between het ensemble averaged RMS over the bubble diameter of (a) cylinder 7 and (b) cylinder 4 for each pitch velocity U_p (see Table 1) and the polynomial chaos models for the expansion order ranging from 1 to 3.

The descriptive statistics of the RMS vibration amplitude for both cylinders are summarized in Table 2. The convergence in terms of polynomial order is confirmed to be good, evidenced by the consistent values obtained here. A coefficient of variation of U_p of 4.27 % is seen to lead to an output coefficient of variation of the vibration amplitude of about 6.5 %.

A Gaussian kernel density estimator (KDE) is constructed in Chaospy by a Monte Carlo sampling of the polynomial chaos expansion, which serves as a surrogate model between the uncertain input and output. It can be used to visualize the probability density function, as is done in Figure 7. It can again be seen that the results are consistent over the different expansion orders. The 1st order approximation of the uncertainty of the vibration of cylinder 4 deviates the most, predicting a slightly higher mean value than the other PDFs as was observed in Table 1 as well.

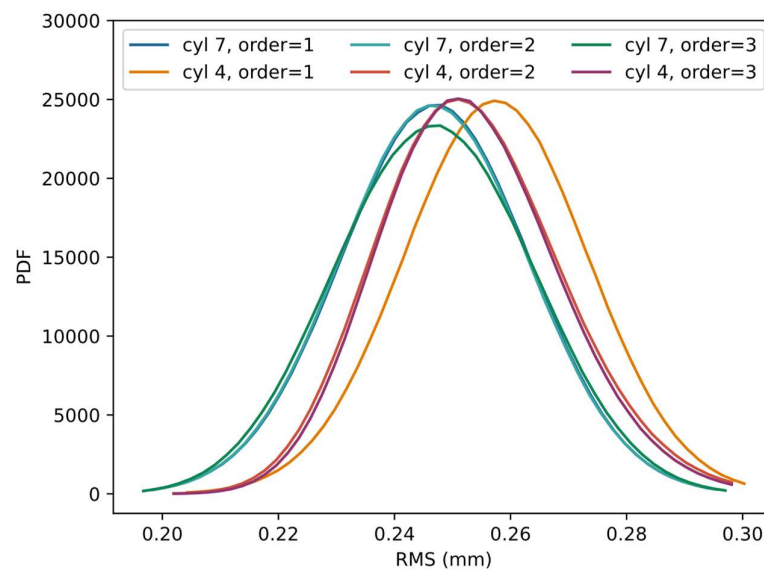


Figure 7: Probability density function of the vibration amplitude of cylinder 7 and cylinder 4, obtained through a KDE.

1.4.3 Comparison with TITAN experiment

Figure 8 compares the simulation data used to fit the polynomial chaos model to the experimental measurements taken from the TITAN experimental setup. It can be seen from this figure that the RMS amplitudes are underestimated by a factor 3 at lower velocities to 5 at higher velocities. One possible reason is the use of the implicit VOF approach, together with a 1st order discretization schemes. These modelling choices may have been overly dissipative.

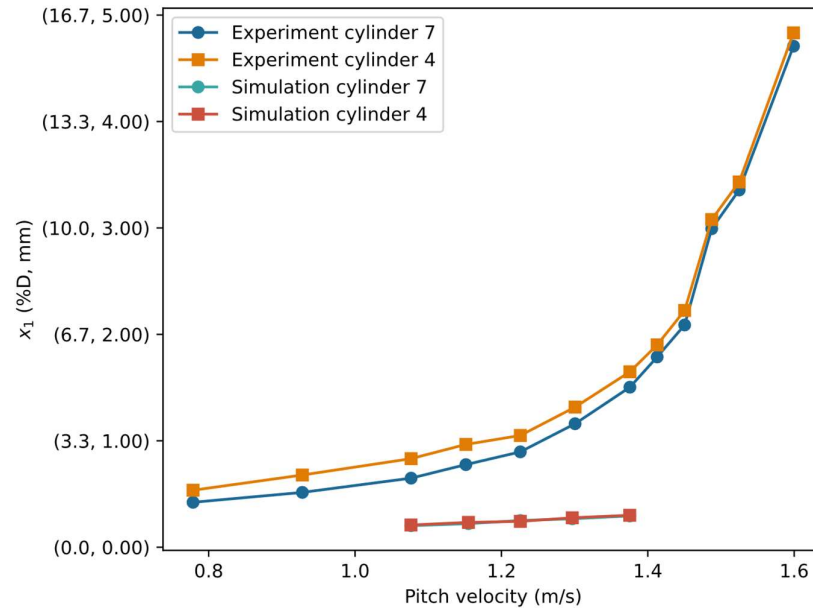
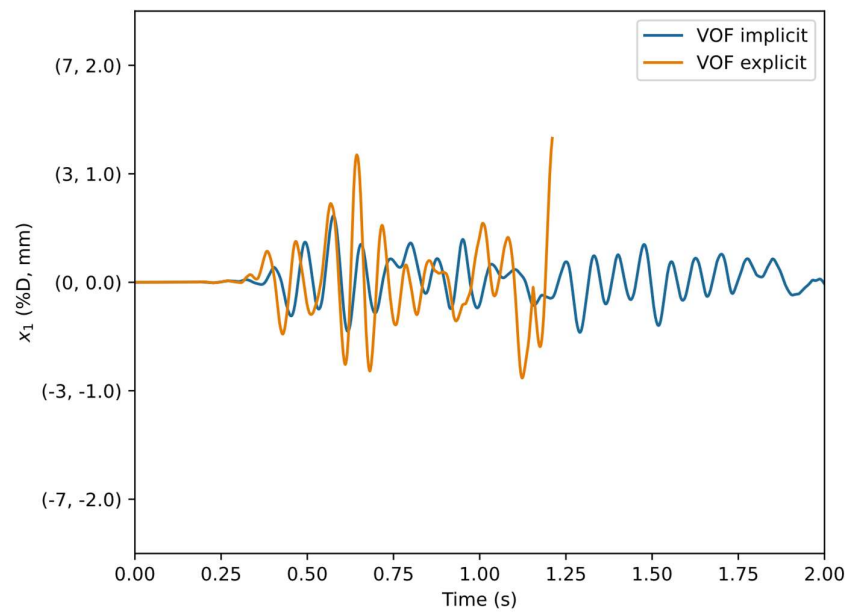
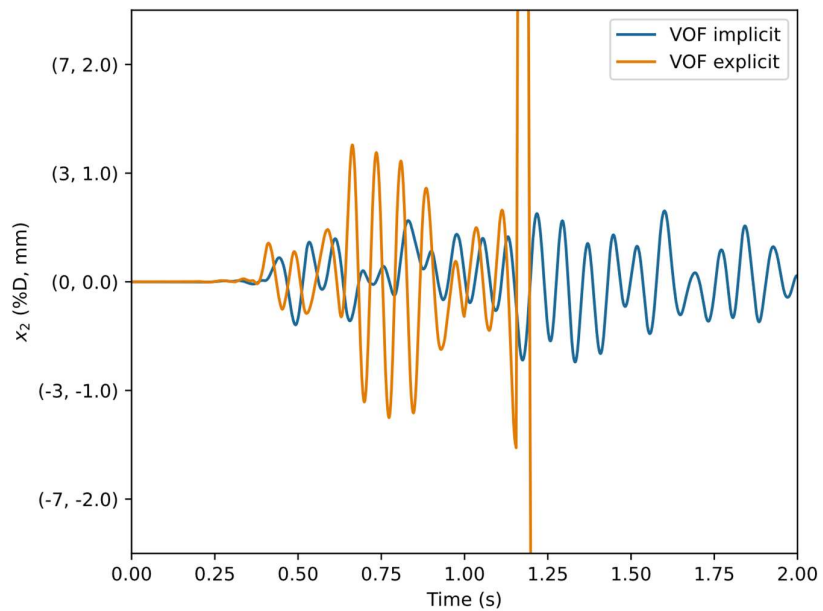


Figure 8: Comparison between the RMS vibration amplitude obtained via the FSI simulations and experimental measurements for cylinder 7 and 4 of the TITAN setup.

Figure 9 shows the displacements obtained from a simulation with an explicit VOF approach, which can be seen to be larger. This results from the larger forces, as evidenced by Figure 10. Unfortunately, no reliable convergence could be achieved with the explicit approach, such that only a simulation time of 1.21 s could be obtained. This is insufficient to obtain a converged value of the RMS vibration amplitude. This is illustrated by Figure 11, showing how the value of the RMS of cylinder 7 changes in a longer simulation. Even at the total simulation time of 7.6 s, changes in RMS value can be perceived. Two longer simulations were run as a test, but also their RMS values still exhibit variation. The slow convergence of the RMS value with respect to time is one of the major challenges of performing UQ for a vibration problem, and could be the reason 4th order polynomial chaos lead to overfitting.

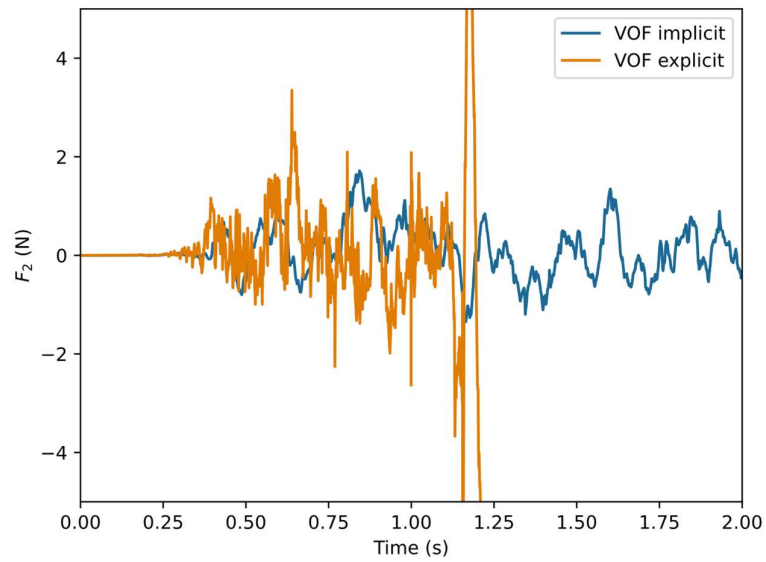


(a)

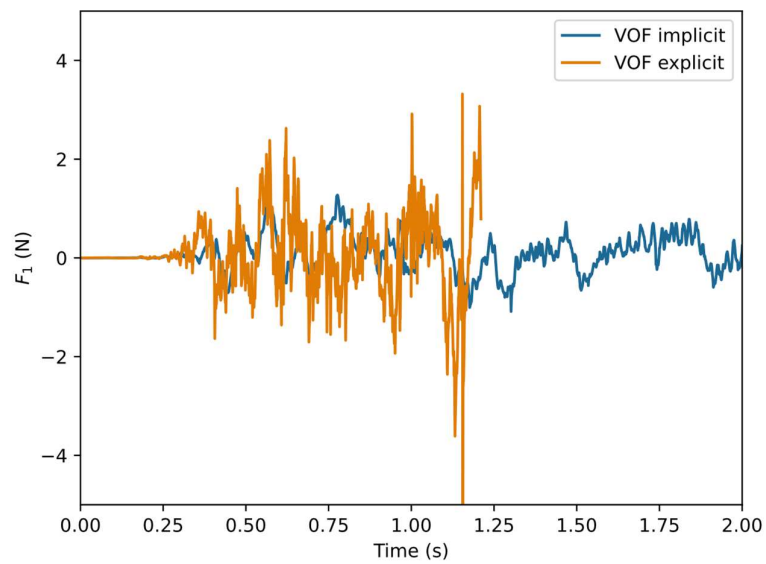


(b)

Figure 9: Displacement versus time resulting from the implicit VOF approach compared to the explicit VOF approach for (a) cylinder 7 and (b) cylinder 4.



(a)



(b)

Figure 10: Force versus time time resulting from the implicit VOF approach compared to the explicit VOF approach for (a) cylinder 7 and (b) cylinder 4.

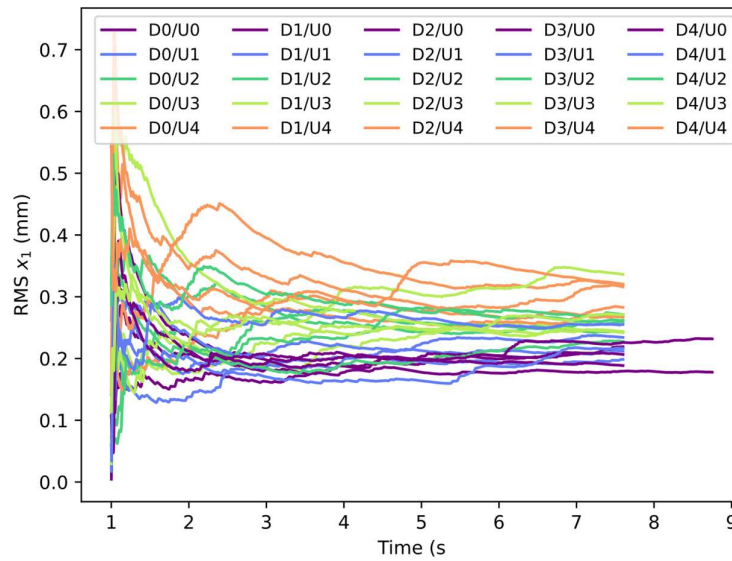


Figure 11: Convergence of the value of the RMS vibration amplitude for cylinder 7 w.r.t. the final time step included in its calculation, for all simulations included in the polynomial chaos model. The legend indicate the different diameters and velocities.

The numerical dissipation caused by the modelling choices is not deemed the sole explanation. Modelling the tubes as two coupled 1DOF rigid bodies imposed some sacrifices to be made, such as the single value for the stiffness to be used. This value was derived from the displacement from the middle of the tube. However, in reality, the tip exhibits larger displacements, of which the FSI model is agnostic. A non-linear response to this vibration amplitude, could cause the cylinder to vibrate in the subcritical regime in the simulation, while the experiments show the onset of fluid-elastic instability, as indicated in Figure 8.

Other modelling choices that could be worthwhile to investigate are using a finer mesh and smaller time step, as well as simulating the full depth of the domain instead of $1/3^{\text{rd}}$. Also using smaller bubble diameters was not feasible using the current models, so the effect of bubble diameter could not be investigated. These aspects are however beyond the computational limitations and human resources of UGent in this project. Partners participating in WP4 specifically aim at reproducing TITAN numerically in the best possible way. Feeding their simulation results to the UQ methodology could yield improved results.

1.5 Conclusion

This deliverable presents the demonstration of the UQ techniques to the WP4 TITAN experiment of GO-VIKING, containing two flexibly mounted cylinders in a rigid tube bundle, subject to two-phase cross-flow. The creation of the FSI simulation model required modifications to the Synthetic Bubble Model and the implementation of a 2-DOF rigid body solver.

The polynomial chaos method was used to propagate an uncertain pitch velocity in the RMS vibration amplitude of both flexibly mounted cylinders. The main difficulty to overcome was

the high computational cost of an unsteady flow simulation, as the uncertainty quantification requires an estimate of the RMS that is sufficiently accurate. The bubble diameter did not have a significant effect.

Parallelization was used as much as possible, by partitioning the simulation mesh over 256 cores and running the separate samples simultaneously. However, due to the slow convergence of the RMS and no possibility to parallelize in time, ensemble averaging was applied to get a better estimate of the RMS faster.

Polynomial chaos of 4th order (and beyond) was not feasible, as overfitting to the data leads to a distorted outcome, owing to the RMS-value of the tip displacement not being completely converged. For future work it is advised to use nested quadrature rules, such that different PCE orders can be investigated with spectral projection methods too, which rely on quadrature.

In this work the PCE coefficients were obtained using the least-squares method instead. The accuracy of the RMS was sufficient up to 3rd order polynomial chaos expansions. The polynomial chaos surrogate models, along with the descriptive statistics and probability density function, converged well with the polynomial order. A variability of the pitch velocity of 4.27 % is seen to lead to an output variability of the vibration amplitude of about 6.5 %.

One suggestion for future work is to consider an uncertain void fraction, since this can lead to large uncertainty in the stability threshold prediction for fluid-elastic instability [33].

2. Uncertainty Quantification and Bayesian Calibration of Turbulence Model Parameters in URANS Simulations

2.1 Introduction

2.1.1 Motivation

Turbulence-induced vibration (TIV) and flow-induced vibration (FIV) phenomena represent a major source of structural loading and uncertainty in nuclear fuel assemblies and related engineering systems [1]. Accurately predicting these vibrations requires reliable estimates of the fluctuating fluid forces, which in turn depend on the fidelity of the underlying turbulence modelling. In practical simulations, the Unsteady Reynolds-averaged Navier-Stokes (URANS) equations together with turbulence closures such as the SST $k - \omega$ (SST) model remain the primary tools for predicting mean flow fields and second-order turbulence statistics. However, these closures carry intrinsic model-form uncertainty, originating from empirical coefficients, simplified physical assumptions and limited transferability across flow regimes.

Task 5.2 of the GO-VIKING project addresses this challenge by developing an uncertainty quantification (UQ) framework for turbulence modelling in the context of FIV. A central component of this task is the quantification of turbulence-closure uncertainty and its impact on quantities of interest (QoIs) relevant for vibration prediction. This includes variability in



reconstructed turbulence fluctuations, pressure-fluctuation intensities, turbulent kinetic energy (TKE), and Reynolds-stress components, all of which influence the forcing experienced by structures. By estimating uncertainty in these quantities, Task 5.2 provides the foundation for improved reliability of FIV analyses performed elsewhere in the project.

In order to achieve this, this task combines several elements: Bayesian estimation of turbulence-model corrections based on high-fidelity reference data; non-intrusive UQ techniques such as Monte-Carlo sampling and surrogate-based approaches; and global sensitivity analysis (SA) to identify the most influential turbulence-model parameters. While some activities in Task 5.2 involve coupled FSI simulations, the present deliverable focuses on the fluid-side UQ, calibrating the SST turbulence-model parameters in three representative URANS configurations. These cases—turbulent channel flow, turbulent annular flow, and a blunt-end cantilevered-rod geometry—provide increasing levels of geometric and physical complexity, while remaining sufficiently controlled to isolate model-form uncertainty associated with turbulence closures.

The motivation for this deliverable is therefore twofold. First, it develops and applies a complete UQ pipeline for turbulence-model parameter uncertainty, enabling Bayesian calibration and predictive UQ for selected flow quantities. Second, it provides the uncertainty-aware fluid-dynamics input needed for subsequent FIV-focused simulations in the GO-VIKING project, ensuring that structural analyses in future work stages are informed by quantified uncertainties in the underlying turbulence modelling.

2.1.2 Link to GO-VIKING D5.3

Deliverable D5.3 provided a broad theoretical and methodological overview of parameter estimation and UQ in RANS turbulence modelling. It introduced the fundamental statistical principles and concepts used throughout Work Package (WP) 5, including Bayes' theorem, likelihood construction, model inadequacy, Monte-Carlo sampling, and surrogate-model acceleration techniques. In addition, D5.3 reviewed classical and Bayesian approaches to turbulence-closure coefficient identification, with examples drawn from canonical RANS applications such as isotropic turbulence decay, free shear flows, and flat-plate boundary layers. The deliverable also presented several strategies for estimating Reynolds stresses and addressed model selection and model averaging from a Bayesian perspective.

The present deliverable builds directly on this theoretical foundation. Whereas D5.3 focused on general principles and illustrative examples drawn from classical turbulence-modelling literature, D5.4 applies these ideas within the context of the GO-VIKING project. Specifically, the methods introduced in D5.3—Bayesian calibration, surrogate modelling, model inadequacy treatment, and global SA—are implemented here for three URANS-based test cases of increasing complexity: a turbulent channel flow, a turbulent annular flow, and a cantilevered-rod configuration. D5.4 therefore represents the practical counterpart to the conceptual framework of D5.3, translating the general methodology into a complete end-to-end UQ workflow tailored to the needs of TIV modelling within WP5.

