DAMAGE DETECTION OF THE ROD IN THE CROSSFLOW USING SURROGATE-BASED MODELLING

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An effective and accurate methodology is developed to create an inverse surrogate model for the mass reduction analysis of the rod in the rod bundle inserted in the crossflow. The performance of two surrogate modelling approaches has been evaluated. These models are the Response Surface Method and Legendre polynomial approximations. The relationship between dominant frequencies, support stiffness and rod mass derived from Computational Fluid Dynamics simulations is used as input data for approximations. The selection of sample points is implemented with a new type of orthogonal design. The results have shown that the proposed methodology can reliably replace the finite volume model and drastically reduce computational time.

Keywords: *CFD, inverse model, rod bundle, surrogate model.*

1. INTRODUCTION

For the safe operation of engineering equipment, it is necessary to continuously monitor whether the system does not exceed its operational limits and does not compromise its structural integrity. Relatively frequently it is not possible to measure changes in the internal elements of the system directly during the operation of the equipment, for example, in heat exchangers or nuclear reactor assembly. For complex systems, their behaviour as a function of the input parameters is generally not known. In such situations, physical and numerical experiments can often be the only way to

determine the relevant relationships. Nevertheless, full-model simulations would require long calculations from several hours to several days or weeks, even using high-performance computing resources. That approach is not applicable to the monitoring of the system during its operation. Therefore, to reduce computing time, simplified models – surrogate models or metamodels – are used that approximate the original model. Adequate mathematical models can be used to detect as early as possible changes in the typical behaviour of the system that could indicate its malfunction and structural integrity problems.

This study focuses on heat exchangers consisting of a bundle of rods placed in a highly turbulent crossflow. Flow induces rod vibrations with a typical spectrum that can be used to indirectly detect changes in system parameters. The decrease in the mass of the rod may be one of the parameters indicating that damage has occurred in the installation. Therefore, Computational Fluid Dynamics (CFD) simulations and surrogate modelling approaches are used to find the relationship between the mass of the rod and the dominant frequencies.

In the literature, various types of engineering problems are solved through surrogate models such as design optimization, uncertainty quantification, parameter identification, sensitivity analysis or inverse problems. Available surrogate models include, e.g., Response Surface Method (RSM), Kriging (or Gaussian process modelling), radial basis functions and artificial neural networks. RSM is predicated on the assumption that many physical systems are smooth and continuous and can be well approximated, at least in the region of interest, by low-order polynomials [1]. As follows from [2], the polynomial approximation is not applicable to highly non-linear functions, but in cases of low non-linearity and low dimensions, it is an effective approach. The Kriging method is of most use when the true function is particularly computationally intensive, e.g., a CFD-based calculation [3]. As an example, we can mention the minimization of vortex-induced vibrations using Kriging described by Filho et al. [4]. Banyay et al. [5], [6] used Kriging surrogate for global sensitivity analysis of flow-induced vibrations. In the present paper, low-order (less than 4th order) polynomials and Legendre polynomial were investigated. Two-factor forward and inverse surrogate models were created.

The training data set for the surrogate model development is generated by exercising complex high accuracy models such as finite volume or finite element models. The selection of sample points can be implemented through the design of experiments. The design of experiments is very important for a high-quality surrogate model. There are several metrics to determine the adequacy and goodness of fit of the model, such as a root mean square error, cross-validation error, T-tests or Pearson's χ^2 test, etc. As mentioned by Greenwood and Nikulin [7], when the amount of data is small, no test is very good, and when there are a lot of high-quality data almost any test, properly designed and applied, will give good results. However, when addressing problems with high computational costs, an effective sampling plan must be sought, which means a minimum number of points that provide a surrogate model with good precision. Techniques that are commonly considered are Latin Hypercube Sampling, Central Composite Design (CCD), orthogonal arrays, factorial designs. In this study, a new type of orthogonal design [8] is used. Based on the obtained sample points, the selection of initial conditions for the full-order model is carried out.

The paper is structured as follows. In

Section 2, the CFD approach applied to obtain the results of the full model is formulated. Section 3 describes the types of employed surrogate models, the sampling method and the model accuracy metrics. Verification results are presented in Section 4. Finally, concluding remarks are given in Section 5.

