UNCERTAINTY EVALUATION OF CFD SIMULATION USING OPTIMAL STATISTICAL ESTIMATOR

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ABSTRACT

Uncertainty methods are widely applied to evaluate the uncertainty of thermalhydraulic system codes, being the main safety analysis tool in past decades. Rapid increase of computational power along with continuous development of local mechanistic models opens the space for detailed Computational Fluid Dynamics (CFD) codes. Like system codes, CFD predictions can also be affected by uncertainties. Uncertainty evaluation methods for CFD codes are still under development. The main purpose of this study was the uncertainty evaluation of NEPTUNE_CFD results for Generic Mixing eXperiment (GEMIX). A method called Optimal Statistical Estimator (OSE) has been proposed for response surface generation of CFD predictions, which replace code calculations when using Monte Carlo method to randomly sample the input parameters to quantify the uncertainty. The turbulent mixing experiment GEMIX performed at Paul Scherrer Institute was used as a benchmark case. In the GEMIX experiment two turbulent horizontal channel flows with the same fluid properties and inlet velocities have been mixed together to form a mixing layer flow. Two uncertain input parameters were considered as uncertainty variables: inlet velocity profile and inlet turbulence intensity. The calculational matrix consisted of 30 CFD calculations. The parameter turbulence intensity was varied in equidistant steps of 1% and the parameter alpha ($0 \leq \alpha \leq 1$) was varied in steps of 0.2. The results of the uncertainty analysis are presented. It has been demonstrated that OSE is a very efficient and accurate method for uncertainty evaluation of CFD calculations when a few parameters are being varied.

KEYWORDS
CFD simulation, uncertainty evaluation, turbulent flow

1. INTRODUCTION

Uncertainty methods are widely applied to evaluate the uncertainty of system codes [1], being the main safety analysis tool in past decades. Rapid increase of computational power along with continuous development of local mechanistic models opens the space for detailed Computational Fluid Dynamics (CFD) codes. Like system codes, CFD predictions can also be affected by uncertainties. Uncertainty of results can be associated by inlet boundary conditions (e.g. the mass flow rate is known but not the velocity distribution or turbulence intensity at the inlet), fluid properties or modelling parameters. Uncertainty evaluation methods for CFD codes are still under development hence a simple single-phase test case is needed as a starting point. In this work a turbulent mixing experiment GEMIX (Generic Mixing eXperiment) [2] performed at Paul Scherrer Institute (PSI) was used as a benchmark case. In the GEMIX experiment two turbulent horizontal channel flows with the same fluid properties and inlet velocities are mixed together to form a mixing layer flow.

Very accurate predictions of the turbulent mixing flow can be provided by the Direct Numerical Simulation (DNS) or by the Large Eddy Simulation (LES) method. However, these methods are computationally too demanding. Much faster but also less accurate method is based on the solving of Reynolds Averaged Navier Stokes (RANS) equations. RANS methods require modelling of the entire turbulence spectrum that is based on various assumptions. In the present work the widely used k-ε turbulence model is adopted for turbulence modelling.

The presented work is performed within the frame of the NURESAFE project (7^{th} FP EURATOM). The main objective of the study is to evaluate the uncertainty of the NEPTUNE_CFD code [3] that is one of the NURESIM platform codes. Two uncertain input parameters are considered in this study: variation of inlet velocity profile and variation of inlet turbulence intensity. In this respect 30 “steady-state” calculations were performed varying these two parameters. NEPTUNE_CFD code version 2.0.1 [3] was used for CFD simulations. In the following the methods are explained first. The GEMIX experiment with NEPTUNE_CFD input model and the Optimal Statistical Estimator (OSE) method, which was used for uncertainty analysis, are described. The calculations needed for uncertainty analysis are also briefly described. In the results section the CFD calculated results and the results of the uncertainty analysis by OSE method are presented.

2. BENCHMARK AND METHODS USED

First the GEMIX experiment is presented. A brief information on the NEPTUNE_CFD input model for GEMIX experiment is given and the rationale for selection of uncertain parameters are provided. Finally, OSE method and the calculation matrix for uncertainty analysis are described.

2.1. Gemix Experiment

The GEMIX test section consists of a Y-shaped horizontal square channel, where the two streams with the same inlet velocities and fluid densities mix together forming a turbulent mixing region downstream the splitter plate. Measured data at several horizontal locations downstream the splitter plate include cross-sectional profiles of velocity, turbulent kinetic energy and concentration in the mixing region. It is assumed that the main source of uncertainties arises from the inlet boundary conditions and from the turbulence models in the CFD code. The inlet mass flow rate is known, but the inlet distributions of velocity and turbulence intensity are not measured therefore they are considered as uncertainty parameters. The layout of GEMIX mixing experiment is shown in Figure 1. The experiment consists of two rectangular ducts, through which the water is introduced into a rectangular mixing section with a mass flow rate of 0.8 kg/s. As the two flows pass the splitter plate, they interact with each other and form turbulent mixing layer. Detailed description of experiment is given in [2].