2.1.3 Objectives



The main objective of this deliverable is to apply a complete UQ workflow to three turbulent flow configurations of increasing complexity: a plane turbulent channel flow, a turbulent annular flow, and a cantilevered-rod configuration with a blunt end. Together, these cases provide a systematic progression from canonical wall-bounded turbulence to a geometry representative of fluid–structure-interaction (FSI) applications.

A first goal is to identify the most influential parameters in the SST turbulence model for these flows. Global SA is used to determine which model coefficients significantly affect the predicted QoIs, enabling a reduction of the original parameter set to a smaller subset that still captures the dominant sources of model-form uncertainty.

A second objective is the construction of surrogate models that can emulate the dependence of the QoIs on the selected turbulence-model parameters at a fraction of the computational cost of full URANS simulations. For the turbulent channel flow and annular flow cases, Gaussian-process (Kriging) surrogates are employed. For the cantilevered-rod case, both Kriging and polynomial chaos expansion (PCE) are used, allowing a comparison of two surrogate strategies in a more complex flow configuration.

The third objective is to perform Bayesian calibration of the influential turbulence-model parameters using the surrogate models in combination with reference data. This yields posterior probability distributions and recommended calibrated values for the SST coefficients, separately for the canonical flows and for the cantilevered-rod case. These calibrated parameter sets are intended as input for FSI simulations within GO-VIKING.

Finally, the deliverable aims to provide uncertainty-bounded predictions for engineering-relevant flow quantities such as reconstructed pressure fluctuations, TKE, and Reynolds-stress components in the channel and annular flow cases, and predictive posteriors for mean-flow quantities, including the streamwise velocity and TKE, in the fluid-only cantilevered-rod configuration. In this way, the work reported here lays the foundation for uncertainty-aware extensions toward coupled FSI simulations.

2.1.4 Deliverable structure

The remainder of this chapter is organized according to the methodological steps of the UQ workflow and the three computational fluid dynamics (CFD) test cases considered. Section 2.2 introduces the methodological framework used throughout the report. It summarizes the principles of global SA, surrogate modelling and Bayesian inference, and outlines the set of SST turbulence-model parameters considered in the study. Only the information required for reproducibility is provided here, as the theoretical background underlying these methods has already been presented in D5.3.

Section 2.3 presents the three CFD case studies to which the UQ framework is applied. The turbulent channel flow case is introduced first, serving as the canonical configuration used to investigate parameter behaviour across multiple Reynolds numbers. This section describes the numerical setup, the SA performed across four friction Reynolds numbers, and the construction of Gaussian-process surrogate models for the reference case $Re_\tau = 640$. The subsequent Bayesian calibration and predictive posterior analysis are then detailed.



The turbulent annular flow case is discussed next. The same UQ workflow is applied, including SA, surrogate construction and Bayesian calibration, allowing direct comparison with the channel-flow results. Differences in parameter informativeness and predictive behaviour between the two canonical configurations are highlighted.

The third case concerns a blunt-end cantilevered-rod configuration. Owing to its higher computational cost and the absence of high-fidelity fluctuation data, this case is treated as a fluid-only configuration without anisotropic pressure fluctuation model (AniPFM) coupling. Surrogate models based on both Gaussian-process regression (GPR) and PCE are constructed for the two dominant SST parameters identified from the canonical cases. A reduced-dimension Bayesian calibration is then performed, and predictive posteriors for relevant mean-flow quantities are presented.

Section 2.4 provides a cross-case comparison of the dominant parameters, posterior distributions and predictive uncertainties obtained in the three flow configurations. The consistency of parameter influence, the agreement between different surrogate approaches and the overall computational efficiency of the workflow are discussed. Remaining limitations of the current analysis and anticipated next steps within the GO-VIKING project are also outlined.

Finally, Section 2.5 summarizes the main findings and contributions of the deliverable, including the identification of key turbulence-model parameters, the development of surrogate-based UQ tools and the generation of calibrated parameter sets suitable for future FIV-oriented FSI simulations.

2.2 Methodological framework

2.2.1 Sensitivity analysis framework

The first step in the UQ workflow is a global SA designed to determine how uncertainty in the turbulence-model parameters influences the variability of the selected flow quantities. This analysis is carried out using a fully non-intrusive approach [2]: model parameters are sampled from prescribed input distributions, independent CFD simulations are performed for each parameter set, and sensitivity indices are computed from the resulting input–output data.

The procedure begins with the definition of an input parameter space associated with the turbulence model under consideration. Each parameter is assigned an interval that reflects plausible variability based on prior knowledge or literature-reported ranges. Together, these intervals form a multidimensional hyper-rectangle representing the domain of uncertain inputs. No assumptions are made about parameter interactions at this stage; the SA focuses exclusively on the individual effect of each parameter on the QoIs.

Sampling of the parameter domain is performed using Sobol’ low-discrepancy sequences, as implemented in the *SALib* library [3]. This quasi-random sampling method provides uniform coverage of high-dimensional spaces and is well suited for variance-based sensitivity estimation. The number of samples used is selected as a power of two, which improves the convergence behaviour of the Sobol’ sequence. For each sampled input vector, a new CFD case directory is generated automatically from a baseline configuration (default parameter values in OpenFOAM for the turbulence model), and a complete simulation is carried out. The resulting ensemble of simulations forms the dataset used to quantify the sensitivity of the output quantities to the uncertain parameters.

The SA relies on the first-order Sobol’ index, which measures the isolated contribution of a parameter to the variance of a model output. For an output quantity $Y = f(\theta)$, depending on the vector of uncertain inputs $\theta = (\theta_1, \theta_2, \dots)$, the first-order index for parameter θ_i is defined as

$$S_i = \frac{\text{Var}(\mathbb{E}[Y|\theta_i])}{\text{Var}(Y)} \quad (1.2.1)$$

This quantity represents the fraction of the total output variance that can be attributed to variations in θ_i alone, with all other parameters integrated out. The indices are computed independently at each spatial location or QoI, using the *SALib* implementation of the Sobol’ method. Because only first-order indices are considered, no estimation of higher-order interaction terms is required, which reduces the computational cost of the analysis.

In flow configurations where the CFD simulations are expensive—such as geometries involving complex three-dimensional structures—a direct sampling-based SA may be infeasible. In these cases, the same Sobol’ method is applied to a surrogate model trained to approximate the CFD response surface. Once trained, the surrogate can be evaluated repeatedly at

negligible cost, enabling sensitivity estimation without requiring a large number of full CFD simulations.

Overall, this sensitivity-analysis framework provides a systematic and reproducible means of identifying how uncertainty in turbulence-model parameters influences the outputs of interest. The results of this step guide the parameter reduction and surrogate-modelling strategies employed in subsequent stages of the UQ workflow.

2.2.2 Surrogate modelling approaches

Surrogate models are introduced in the UQ workflow to overcome the high computational cost of repeated CFD simulations. In this deliverable, they serve as fast, non-intrusive emulators of the CFD solver, enabling tasks that would otherwise be infeasible using direct simulations—such as Monte-Carlo uncertainty propagation, Bayesian calibration with thousands of likelihood evaluations, and global SA. The basic idea is to approximate the mapping $\theta \mapsto y(\theta)$, where θ denotes the vector of uncertain turbulence-model parameters and $y(\theta)$ denotes the corresponding CFD QoIs. Since full simulations require several hours per evaluation, a surrogate model is trained on a set of CFD samples and then used as a computationally inexpensive substitute for further evaluations. This makes it possible to explore the parameter space extensively and to quantify uncertainty in a statistically robust way.

The surrogate modelling stage is applied after the global SA. Only the parameters identified as influential are retained for surrogate construction. This reduction of dimensionality improves the accuracy and stability of the surrogate models and ensures that computational effort is concentrated on the most relevant physical mechanisms.

To build the surrogates, a set of training samples covering the reduced parameter space is generated using a space-filling design. A Latin Hypercube Sampling (LHS) [4] approach is adopted, providing uniform coverage of the input domain and avoiding clustering of sample points. Each sample defines a distinct CFD case in which the parameter file is modified and the simulation is executed automatically.

Once the ensemble of simulations is completed, the outputs are assembled into a training dataset. This dataset is then used to construct the surrogate models described in the subsequent subsections. GPR is employed for the channel-flow and annular-flow cases, while both GP and polynomial-chaos surrogates are constructed for the cantilevered-rod case. The surrogate models generated in this stage form the backbone of the Bayesian inference and uncertainty-propagation procedures presented later in the following subsections.

Following the sensitivity-analysis stage, surrogate models are built using only the reduced set of influential parameters. As mentioned above, the training data required for these surrogates is generated by sampling the reduced parameter space with LHS. LHS divides each parameter range into equiprobable intervals and draws one sample per interval, ensuring good uniformity and avoiding the clustering effects typical of simple random sampling.

Let $\theta = (\theta_1, \dots, \theta_d)$ denote the reduced parameter vector, where each parameter θ_i lies within a prescribed interval $[a_i, b_i]$. The LHS procedure generates N parameter vectors $\theta = \{\theta^{(1)}, \dots, \theta^{(N)}\}$, with uniform one-dimensional marginals. The number of CFD samples N is selected according to the heuristic $N \approx c d \ln(m)$, where d is the number of retained parameters, m is the number of QoIs for which surrogate models will be constructed, and c is a proportionality constant chosen to achieve the desired accuracy. This guideline provides a moderate growth in sample size as the number of outputs increases, which is important in multi-output surrogate modelling.

For each sample, a dedicated CFD case is generated automatically: the baseline case directory is copied, the parameter file is rewritten with the sampled values, and the solver is executed. After all simulations complete, the outputs $y^{(k)}$ are collected at all sampling locations, forming a dataset of the form $Y = \{y^{(k)}(x_j)\}$, where $k = 1, \dots, N$ indexes simulations and j indexes the QoI output channels. This dataset serves as the input for the surrogate-modelling methods.

2.2.2.1 Kriging/Gaussian Process Regression (GPR)

GPR [5], also known as Kriging, is used in this deliverable to construct non-intrusive surrogate models that approximate the mapping between the selected turbulence-model parameters and the CFD QoIs. The approach provides not only point predictions, but also a measure of epistemic uncertainty associated with the surrogate. This makes GPR naturally compatible with Bayesian inference, where repeated evaluations of the likelihood would otherwise require expensive CFD simulations.

Gaussian-process prior and kernel specification

A Gaussian process defines a prior over functions, $f(\theta) \sim \mathcal{GP}(m(\theta), k(\theta, \theta'))$, where $m(\theta)$ is the prior mean (taken as zero after normalization) and $k(\theta, \theta')$ is the covariance kernel. In this work, each QoI is modelled with a GPR surrogate using a kernel of the form

$$k(\theta, \theta') = C \cdot \exp\left(-\frac{1}{2\ell^2} \|\theta - \theta'\|^2\right) + \sigma_n^2 \delta_{\theta\theta'}, \quad (1.2.2)$$

which corresponds to a scaled radial-basis function (RBF) kernel combined with a white-noise term. The RBF kernel provides a smooth approximation of the CFD response, while the white-noise component accounts for unresolved numerical noise in the data. All input parameters are normalized to zero mean and unit variance before training; similarly, all QoIs are standardized component-wise.

Hyperparameter estimation

Each QoI surrogate is trained independently. Kernel hyperparameters $\{C, \ell, \sigma_n^2\}$ are obtained by maximizing the marginal log-likelihood, $\log p(Y | \theta, C, \ell, \sigma_n^2)$, using multi-start optimization to avoid local minima. This ensures an optimal balance between fidelity to the training data and smoothness in the function estimate.

Multi-output Kriging

The CFD solver produces many QoIs per simulation (e.g., velocities, pressures, Reynolds-stress components at multiple spatial locations). Instead of building a single joint GP model, which would be prohibitively expensive, a multi-output surrogate is constructed by training a separate scalar GP for each QoI.

Let $Y = [y_1, \dots, y_M]$ denote the set of M QoIs. For each y_j , a scalar surrogate $\hat{y}_j(\theta)$ is trained independently. These scalar models are then grouped into a lightweight multi-output wrapper: $\hat{Y}(\theta) = (\hat{y}_1(\theta), \dots, \hat{y}_M(\theta))^T$, which returns predictions for all QoIs simultaneously. This strategy avoids the cubic scaling associated with fully correlated multi-output kernels, while allowing each QoI to have its own optimized hyperparameters.

Train/validation split and surrogate validation

To assess the predictive accuracy of the surrogate, the available CFD dataset is partitioned into: a training set, a validation set, and a test set, using a stratified random split. For each QoI, surrogate accuracy is quantified using the root-mean-square error (RMSE) on both the training and validation data. Global surrogate quality is summarized using a normalized RMSE (NRMSE) averaged across QoIs:

$$NRMSE = \frac{1}{M} \sum_{j=1}^M \frac{\sqrt{MSE_j}}{\sigma_j}, \quad (1.2.3)$$

where σ_j is the standard deviation of QoI j . This metric is reported for both training and validation sets to monitor overfitting.

Gaussian-process model-inadequacy correction

Although Kriging approximates the general relationship between parameters and QoIs, small systematic residuals remain due to structural model error of the turbulence model, numerical discretization error, or insufficient smoothness for certain QoIs. To account for this, a second set of GP models is trained on the residuals of the Kriging surrogate:

$$r_j(\theta) = y_j(\theta) - \hat{y}_j(\theta), \quad (1.2.4)$$

for each output channel j . These residual models use a separate RBF-based kernel and are trained on the combined (training + validation) datasets to maximize available information. The corrected surrogate used for Bayesian inference is therefore:

$$\tilde{y}_j(\theta) = \hat{y}_j(\theta) + \hat{r}_j(\theta), \quad (1.2.5)$$

where $\hat{f}_j(\theta)$ is the GP prediction of the inadequacy term. This formulation mirrors the classical Bayesian Model Inadequacy approach, described in D5.3, and ensures that the surrogate represents both interpolation uncertainty and model-form error.

Role of the Kriging surrogate in Bayesian inference

The final multi-output surrogate, augmented with a GP model-inadequacy correction, replaces the CFD solver during Bayesian calibration and enables rapid evaluation of the model response for any parameter vector. It provides fast predictions of all QoIs together with predictive uncertainty derived from the GP kernel and an explicit correction term that accounts for unresolved physical or numerical discrepancies. This combination allows the likelihood $p(y_{\text{obs}} | \theta)$ to be evaluated thousands of times at negligible computational cost, making it feasible to perform efficient Markov Chain Monte Carlo (MCMC) sampling and obtain reliable posterior estimates of the turbulence-model parameters.

2.2.2.2 Polynomial Chaos Expansion (PCE)

PCE [6, 7] is employed as an alternative surrogate-modelling technique for approximating the dependence of CFD QoIs on a reduced set of uncertain model parameters. Unlike GP surrogates, which rely on stochastic process priors, PCE constructs an explicit polynomial representation of the model response in terms of the input parameters. This representation offers excellent efficiency for smooth, low-dimensional input–output maps, which is particularly advantageous when only a small number of parameters remain after the sensitivity-analysis stage.

Polynomial representation on normalized parameter space

Let $\theta = (\theta_1, \theta_2)$ denote the reduced parameter vector retained for surrogate modelling. To utilize classical Legendre polynomials, each physical parameter is linearly mapped to the interval $[-1, 1]$:

$$\xi_i = \frac{2(\theta_i - \theta_i^{\min})}{\theta_i^{\max} - \theta_i^{\min}} - 1, \quad i = 1, 2. \quad (1.2.6)$$

This transformation preserves the uniform input distribution implied by the sampling process. The model response for a given QoI, denoted $y(\theta)$, is approximated as:

$$y(\theta) \approx \sum_{(p,q) \in \mathcal{J}} c_{pq} P_p(\xi_1) P_q(\xi_2), \quad (1.2.6)$$

where $P_p(\cdot)$ and $P_q(\cdot)$ are 1D Legendre polynomials, c_{pq} are deterministic coefficients, $\mathcal{J}$ is the set of index pairs satisfying the total-order constraint $p + q \leq p_{\max}$. The choice of Legendre polynomials follows naturally from their orthogonality under a uniform measure on $[-1, 1]$.

Polynomial-basis construction and truncation



The multivariate polynomial basis is defined using a total-order truncation scheme, which includes all combinations of polynomial degrees satisfying $p + q \leq p_{\max}$. This ensures that the number of basis terms grows moderately with the polynomial order, making PCE practical for low-dimensional parameter spaces. For each candidate order $p_{\max}$, a design matrix Φ is assembled by evaluating every basis function at every sample point. Let N denote the number of CFD samples and n_{terms} the number of basis functions. Then $\Phi \in \mathbb{R}^{N \times n_{\text{terms}}}$, $\Phi_{k,j} = P_{p_j}(\xi_{1,k}) P_{q_j}(\xi_{2,k})$. This matrix is constructed once per polynomial degree.

Coefficient identification via regularized least squares

Each QoI is approximated independently. Given the scaled QoI vector $y \in \mathbb{R}^N$, the polynomial coefficients satisfy:

$$\min_c \quad \|\Phi c - y\|^2 + \alpha \|c\|^2, \quad (1.2.7)$$

where α is a small Tikhonov regularisation parameter used to stabilize the least-squares fit and to limit the effect of near-collinearity between basis terms. This yields the closed-form ridge solution; $c = (\Phi^T \Phi + \alpha I)^{-1} \Phi^T y$. Regularization is particularly useful when the number of samples is close to the number of basis terms.

Model-order selection using K-fold cross-validation

The appropriate polynomial degree is determined through K-fold cross-validation. For each candidate degree $p_{\max}$, the following procedure is applied:

1. Split the dataset into K folds.
2. For each fold:
 - Fit the PCE model on the $K - 1$ training folds.
 - Predict on the held-out fold.
 - Compute RMSE for each QoI.
3. Average RMSE across folds and across QoIs.

The degree $p_{\max}$ minimising the cross-validated RMSE is selected as the optimal order. A final PCE model is then retrained using all available CFD samples and the chosen polynomial order. This provides a principled and data-driven selection of polynomial complexity, preventing both underfitting and overfitting.

Final surrogate and prediction

Once the PCE coefficients are determined, prediction for any parameter value involves:

1. Mapping the parameters to $\xi \in [-1, 1]$.
2. Evaluating the polynomial basis at ξ .
3. Computing: $\hat{y} = \sum_{(p,q)} c_{pq} P_p(\xi_1) P_q(\xi_2)$.

Because this evaluation is purely algebraic and requires no optimisation, PCE prediction is extremely fast and therefore well-suited for Monte-Carlo uncertainty propagation and repeated evaluations within Bayesian inference.

Variance decomposition and Sobol sensitivity indices

The orthogonality of Legendre polynomials enables direct computation of variance contributions from the polynomial coefficients. For a model $y(\theta) \approx \sum_{p,q} c_{pq} P_p(\xi_1) P_q(\xi_2)$, the total variance is

$$\text{Var}(y) = \sum_{(p,q) \neq (0,0)} c_{pq}^2 \langle P_p^2 \rangle \langle P_q^2 \rangle, \quad (1.2.8)$$

where $\langle P_n^2 \rangle = \frac{2}{2n+1}$. The first-order Sobol index for parameter 1 is:

$$S_1 = \frac{\sum_{p>0, q=0} c_{pq}^2 \langle P_p^2 \rangle \langle P_q^2 \rangle}{\text{Var}(y)}. \quad (1.2.9)$$

Interaction and total-order indices follow analogously. Because the computation is analytical, the indices are obtained at virtually no additional cost once the PCE coefficients are known.

Summary and role of the PCE in the workflow

PCE serves in this workflow as a deterministic, closed-form surrogate model that can be evaluated extremely quickly, and therefore, enables efficient uncertainty propagation and Bayesian inference. Its polynomial structure provides robust performance in low-dimensional parameter spaces and offers smooth approximations that are well suited to CFD responses that vary continuously with the inputs. A key advantage is that sensitivity measures, including first-order and total-effects Sobol indices, can be computed analytically from the polynomial coefficients without requiring additional sampling. Within this deliverable, PCE is used as an alternative to GP surrogates for a reduced-parameter case, providing a complementary approximation of the CFD response, facilitating cross-validation of surrogate accuracy, and strengthening the overall UQ framework.