2. HIGH-FIDELITY COMPUTATION

The full model uses the configuration of the rod bundle described in Upnere et al. [9], in which laboratory experiments were carried out to examine the vibrations of single flexible-mounted rod caused by the crossflow in the rigid rod array. The configuration has a triangular array with pitch-to-diameter ratio, $P/d = 1.1$. The rod diameter is 8 mm and it is made of steel (in the laboratory experiment).

The open-source CFD tool OpenFOAM 2.4.x was used to solve differential equations of mass and momentum. Unsteady Reynolds-Averaged Navier–Stokes (URANS) equations are solved using the k-ω SST turbulence model to ensure the closure of the equation system. A lowReynolds turbulence model approach was used. The 2D problem was addressed to simplify numerical calculations.

2.1 Description of the Numerical Model

The investigation of an appropriate computational domain was achieved through a decoupling approach. The number of cylinders was reduced by columns in the in-flow direction and by rows in the crossflow direction. Several computational domains were analysed to find an optimal case given both the accuracy of the results and the cost of computing. The columns and rows of the cylinder arrays were decreased step by step with a decrement 1. Other conditions remained the same. The drag force F_x was used to compare the impact of array rows and columns.

The largest analysed domain was a 4×5 cylinder array, see the domain A in Fig. 1. Decreasing rows from four to two changes the force F_x by less than 1 %. The boundary condition at the top and bottom is simplified as a symmetry condition. The reduction of columns in the direction of flow by removing one column behind the test cylinder causes a non-significant change in the calculated force. In contrast, the reduction of one column in the direction of upstream causes a change of approximately 4 %. Because of the above, the domain B (see Fig. 1) can be considered an optimal computational domain for the analysed Reynolds numbers and array configuration.
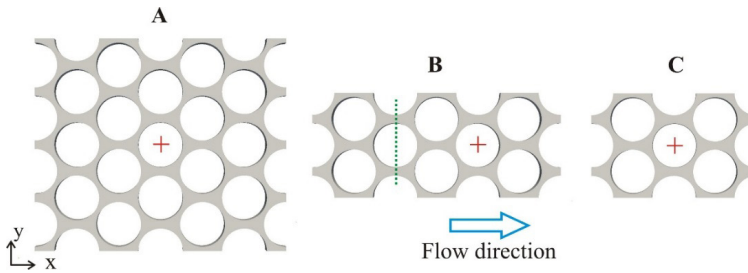

Fig. 1. Analysed computational domains. The centre of the test cylinder is marked with the red cross.

As RANS-type calculations are performed that are time-averaged, it is possible to determine a typical distribution of flow between two adjacent cylinders, see the green dotted line in the domain B. Using the found flow profile as an inflow boundary condition, the computational domain can be reduced to a 2×2 array of cylinders, see the domain C in Fig. 1. This approach is useful because the developed surrogate models require a set of calculations that change only the mass and support stiffness of the test cylinder and not the characteristic of the inlet flow. Operating pressure $p = 0$ Pa was defined on the outflow boundary.

Different mesh refinements were studied to avoid the influence of the cell size on the numerical simulations. As a low-Reynolds turbulence model was used, particular attention was paid to the correct description of the boundary layer around cylinders. The final version of the mesh contains 476 000 cell elements. Around cylinders, it contains 25 layers with an expansion ratio of 1.05, providing y^+ less than 1.

Based on studies available in the literature, it is known that the largest oscillations are in a direction perpendicular to the flow and therefore the movement of the test cylinder is only allowed in the transverse direction. The rotation of the test cylinder is also not allowed. The movement of the test cylinder in crossflow was studied by mounting it as a massspring system, where m is the mass of the oscillating part and k is the stiffness coefficient of the mounting.