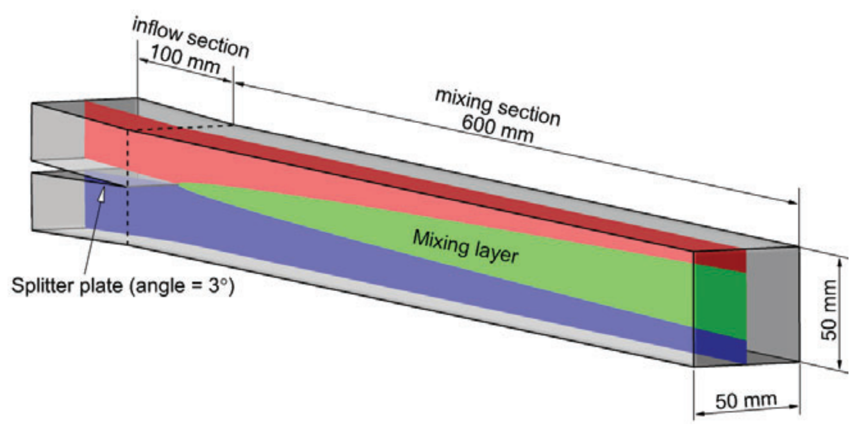


Figure 1. Setup of the GEMIX experiment (Courtesy of PSI).

2.2. NEPTUNE_CFD Model

The simulations were carried out with the NEPTUNE_CFD computational program, version 2.0.1 [3, 4]. The standard k-ε model with the logarithmic wall function near the walls was used for turbulence modelling. The calculations were performed on the computational mesh with 475,000 hexagonal elements with moderate mesh refinement near the channel walls and the splitter plate. The cross-section of the mesh is presented in Figure 2.

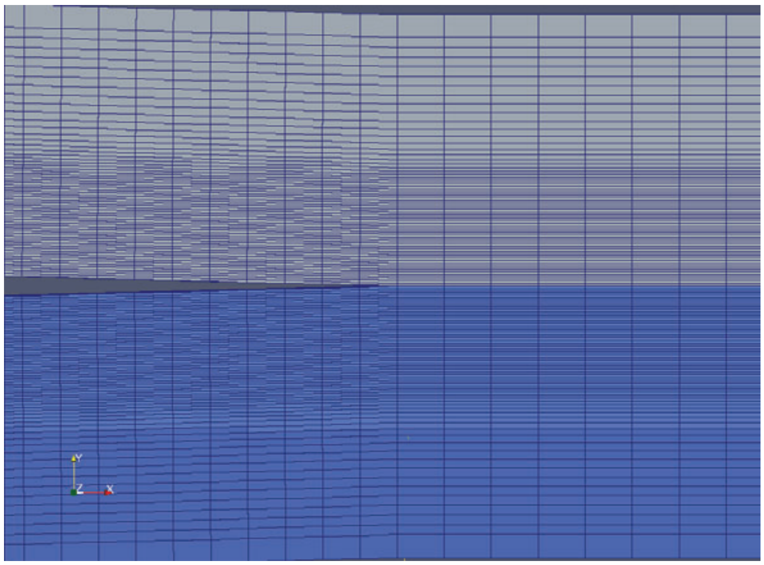


Figure 2: Cross-section of the computational mesh

The selected mesh is the same as the one used in the FLUENT code calculations carried out by the Paul Scherrer Institute (PSI) [2]. Beside mesh also the same turbulence model was used, aiming to compare the results of both codes within the NURESAFE project.

It should be noted that the NEPTUNE_CFD code is primarily developed for the simulation of two-phase flow transients. Therefore, the single-phase simulation in the NEPTUNE_CFD can be activated by prescribing the value of 1 for the liquid void fraction in the computational domain. The mass flow at the inlet is the same in both legs (1 kg/s), which corresponds to the average liquid velocity of 0.8 m/s. Density of the water at the inlet of both legs is 998 kg/m^3 at the temperature of 23 ^{o}C. Besides the velocity, also the turbulence intensity has to be prescribed at the inlet. No-slip boundary conditions are used on the wall and constant pressure is set at the outlet of the domain.

The constant time step of 0.02 seconds was used for calculations. About 100 iterations was sufficient to reach the converged solution. Default numerical schemes were used for the calculations. Time development of downstream velocity W is presented in Figure 3.