2.2.3 Bayesian inference framework

The Bayesian inference stage combines the surrogate model, the observational/reference data, and prior information on the model parameters to obtain posterior distributions and predictive uncertainty [8]. The overall workflow is identical for all cases, with only the surrogate type (Kriging or PCE) changing. The inference process consists of four components: the likelihood formulation, the prior specification, posterior sampling, and posterior predictive estimation. All steps operate entirely in the reduced parameter space defined after the sensitivity-analysis stage.

Likelihood formulation



For both surrogate types, the likelihood is constructed in the normalized output space, ensuring exact consistency with the scaling used during surrogate training. Given a parameter vector, the surrogate is evaluated, the result is combined with the model-inadequacy correction (for Kriging-based surrogates) if applicable, and residuals with respect to the normalized reference data are computed.

To define the noise model, a residual analysis is performed prior to MCMC. The surrogate is evaluated at all available training inputs, and residuals against the reference data are collected. Two noise representations are extracted:

1. A global scalar variance, used in the Gaussian log-likelihood.
2. A per-output variance, obtained by computing the standard deviation of residuals at each output location.
 - These variances are smoothed, capped, and tapered near boundaries to avoid local overfitting to training artefacts.
 - They are then mapped back to physical units using the stored output scaling.

The resulting likelihood corresponds to a multivariate Gaussian with diagonal covariance. For each parameter vector θ ,

$$\log p(y | \theta) = -\frac{1}{2} \sum_i \left[\left(\frac{y_i - \hat{y}_i(\theta)}{\sigma_i} \right)^2 + \log (2\pi\sigma_i^2) \right], \quad (1.2.10)$$

where, $\hat{y}(\theta)$ is the surrogate prediction and σ_i is either the global or per-output variance depending on the implementation.

The model-inadequacy term appears only in the Kriging workflow. After training the deterministic multi-output GP, residuals are modelled using independent GPRs, and this correction is added at inference time to the surrogate prediction. In this work, the deterministic GP mean (together with the model-inadequacy correction) is used inside the likelihood, rather than the full GP predictive variance. This is consistent with standard CFD surrogate-based UQ practice, where interpolation uncertainty is handled through a separate model-inadequacy term and where using full GP variance in the likelihood is known to be overly conservative.

Prior distribution

A uniform prior is used over the admissible parameter domain. The inference code enforces this by returning $-\infty$ for the log-likelihood whenever a proposed parameter falls outside its prescribed bounds. Thus,

$$p(\theta) \propto \begin{cases} 1, & \theta \in \Theta_{\text{admissible}}, \\ 0, & \text{otherwise.} \end{cases}$$

Posterior sampling

Posterior sampling uses an Adaptive Metropolis algorithm [9]:

1. An initial Gaussian proposal distribution is chosen.
2. The chain proceeds with a Random-Walk Metropolis update.
3. After a burn-in phase, the empirical covariance of the chain is used to adapt the proposal covariance matrix.
4. Samples falling outside the admissible parameter bounds are automatically rejected.
5. The acceptance rate, trace evolution, and distributional stability provide the convergence assessment. (The implementation monitors chain stability rather than relying on automated $\hat{R}$ metrics.)

After burn-in, the remaining samples form an empirical approximation to the posterior;

$$p(\theta | y) \propto p(y | \theta)p(\theta).$$

The method is identical for Kriging-based and PCE-based surrogates, with the only difference being the surrogate evaluation step inside the likelihood.

Posterior predictive distribution

Posterior predictive estimation is performed by Monte Carlo sampling:

$$p(\hat{y} | y) = \int p(\hat{y} | \theta) p(\theta | y) d\theta.$$

For each draw $\theta^{(s)}$ from the posterior:

1. The surrogate model is evaluated in normalized output space.
2. The result is transformed back to physical units.
3. Blocks corresponding to physical probe locations or spatial points are reconstructed in their original ordering.
4. The ensemble of surrogate evaluations is aggregated into posterior means, credible intervals (CIs), and uncertainty bands.

When the Kriging surrogate is used, both deterministic GP predictions and GP inadequacy corrections contribute to the predictive mean. The residual-based standard deviation is inflated slightly to obtain robust uncertainty envelopes. When the PCE surrogate is used, the deterministic PCE prediction directly forms the predictive distribution, with uncertainty arising solely from parameter uncertainty and the residual-based noise model.

Summary of the Bayesian inference framework

The Bayesian inference stage provides the link between surrogate modelling and UQ. Using a likelihood constructed in the surrogate's normalized output space—augmented with a residual-based noise model—and uniform priors defined over the admissible parameter domain, the posterior distribution is obtained through an Adaptive Metropolis sampler that automatically tunes its proposal covariance. The surrogate replaces the CFD solver inside the likelihood, enabling thousands of evaluations at negligible cost while retaining consistency with the original model outputs. Posterior samples are then propagated through the surrogate to construct predictive distributions for all QoIs, yielding posterior means, CIs, and uncertainty envelopes that reflect both parameter uncertainty and surrogate discrepancy. This framework

provides a fully probabilistic calibration approach applicable to all surrogate types used in the deliverable.

2.2.4 Turbulence modelling: Parameter set

The UQ framework in this deliverable requires a clear specification of the turbulence-model parameters that influence the governing equations and that are treated as uncertain in the UQ pipeline. This section summarizes the full set of parameters of the turbulence model used throughout the CFD simulations, presents the relevant equations, and clarifies the physical meaning of each coefficient. All notation follows the conventions used in this deliverable, where coefficients of the k -equation and the ω -equation are denoted by α_{k1}, α_{k2} and $\alpha_{\omega1}, \alpha_{\omega2}$, respectively.

Governing transport equations

The turbulence closure is based on the two-transport-equation k – ω formulation [10] with a cross-diffusion term and a blending function that transitions between near-wall and outer-layer behaviour. The modelled transport equations for the TKE (k) and the specific dissipation rate (ω) are:

- TKE equation

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = P_k - \beta^* \rho k \omega + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\alpha_k} \right) \frac{\partial k}{\partial x_j} \right], \quad (1.2.11)$$

where: $\alpha_k = \alpha_{k1} F_1 + \alpha_{k2} (1 - F_1)$

- Specific dissipation-rate equation

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \frac{\gamma}{\nu_t} P_k - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\alpha_\omega} \right) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \frac{\rho}{\omega} \sigma_{\omega 2} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (1.2.12)$$

where $\alpha_\omega = \alpha_{\omega 1} F_1 + \alpha_{\omega 2} (1 - F_1)$ and $\sigma_{\omega 2} = 1/\alpha_{\omega 2}$.

- Production term

$$P_k = \tau_{ij} \frac{\partial u_i}{\partial x_j}, \tau_{ij} = \mu_t \left(2S_{ij} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij}, \quad (1.2.13)$$

where the strain-rate tensor is $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$. The turbulent eddy viscosity is given by

$$\mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, S F_2)}. \quad (1.2.14)$$

- Blending functions and auxiliary quantities

The formulation transitions between the near-wall k – ω branch and the outer-layer modified k – ε behaviour using blending functions F_1 and F_2 .

Model coefficients and parameter set



The turbulence model contains nine independent coefficients which determine the character of production, diffusion, cross-diffusion, and dissipation in the closure model. These parameters constitute the full uncertainty space used for the global SA [11]. All subsequent sampling (Sobol SA and surrogate-model training) uses these ranges as the prior support.

Table 3: Independent SST turbulence-model parameters used in the UQ workflow, together with the sampling intervals adopted in this deliverable. The coefficients γ_1 and γ_2 are derived from these parameters and are therefore not sampled.

Parameter	Description	Normal value	Sampling interval2
$\alpha_{\omega 1}$	Specific dissipation rate coefficient	0.5	[0.3, 0.7]
$\alpha_{\omega 2}$	Specific dissipation rate coefficient	0.856	[0.7, 1.0]
α_{k1}	TKE coefficient	0.85	[0.7, 1.0]
α_{k2}	TKE coefficient	1.0	[0.8, 1.2]
β_1	Destruction coefficient for ω	0.075	[0.06, 0.09]
β_2	Destruction coefficient for ω	0.0828	[0.07, 0.1]
β^*	Dissipation coefficient for k	0.09	[0.784, 0.1024]
a_1	Cross-diffusion term coefficient	0.31	[0.31, 0.4]
κ	von Kármán constant	0.41	[0.38, 0.42]
γ_1	Derived coefficient	computed	computed
γ_2	Derived coefficient	computed	computed

Derived coefficients γ_1 and γ_2

Two additional model constants enter the ω -equation via the destruction term. They are computed, not sampled. Using the notation in this deliverable:

$$\gamma_1 = \frac{\beta_1}{\beta^*} - \alpha_{\omega 1} \frac{\kappa^2}{\sqrt{\beta^*}}, \gamma_2 = \frac{\beta_2}{\beta^*} - \alpha_{\omega 2} \frac{\kappa^2}{\sqrt{\beta^*}}. \quad (1.2.15)$$

These expressions enforce consistent near-wall behaviour and ensure that the modelled dissipation scales correctly with shear.

Physical interpretation of key parameters

Although all nine coefficients affect the turbulence closure, several play particularly important physical roles:

- β^* — controls the dissipation rate of TKE; directly influences k - ω equilibrium predictions.
- $\alpha_{\omega 1}$ — regulates the strength of the ω -equation in the near-wall region; strongly coupled to shear-layer behaviour.
- β_1 — governs the destruction of ω , affecting the balance between production and dissipation.

- κ — the von Kármán constant, essential for reproducing the log-law; its value impacts both the eddy viscosity and the derived coefficients γ_1, γ_2 .

Together, the parameters determine the shape of the mean velocity profile, the magnitude of turbulent stresses, and the interaction between near-wall and outer-layer turbulence physics.

Use in the UQ workflow

The nine parameters above form the full parameter space for the initial SA. Based on that analysis, only a reduced subset is used for surrogate modelling and Bayesian calibration, but the formulation presented here defines the complete, physically consistent parameter set for the turbulence model.

2.2.5 Summary

Section 2.2 described the methodological framework underlying the UQ workflow used throughout the deliverable. A global Sobol SA strategy was introduced to identify the influential SST model parameters and to reduce the dimensionality of the parameter space. Two surrogate-modelling approaches—Kriging surrogates and PCE—were outlined as fast emulators enabling large-scale sampling and Bayesian inference at negligible computational cost. The Bayesian calibration framework, based on an Adaptive Metropolis MCMC scheme and a residual-based noise model, was presented for estimating posterior parameter distributions and predictive uncertainty. Finally, the full SST parameter set and its role in turbulence production, dissipation, and transport were summarized to motivate the parameter choices used in all subsequent case studies.

2.3 Case studies

2.3.1 Turbulent channel flow case

2.3.1.1 Case setup

The turbulent channel flow is selected as the first configuration for the UQ study because of its geometric simplicity, statistical homogeneity, and the availability of high-fidelity DNS databases. These properties make it a well-established benchmark for evaluating the influence of turbulence-model parameters without complicating geometric effects. To explore the behaviour of the SST model across different turbulence intensities, simulations were performed at four friction Reynolds numbers $Re_\tau = 180, 395, 640, 1020$. These Reynolds numbers correspond to canonical DNS datasets from [12], [13] and [14], which are used for validation of mean velocity, Reynolds stresses, and pressure-fluctuation statistics.

Domain and Boundary Conditions

The computational domain consists of two parallel plates separated by a distance 2δ , where δ is the channel half-height. The streamwise, wall-normal, and spanwise dimensions of the domain are set to 6δ , 2δ , and 3δ , respectively. Periodic boundary conditions are imposed in both the streamwise (x) and spanwise (z) directions, while no-slip velocity boundary conditions are applied at the walls. The flow is driven by a constant body force that is adjusted dynamically so that the resulting friction velocity u_τ matches the target Reynolds number, defined as $Re_\tau = \frac{u_\tau \delta}{\nu}$, where $\nu = 2 \times 10^{-5} \text{ m}^2\text{s}^{-1}$ is the kinematic viscosity.

Figure 12 provides a geometric illustration of the channel-flow configuration described above. The upper schematic shows the full planar channel, while the highlighted rectangular region indicates the portion selected for simulation. The lower diagram zooms into this computational subdomain and visually identifies the streamwise, wall-normal, and spanwise directions. The periodic loops denote the directions in which periodic boundary conditions are applied, and the arrows indicate the mean flow direction. The figure is included to clarify how the mathematically idealized channel-flow geometry is mapped to the three-dimensional CFD domain used in the UQ study.

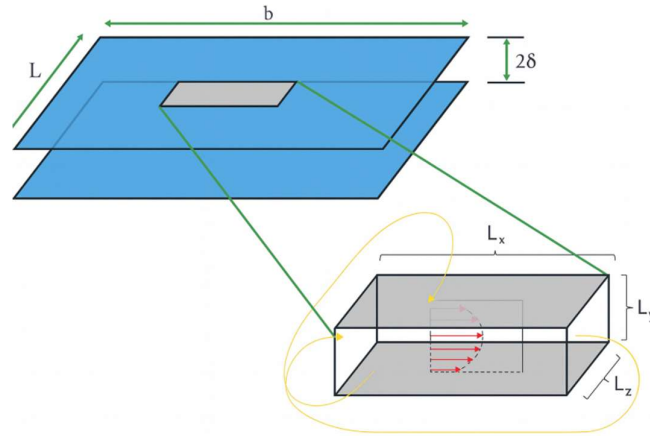


Figure 12: Schematic representation of the turbulent channel-flow configuration. The upper panel shows the canonical two-plate channel, while the lower panel highlights the three-dimensional computational domain used in the simulations, including the periodic directions and mean-flow orientation [15].

Mesh Resolution

A structured hexahedral mesh is used in all simulations. The grid is uniform in the statistically homogeneous directions and geometrically stretched in the wall-normal direction to ensure that the first cell centre lies within $y^+ = \frac{u_\tau y}{\nu} \leq 1$, so that the viscous sublayer is fully resolved. A mesh-independence study is performed for the case $Re_\tau = 640$, using the following three resolutions:

- Coarse mesh: $40 \times 80 \times 30$
- Medium mesh: $50 \times 96 \times 40$
- Fine mesh: $80 \times 112 \times 60$

The medium and fine meshes produce nearly identical mean and RMS flow statistics, while the coarse mesh still captures the essential flow behaviour. Because the UQ pipeline requires a large number of simulations, all SA, surrogate-model training, and Bayesian-inference computations are performed using the coarse mesh. The remaining three Reynolds-number cases ($Re_\tau = 180, 395, 1020$) are used only in the global SA of turbulence-model parameters and do not participate in surrogate or Bayesian modelling.

Figure 13 illustrates the structured hexahedral mesh used in the channel-flow simulations. The figure highlights the uniform grid spacing in the streamwise and spanwise directions, as well as the progressive refinement toward the wall in the wall-normal direction. This mesh layout reflects the resolution strategy described above: uniform cells along the homogeneous directions and a stretched distribution normal to the wall to ensure correct near-wall resolution. The figure is included to visually convey the smooth mesh stretching and overall grid topology used for all mesh-independence and UQ simulations.

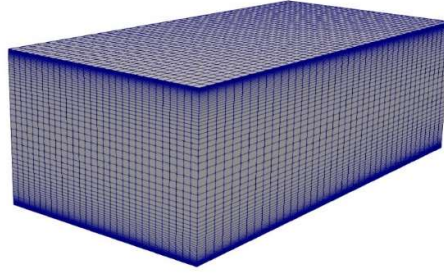


Figure 13: Structured hexahedral mesh employed in the channel-flow case. The grid is uniform in the streamwise and spanwise directions and stretched in the wall-normal direction to achieve adequate near-wall resolution ($y^+ < 1$ at the first cell centre) [15].

Solver Configuration

All computations are carried out using OpenFOAM (OpenFOAM foundation v8). The solution procedure consists of two stages. First, a steady-state RANS calculation is performed using *simpleFoam* with the SST model to initialize the velocity, pressure, and turbulence fields at the desired Reynolds number. This is followed by an unsteady URANS simulation using *pimpleFoam* with second-order backward time integration coupled with the Anisotropic Pressure Fluctuation Model (AniPFM) [15, 16]. The reason for the use of a pressure fluctuation model is that the turbulent fluctuations are not resolved in the RANS approach. In the initial Pressure Fluctuation Model (PFM) [36] local average velocity and turbulence fields are used to create instantaneous velocity fluctuations. With these velocity fluctuations, the pressure fluctuations are calculated and these are added to the averaged pressure and sent to the structural solver as boundary conditions. However, one of the major shortcomings of this initial PFM is that the spatial and temporal correlation of the produced turbulent velocity fluctuations is underpredicted, resulting in a significant underestimation of the Root-Mean Square (RMS) pressure fluctuations. A second shortcoming is that the PFM assumes isotropic turbulence, while the vibrations in fuel rods subjected to axial flow are caused by the turbulence generated at the walls, which is anisotropic in nature. To overcome these limitations, an improved pressure fluctuation model, called AniPFM, has been created [37] and further developed and tested [15, 16]. AniPFM reconstructs the wall-pressure fluctuation spectrum from URANS mean-flow quantities and Reynolds stresses, enabling the prediction of unsteady pressure loads without the computational cost of scale-resolving simulations. The model explicitly incorporates turbulence anisotropy, making it suitable for flows where isotropic assumptions are inadequate. In the present simulations, AniPFM is fully integrated within the URANS framework and evaluated in a one-way coupled manner, where the flow field provides the required turbulence statistics for pressure fluctuation reconstruction.

A Courant-number constraint $CFL \leq 0.5$ is imposed throughout the simulation. Each URANS run is advanced for approximately 10–15 flow-through times, corresponding to 300s of physical time for the $Re_\tau = 640$ case. This duration is sufficient to obtain statistically converged averages. The AniPFM pressure-fluctuation model is enabled, but its parameters

are kept fixed throughout the deliverable, as the present study focuses exclusively on uncertainty in the SST turbulence-model parameters.

Quantities of Interest

For surrogate modelling and Bayesian calibration at $Re_\tau = 640$, several QoIs are extracted at 40 wall-normal locations, giving 160 outputs per simulation. These include the normal Reynolds-stress components $\overline{u'u'}, \overline{v'v'}, \overline{w'w'}$, and the pressure root-mean-square fluctuations, $p'_{\text{rms}} = \sqrt{\overline{p'p'}}$. These QoIs provide direct comparison with DNS results and form the basis for surrogate training and Bayesian inference.

Overall, the channel-flow configuration establishes the foundational behaviour of the SST turbulence-model parameters across multiple Reynolds numbers, provides the data required to identify the dominant parameters, and supports the construction and validation of surrogate models. The $Re_\tau = 640$ case in particular forms the basis for the Bayesian calibration performed later in this deliverable, while the lower and higher Reynolds numbers contribute to assessing parametric trends in the SA.

2.3.1.2 Global sensitivity analysis

A global SA was carried out to determine which of the nine independent turbulence-model parameters of the SST model exert the strongest influence on the channel-flow QoIs. The analysis was conducted at four friction Reynolds numbers, $Re_\tau = 180, 395, 640, 1020$, so that trends across different turbulence intensities could be identified. For each Reynolds number, the nine parameters were assigned independent uniform distributions within literature-supported bounds, and a Sobol low-discrepancy sequences was used to generate the parameter sets for the URANS simulations. For each Reynolds number, the baseline case combined with the 1408 simulations required approximately 15,000 CPU hours, representing the main computational cost of the sensitivity-analysis stage.

The QoIs in this analysis are those produced by the AniPFM reconstruction, rather than the raw URANS fields. AniPFM reconstructs stochastic fluctuations from the mean URANS solution, and therefore its outputs directly reflect the influence of the turbulence-model parameters on the fluctuating part of the solution. The QoIs used in the SA are:

- Root-mean-square pressure fluctuations: $p'_{\text{rms}} = \sqrt{\overline{p'p'}}$
- TKE, $k = \frac{1}{2}(\overline{u'u'} + \overline{v'v'} + \overline{w'w'})$
- Normal Reynolds-stress components reconstructed by AniPFM: $\overline{u'u'}, \overline{v'v'}, \overline{w'w'}$.