2.2 Verification and Validation of the Model

According to Roache [10], the quantification of uncertainty in numerical simulations contains the three most important items: verification of codes, verification of calculations and validation. Since standard OpenFOAM solvers are used in the modelling process, the verification of the code is not carried out in this case. Solution verification is carried out using flow simulation around a single cylinder at Re = 11000 and comparing integral parameters with data available in the literature. Table 1 shows a summary of the drag coefficient, $C_d = 2F_x/(u^2S)$, where u is flow velocity, S is an area that interacts with the flow and Strouhal number, St, from the various studies.

Table 1. Comparison of the Modelled and Experimental Results of the Drag Coefficient C_d and Strouhal Number St

The study	C_d	St
Khan et al. [11], RANS, 2D	1.150	0.201
Khan et al. [11], RANS, 3D	1.210	0.203
Dong et al. [12], DNS	1.208	0.209
Wornom et al. [13], LES	1.22	0.20
Nguyen and Nguyen [14], DES	1.133	0.200
Gopalkrishnan [15], Exp	1.186	0.193
Norberg [16], Exp	-	0.202
Present study, URANS, 2D	1.19	0.21

The analysis of the test case allows selecting the optimal turbulence model, boundary conditions and computational cell size.

The model validation was implemented by comparing the numerical results with the experimental drag force values, C_d, the natural frequency of the test rod in the flow, f_n and the flow-induced frequency f_t. The results obtained are summarised in Table 2.

Table 2. Validation of the Full Numerical Model

The study	f_n	f_t	C_d
Experiment (Upnere *et al.*, 2020)	58.50	27.30	0.346
CFD, 2D	59.32	28.66	0.359
CFD, 3D	-	28.56	0.352

As shown in Table 2, the difference between the results of CFD and the experimental measurements obtained is less than 5 %.

2.3 Dominant Frequencies

The dominant frequencies were determined using the movement of the test cylinder and the calculated lift coefficient. The fast Fourier transform (FFT) and inverse FFT method were applied to time series obtained from numerical simulations. The FFT approach was implemented in Matlab.

3. SURROGATE MODELLING

3.1 Design of Experiments

The selection of sampling points has a major effect on building a reliable surrogate model. Space-filling designs become a primary consideration for the design of computer simulation experiments [1]. Space-filling design allows selecting those sample points that are distributed within the entire domain.

In this study, the new class of experimental designs described in [8] is used. Unlike classical CCD designs, in this case, all design points are within the research domain. Orthogonal designs of this type are particularly suitable for use with orthogonal Legendre polynomials detailed in the next subsection. This approach allows avoiding problems related to the optimal selection of significant terms, for example, in cases where the number of points is not much larger than the total number of possible terms. The following constraints were used to develop the experimental design [8]: 1) all experimental points were located in the unit cube [-1, 1]^l; 2) designs had central symmetry, axial symmetry and 90-degree rotation symmetry properties; 3) designs were invariant to the permutation of input variables; 4) designs gave replications of centre point; 5) designs were orthogonal; 6) designs were D-optimal.

Figure 2 shows the 13-point orthogonal design used in the study to create a surrogate model with mass m = [0.2765; 0.3253] and stiffness coefficient k = [15725; 18500] as factors.
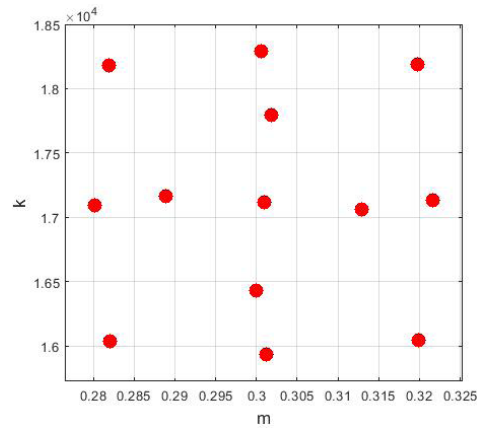

Fig. 2. The two factors (mass m and stiffness coefficient k) orthogonal design with 13 points.

3.2 Response Surface Method

Polynomial approximations produce surrogate models using low-order polynomials in a relatively small region of parameter space [2]. If the response function to be studied is expected to be linear, the first-order polynomial approximation can be used, defined as [17]:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n + \varepsilon, \tag{1}$$

where $\hat{y}$ is the system response, x_i, $i = 0, 1, \ldots, n$, are independent variables, the parameters β_i are called the regression coefficients, ε represents the noise or error observed in the response y assumed to be independent and normally distributed with mean zero and constant variance σ^2.