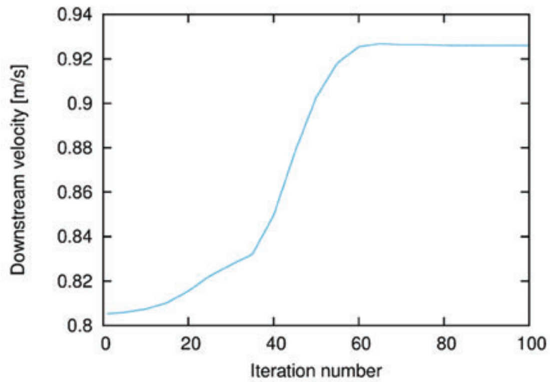


Figure 3. Time history for the downstream velocity in the NEPTUNE_CFD calculation

2.3 Selection of Uncertain Parameters

Inlet boundary conditions represent the major source of uncertainty. Namely, in the experiment only the mass flow rate was measured, while the velocity and turbulence intensity at the inlet remain unknown. Therefore these two variables were considered as uncertain parameters. The inlet velocity profile was varied between the uniform and fully developed turbulent profile shape, by taking into account the parameter α:

$$U(x,y) = \left(\frac{\alpha}{U_d(x,y)} + \frac{1-\alpha}{U_u}\right)^{-1}, \tag{1}$$

where $U_d(x,y)$ stands for fully developed velocity profile and U_u for the uniform velocity. Fully developed velocity profile was obtained from a separate run in a single long rectangular channel of the same cross-section and was imposed on both inlet legs. However, in the NEPTUNE_CFD it is not possible to impose an array of pre-calculated values for boundary conditions. Therefore the profile was approximated by trigonometric mathematical functions that are exactly zero at the wall. The product of two series of cosine functions (Fourier series) was used:

$$U_d(x,y) = \left(\sum_{n=1}^{26}\left(a_n\, cos\,\frac{n\pi x}{L_x}\right)\right)\left(\sum_{n=1}^{26}\left(b_n\, cos\,\frac{n\pi y}{L_y}\right)\right), \tag{2}$$

where a_n and b_n are coefficients obtained with least-squares method and L_x and L_y represent the dimensions of the channel. The parameter α in Eq. (1) is varied between 0 and 1 (0 represents uniform and 1 fully developed axial velocity profile) in steps of 0.2. The second uncertainty parameter is turbulence intensity β which is varied between 0% and 4% in steps of 1%.

2.4 Description of OSE for Uncertainty Analysis

When hundreds of complex computer code runs are needed for statistical analysis, the response surface can be used to replace numerous code simulations. In this way, the response surface can be applied for uncertainty analysis in order to derive the probability statement (for example, 5% and 95% probability). The use of response surface for uncertainty analyses of system codes in nuclear engineering was successfully demonstrated by Haskin et al. [5] and by Prošek and Mavko [6]. In the treatment of uncertainty by Duffey [7], the probability distribution function, for each output parameter as a function of two parameters, was obtained by fitting second order polynomials. There were also attempts to replace response surface functions with Latin hypercube sampling [8]. In the work of Prošek and Mavko [9] the response surface was generated by the OSE, which enables its use also for continues-valued parameters and can be applied for multidimensional space.

Basic equations for response surface generation with OSE are provided herein, details are provided in [9]. OSE is expressed as a linear combination of code calculated output values (or their corrected values) and coefficients representing the similarity between the code and a given input data. In the case of uncertainty evaluation this linear combination is used to replace the code-calculated value when Monte Carlo method is used to generate an approximate distribution that characterizes uncertainty of an input parameter. The optimal statistical estimator $\hat{H}_O(G)$ and the coefficients C_n are defined as:

$$\hat{H}_O(G) = \sum_{n=1}^{N} C_n H_n, \tag{3}$$

$$C_n \equiv \frac{\delta_a(G - G_n)}{\sum_{n=1}^{N} \delta_a(G - G_n)}, \tag{4}$$

where $G=(x_1, x_2,...,x_M)$ is a given input data vector, $G_n=(x_{n1}, x_{n2},...,x_{nM})$ and $H_n=(x_{n(M+1)}, x_{n(M+2)},...,x_{nI})$ are input and ouput data vectors for n-th calculation, respectively, M is number of input parameters, I number of input and output parameters and N is the number of calculated (or measured) values. The coefficients C_n represent the measure of similarity between a given vector of input data G and the vector G_n for n-th calculation. The approximation of δ function is Gaussian function:

$$\delta_a(G - G_n) = \left(\prod_{i=1}^{M} \frac{1}{\sqrt{2\pi} \cdot \sigma_i} \right) \exp\left(-\frac{1}{2} \sum_{i=1}^{M} \left(\frac{x_i - x_{ni}}{\sigma_i} \right)^2 \right), \tag{5}$$

where σ_i is width of the Gaussian curve selected by the user. The contribution of each calculated data point to the final output parameter estimation can be adjusted by this function as shown in [9].