These quantities are evaluated at 40 wall-normal locations across the channel, giving a total of 200 scalar outputs for each simulation. Because these outputs are generated entirely by AniPFM, they are particularly sensitive to the interaction between URANS mean-flow predictions and the choice of turbulence-model parameters.

A variance-based Sobol analysis was used to determine the contribution of each parameter to the variability of the QoIs. For a model output Y depending on the vector of parameters $\theta = (\theta_1, \dots, \theta_9)$, the total variance is decomposed as:



$$\text{Var}(Y) = \sum_{i=1}^9 V_i + \sum_{i < j} V_{ij} + \dots + V_{12\dots 9}, \quad (1.3.1)$$

where V_i denotes the variance attributed solely to the parameter θ_i , and the higher-order terms correspond to parameter interactions. The first-order and total-order Sobol indices are defined as

$$S_i = \frac{V_i}{\text{Var}(Y)}, S_{T,i} = 1 - \frac{V_{\sim i}}{\text{Var}(Y)}. \quad (1.3.2)$$

As shown in Figure 14, the first-order Sobol indices reveal a clear and highly consistent hierarchy among the nine SST turbulence-model parameters. Across all five reconstructed quantities—pressure fluctuations, TKE, and the three normal Reynolds-stress components—the dominant contributors to output variability is the parameter β^* . This coefficient directly controls the balance between production and dissipation in the turbulence-model transport equations, and therefore exerts the strongest influence on the URANS mean solution. Since AniPFM generates its fluctuating fields conditioned on the mean flow, this dominance naturally propagates into all reconstructed QoIs.

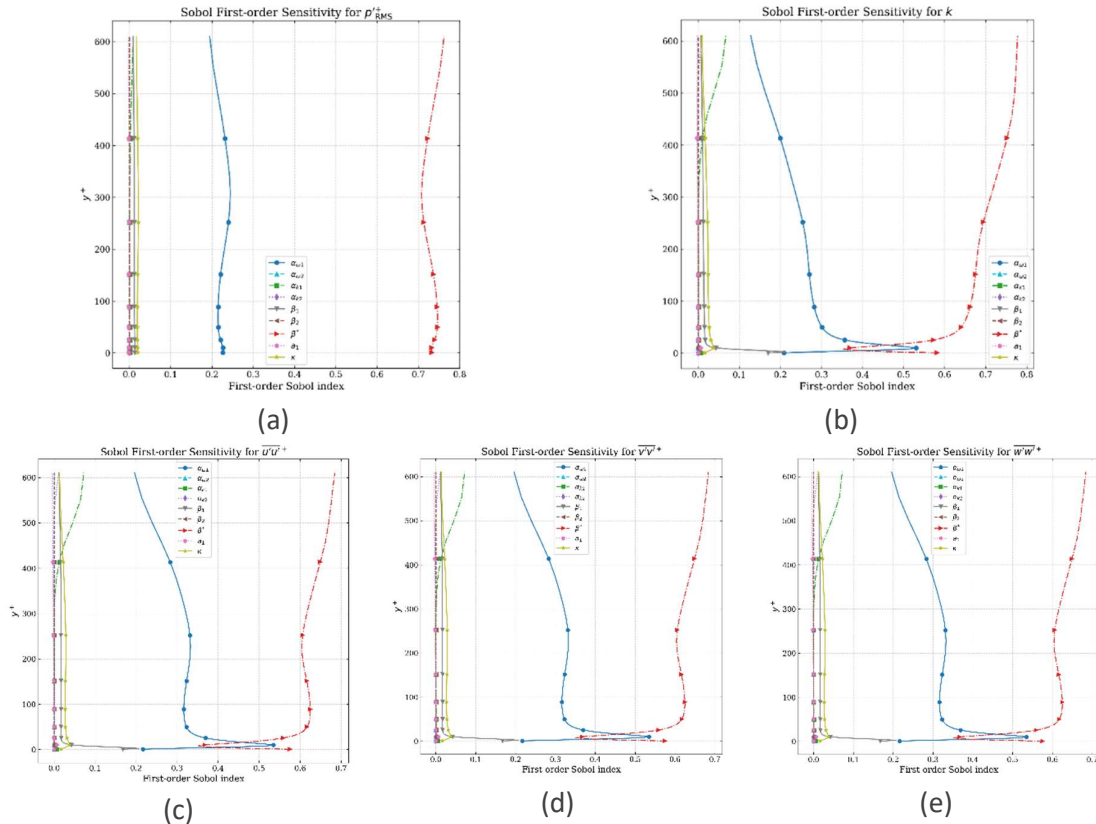


Figure 14: First-order Sobol sensitivity indices for (a) p'_{rms} , (b) k , (c) $\overline{u'u'}$, (d) $\overline{v'v'}$, and (e) $\overline{w'w'}$ across wall-normal locations y^+ .

A second tier of influence is associated with $\alpha_{\omega 1}$ which exhibits non-negligible sensitivity across the entire channel, albeit with consistently lower Sobol index values compared to β^* .

This parameter governs the diffusion and transport of the specific dissipation rate ω , and thus affects the large-scale structure of the reconstructed fluctuations. Its contribution is most visible in the TKE and Reynolds-stress components, especially at higher y^+ values. Closer to the wall, a moderate sensitivity to the von Kármán constant κ and β_1 is observed. This is consistent with κ 's role in shaping the logarithmic-layer velocity gradient, which in turn affects the forcing provided by the mean flow to the AniPFM reconstruction. In addition, β_1 exhibits localized sensitivity in the immediate near-wall region, most notably in the TKE and, consequently, in the normal Reynolds-stress components, reflecting its influence on near-wall turbulence production and dissipation. Although their overall influence remains smaller than that of the leading parameters, they consistently appear across some Qols.

All remaining parameters— α_{k1} , α_{k2} , $\alpha_{\omega2}$, β_2 , α_1 —exhibit negligible contributions for every quantity and across all wall-normal locations. Their Sobol indices remain close to zero, indicating that variability in these parameters does not meaningfully propagate into the reconstructed fluctuations (in particular, although α_{k1} shows marginal sensitivity away from the wall, its consistently low Sobol indices, combined with computational feasibility considerations and the number of simulations required for the UQ study, motivated its exclusion from the set of effective parameters). This finding provides strong justification for reducing the parameter space in subsequent surrogate-model development and Bayesian inference steps to the subset $\{\beta^*, \beta_1, \alpha_{\omega1}, \kappa\}$. The spatial redistribution of sensitivity within the channel also follows a physically interpretable pattern. Near-wall regions are influenced most strongly by parameters affecting shear and the logarithmic-layer structure (primarily κ and β_1), whereas parameters controlling turbulence transport and dissipation (β^* and $\alpha_{\omega1}$) gain prominence farther from the wall. Importantly, despite these spatial variations, the same four parameters dominate the sensitivity structure everywhere, highlighting the robustness of this ranking.

This consistent behaviour across all Qols and wall-normal positions motivates a deeper investigation into how these sensitivities vary with Reynolds number. The next figure therefore compares the aggregated Sobol indices across the four friction Reynolds numbers studied, providing additional insight into how turbulence-model parameter influence evolves with increasing turbulence intensity.

The Sobol sensitivity results remain remarkably consistent across all four friction Reynolds numbers investigated— $Re_\tau = 180, 395, 640, 1020$. At every Reynolds number, only four SST turbulence-model parameters exhibit any meaningful influence on the AniPFM-generated Qols: $\alpha_{\omega1}, \beta_1, \beta^*, \kappa$. Among these, β^* and $\alpha_{\omega1}$ consistently display the largest first-order Sobol indices, confirming their dominant role in controlling the variability of both the reconstructed pressure fluctuations and the Reynolds-stress components. The parameters β_1 and κ show secondary yet non-negligible influence, with their impact concentrated near the wall where they modulate shear production and the logarithmic-layer structure.

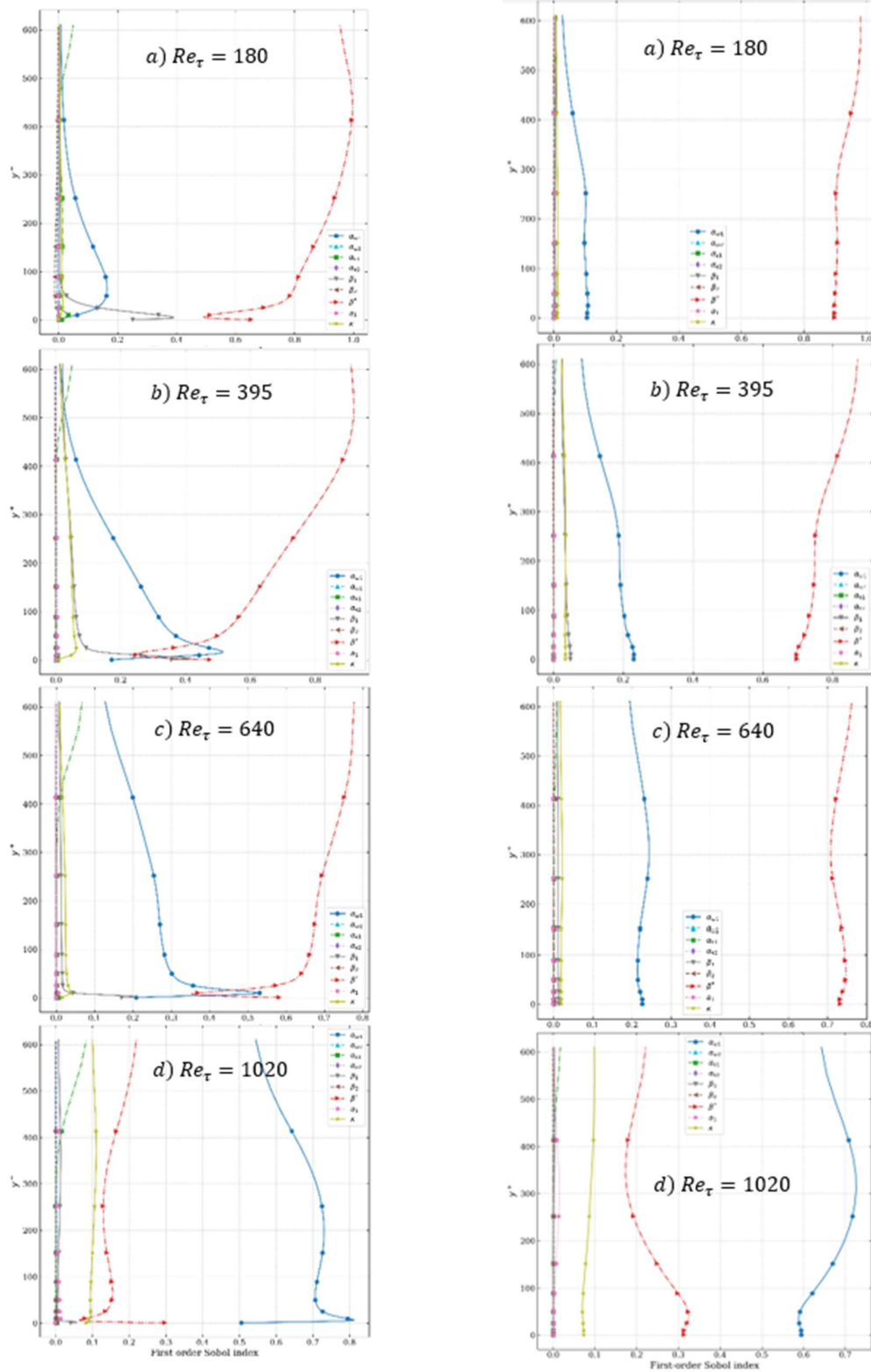


Figure 15: First-order Sobol sensitivity indices for the dominant SST model parameters at (a) $Re_\tau = 180$, (b) $Re_\tau = 395$, (c) $Re_\tau = 640$, and (d) $Re_\tau = 1020$. Results are shown as a function of wall-normal location y^+ for k (left column) and p'_{rms} (right column).

The remaining five parameters maintain Sobol indices close to zero at all wall-normal positions and for all Reynolds numbers, demonstrating that they do not contribute meaningfully to the variability of the URANS+AniPFM outputs. The robustness of this ranking across increasing turbulence intensity indicates that the effective dimensionality of the underlying parametric space is inherently low.

This finding justifies reducing the nine-parameter SST model to a four-parameter subset for all subsequent steps of the UQ workflow for the investigated case. The surrogate modelling and Bayesian inference procedures presented later for this case in this deliverable focus exclusively on these four influential parameters, allowing a significant reduction in computational cost while fully preserving the essential parametric dependence of the reconstructed fluctuations. The analysis therefore establishes a clear, Reynolds-number-independent hierarchy among the turbulence-model parameters and motivates the reduced-parameter Bayesian calibration performed for the $Re_\tau = 640$ case.

2.3.1.3 Surrogate model construction

For the turbulent channel-flow case, surrogate models were constructed to emulate the dependence of the AniPFM-reconstructed quantities on the four influential SST turbulence-model parameters identified in the global SA. The surrogate enables rapid evaluation of the QoIs during Bayesian inference, replacing the expensive URANS–AniPFM simulations while preserving the key parametric dependencies.

Quantities of interest

At each simulation, AniPFM produces: p'_{rms} , $\overline{u'u'}$, $\overline{v'v'}$ and $\overline{w'w'}$, evaluated at 40 wall-normal locations. This results in 160 scalar QoIs per simulation:

$$\text{QoIs} = 4 \text{ parameters} \rightarrow 160 \text{ outputs.}$$

Each QoI is treated as a separate scalar response during surrogate construction, and the resulting models are collected into a lightweight multi-output wrapper.

Training dataset generation

The surrogate was trained using CFD simulations generated via a LHS design in the reduced four-dimensional parameter space:

$$\theta = (\alpha_{\omega 1}, \beta_1, \beta^*, \kappa).$$

The LHS design provides good dispersion across the input space and avoids clustering. Each LHS sample corresponds to a full URANS–AniPFM simulation performed on the coarse mesh, which provides a balance between accuracy and computational affordability. In total, 222 simulations were carried out, corresponding to approximately 2,200 CPU hours. These simulations form the training dataset: $Y = \{y^{(k)}(x_j) : k = 1, \dots, 222, j = 1, \dots, 160\}$. All inputs were normalized, and each QoI was standardized to zero mean and unit variance prior to surrogate training.

Gaussian-process (Kriging) surrogate



A separate Gaussian-process surrogate was fit for each of the 160 QoIs. The surrogate uses a zero-mean GP with an RBF kernel and an added white-noise term to account for small residual inconsistencies in the CFD outputs:

$$k(\theta, \theta') = C \exp\left(-\frac{\|\theta - \theta'\|^2}{2\ell^2}\right) + \sigma_n^2 \delta_{\theta\theta'}. \quad (1.3.3)$$

Each QoI has its own set of kernel hyperparameters (C, ℓ, σ_n^2) , enabling the model to adapt to differences in sensitivity and spatial distribution across the 40 wall-normal locations.

Hyperparameter optimization and validation

Hyperparameters were obtained by maximizing the marginal log-likelihood using multi-start optimization to avoid local minima. For each QoI, convergence to a smooth length scale (consistent with the physics of the response surface) was achieved. To assess predictive performance:

1. Training/Validation Split: The dataset was partitioned into training and validation subsets, and a normalized RMSE was computed for each QoI.
2. Leave-One-Out (LOO) Cross-Validation: A LOO error estimate was calculated using the analytic GP LOO formula, which provides a sensitive measure of local interpolation quality. The resulting LOO error curves across the 40 wall-normal locations were inspected to ensure that: surrogate accuracy remains consistent, no region exhibits excessive extrapolation error, QoIs near the wall (where gradients are sharpest) remain well represented.

Overall, the Kriging surrogate achieved low validation and LOO error for all QoIs, demonstrating that the training dataset provides sufficient coverage of the reduced parameter space.

Final multi-output surrogate

The 160 scalar Kriging models are combined into a multi-output predictor: $\hat{Y}(\theta) = (\hat{y}_1(\theta), \hat{y}_2(\theta), \dots, \hat{y}_{160}(\theta))^T$, which returns the full set of AniPFM-reconstructed quantities at any new parameter value. This surrogate is used throughout the subsequent Bayesian-calibration and UQ stages, replacing expensive CFD evaluations with millisecond-level GP predictions.

2.3.1.4 Secondary sensitivity analysis on surrogate models

To verify that the Kriging surrogate developed for the turbulent channel-flow case accurately reproduces the parametric dependencies present in the full URANS–AniPFM simulations, a secondary global SA was performed directly on the trained surrogate model. The goal of this analysis is to confirm that the surrogate preserves the structure of the Sobol indices obtained from the high-fidelity simulations and therefore can be used reliably in the subsequent Bayesian-inference and predictive-UQ stages.

The comparison is shown in Figure 16 for the reconstructed pressure-fluctuation intensity p'_{RMS}^+ , which serves as a representative QoI. On the left, the first-order Sobol indices computed from the full CFD simulation database are shown; on the right, the corresponding indices calculated using the surrogate model are presented.

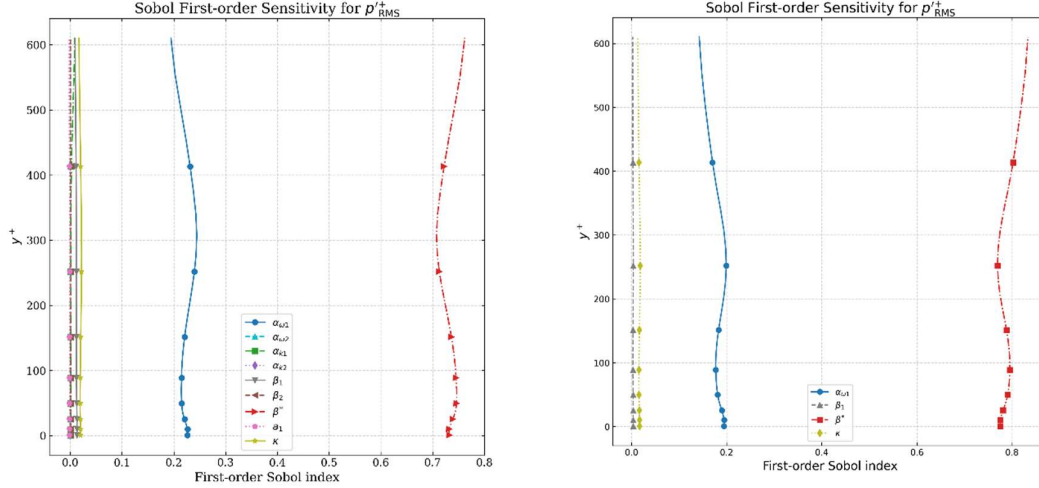


Figure 16: Comparison of first-order Sobol sensitivity indices for p'_{RMS}^+ in the turbulent channel-flow case. Left: Sobol indices computed from the full set of URANS–AniPFM simulations. Right: Sobol indices obtained from the Gaussian-process surrogate model.

The surrogate-based Sobol indices closely match those obtained from the CFD simulations. Both analyses identify β^* and $\alpha_{\omega 1}$ as the dominant contributors across the entire wall-normal domain, with κ and β_1 showing only minor sensitivity localized near the wall. The negligible parameters in the CFD-based analysis remain negligible in the surrogate-based analysis. Importantly, the surrogate does not introduce any spurious sensitivities or suppress any physically meaningful contributions.

The close agreement between the two sets of Sobol indices demonstrates that the surrogate model accurately captures not only the magnitude of the reconstructed pressure fluctuations, but also the way in which these fluctuations depend on the SST model coefficients. This validates the use of the surrogate as a reliable drop-in replacement for the URANS–AniPFM solver in the calibration and UQ workflow, enabling substantial reductions in computational cost while preserving the essential parameter–response relationships.