If the system under investigation is nonlinear, a higher-order polynomial should be used. For example, in the general case, a second-order polynomial regression model with n simulation inputs is as shown below:

$$\hat{y} = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii} x_i^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} x_i x_j + \varepsilon. \tag{2}$$

Regression coefficients β in Eq. (2) are estimated applying the least-squares criterion

$$\hat{y} = (X'X)^{-1} X'w, \tag{3}$$

where w denotes the n-dimensional vector with the simulation outputs. The least-squares estimator $\hat{\beta}$ exists if and only if the inverse of $X'X$ exists; e.g., $\hat{\beta}$ exists if X is orthogonal [18]. The method of the least squares returns the vector of the regression model parameters, which minimizes the sum of squared errors between the predictions of the regression model and the values of the true function.

3.3 Legendre Polynomial Approximation

The Legendre polynomials $P_i(x)$ are defined over $x \in [-1; 1]$ by the recurrence relation as [19]:

$$\begin{cases} P_0(x) = 1 \\ P_1(x) = x \\ (i+1)P_{i+1}(x) = (2i+1)xP(x) - iP_{i-1}(x), i-1,2,\ldots \end{cases} \tag{4}$$

The classic and discrete Legendre polynomials are orthogonal. In this study, orthonormal Legendre polynomials are used, which means that all terms must be multiplied by $\sqrt{\frac{2i+1}{2}}$. For onedimensional problem the first 4 orthonormal polynomials are:

$$\begin{cases} P_0(x) = \sqrt{\frac{1}{2}} \\ P_1(x) = \sqrt{\frac{3}{2}}x \\ P_2(x) = \sqrt{\frac{5}{2}}(3x^2 - 1)/2 \\ P_3(x) = \sqrt{\frac{7}{2}}(5x^3 - 3x)/2 \end{cases} \quad . \qquad (5)$$

The multivariable polynomial terms are the product of single variable polynomials and they are orthonormal. The property of orthonormality allows for optimal selection of significant terms in the approximation polynomial function [8]. This is useful in cases where multivariate high order polynomials are used since in such situations the number of terms is rapidly increased and makes the application more difficult. The cross-validation criterion is used to decide whether to eliminate or keep the term with a small Euclid norm [8]:

$$\|P_i(x)\| = \sqrt{\int_{-1}^{1} P_i^2(x)dx} = \sqrt{\frac{2}{2i+1}}. \qquad (6)$$

In surrogate models, assessment methods should be applied to check if the developed models are adequate. The selection of approximations here is based on strategies described in the next subsection.

3.4 Surrogate Model Adequacy and Fitting

Myers et al. [1] define two steps for checking the response surface: 1) to examine the fitted model to ensure that it provides an adequate approximation to the true system and 2) to verify that none of the least-squares regression assumptions is violated.

One of the techniques for checking model adequacy is residual analysis. In the context of surrogate modelling, the residual is defined as

$$e_i = y_i - \hat{y}_i, i = 1, 2, \ldots, n. \qquad (7)$$

In the plot of residuals e_i versus the predicted response $\hat{y}_i$, the residuals should scatter randomly, suggesting that the variance of the original observations is constant for all values of y.

To estimate the generalization error, leave-k-out cross-validations commonly used. The cross-validation error can be used for surrogate model parameter estimation, model selection and validation when it is too costly to employ a separate validation data set [3]. Based on the study of Meckesheimer et al. [20], the value of $k = 1$ is recommended for providing a prediction error estimate for low-order polynomials, and for Kriging surrogate models it is rec-

ommended to select k as a function of the fitting design size, for example, $k = 0.1N$ or $k = \sqrt{N}$. In this study, the relative cross-validation error is expressed as:

$$\sigma_{cr\%} = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_{-i} - y_i)^2}}{\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2}} 100\,\%, \qquad (8)$$

where $\hat{y}_{-i}$ denotes the prediction of the response using the surrogate model created without the point i ($i=1, 2, \ldots, n$) and $\bar{y}$ is the average value of y.