Using the derived optimal statistical estimator $\hat{H}_0$ the complete estimated vector can be defined as

$$Y = \left(G \oplus \hat{H}_0\right) = Y(X) \tag{6}$$

The function Y(X) is modeled by the OSE computer code. Vector Y is influenced by input parameters, which are directly transferred to the output, while optimal statistical estimator determines the complementary values $\hat{H}_0(G)$. One of the most important characteristics of this estimator is that involves the highly non-linear coefficients C_n, therefore response surface for highly non-linear functions can be efficiently generated.

For assessing the adequacy and predictive capability of the optimal statistical estimator the root mean square error and coefficient of determination for m-th parameter are used:

$$RMS_m = \left(\frac{\sum_{n=1}^{N} \left(x_{nm} - x_{est_n,m}\right)^2}{N} \right)^{1/2} \tag{7}$$

$$R_m^2 = \frac{\sum_{n=1}^{N}\left(x_{est_n,m} - x_{avg,m}\right)^2}{\sum_{n=1}^{N}\left(x_{nm} - x_{avg,m}\right)^2} \tag{8}$$

for m=(M+1), (M+2),...,I, where M is the number of input uncertain parameters and I is the number of the input and output parameters. Here x_{nm} is the n-th code calculated value of the m-th output parameter, $x_{est_n,m}$ is n-th estimated value with the optimal statistical estimator (see eq. 3) and $x_{avg,m}$ is the mean of the N code calculated values of the m-th output parameter. The predictive capability of the optimal statistical estimator assessing with the two proposed statistics is perfect when RMS_m=0 and $R_m^2 = 1$.

To produce output results the values of the input parameters $(x_1,x_2,...,x_M)$ are randomly sampled (e.g. by Monte Carlo method) each time and then the corresponding unknown output values are estimated by the optimal statistical estimator using Eqs. (3) through (8). Each time new coefficients C_n are calculated, while the values of H_n are data points, determined in the phase of response surface generation by OSE. The values are based on computer code calculation values appropriately corrected (if needed) to achieve the desired predictive capability of OSE in the code calculated values. If estimated value $x_{est_n,m}$ exceeds the code calculated value x_{nm} the code calculated value is decreased for the difference between estimated and code calculated value, and vice versa. This is done in the iterative steps until the desired accuracy of estimated value is obtained in the points (i.e. values of input parameters) used in N code calculations.

2.5 Calculational Matrix for Uncertainty Analysis

The relevant output quantities for our investigation are turbulent kinetic energy k and velocity in downstream direction at two locations: 0.07 m and 0.45 m downstream from the edge of the splitter plates. To use the response surface technique, each of the input parameters must have an associated range of variation and have an underlying probability distribution function. The uniform distribution requires only that the end points (the range) be specified. It is often referred to as the distribution that maximizes lack of knowledge.

Overall 30 calculations have been carried out at different combinations of parameters α and β representing the velocity profile and turbulence intensity, respectively. The parameter α is varied in range between 0 and 1 in steps of 0.2 what gives 6 runs at given β value. The second input uncertain parameter is turbulence intensity β which is varied in range between 0% (value 0.1% used) and 4% in steps of 1%, what gives 5 runs at given α value. The dimension of calculational matrix is 6 times 5, and the code runs were performed for all combinations in order to have more points for response surface generation (more points mean more information for uncertainty analysis). All calculations have been performed at constant turbulent Schmidt number Sc=0.7.

3. RESULTS

3.1 NEPTUNE_CFD Simulations

The NEPTUNE_CFD simulations results are presented and discussed in Figures 4 to 5.

Axial velocities 0.07 m and 0.45 m downstream the splitter plate are shown in Figure 4. In general, a good agreement with experiment is obtained. The variation of α produces significant variations in downstream velocity just after the splitter plate (Figure 4 (a)), which diminish as the flow develops (Figure 4(b)).