2.3.1.5 Bayesian calibration

Following surrogate-model construction, Bayesian inference was performed to infer the posterior distributions of the four influential SST turbulence-model parameters,

$$\theta = \{\alpha_{\omega 1}, \beta_1, \beta^*, \kappa\},$$

using the DNS data at $Re_\tau = 640$. The likelihood compares the DNS QoIs (pressure fluctuations, and Reynolds-stress components) with their surrogate-model predictions. The

Gaussian-process surrogate—augmented with a GP model-inadequacy correction—provides the model output required for evaluating the likelihood efficiently during MCMC sampling.

Trace plots and convergence

A Metropolis-adjusted Langevin algorithm with adaptive tuning was used to draw posterior samples. The chain was run for 40,000 iterations after burn-in, giving a dense, well-mixed set of posterior samples for all four parameters. The trace plots (Figure 17) demonstrate excellent mixing across the entire chain for all parameters. No long-term drift or persistent autocorrelation is visible, indicating that the sampler effectively explores the support of the posterior distribution. The samples fill the prior ranges without becoming trapped, confirming that the parameter space is well informed by the data and that the surrogate likelihood is smooth and well-behaved.

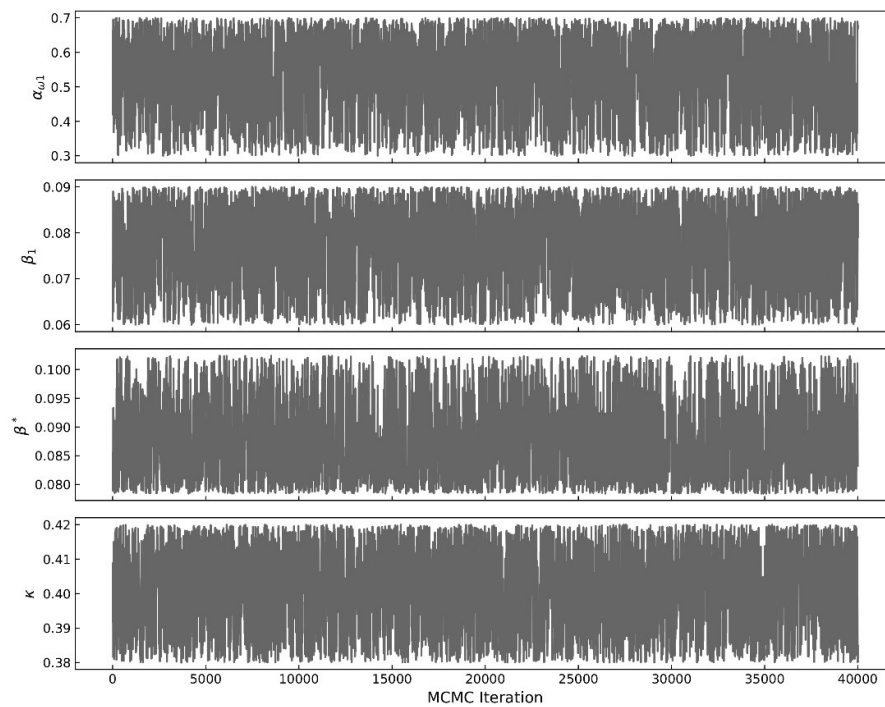


Figure 17: Trace plots of the four SST turbulence-model parameters over 40,000 MCMC iterations.

Posterior dependence structure

The joint posterior distributions shown in the corner plot (Figure 18) reveal distinct dependence patterns between parameters:

- $\alpha_{\omega 1}$ exhibits a moderate correlation with β_1 and β^* , reflecting the interplay between dissipation-rate transport and production-dissipation balance in shaping the reconstructed fluctuations.
- β_1 and β^* show a weak, but noticeable correlation, consistent with their combined role in the turbulent kinetic-energy equation.

- κ is largely independent of the other parameters, with tight uncertainty bounds, reflecting the strong physical constraint imposed by the DNS mean-flow profiles.

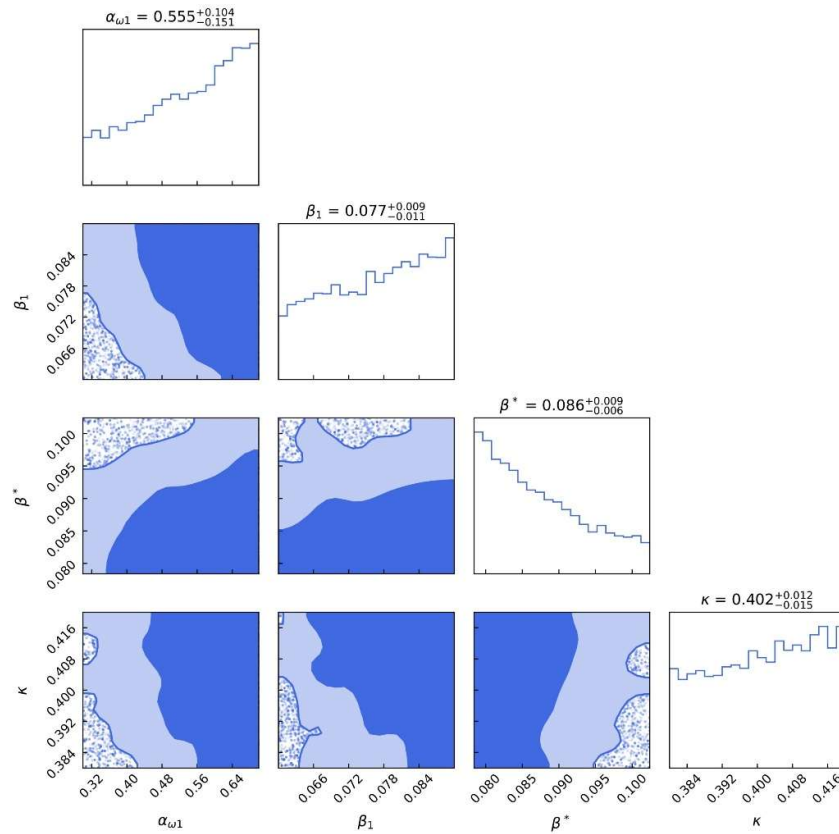


Figure 18: Joint posterior distributions of the four calibrated SST parameters obtained from MCMC samples. Diagonal panels show marginal densities with modes and 68% CIs; off-diagonal panels show bivariate contours revealing correlation structure among parameters.

These correlations highlight the physical compensations that occur when adjusting turbulence-model coefficients while matching the DNS data.

Marginal posterior PDFs

The marginal posterior densities for the four parameters (Figure 19) provide quantitative uncertainty estimates. The posterior modes and 68% CIs (CI) are:

- $\alpha_{\omega 1} = 0.555^{+0.104}_{-0.151}$: A clearly shaped and moderately peaked posterior, substantially narrower than its prior interval. This indicates meaningful parameter learning, with the DNS data suppressing low-valued regions and favouring higher $\alpha_{\omega 1}$, consistent with sensitivity to ω -transport dynamics.
- $\beta_1 = 0.077^{+0.009}_{-0.011}$: A relatively broad and only mildly tilted posterior. The distribution shows weak–moderate identifiability, with parameter values across much of the prior still admissible.

- $\beta^* = 0.086^{+0.009}_{-0.006}$: The sharpest and most concentrated posterior among all parameters. This reflects strong identifiability of β^* from the DNS data and confirms its dominant influence on the reconstructed turbulent kinetic-energy field.
- $\kappa = 0.402^{+0.012}_{-0.015}$: The least informed posterior distribution. The density remains broad and nearly flat, indicating limited learning relative to the prior and highlighting residual structural uncertainty in the near-wall and log-layer representation.

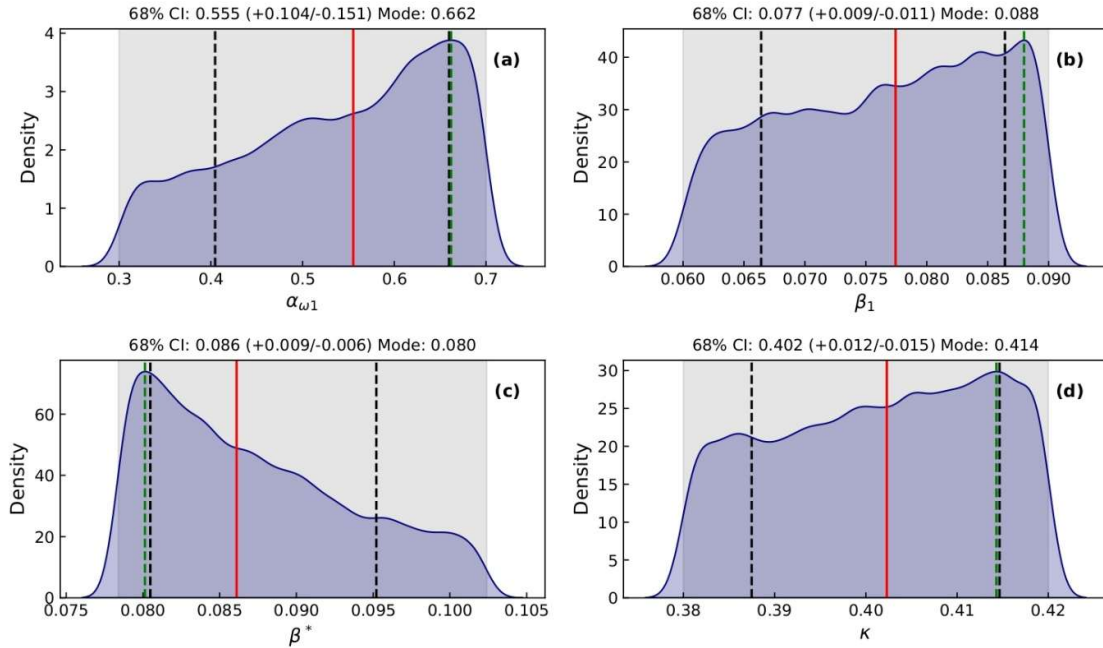


Figure 19: Marginal posterior probability density functions for (a) $\alpha_{\omega 1}$, (b) β_1 , (c) β^* , and (d) κ . Shaded regions denote the 68% CIs, red and green lines indicate posterior median and mode, respectively, and dashed lines mark the credible-interval limits.

Overall, the posterior PDFs differ markedly in sharpness and contraction relative to their prior ranges. The parameters β^* and $\alpha_{\omega 1}$ show clear information gain, with β^* being the most strongly constrained. In contrast, β_1 is only moderately informed, and κ remains weakly constrained, with a posterior shape close to the prior. This hierarchy reflects the respective roles of these parameters in the SST model and aligns with the dominant-parameter trends identified through the global and reduced sensitivity analyses.

Predictive posteriors

After obtaining the posterior distribution of the turbulence-model parameters, predictive posterior distributions were generated for the four key reconstructed QoIs in the turbulent channel flow:

- pressure fluctuations p'_{rms} ,
- streamwise Reynolds stress $\overline{u'u'}$,
- wall-normal Reynolds stress $\overline{v'v'}$,
- spanwise Reynolds stress $\overline{w'w'}$.

For each QoI, the posterior predictive mean and the associated 95% CI were computed by drawing samples from the calibrated parameter posterior and evaluating the multi-output Kriging surrogate. The resulting uncertainty bands quantify the combined effect of parametric uncertainty, surrogate interpolation error, and model-inadequacy correction. The predictive posteriors are shown in Figure 20 (subplots a-d), together with the corresponding DNS reference data.

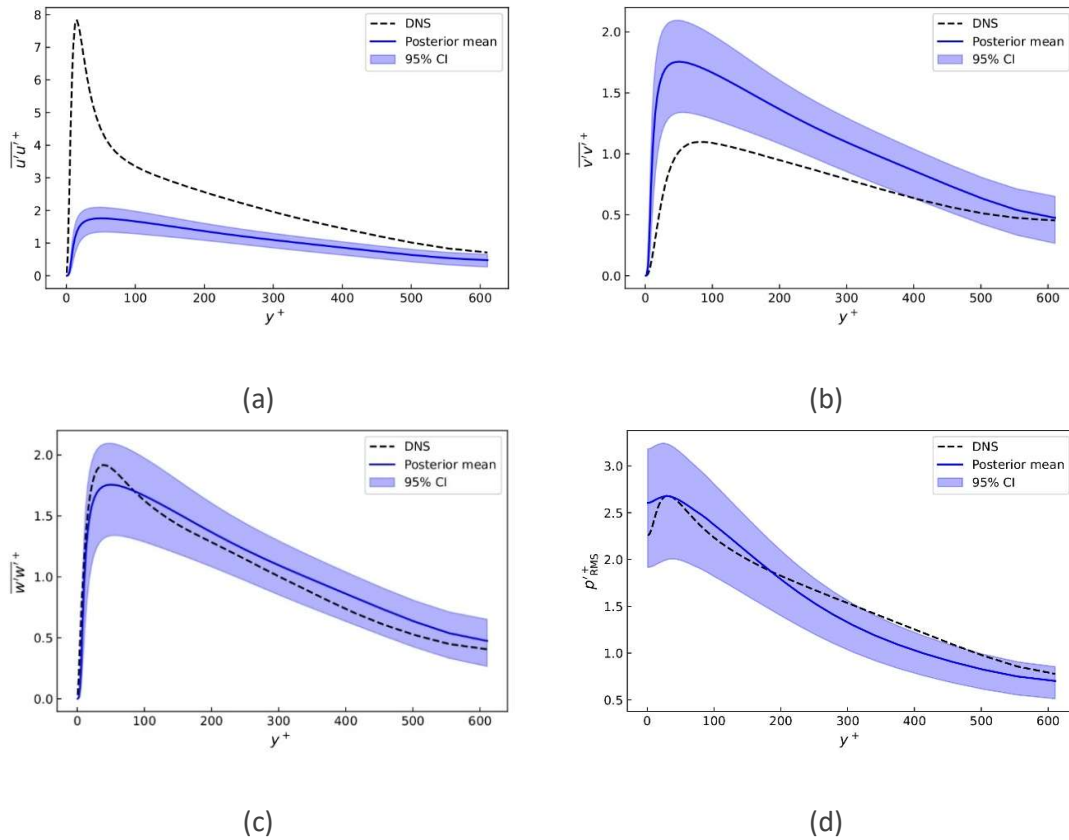


Figure 20: Posterior predictive distributions for the (a) streamwise Reynolds stress $\overline{u'u'}$, (b) wall-normal Reynolds stress $\overline{v'v'}$, (c) spanwise Reynolds stress $\overline{w'w'}$, and (d) pressure fluctuations p_{rms}' in turbulent channel flow at $Re_\tau = 640$. Solid blue lines denote the posterior mean, shaded regions show the 95% CI, and dashed black lines represent DNS reference data.

Comparison with DNS

The predictive posterior bands exhibit several consistent features across all quantities:

- Streamwise Reynolds stress ($\overline{u'u'}$): The posterior mean underpredicts the near-wall peak and the logarithmic-layer decay relative to DNS. Although the uncertainty band widens with wall distance, it remains largely below the DNS curve, indicating that calibration of the four SST coefficients is insufficient to reproduce the true DNS level of streamwise turbulence intensity.

- Wall-normal Reynolds stress ($\overline{v'v'}$): The predictive posterior significantly overpredicts the $\overline{v'v'}$ peak compared to DNS. This behaviour reflects the structural limitations of the URANS–AniPFM coupling: the URANS mean-flow field does not contain sufficient information to reconstruct the correct wall-normal fluctuations, even after parameter calibration.
- Spanwise Reynolds stress ($\overline{w'w'}$): The posterior predictive distribution shows very good agreement with the DNS profile across the entire wall-normal extent. The DNS curve lies well within the 95% credible interval for all y^+ , and the posterior mean reproduces the correct peak location and decay trend. The uncertainty band remains narrow in the viscous sublayer and widens only moderately toward the outer region, reflecting limited parameter sensitivity there. Overall, this result indicates that the calibrated SST model provides a credible and consistent representation of the spanwise Reynolds stress without significant model-form discrepancy.
- Pressure fluctuations (p'_{rms}): The posterior predictive distribution captures the qualitative behaviour of the DNS pressure fluctuations, including the near-wall peak and gradual decay toward the channel centre. The posterior mean slightly underpredicts the DNS curve beyond $y^+ \approx 80$, but the DNS profile remains partially enclosed within the 95% credible interval, particularly in the near-wall and outer regions. This indicates that the calibrated parameters improve the agreement compared to the prior model, although some residual model-form discrepancy persists in the mid-channel region. The width of the uncertainty band reflects the moderate sensitivity of pressure fluctuations to the calibrated parameters and suggests that remaining errors are linked mainly to structural limitations of the turbulence model rather than parameter uncertainty.

Discussion: evidence of model-form error

Taken together, the predictive posteriors for the four QoIs show that parameter calibration improves the agreement with DNS in several regions of the flow, but notable discrepancies remain for certain components. In particular, the calibrated model reproduces the spanwise Reynolds stress well across the full wall-normal extent and partially captures the DNS behaviour of pressure fluctuations. In contrast, the streamwise and wall-normal Reynolds stresses exhibit persistent mismatch with DNS despite parameter adjustment.

These patterns indicate that, for the turbulent channel-flow case, the remaining errors in the predictive posteriors are dominated by structural limitations of the URANS–SST model and the AniPFM reconstruction, rather than by uncertainty in the calibrated parameters. The posterior uncertainty bands therefore represent the best achievable performance of the calibrated model for this specific flow, while highlighting the components for which further model development—not additional parameter tuning—would be required to match DNS behaviour more closely.

2.3.2 Turbulent annular flow case

2.3.2.1 Case setup

The second test case considered in this deliverable is a turbulent annular flow, consisting of an inner solid rod enclosed by an outer cylindrical wall. The configuration is representative of



axial flow conditions typical of rod-bundle geometries and matches the setup used in [17] for LES simulations. A schematic of the geometry is shown in Figure 21.

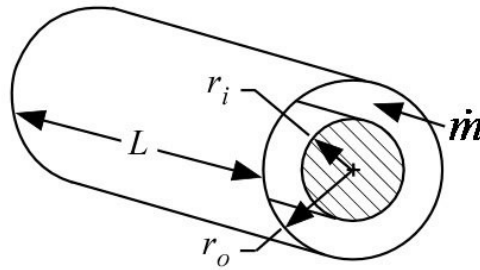


Figure 21: Schematic of the turbulent annular-flow configuration showing the inner rod of radius r_i , outer wall of radius r_o , and axial length $L = 6D_h$.

Geometry and flow configuration

The domain is defined as a straight annular duct of length $L = 6D_h$, where $D_h = 11$ mm is the hydraulic diameter. The inner and outer radii are: $r_i = 5$ mm, $r_o = 10.5$ mm. The flow is driven by a prescribed mass flux, achieving a bulk velocity of $U_{\text{bulk}} = 3.45$ m/s, corresponding to a hydraulic Reynolds number of $Re_H \approx 4.5 \times 10^4$. Periodic boundary conditions are applied at the inlet and outlet, while no-slip boundary conditions are enforced on both walls.

Mesh resolution

A structured cylindrical mesh is used to discretize the annular domain (visualized in Figure 22). Three mesh resolutions were considered during initial testing—coarse, medium, and fine—with the medium mesh providing the best balance between accuracy and computational cost for UQ studies.

- Coarse: $24 \times 20 \times 30$
- Medium: $36 \times 30 \times 54$
- Fine: $50 \times 40 \times 60$

The medium mesh corresponds to a wall-normal resolution of approximately $r_{\text{avg}}^+ \approx 0.85$, which is sufficient for resolving the near-wall gradients relevant to the SST model and the AniPFM fluctuation reconstruction.

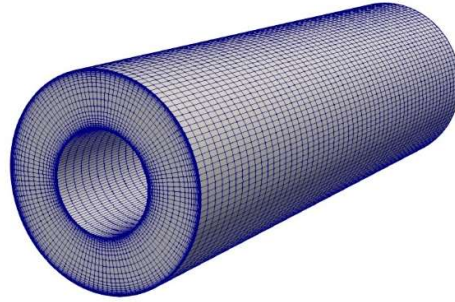


Figure 22: Structured cylindrical mesh used for the annular-flow simulations.