For regression models, R^2-type metrics (R^2 is the coefficient of determination) are the commonly used goodness-of-fit measure. An adjusted coefficient of determination R^2_{adj} is used to avoid the fact that adding a variable to the model always increases the value of R^2. Pearson's χ^2 test is another commonly used metric. The χ^2 test is a goodness-of-fit test to see whether the data are in concordance with the null hypothesis H_0 [7]. Pearson's χ^2 test indicates whether the frequency distribution of specific events observed in the sample corresponds to a theoretical distribution.

4. RESULTS

CFD simulations are used to obtain the response values in the sampling points. The values from the high-fidelity model are applied to construct an approximation model that would indirectly detect a change in the mass of the rod.

4.1 Forward Model

Based on the results of the laboratory experiments described in Upnere et al. [9], the frequency ratio between the natural frequency of the rod in the flow f_n and the flow-induced frequency f_t is selected as a response for the surrogate modelling.

As the design of experiments (see Fig. 2) is orthogonal, Legendre polynomials can be used as an approximation. The transformation from physical units to the unit cube $[-1; 1]^2$ is as follows:

$$x_1 = 40.983896062695m - 12.332054325265,$$
$$x_2 = 0.0007207207207207k - 12.333333333333, \tag{9}$$

where $m = [0.2765, 0.3253]$ and $k = [15725, 18500]$.

Analysis of the significance of polynomial terms based on Euclid norm in Eq. (6) shows that the coefficient per term does not depend on the number of terms used for approximation. This is due to the orthogonality of the design of experiments. From the relative cross-validation error depending on the number of terms of the Legendre polynomials presented in Fig. 3a, it follows that half of the polynomial terms can be discarded without affecting the outcome.
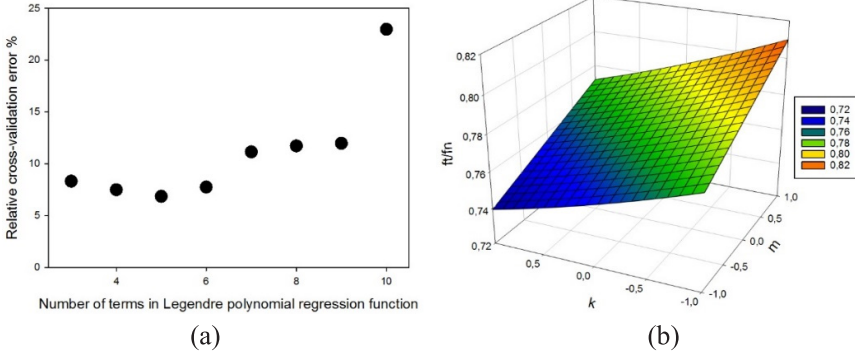

Fig. 3. Legendre polynomials: (a) the relative cross-validation error depending on the number of orthogonal terms; (b) response surface of 5-term Legendre polynomials in the unit cube.

The response surface of the 5-terms polynomial model in the unit cube is shown in Fig. 3b and the corresponding Legendre polynomial can be described as follows:

$$\hat{y}(x_1, x_2) = 1.544039P_0P_0 + 0.020323P_0P_1(x_1) - 0.020521P_0P_1(x_2) + 0.001028P_0P_2(x_2) - 0.000967P_1(x_1)P_1(x_2). \tag{10}$$

In addition to Legendre polynomials, the first, second and third-order polynomials are investigated. The comparative results of the model quality metrics are summarised in Table 3.

Table 3. Approximation Quality Indicators of the Forward Model

Approximation	$\sigma_{cr\%}$	R^2_{adj}
First-order	8.31	0.996
Second-order	8.16	0.998
Third-order	22.96	0.998
Legendre	6.85	0.998

Table 3 shows that there is a small difference between the first- and second-order polynomial approximation which gives 8.31 % and 8.16 % cross-validation error, respectively. From Fig. 3a and Table 3 it follows that the lowest error – 6.85 % is obtained by 5-term Legendre polynomials.