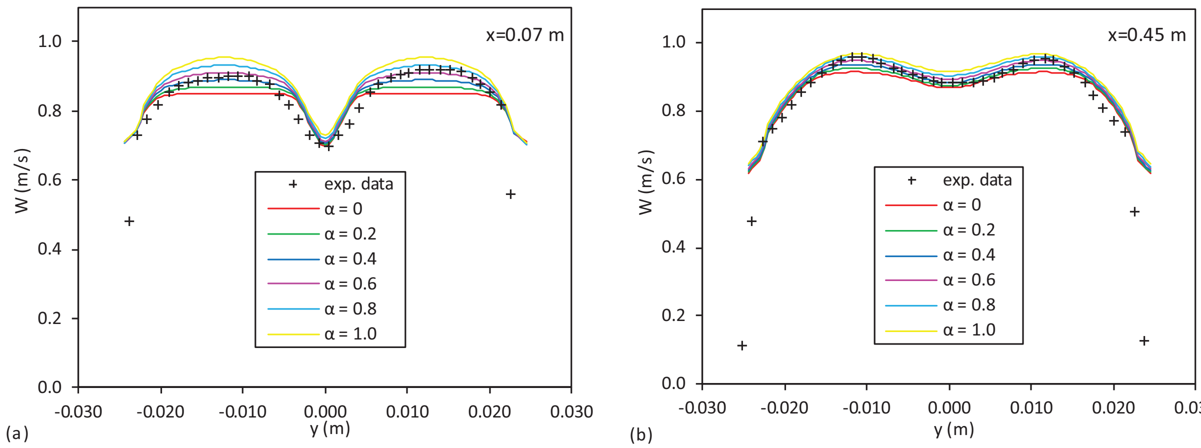


Figure 4: Downstream velocity W for β = 4%: (a) 0.07 m downstream of the splitter plate, (b) 0.45 m downstream of the splitter plate.

Figure 5 shows the turbulence kinetic energy k at two locations. In Figure 5(a) showing turbulence kinetic energy at location 0.07 m downstream of the splitter plate and Figure 5(b) showing turbulence kinetic energy at location 0.45 m downstream of the splitter plate we can see that the production of turbulence kinetic energy at walls is slightly overestimated on left side and slightly underestimated on the right side of Figures 5(a) and 5(b). This can be attributed to the weakness of the *k-ε* model to correctly predict the turbulence in non-circular ducts. At the same time the turbulent energy is underestimated in the intermediate region between the wall boundary layer and the flow center for both meshes. The k profiles in Figure 5(b) also show that the region of overestimated k widens with the flow moving downstream. The variation of the turbulence kinetic energy intensity at the inlet also plays a significant role, as can be seen in Figure 5(a).

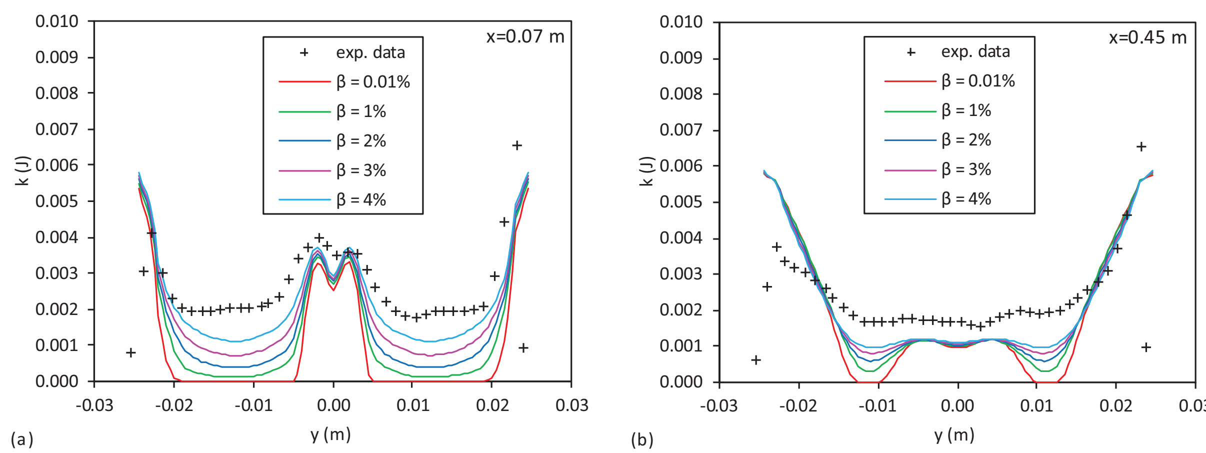


Figure 5: Turbulence kinetic energy k for α = 1: (a) 0.07 m downstream of the splitter plate, (b) 0.45 m downstream of the splitter plate.

3.2 Response Surface Generation by OSE

Figure 6 shows the downstream velocity W at x=0.07 m at three y locations (-0.01 m, 0 m and 0.0245 m) as a function of parameters α and β. On the left side the NEPTUNE_CFD code calculations are shown (graph is created based on 30 calculated data points). The calculated results of output parameters are available in the interval (-0.0245 m, 0.0245 m) with step size 0.0005 m. This gives 99 points (y axis position values) at x=0.07 m and x=0.45 m. At each point (given x and y value) there is a surface (function of α and β), which has to be generated by OSE for uncertainty analysis using Monte Carlo. The response surfaces generated by OSE for three points (x=0.07 m, y=-0.01m), (x=0.07 m, y=0 m) and (x=0.07 m, y=0.0245 m) are shown on the Figure 6. It can be seen that agreement between NEPTUNE_CFD calculation (Figure 6(a)) and response surface generated by OSE (Figure 6(b)) is very good. In Figure 7 similarly the turbulence kinetic energy k is compared between NEPTUNE_CFD calculated surface and response surface generated by OSE as a function of parameters α and β, this time at x=0.45 m for the same y locations (-0.01 m, 0 m and 0.0245 m).