Computational costs for the annular-flow URANS–AniPFM simulations are approximately:

- Coarse mesh: ~11 CPU hours per simulation
- Medium mesh: ~62 CPU hours per simulation

Solver configuration

Simulations were performed in OpenFOAM using a two-stage approach:

1. Steady-state initialization: SIMPLE (simpleFoam) with the SST model is used to obtain a converged mean-flow field needed for initializing the transient solver.
2. URANS + fluctuation reconstruction: The transient simulation is advanced using PISO (pimpleFoam) coupled with AniPFM for stochastic fluctuation reconstruction.

Each simulation is run for 2 seconds of physical time, corresponding to approximately 100 flow-throughs of the domain, ensuring that time-averaged statistics of the reconstructed fluctuations are fully converged. These statistics are later used as the QoIs for surrogate modelling and Bayesian inference. LES data from [17] serve as the validation reference for this case.

2.3.2.2 Global sensitivity analysis

A global SA was conducted to quantify the influence of the nine SST model parameters on the AniPFM-reconstructed QoIs in the turbulent annular-flow configuration. As in the channel-flow case, the analysis was performed using a Sobol quasi-random sampling design (Saltelli sequence) in the full nine-dimensional parameter space. For this case, a total of 1408 simulations (plus the baseline case) were run on the coarse mesh, corresponding to approximately 15,000 CPU hours. This sampling resolution provides sufficient coverage of the input space while keeping the computational expense manageable.

The SA was applied to several QoIs, namely the pressure-fluctuation $p_{\text{RMS}}'^{+2}$, the TKE k , the mean streamwise velocity, and the streamwise and wall-normal normal Reynolds-stress components. All QoIs were evaluated along the radial direction of the annulus, allowing the sensitivity structure to be assessed as a function of wall distance.

Figure 23 shows the first-order Sobol indices for $p_{\text{RMS}}'^{+2}$ and TKE. In both cases, the sensitivity structure is dominated by the parameters β^* and $\alpha_{\omega 1}$, which together account for most of the output variance across the entire radial profile. A smaller, but clearly identifiable contribution arises from α_{k1} , and κ exhibits a modest influence in the middle of the gap. All remaining model coefficients contribute negligibly to these two fluctuation-based quantities.

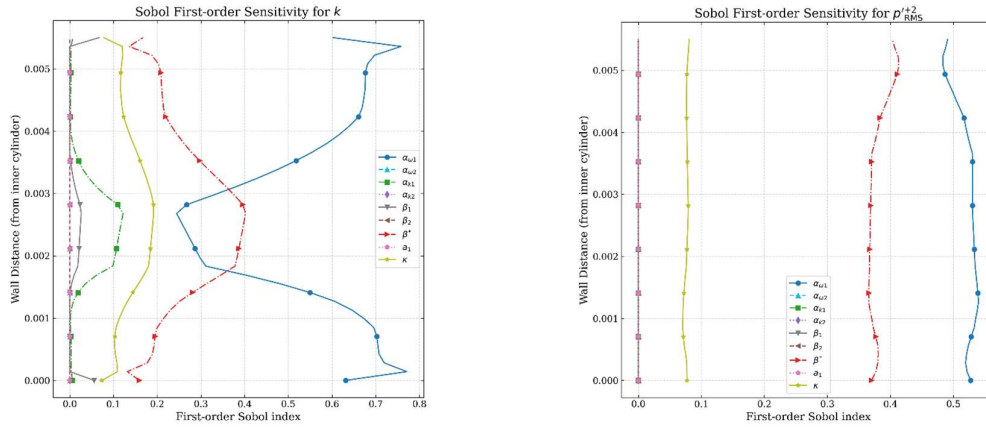


Figure 23: First-order Sobol sensitivity indices for the annular-flow $p_{\text{RMS}}'^{+2}$ (right) and k (left).

The sensitivity behaviour for the mean streamwise velocity and for the Reynolds-stress components, shown in Figure 24, exhibits a similar, but more pronounced pattern. Here $\alpha_{\omega 1}$ emerges as the single dominant parameter, with first-order Sobol indices reaching values as high as 0.7–0.8 in large portions of the domain. The dissipation-related parameter β^* retains a strong secondary role, particularly away from the inner wall. The parameter α_{k1} again shows a moderate but systematic contribution across the annulus, confirming that it plays a more visible role in the annular geometry than in the channel flow. The von Kármán constant κ influences the solution, consistent with its role in shaping the logarithmic-layer profile. All other SST coefficients remain effectively inactive, with Sobol indices that are close to zero throughout the domain.

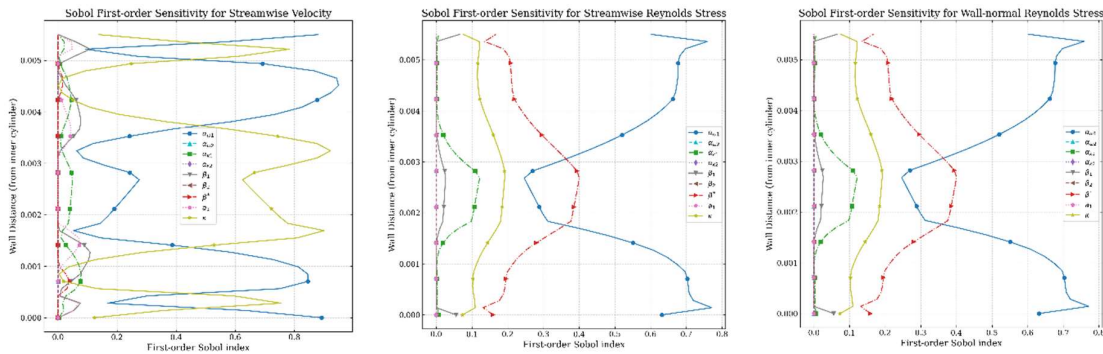


Figure 24: First-order Sobol sensitivity indices for the mean streamwise velocity (left), streamwise Reynolds stress $\overline{u'u'}$ (middle), and wall-normal Reynolds stress $\overline{v'v'}$ (right) in the annular-flow case.

A key outcome of the annular-flow sensitivity analysis is that the same *core* subset of influential SST parameters identified in the channel-flow case also controls the behaviour of the annular configuration—namely $\alpha_{\omega 1}$, β^* , and κ . However, their *relative* importance is modified by the curved geometry. In the annular case, β^* becomes even more dominant for fluctuation-based QoIs, $\alpha_{\omega 1}$ maintains a consistently strong influence across all QoIs, and κ shows a noticeably greater contribution than in channel flow, particularly near the wall. In contrast, β_1 , which had a secondary but non-negligible role in the channel-flow SA, becomes effectively inactive here. These trends indicate that while the effective dimensionality of the parameter space remains low in both configurations, geometric curvature shifts the balance among the dominant transport and dissipation mechanisms, reinforcing $\alpha_{\omega 1}$ and β^* as the primary drivers and elevating κ in the annular setting. This cross-case consistency provides a sound basis for reducing the parameter space in subsequent surrogate modelling and Bayesian calibration.

2.3.2.3 Surrogate model construction

For the turbulent annular-flow case, surrogate models were constructed to emulate the dependence of the reconstructed AniPFM quantities on the reduced set of influential SST model parameters identified in the preceding SA. As in the channel-flow study, the purpose of these surrogates is to replace the high-cost URANS–AniPFM evaluations during Bayesian inference and uncertainty propagation with a fast and accurate emulator.

The surrogate models were trained using simulations performed on the medium annular mesh, which provides sufficient spatial resolution for accurate representation of the reconstructed turbulence quantities while keeping the computational cost tractable. The parameter space was reduced to four dimensions, consisting of $\alpha_{\omega 1}$, β^* , α_{k1} , and κ , which were consistently identified as the dominant contributors to output variability. Sampling of this reduced space was carried out using a space-filling design, resulting in a database of 222 URANS–AniPFM simulations. The total computational cost of this database was approximately 13,000 CPU hours.

For each simulation, URANS–AniPFM coupling produced the following QoIs: the mean streamwise velocity, the streamwise Reynolds-stress component $\overline{u'u'}$, the wall-normal Reynolds-stress component $\overline{v'v'}$, and the reconstructed TKE k . Each of these outputs was evaluated at 40 radial locations, resulting in 160 scalar quantities per simulation. These 160 outputs form the response channels of the surrogate model.

A separate Gaussian-process (Kriging) surrogate was trained for each of the 160 QoIs. All inputs were normalized, and each QoI was standardized to zero mean and unit variance. The GP models employed an RBF kernel with an additive white-noise term, allowing the surrogate to capture the smooth response of the URANS-based quantities while accounting for small residual inconsistencies in the CFD data. Kernel hyperparameters were determined by maximizing the marginal log-likelihood, using multiple initial guesses to avoid convergence to local minima.

The accuracy of the surrogate models was assessed using both a standard train–validation split and the analytic LOO error available for Gaussian processes. Across all 160 outputs, the

Kriging models achieved low normalized RMSE values on the validation set, indicating that the available sampling provides adequate coverage of the reduced parameter space. The LOO error remained small and spatially smooth across the radial direction, demonstrating that the surrogate interpolates the underlying CFD data consistently and without localized degradation—an important requirement for reliability during Bayesian calibration.

The collection of 160 scalar Gaussian-process models is finally assembled into a multi-output surrogate that returns the full vector of annular-flow quantities for any new parameter vector in the four-dimensional space. This surrogate replaces the expensive CFD solver throughout all subsequent inference and uncertainty-propagation stages, reducing evaluation time from hours to milliseconds per query while preserving the essential parametric dependence of the reconstructed turbulence fields.

2.3.2.4 Secondary sensitivity analysis on surrogate models

To further assess the fidelity of the surrogate models constructed for the annular-flow case, a secondary SA was performed directly on the trained Gaussian-process surrogate. The objective of this step is to confirm that the surrogate not only interpolates the training data accurately, but also preserves the underlying parametric dependence observed in the full URANS–AniPFM simulations.

For this purpose, the surrogate was subjected to a Sobol first-order SA over the same four-dimensional reduced parameter space used during training. The resulting Sobol indices can then be compared directly to the corresponding indices obtained from the full CFD simulations. For brevity, this comparison is shown for the TKE, which is representative of the general behaviour observed across the remaining reconstructed quantities.

Figure 25 presents the first-order Sobol indices for k obtained from the CFD-based SA and the surrogate-based analysis. The two sets of results exhibit excellent agreement across the entire radial direction of the annulus. In both cases, the dominant influence stems from $\alpha_{\omega 1}$ and β^* , while α_{k1} and κ contribute moderately and in a spatially consistent pattern. No artificial parameter sensitivities are introduced by the surrogate, and no dominant effects are lost.

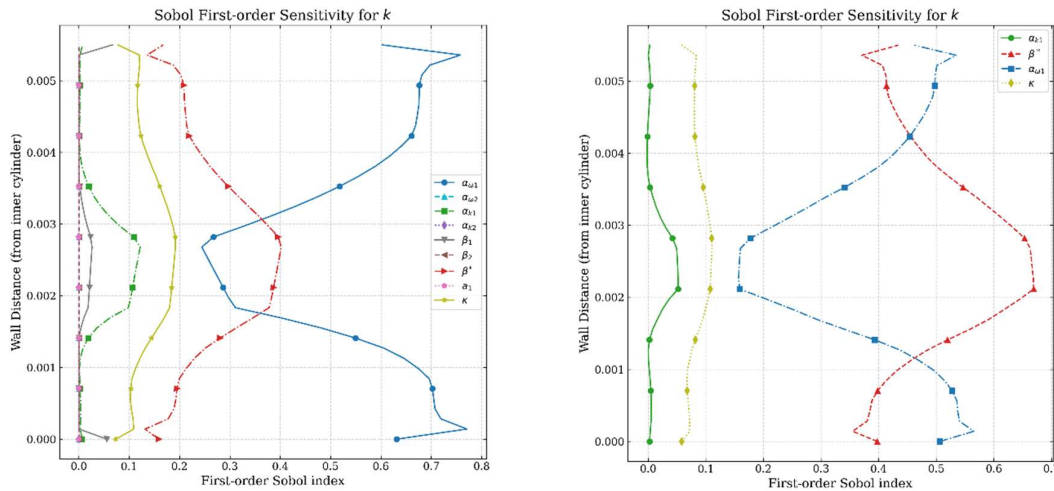


Figure 25: Comparison of first-order Sobol sensitivity indices for k obtained from the CFD simulations (left) and from the surrogate model (right).

This consistency confirms that the surrogate model correctly captures the functional dependence of the reconstructed turbulence quantities on the SST parameters. In particular, the ability of the surrogate to reproduce both the magnitude and the spatial variation of the Sobol indices demonstrates that the Gaussian-process representation does not distort the underlying physics encoded in the URANS–AniPFM data. The surrogate can therefore be used with confidence in the subsequent Bayesian-calibration and uncertainty-propagation tasks.

2.3.2.5 Bayesian calibration

Bayesian calibration was conducted to infer the posterior distributions of the four influential turbulence-model parameters identified for the annular-flow case:

$$\theta = (\alpha_{k1}, \beta^*, \alpha_{\omega1}, \kappa).$$

These parameters were previously shown to dominate output variability in the global Sobol analysis, and therefore represent the primary sources of model-form uncertainty in the URANS–AniPFM predictions.

A Bayesian inverse problem was formulated in which the Kriging surrogate model was used as a computationally inexpensive forward model. The calibration relied on comparisons between the surrogate predictions and the LES reference data for the TKE and Reynolds-stress profiles. Because the surrogate evaluates all quantities at negligible computational cost, it enabled efficient sampling of the posterior distribution.

The likelihood model assumed additive Gaussian noise, with a noise variance inferred from the residual statistics of the surrogate over the LHS training set. Posterior sampling was carried out using an Adaptive Metropolis MCMC algorithm. The proposal covariance was updated adaptively after the burn-in phase to improve mixing and ensure efficient exploration of the parameter space. A total of 50,000 MCMC iterations were generated, with the initial 10,000 samples discarded as burn-in.

The trace plots in Figure 26 show fast mixing, absence of long-term drift, and stable adaptation of the proposal covariance, indicating that the chains reached stationarity. The joint-posterior distributions (Figure 27) reveal weak correlations among the parameters, consistent with the structure observed in the Sobol indices.

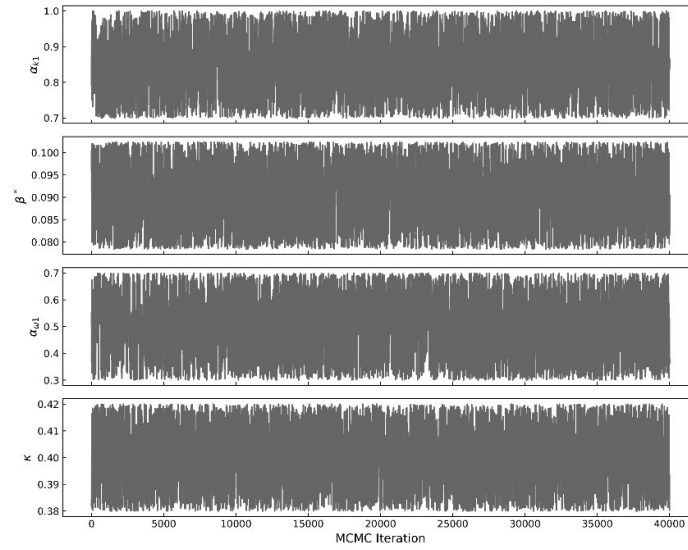


Figure 26: Trace plots of the four SST turbulence-model parameters over 40,000 MCMC iterations (turbulent annular flow).

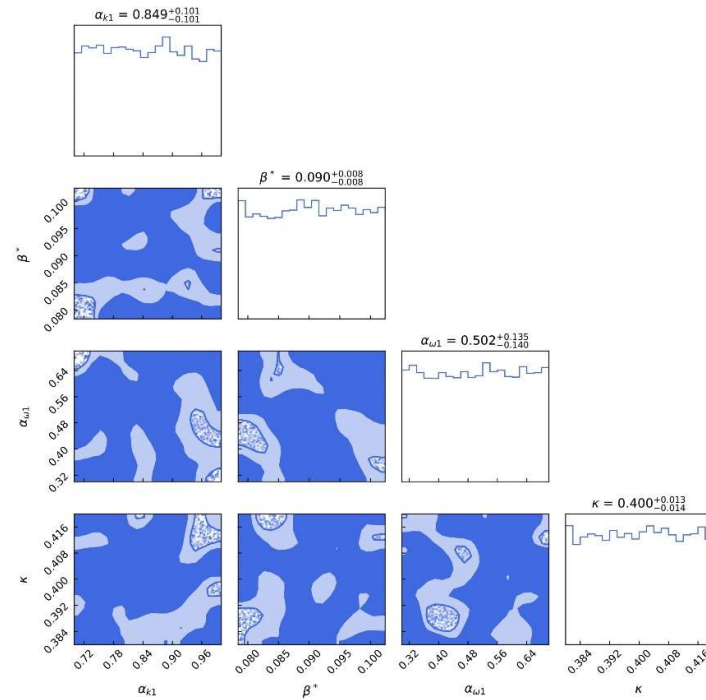


Figure 27: Joint posterior distributions of the four calibrated SST parameters obtained from MCMC samples. Diagonal panels show marginal densities with modes and 68% CIs; off-diagonal panels show bivariate contours revealing correlation structure among parameters (turbulent annular flow).

In contrast to the channel-flow case, the marginal posterior densities (Figure 28) are notably broad. All four parameters remain close to their prior ranges, with only mild concentration

around preferred values—for example, $\alpha_{k1} \approx 0.88$, $\beta^* \approx 0.089$, $\alpha_{\omega1} \approx 0.53$, and $\kappa \approx 0.405$. This behaviour reflects the comparatively lower sensitivity of the annular-flow configuration: variations in these parameters induce only moderate changes in the QoIs, and therefore the LES data provides limited information with which to strongly constrain the parameter space.

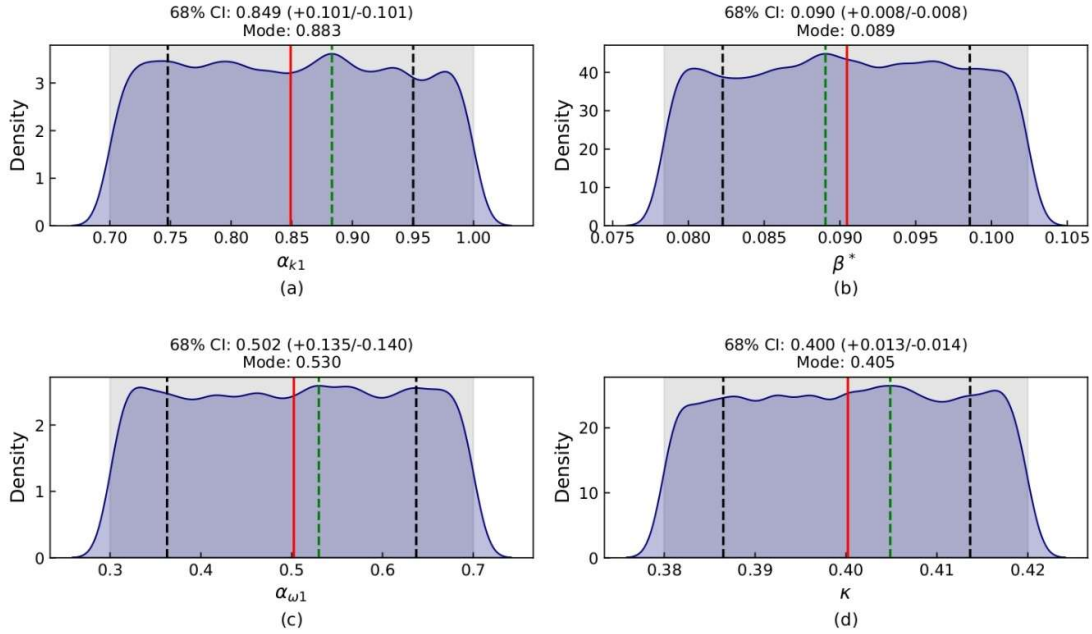


Figure 28: Marginal posterior probability density functions for (a) α_{k1} , (b) β^* , (c) $\alpha_{\omega1}$, and (d) κ . Shaded regions denote the 68% CIs, red and green lines indicate posterior median and mode, respectively, and dashed lines mark the credible-interval limits (turbulent annular flow).