The adequacy of the model is also confirmed by plots of residuals that are randomly scattered (see Fig. 4). The residual versus response f_t/f_n is shown in Fig. 4a. The residual values are not correlated with factors x_1 and x_2. The example of the residual versus input x_1 is presented in Fig. 4b.

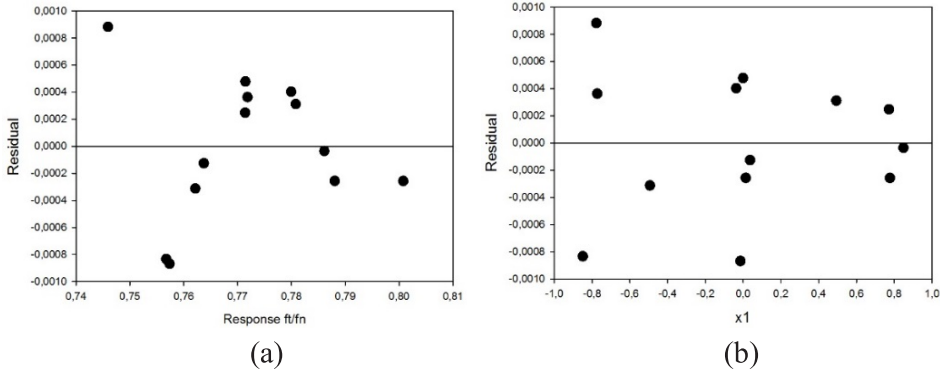(a)   (b)

Fig. 4. The residual and regression line: (a) the residual values vs. response; (b) the residual vs. factor x_1.

4.2 Inverse Model

The inverse surrogate model for predicting changes of the oscillating cylinder mass was created using f_t/f_n and k as factors. The formulas for transformation to unit cube for Legendre polynomials are:

$$x_1 = 37.2562667089699 f_t/f_n - 28{:}8236008539,$$
$$x_2 = 0.0008489240339426k - 14{:}52721253084, \quad (11)$$

where f_t/f_n = [0.746816665, 0.800498909] and k = [15934.5382978725, 18290.4617021275].

As the design of experiments is not orthogonal, the coefficients for the terms of the Legendre polynomials vary depending on the number of terms. Therefore, the use of Legendre polynomials is not as effective as in the forward model. The comparative results of the model quality metrics are summarised in Table 4.

Table 4. Approximation Quality Indicators of the Inverse Model

Approximation	$\sigma_{cr\%}$	R^2_{adj}
First-order	11.52	0.992
Second-order	11.37	0.996
Third-order	36.41	0.995
Legendre	8.95	0.997

As can be seen from Table 4, there is only one method of approximation, for which the crossvalidation error is less than 10 %, the 4-term Legendre polynomials. Therefore, the Legendre polynomials were selected for building the surrogate model. Figure 5 presents response surfaces of 4-term Legendre polynomials and the relative cross-validation error depending on the number of terms.
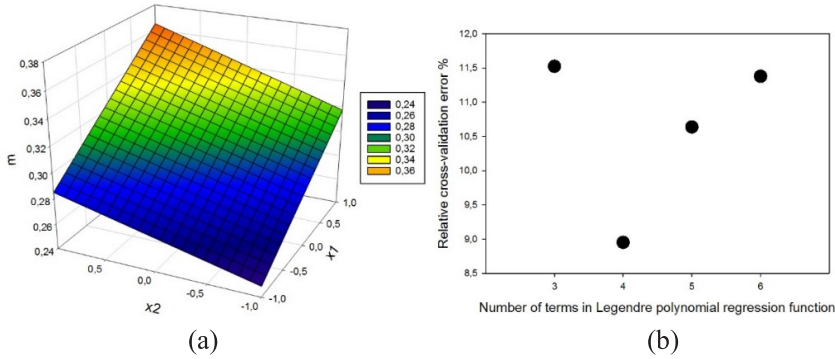

Fig. 5. Legendre polynomials of inverse surrogate model: (a) the response surface designed using 4 terms; (b) the relative cross-validation error vs. terms of the polynomial.