As there are two output parameters at two axial locations for each run this means that 4 times 99 response surfaces were automatically generated by OSE. The coefficients of determination R^2 achieved after 10 corrections were above 0.9996 for all 99 calculated points for both output parameters at both locations indicating high accuracy of response surface generation in known NEPTUNE_CFD calculated points.

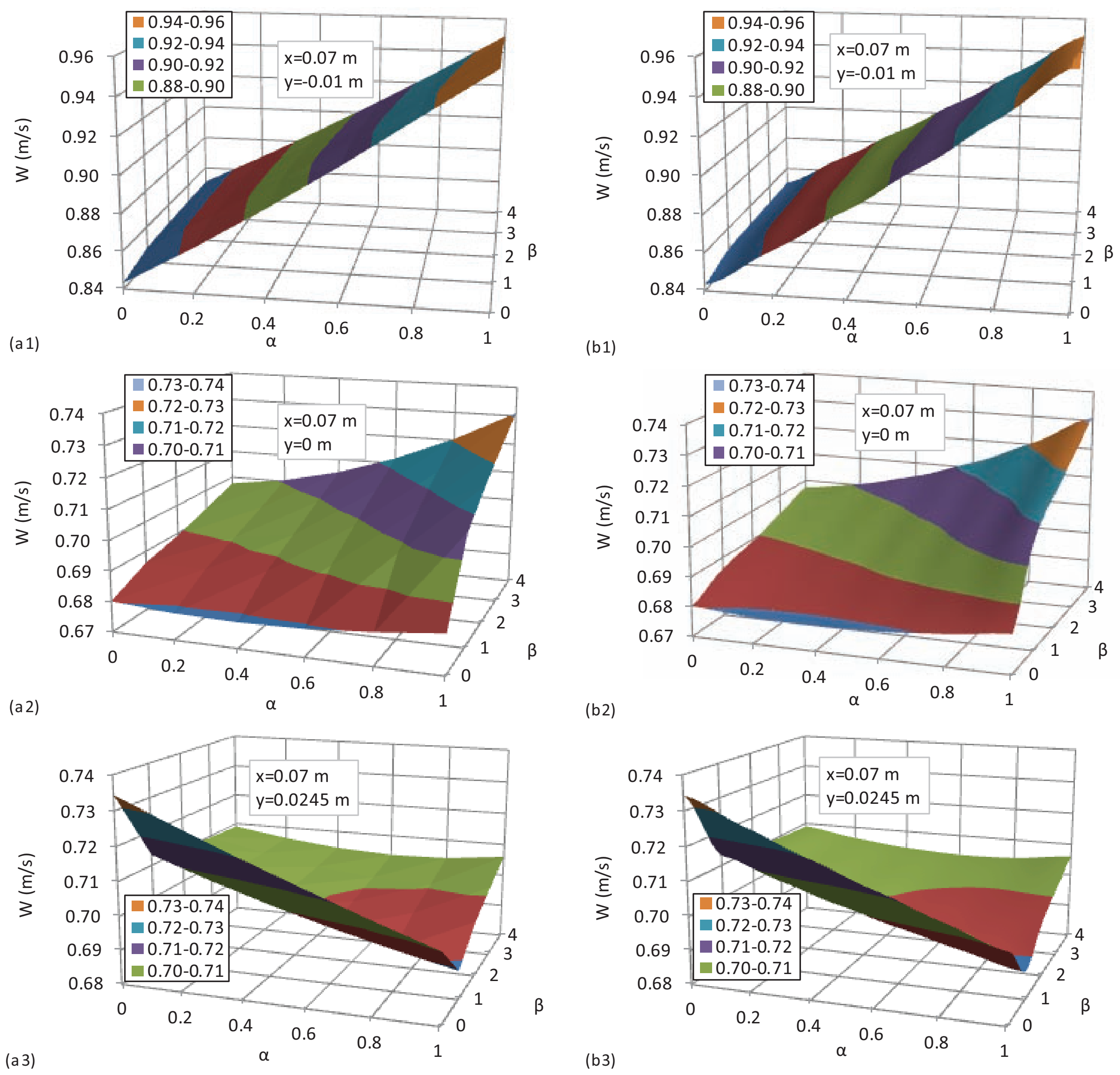


Figure 6: Downstream velocity W dependence on α and β at downstream location 0.07 m for three y axis positions: (a) NEPTUNE_CFD calculation and (b) response surface generated by OSE.