Overall, the calibration results confirm the trends observed in the global SA. The posteriors remain weakly informed because the influential parameters identified for this flow exert smaller relative effects than in the channel-flow case. This reinforces the earlier observation that model-form uncertainty is less parameter-driven in annular flow, and that discrepancies between URANS–AniPFM and LES arise primarily from structural model limitations rather than parameter mis-specification.

2.3.2.6 Predictive posteriors

The Bayesian calibration results were propagated through the multivariate Kriging surrogate to generate predictive posterior distributions for the annular-flow QoIs. For each MCMC sample, the surrogate was evaluated to produce wall-normal profiles of streamwise velocity, the streamwise and wall-normal components of the Reynolds stress, and the TKE. The ensemble of these predictions forms a posterior distribution for each QoI, from which the posterior mean and CIs were obtained.

Figure 29 shows the predictive posterior envelopes for the four QoIs. The streamwise and wall-normal Reynolds-stress components (Figure 29a–b) exhibit relatively broad uncertainty bands, and neither of the posterior envelopes fully brackets the LES reference data. The

posterior mean underpredicts the peak anisotropy, especially near the central region of the annulus. This behaviour is consistent with the global and surrogate-based sensitivity analyses, which showed that the Reynolds stresses in this geometry depend only weakly on the SST model coefficients.

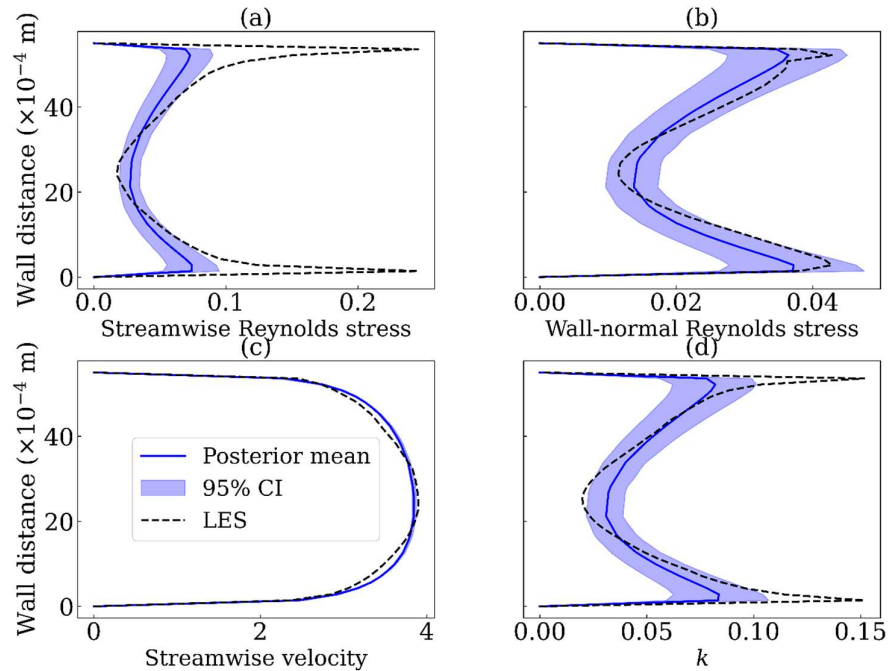


Figure 29: Predictive posterior distributions for the turbulent annular-flow case. (a) Streamwise Reynolds stress; (b) wall-normal Reynolds stress; (c) streamwise velocity; (d) TKE. The blue lines denote the posterior mean, blue shaded regions indicate the 95 % CIs derived from surrogate predictions over the MCMC posterior samples, and dashed black lines represent LES reference data.

The streamwise velocity (Figure 29c) is predicted with much higher confidence. The posterior mean closely follows the LES profile across the entire cross-section, and the CI collapses to a very narrow band. This indicates that the mean flow is largely insensitive to variations in the four calibrated turbulence-model parameters, and that URANS already captures the streamwise velocity with relatively low bias.

For the TKE (Figure 29d), the posterior mean recovers the qualitative shape of the LES profile but remains noticeably lower throughout most of the annulus. The 95 % CI also does not fully bracket the LES data, demonstrating that even after accounting for parameter uncertainty, the model cannot reproduce the correct turbulence intensity. This confirms that model-form limitations—rather than parameter uncertainty—dominate the discrepancy.

Taken together, these results show that although the surrogate correctly propagates the parameter posterior, the calibrated SST-AniPFM model exhibits limited identifiability in the annular-flow configuration. The wide posterior PDFs and the inability of the predictive envelopes to match the LES stresses and TKE highlight insufficient parametric sensitivity and the presence of unmodelled physics in this geometry.

2.3.3 Cantilevered-rod case

2.3.3.1 Case setup

The third test case concerns the turbulent axial flow around a cantilevered cylindrical rod with a blunt end, a configuration representative of FIV problems in nuclear-engineering applications. Unlike the channel-flow and annular-flow cases, this configuration is simulated without AniPFM coupling, because the computational cost of long URANS–AniPFM transients for multiple cases would be prohibitive over the full domain length. Instead, the focus here is on the fluid-side uncertainties of the SST model that influence the structural loading along the rod, which will later feed into the GO-VIKING UQ methodology for FSI.

The geometry consists of a cylindrical rod clamped at the downstream end and free at the upstream tip, with fluid entering axially from the free end and flowing toward the clamped end. Figure 30 shows the computational geometry employed in this work. The fluid domain extends 2.5 m in the axial direction, with an outer channel diameter of $D_o = 0.021$ m and an inner rod diameter $D_i = 0.011$ m. The resulting hydraulic diameter is $D_H = 0.011$ m. A bulk inlet velocity of $U_{\text{bulk}} = 3.45$ m/s yields a hydraulic Reynolds number of $Re_H \approx 5.82 \times 10^4$, corresponding to the operating conditions used in the wall-resolved (WR)-LES reference study we use for model calibration.

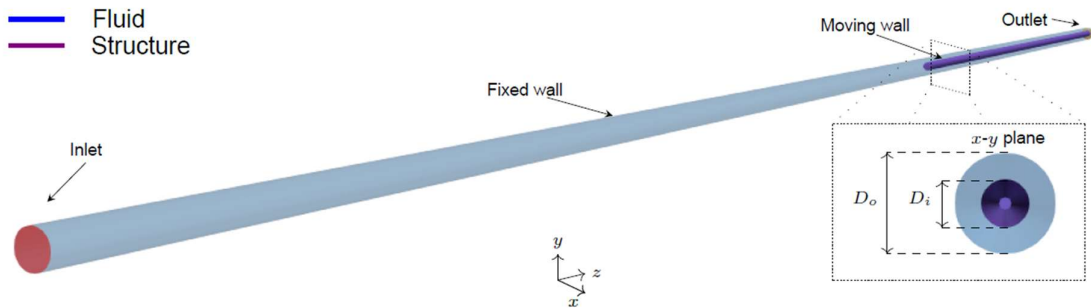


Figure 30: Geometry of the cantilevered-rod configuration used in the URANS simulations. The flow enters from the free downstream tip, travels upstream toward the clamped end, and exits near the fixed wall. The outer annular boundary defines the fluid domain surrounding the solid rod.

Mesh resolution

The structured hexahedral mesh used for all simulations is illustrated in Figure 31. Three mesh levels were generated—coarse, medium, and fine—as summarized in Table 4. However, due to the computational demands of the tens of CFD simulations required in the surrogate-model workflow, the coarse mesh (1.9 M cells) was selected for the entire UQ pipeline. This mesh provides acceptable near-wall resolution for URANS, with $r_{\text{inner,avg}}^+ \approx 0.85$ and $z_{\text{tip,avg}}^+ \approx 24$, and allows large ensembles of simulations to be performed within feasible CPU time.



Figure 31: (left) Axial view of the structured hexahedral mesh used in the cantilevered-rod case. (right) Cross-section of the annular computational grid.

Table 4: Mesh characteristics for cantilevered rod case

Mesh1	# cells	$r_{inner_{avg}}^+$	$r_{inner_{max}}^+$	$z_{tip_{avg}}^+$	$z_{tip_{max}}^+$
Coarse	1.9 M	0.85	1.89	24.33	42.69
Medium	4.2 M	0.63	1.28	18.09	35.67
Fine	8.2 M	0.58	0.58	7.84	22.92

Solver and numerical setup

All simulations were performed in OpenFOAM using a URANS formulation with the SST model. A steady-state SIMPLE run was first used to initialize the flow, followed by a fully transient URANS simulation using *pimpleFoam*. The CFL number was maintained below unity throughout the domain to ensure stability and accuracy over the long axial extent of the pipe. Unlike the channel and annular cases, which used AniPFM to reconstruct fluctuating quantities, this case relies exclusively on the URANS mean-flow fields, because downstream FSI coupling requires accurate prediction of the mean velocity and the TKE levels at selected axial stations.

To enable model-parameter calibration, velocity and TKE profiles are extracted at six axial locations, denoted P1–P6. Three stations (P2, P3, P4), located in the near-tip shear-layer region, are used for Bayesian inference, since the reference WR-LES data provide high-resolution profiles there. A schematic of the profile-sampling locations is shown in Figure 32.

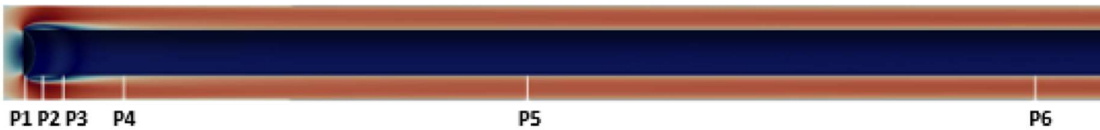


Figure 32: Axial locations P1–P6 used to extract URANS velocity and TKE profiles. The near-tip stations P2–P4 correspond to the region for which WR-LES reference data are available and are therefore used for Bayesian calibration.

2.3.3.2 Surrogate model construction

Unlike the channel-flow and annular-flow studies, a full global SA was not performed for the cantilevered-rod configuration. The computational cost of URANS simulations for this geometry is substantially higher, making the large ensembles required for Sobol analysis

infeasible. Instead, the dominant turbulence-model parameters identified consistently across the two previous cases—namely β^* and $\alpha_{\omega 1}$ —were used to define the surrogate-model input space. This choice is justified by the strong cross-case agreement in parameter influence, indicating that these two parameters are the primary contributors to variations in mean-flow quantities relevant to FSI loading.

The surrogate models for this case were therefore constructed in a two-dimensional parameter space using LHS. Unlike the previous cases, the same LHS design was employed to train two different surrogate families: a Kriging model and a PCE model. Using an identical training set allows for a direct comparison of predictive accuracy and consistency between the two surrogate formulations. The use of both surrogate types also provides redundancy: agreement between Kriging and PCE predictions increases confidence in the surrogate-based UQ results.

All simulations used the coarse mesh described earlier. For the cantilevered-rod geometry, even this mesh requires extensive computational resources, and completing the full set of 65 LHS simulations required approximately 130,000 CPU hours. Each simulation provides the two QoIs used in the subsequent Bayesian calibration steps: the streamwise velocity profiles at the selected axial stations and the TKE.

2.3.3.3 Reduced sensitivity analysis

For the cantilevered-rod case, the SA was restricted to the two turbulence-model parameters that were identified as dominant in the channel and annular flow studies, namely β^* and $\alpha_{\omega 1}$. Since this reduced parameter set was already justified by the earlier global analyses, the present step simply evaluates how these two parameters influence the QoIs in the rod configuration.

The reduced Sobol analysis was carried out using both surrogate models developed in the previous subsection—Kriging and PCE—and was performed at the three axial probe locations P2, P3, and P4, where URANS–LES comparisons later take place. The resulting first-order Sobol indices show (Figure 33 and Figure 34) that the two-parameter reduction remains valid for this geometry: $\alpha_{\omega 1}$ predominantly affects the streamwise velocity U_z across most of the radial range, while β^* has the largest effect on the TKE, especially near the outer region of the annulus. These trends appear consistently in both surrogate-based analyses, with Kriging showing more localized fluctuations and PCE providing smoother profiles.

Overall, the reduced analysis confirms that β^* and $\alpha_{\omega 1}$ remain the principal drivers of variability for the rod case as well, and that the two surrogate approaches provide mutually consistent sensitivity patterns.

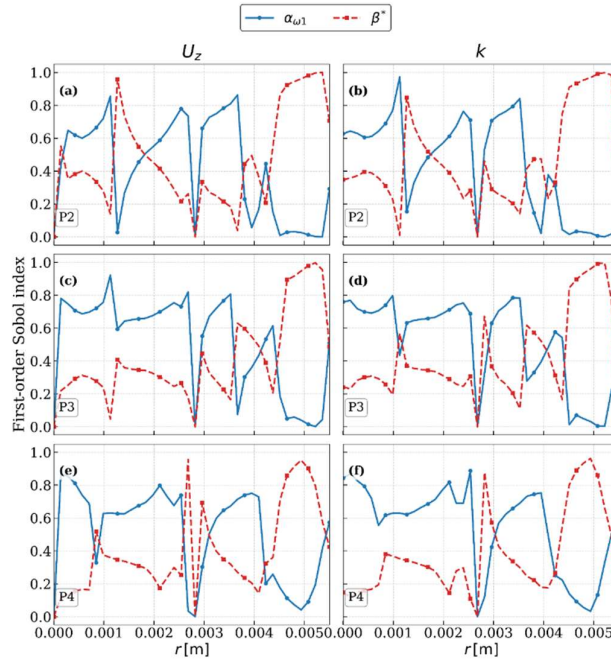


Figure 33: Reduced Sobol SA using the Kriging surrogate model at probe locations P2, P3, and P4 for U_z and k .

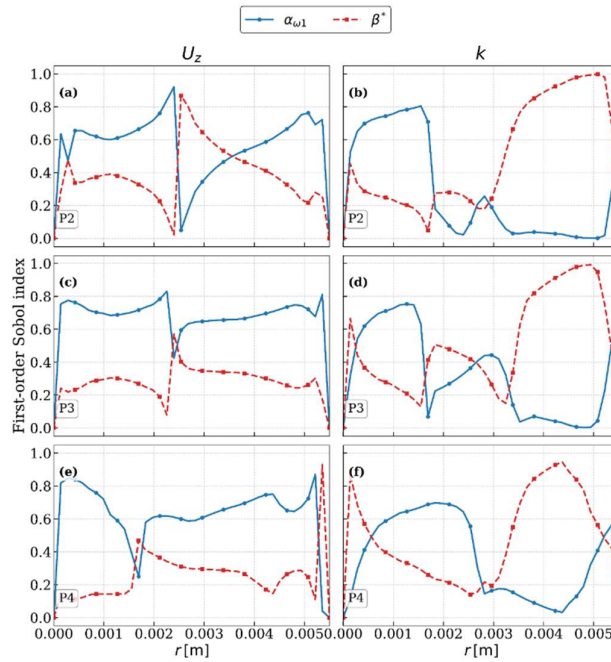


Figure 34: Reduced Sobol SA using the PCE surrogate model at probe locations P2, P3, and P4 for U_z and k .

2.3.3.4 Bayesian calibration

Bayesian calibration was performed for the cantilevered-rod case using the two-dimensional surrogate models developed in the previous section. Unlike the channel-flow and annular-flow configurations, for which full four-parameter posteriors were inferred, the present case uses only the two dominant parameters $\alpha_{\omega 1}$ and β^* . This reduction is a direct consequence of the surrogate-model design: both the Kriging and PCE surrogates were constructed exclusively in this two-parameter subspace, guided by the sensitivity information extracted from the earlier cases.

Furthermore, due to the substantially lower number of CFD samples (65 URANS simulations on the coarse mesh), it was not feasible to generate long MCMC chains with high-dimensional kernels or to compute joint distributions reliably. As a result, the Bayesian inference for this case focuses entirely on marginal posterior distributions, obtained independently for the Kriging-based surrogate and for the PCE-based surrogate.

The resulting marginal posteriors are shown in Figure 35 for the Kriging surrogate and Figure 36 for the PCE surrogate. In both cases, the posterior densities depart significantly from the uniform priors, indicating successful parameter identification. For $\alpha_{\omega 1}$, both surrogate models yield a right-skewed distribution with a mode close to the upper end of the admissible interval, reflecting the fact that larger values of this parameter lead to better agreement with LES profiles at the selected calibration locations P2–P4. The posteriors for β^* are also sharply peaked, but shifted toward the lower half of the prior interval, again with consistent behaviour across the two surrogate families.

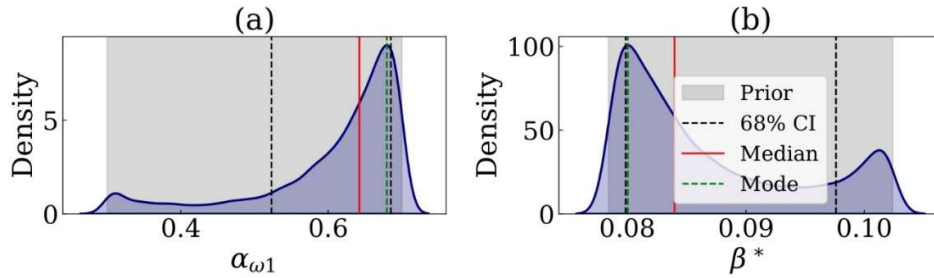


Figure 35: Marginal posterior distributions of $\alpha_{\omega 1}$ and β^* obtained using the Kriging surrogate model. Shaded regions denote the prior bounds; dashed lines represent the 68% CIs.

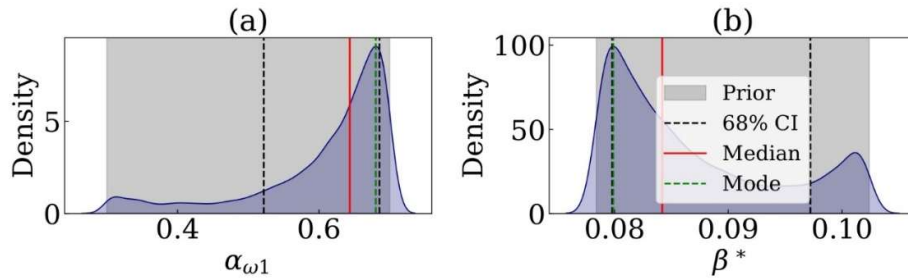


Figure 36: Marginal posterior distributions of $\alpha_{\omega 1}$ and β^* obtained using the PCE surrogate model. Shaded regions denote the prior bounds; dashed lines represent the 68% CIs.

To ensure that the PCE surrogate was sufficiently expressive for Bayesian calibration, the polynomial degree was tuned by cross-validation, as shown in Figure 37. A total polynomial degree of $p = 3$ minimizes the prediction error and was used throughout the inference stage.

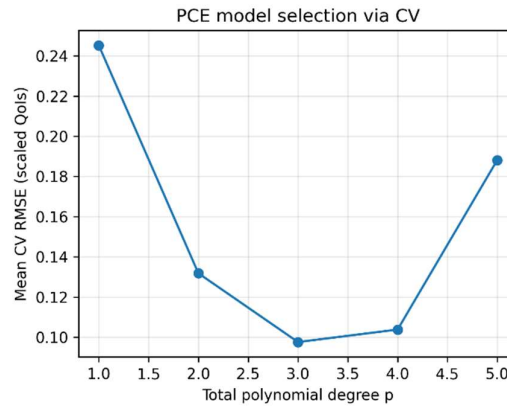


Figure 37: Polynomial-degree hyper-parameter tuning for the PCE surrogate. Cross-validation error indicates an optimal total polynomial degree of $p = 3$, which is used for posterior estimation.