The residual graph shows the absence of correlation between the response and residual values. Examples of residuals are shown in Fig. 6.
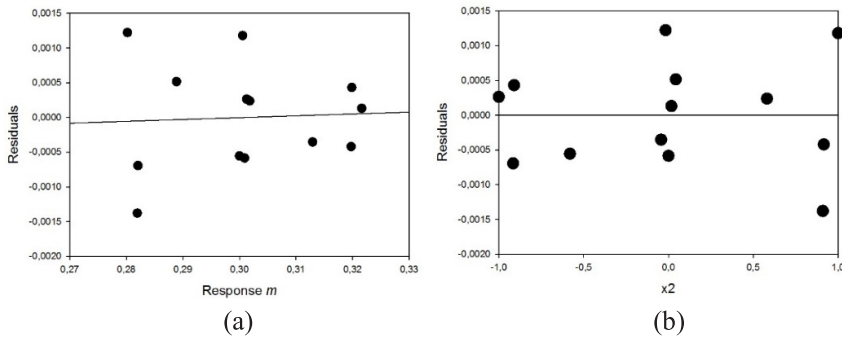

Fig. 6. Residual values and regression line of the inverse surrogate model: (a) the residual versus predicted response; (b) residual values versus input x_2.

The obtained model equation using 4-term Legendre polynomials is as follows:

$$m(f_t/f_n) = -0.11026f_t/f_n - 4.97899 \cdot 10^{-5}k + 8.74349 \cdot 10^{-5}f_t/f_n \cdot k + 0.083652. \quad (12)$$

The inverse model verification was implemented by selecting specific points and comparing the results of the model and numerical experiments at these points. The comparison graph is shown in Fig. 7. The confidence interval *CI* is determined to measure the uncertainty around the estimated values:

$$CI = \bar{y} \pm z \cdot \frac{\sigma}{\sqrt{n}}, \tag{13}$$

where σ is standard deviation and for 95 % *CI* $z = 1.96$. The upper and the lower confidence bound can be seen in Fig. 7 with a dashed blue line.

From Fig. 7, it can be concluded that the resulting surrogate model can predict the behaviour of the analysed model system with high precision – when input factor values are changed within 15 %, the difference is less than 1.5 %.
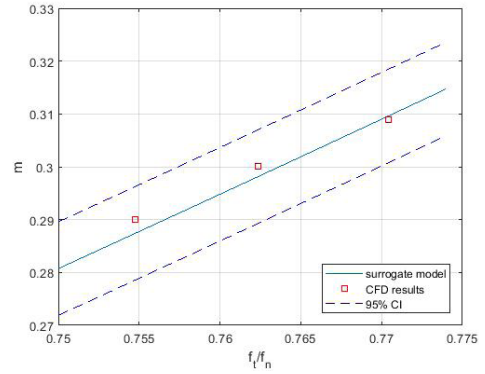

Fig. 7. Verification of the inverse surrogate model if the stiffness coefficient is 17600 N/m.

5. CONCLUSIONS

A methodology was developed for creating a surrogate model for the mass reduction analysis of the rod in the rod bundle inserted in the crossflow. The interaction between mass and stiffness as factors and frequency ratio as the response was applied to build the forward model. The inverse surrogate model was created using mass as a function of stiffness and frequency ratio.

The new third-order orthogonal design of experiments was used to define sample points. Orthogonality of the experimental design allowed for simple elimination of insignificant terms in Legendre polynomial approximations.

Four methods of approximation were investigated: first-, second- and third-order polynomials and Legendre polynomials. The most appropriate approximation for both the direct and inverse models for the problem under study was obtained using Legendre polynomials. The corresponding cross-validation errors were 6.85 % and 8.95 %. Verification of the inverse model showed that the difference between the results of the CFD calculations and the predicted values of the surrogate model was less than 1.5 %.

The analysis carried out showed that the developed method of approximation and the obtained factors-response relationships had a good fit with numerical experiments. The results also demonstrated that the surrogate model could reliably replace the finite volume simulations and drastically reduce computational time. Therefore, the proposed methodology is useful in the monitoring of cooling systems as well as in the design process of such systems.

ACKNOWLEDGEMENTS

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