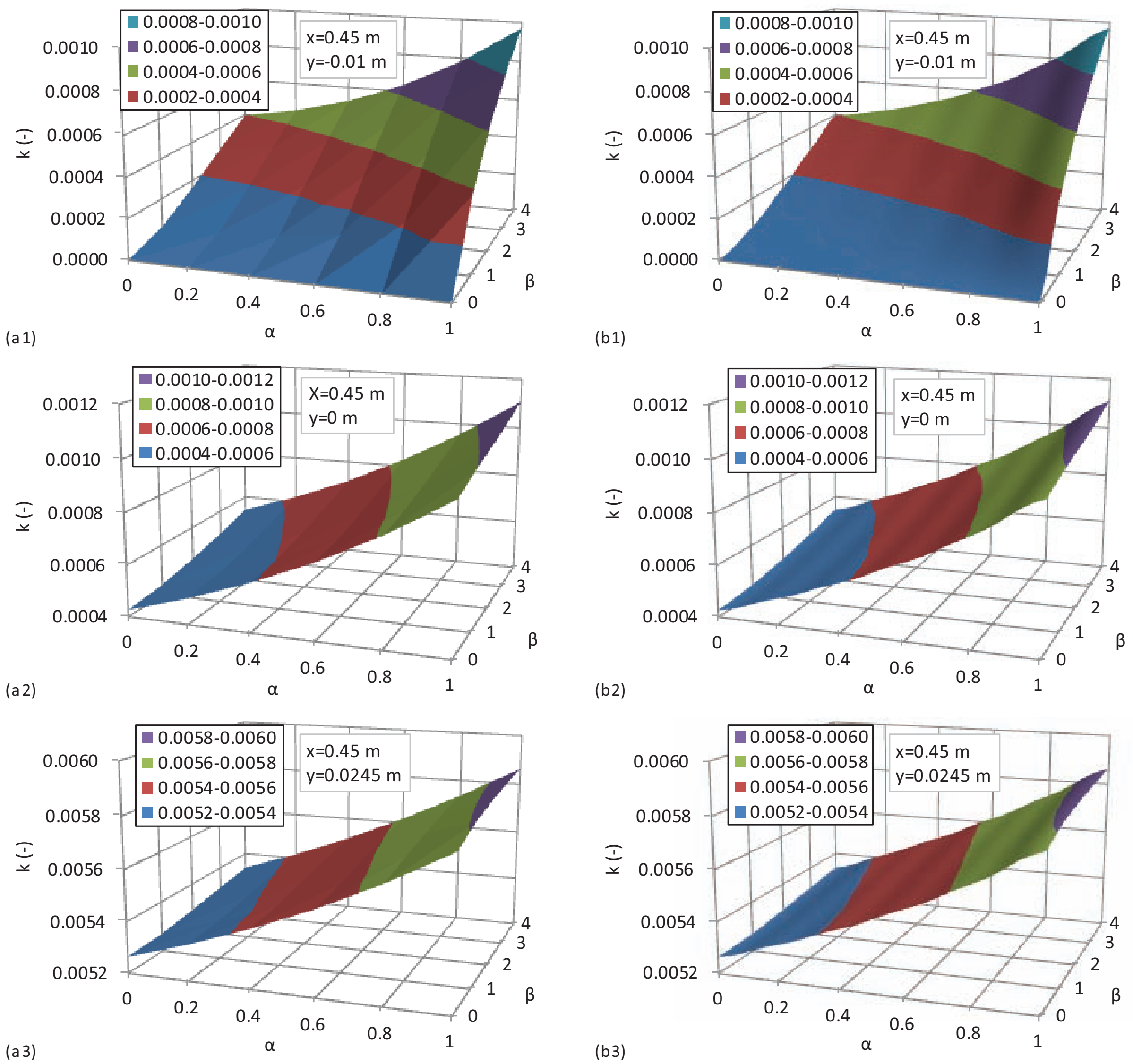
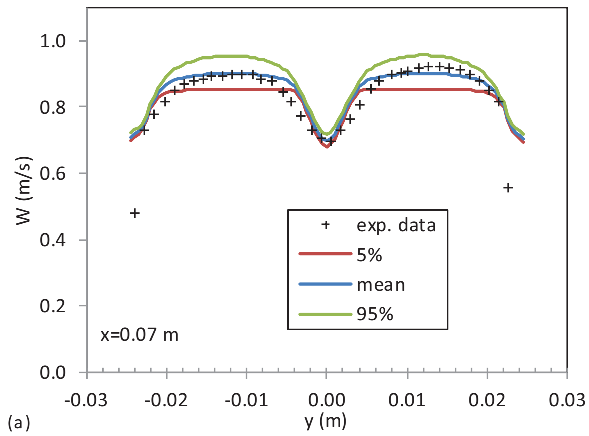


Figure 7: Turbulence kinetic energy k dependence on α and β at downstream location 0.45 m for three y axis positions: (a) NEPTUNE_CFD calculation and (b) response surface generated by OSE.

3.3 Uncertainty Analysis

The results of the uncertainty analysis for downstream velocity and turbulence kinetic energy at two x-axis locations are shown in Figures 8 through 9. For each parameter 100,000 samples were used in uncertainty analysis using Monte Carlo method. The uniform distribution of input parameters was considered like in [2]. The 5 percentile, mean value and 95 percentile were then determined.