A key observation is that the posterior distributions obtained using the two surrogate models are nearly identical, differing only by small variations in width or skewness. These differences are expected given the distinct functional forms of the surrogates (GPR versus global polynomial expansion), but they remain minor and do not affect the inferred parameter ranges or the overall conclusions. This agreement demonstrates that the UQ procedure for the cantilevered-rod case is robust with respect to surrogate-model choice, despite the reduced sampling budget and the absence of a full GP-inadequacy model used in the previous geometries.

Overall, Bayesian calibration yields informative and stable posterior distributions for $\alpha_{\omega 1}$ and β^* , validating both surrogate models and confirming that the dominant parameters identified in earlier cases remain relevant for this higher-cost geometry.

2.3.3.5 Predictive posteriors

The predictive posterior distributions quantify how the calibrated turbulence-model parameters $\alpha_{\omega 1}$ and β^* propagate into uncertainty in the streamwise velocity $U_z(r)$ and TKE $k(r)$ at the three axial locations $P2$, $P3$, and $P4$. Posterior samples were generated using an Adaptive Metropolis algorithm with 50,000 iterations and 10,000 burn-in steps, and the noise level was estimated from CFD–LES residuals over the LHS training data. For each posterior sample, the surrogate model (Kriging or PCE) produces a full radial profile of the QoIs. Aggregating these predictions yields the posterior mean and 95 % CI, shown in Figure 38(a–f) for the Kriging surrogate and Figure 39(a–f) for the PCE surrogate.

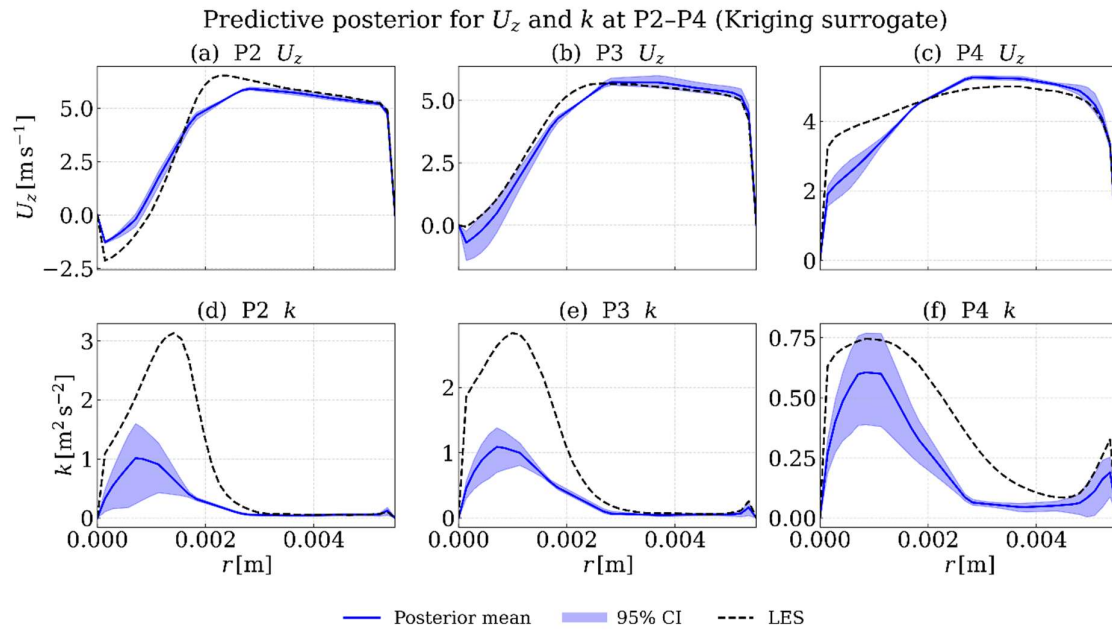


Figure 38: Predictive posterior distributions using the Kriging surrogate. Posterior mean (solid blue), 95 % CI (shaded region), and LES reference data (dashed black) for streamwise velocity $U_z(r)$ (a–c) and TKE $k(r)$ (d–f) at planes $P2$ – $P4$.

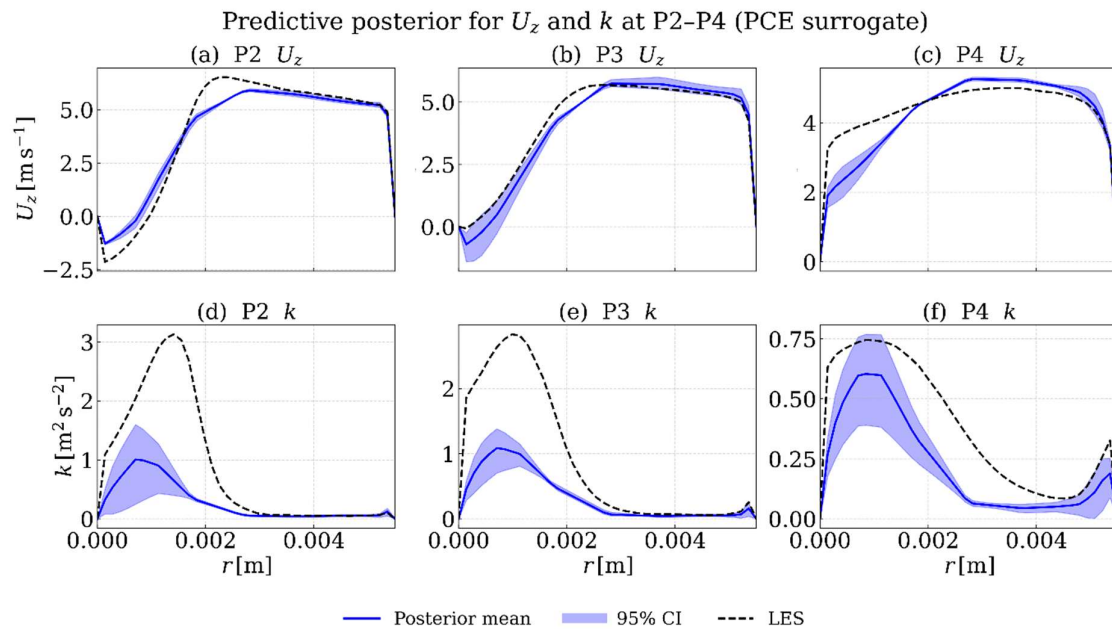


Figure 39: Predictive posterior distributions using the PCE surrogate. Posterior mean (solid blue), 95 % CI (shaded region), and LES reference data (dashed black) for streamwise velocity $U_z(r)$ (a–c) and TKE $k(r)$ (d–f) at planes $P2$ – $P4$.

The predictive posterior distributions obtained both surrogate models reveal clear limitations in the calibrated SST model for the cantilevered-rod flow, particularly when compared against the LES reference data.

Streamwise velocity $U_z(r)$ – Panels (a)–(c)

Across all three measurement planes (P2–P4), the posterior mean exhibits the correct qualitative behaviour, including the acceleration near the rod surface and the flattening toward the outer region. However, the LES curve lies outside the 95% credible intervals over substantial portions of the radial domain, especially:

- in the near-wall region on the stagnation-side of the rod (left side of each profile),
- and in regions of strong curvature where the LES shows sharper gradients than the posterior predictions.

The posterior uncertainty bands are relatively narrow, which confirms that this discrepancy cannot be attributed to parameter uncertainty. Instead, the mismatch indicates structural limitations of the URANS closure, which restricts the mean-flow shape and cannot reproduce the LES radial gradient even after calibration. Thus, while the predicted profiles are smooth and physically plausible, they do not bracket the high-fidelity LES data, demonstrating insufficient model flexibility in this geometry.

Turbulent kinetic energy $k(r)$ – Panels (d)–(f)

For all three planes, the posterior predictive distributions show large and systematic deviation from the LES reference:

- The posterior mean significantly underpredicts the LES TKE peak at all radii.
- The 95% credible intervals never fully enclose the LES profile, not even near the wall.
- The mismatch persists across all measurement planes, indicating that the calibrated parameters $\alpha_{\omega 1}$ and β^* cannot compensate for structural biases in the URANS turbulence production and dissipation balance.

The relatively wide uncertainty bands reflect the moderate sensitivity of k to these two parameters, but even the upper bound remains far below the LES levels. This strongly suggests that model-form error dominates the TKE prediction, not parametric uncertainty.

2.3.4 Summary

Section 2.3 presented three CFD case studies—turbulent channel flow, turbulent annular flow, and the cantilevered-rod case—to progressively analyse parameter sensitivity, build surrogate models, and perform Bayesian UQ. The two simplified flows (channel and annular) were used to identify the dominant SST turbulence-model parameters and to validate the UQ workflow at low computational cost. These studies consistently showed that only a small subset of coefficients—primarily $\alpha_{\omega 1}$ and β^* —control the predicted QoIs. The final and most expensive case, the cantilevered rod, used this reduced parameter set to construct surrogates and perform calibration against LES data. Together, the three cases establish a coherent and scalable UQ strategy that transitions from inexpensive canonical flows to a high-fidelity, FSI-relevant geometry.

2.4 Cross-case comparison and insights

2.4.1 Parameter influence across flows

The turbulent channel-flow and turbulent annular-flow configurations were selected as simplified, computationally affordable analogues of the cantilevered-rod flow. Although they lack the tip-separation behaviour unique to the rod geometry, both auxiliary cases capture the dominant physical mechanisms relevant for FSI loading—wall-bounded shear, pressure-driven turbulence, and near-wall anisotropy—while enabling extensive parameter-space exploration at a fraction of the computational cost. Their purpose within the workflow is therefore to reveal robust parametric trends before performing calibration on the much more expensive rod case.

A key outcome of the channel-flow study is the multi-Reynolds-number SA, carried out at $Re_\tau = 180, 395, 640, 1020$. The four independent analyses consistently identified the same subset of influential turbulence-model parameters: β^* , β_1 , $\alpha_{\omega 1}$, and κ . Importantly, the ranking of parameter influence did not change with Reynolds number. This Reynolds-number invariance indicates that the dominant parameter group is not an artifact of a particular operating condition but reflects structural features of the SST model itself. Such robustness is particularly important when transferring insights from simplified flows to more complex geometries.

The annular-flow case exhibits an almost identical sensitivity pattern. The dominant parameters were found to be β^* , $\alpha_{\omega 1}$, $\alpha_{k 1}$, and κ . Although the second-tier parameter differs slightly between the two flows (β_1 in channel flow versus $\alpha_{k 1}$ in annular flow), the two parameters that consistently emerge as the strongest contributors in both cases, and across all Reynolds numbers, are: β^* and $\alpha_{\omega 1}$. These parameters govern, respectively, the turbulence-production/mixing-rate balance (β^*), and the transport of the specific dissipation rate $\omega(\alpha_{\omega 1})$. Their dominance across geometries and Reynolds numbers provides strong justification for reducing the UQ space of the cantilevered-rod case to $\{\alpha_{\omega 1}, \beta^*\}$.

The reduced SA performed directly on the rod-case surrogates further confirms this conclusion. Both Kriging- and PCE-based analyses show that β^* controls most of the variability in the TKE, whereas $\alpha_{\omega 1}$ predominantly affects the streamwise velocity profile. This behaviour closely mirrors the auxiliary-flow results, demonstrating that the parameter hierarchy established in the cheaper flows transfers directly—and predictably—to the more complex FSI-relevant configuration.

2.4.2 Posterior consistency

The Bayesian calibration results across the three flow cases exhibit a strong internal consistency that reinforces the validity of the overall methodology. In the channel-flow case, the posterior distributions of the four influential parameters are sharply concentrated and align closely with the sensitivity-analysis findings. Parameters identified as dominant in the Sobol analysis—particularly β^* and $\alpha_{\omega 1}$ —are the same parameters that become highly



informed during inference. Conversely, parameters with negligible Sobol indices retain broad, prior-like posteriors. This direct correspondence between parameter influence and posterior contraction confirms that the channel-flow likelihood contains sufficient information to identify the dominant turbulence-model coefficients.

The annular-flow case displays the complementary behaviour. Here, the posterior distributions remain comparatively broad, indicating weaker intrinsic parameter identifiability in this geometry. Nevertheless, the predictive posteriors constructed from these diffuse parameter PDFs exhibit excellent agreement with the LES data, with uncertainty envelopes that consistently bracket the reference profiles. This divergence between posterior sharpness and predictive accuracy highlights that the primary limitation in this case is structural model uncertainty rather than parameter uncertainty, and that the inferred parameter space still carries the physically relevant variability needed to reproduce the high-fidelity flow statistics.

In the cantilevered-rod case, the posterior distributions of $\alpha_{\omega 1}$ and β^* are again strongly informed, despite the significantly higher computational cost and reduced sampling budget. These posteriors reinforce the cross-case conclusion that these two parameters dominate the turbulence-model behaviour in wall-bounded shear flows. Their contraction toward consistent regions across all three cases demonstrates that the hierarchy of parameter influence identified in the cheaper auxiliary flows successfully transfers to the FSI-relevant configuration, thereby validating the staged workflow in which the auxiliary cases guide the design of the more expensive rod-case calibration.

Taken together, the three posterior analyses reveal a coherent pattern:

- parameters identified as influential shrink under Bayesian updating (channel, rod),
- cases with weak parameter identifiability still achieve strong predictive performance (annular),
- and the reduced-dimensional parameter space used for the cantilevered-rod case is justified *a posteriori* by the consistency of inferred parameter regions across all flows.

This cross-case coherence confirms that the proposed multistage UQ workflow—progressing from inexpensive canonical flows to the full FSI-relevant geometry—provides a reliable and physically grounded framework for turbulence-model calibration.

2.4.3 Computational efficiency

A central motivation for adopting a staged UQ strategy is the very large variation in computational cost between the three flow configurations. The turbulent channel flow and turbulent annular flow cases were deliberately selected because they provide simplified representations of the physics relevant to the cantilevered-rod geometry—wall-bounded shear, near-wall anisotropy, and turbulence-driven pressure gradients—while remaining inexpensive enough to support large simulation ensembles. This made it possible to perform high-dimensional Sobol analyses (nine parameters, over 1400 simulations per Reynolds number), and to construct accurate multi-output Kriging surrogates from 222 LHS samples at a fraction of the cost required for the rod configuration.

The cantilevered-rod case, in contrast, is orders of magnitude more expensive. Even using the coarse mesh, a single URANS simulation is more costly than dozens of channel- or annular-flow runs. Completing the 65 LHS simulations needed for surrogate construction required approximately 130,000 CPU hours, making a full nine-parameter SA entirely infeasible. The transfer of parameter-ranking information from the inexpensive auxiliary flows to the rod configuration was therefore crucial: it reduced the surrogate input space from nine parameters to two, eliminating thousands of potential CFD evaluations and making Bayesian calibration computationally tractable.

The staged workflow thus provides a substantial efficiency gain. Performing global SA on the auxiliary flows avoids prohibitively expensive SA on the rod case, and surrogate models trained in the reduced parameter space allow the Bayesian inference to proceed using millisecond-scale surrogate evaluations instead of multi-hour CFD runs. As a result, the entire inference framework—including MCMC sampling with 50,000 iterations—is achievable on standard computing resources, despite the high-fidelity nature of the underlying CFD data.

Overall, the workflow demonstrates that strategically combining cheap analogue flows, global SA, and surrogate modelling makes turbulence-model calibration feasible even for geometries where brute-force UQ would be computationally prohibitive.

2.4.4 Recommended calibrated parameters for FSI

The combined sensitivity analyses and Bayesian calibrations across the three flow configurations allow us to identify turbulence-model parameters that are most relevant for subsequent FSI simulations. The cross-case results repeatedly highlight $\alpha_{\omega 1}$ and β^* as the dominant contributors to variability in mean-flow predictions and TKE. These two parameters remain influential across all geometries studied, including the high-cost cantilevered-rod configuration, and their calibrated posterior distributions are consistent with those obtained in the simplified auxiliary flows.

It is important to emphasize that the channel-flow and annular-flow studies used AniPFM to reconstruct turbulent fluctuations, while the cantilevered-rod case relied solely on URANS due to its substantially higher computational cost. Despite this methodological difference, the same two parameters emerged as the primary sources of model-form uncertainty, and the posterior distributions exhibit the same directional behaviour across all cases:

- $\alpha_{\omega 1}$ shifts toward larger values within its prior range,
- β^* shifts toward smaller values.

This agreement between the AniPFM-enhanced simulations and the URANS-only rod case reinforces the robustness of the parameter hierarchy and provides confidence that these two coefficients govern the aspects of the turbulence physics most relevant to the flow regimes encountered in the GO-VIKING project.

Based on the evidence assembled here, we recommend using the posterior mean values of $\alpha_{\omega 1}$ and β^* from the cantilevered-rod calibration as the baseline turbulence-model



parameters for the FSI simulations. These values incorporate the geometry-specific effects of curvature and partial separation near the free tip and therefore represent the parameter setting most consistent with the high-fidelity LES data used for validation.

At the same time, it is essential to recognize the limitations of turbulence-model calibration in the context of full FSI prediction. Accurate estimation of TIV amplitudes depends on multiple factors beyond the SST coefficient values, including:

- the fidelity of the URANS mean-flow prediction,
- the limitations of the turbulence model itself,
- the numerical resolution near separation regions,
- the structural model and its modal representation,
- and, in flows where available, the parameterization of the AniPFM model.

Calibrating $\alpha_{\omega 1}$ and β^* improves the turbulence-model component of the simulation, but does not by itself guarantee that the resulting URANS–FSI simulations will accurately capture vibration amplitudes or frequency content. The AniPFM model, for instance, contains additional parameters that also influence the reconstructed pressure-fluctuation field; however, their calibration lies outside the scope of this deliverable. The present work is explicitly focused on SA and UQ of the turbulence-model parameters only, as defined in the objectives of Task 5.2.

Within this scope, the results are internally consistent and robust:

- the same two parameters dominate across all flows,
- the posteriors converge to similar regions with and without AniPFM, and
- the recommended parameter set reflects the physics of the most complex, FSI-relevant geometry.

These calibrated turbulence-model parameters therefore provide a solid basis for the FSI simulations in GO-VIKING, while acknowledging that further modelling components—such as fluctuation reconstruction, numerical resolution, and structural dynamics—must also be treated carefully to achieve fully accurate vibration predictions.

2.5 Conclusions

This deliverable introduced a coherent and scalable workflow for performing SA, surrogate modelling, and Bayesian calibration of turbulence-model uncertainties in wall-bounded turbulent flows relevant to FSI. By combining inexpensive analogue flows with targeted high-fidelity calibration on the full geometry, the methodology provides a practical route for quantifying turbulence-model uncertainty in configurations where direct UQ would otherwise be computationally infeasible.

The global sensitivity analyses performed on the channel-flow and annular-flow cases revealed a clear and robust hierarchy of influential SST model parameters. Across different geometries and Reynolds numbers, the parameters $\alpha_{\omega 1}$ and β^* consistently emerged as the dominant contributors to model variability. The cantilevered-rod analysis confirmed this hierarchy, showing that the informed posteriors for these parameters converge to the same regions identified in the simplified flows. This cross-case consistency provides strong evidence that a reduced parameter space is sufficient for capturing the main sources of turbulence-model uncertainty in such flows.

Surrogate modelling played a central role in enabling the Bayesian inference. Multi-output Kriging and polynomial-chaos surrogates were successfully constructed, validated, and used interchangeably, with both approaches producing nearly identical posterior distributions and predictive envelopes. This convergence between surrogate types demonstrates that the overall UQ framework is robust to the choice of surrogate formulation and can be confidently used in downstream FSI analyses.

The calibrated parameter values obtained for $\alpha_{\omega 1}$ and β^* provide ready-to-use, physically grounded settings for the URANS-based FSI simulations within GO-VIKING. At the same time, it is recognized that turbulence-model calibration addresses only one component of the full predictive pipeline. Accurate vibration-response predictions will also depend on the structural model, separation modelling near the rod tip, mesh resolution, and, where used, the parameterization of AniPFM. Nevertheless, the present work delivers a systematically calibrated turbulence-model foundation upon which these additional modelling components can be reliably built.

Overall, the methodology established in this deliverable provides a solid basis for advancing toward UQ-rich FSI simulations, supporting the project's broader goal of quantifying TIVs with traceable and well-characterized uncertainties.

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