The results for downstream velocity show that it is very important to perform a good reference calculation first (here represented by mean value) as uncertainty bands are relatively small. Figure 8 showing downstream velocity is one such example. On the other hand, the velocities near the walls (not accurately predicted) are outside uncertainty bands, as shown in Figure 8. Uncertainty of downstream turbulence kinetic energy is shown in Figure 9. In general, the reference calculations deviate from measured data, therefore only in some intervals the measured data are within uncertainty bands. The results show that in the case of turbulence kinetic energy it is more important the accuracy of reference calculation rather the influence of selected uncertain input parameters. Finally, the obtained results are planned to be used for comparison with the study [2] using the same data.



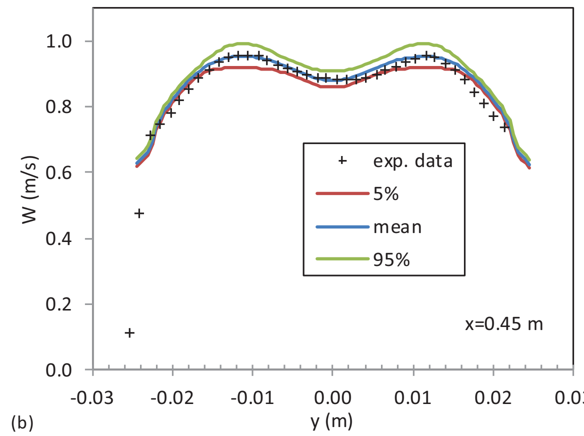
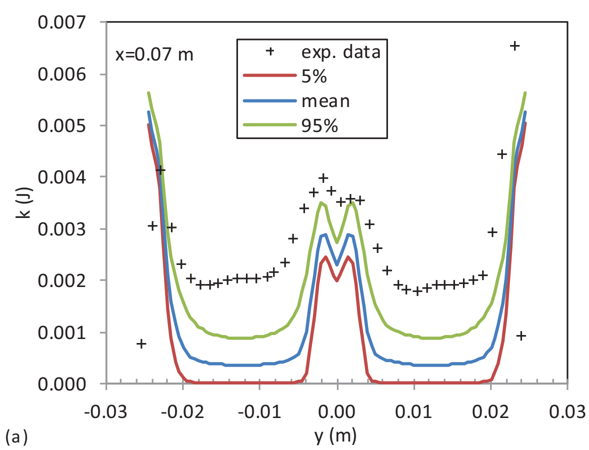


Figure 8: Uncertainty of downstream velocity W: (a) 0.07 m downstream of the splitter plate, (b) 0.45 m downstream of the splitter plate.



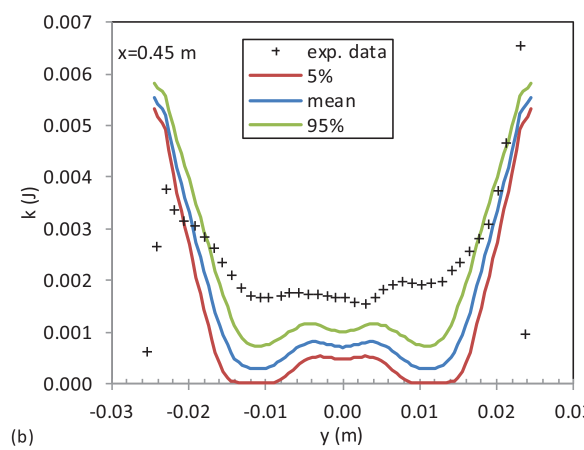


Figure 9: Turbulence kinetic energy k: (a) 0.07 m downstream of the splitter plate, (b) 0.45 m downstream of the splitter plate.

4. CONCLUSIONS

In this study the uncertainty evaluation of NEPTUNE_CFD results for Generic Mixing eXperiment (GEMIX) has been performed. A method called Optimal Statistical Estimator (OSE) has been used for response surface generation of CFD predictions. Two uncertain input parameters were considered as uncertainty variables: inlet velocity profile and inlet turbulence intensity. The calculational matrix consisted of 30 CFD calculations. The parameter turbulence intensity and parameter alpha that describes how much the flow is developed were varied.

The results of the uncertainty analysis show that OSE is applicable for response surface generation of CFD calculations to be used in uncertainty analysis by Monte Carlo method. The method is especially convenient when few parameters are varied. The results suggest that it is very important to perform accurate reference calculation. If this is not the case, the uncertainty may not bound the experimental data. Finally, the aim was achieved to perform the uncertainty analysis of NEPTUNE_CFD calculations for comparison with ANSYS CFD uncertainty analysis simulating the same GEMIX experiment.

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