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Global Sensitivity Analysis of TRACE Physical Model Parameters based on BFBT Benchmark

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Abstract - *Sensitivity analysis (SA) is the study of how uncertain input parameters contribute to the variation in the output. Sensitivity analysis can identify significant input parameters and provide guidance to reduce the response uncertainties most effectively. Global sensitivity analysis aims at quantifying the relative significance of uncertain input parameters. In this paper we compared correlation coefficients and Sobol' indices as Global sensitivity measure. We performed global sensitivity analysis of TRACE void fraction predictions w.r.t. physical model parameters based on the BFBT benchmark. Sobol' indices can directly represent the part of output variance that can be attributed to each parameter and they are preferred over correlation coefficients. Two approaches to compute the Sobol' indices are compared: Polynomial Chaos Expansion (PCE) and Kriging (also known as Gaussian Process emulator) surrogate modeling. The Sobol' indices calculated using PCE and Kriging surrogate models are close to each other, but Kriging surrogate model takes less computational cost. Moreover, it has the potentional to be more applicable when the input dimension gets larger.*

I. INTRODUCTION

Sensitivity analysis (SA) is the study of how uncertain input parameters contribute to the variation in the output. Methods for SA can be generally categorized as local or global [1] [2]. Local SA methods mainly focus on the variation of the model using derivative-based methods around nominal values for the inputs, whereas global methods deal with the variation of the output due to uncertain inputs over the whole domain.

Global SA can be further categorized by regression-based methods and variance-based methods [2]. An example for the former is the input/output correlation coefficient that measures the effect of each input variable by the correlation it has with the model output. Both Pearson Correlation Coefficient (PCC) and Spearman Rank Correlation Coefficient (SRCC) have been used widely as sensitivity measure in previous sensitivity study of nuclear engineering [3] [4].

The variance-based methods [1] [2] mainly use ANOVA (ANalysis Of VAriance) decomposition which represents the variance of the output as a sum of contributions of each input variable or their combinations. For example, Sobol' indice [5] is a popular measure using variance-based methods.

In this work, we perform global sensitivity analysis of TRACE physical model parameters based on the BFBT benchmark. Global sensitivity measures like Sobol' indice and correlation coefficients will be compared to show the superiority of the former over the latter. Finally, both Polynomial Chaos Expansion (PCE) and Kriging surrogate model will be developed for TRACE to calculate the Sobol' indice.

II. GLOBAL SENSITIVITY ANALYSIS

1. Sobol' indices

In the following, we follow the notation in [6] to briefly introduce the formulation of Sobol' indices. We define a model:

$$Y = f(X_1, X_2, \ldots, X_d) = f(\mathbf{X}) \tag{1}$$

where Y and $\mathbf{X}$ are model output and input, respectively. Without loss of generality, Y is assumed as a scalar output and the input vector $\mathbf{X}$ is of dimension d. We define the variance of Y with respect to a generic input factor X_i as:

$$\text{Var}_{(X_i)}\left\{\mathbb{E}_{(\mathbf{X}_{\sim i})}(Y|X_i)\right\} \tag{2}$$

In the above definition $\mathbf{X}_{\sim i}$ represents list of all input factors except for X_i. The inner expectation operator means that the mean of Y is taken over all possible values of $\mathbf{X}_{\sim i}$ given a fixed X_i, while the outer variance is taken over all possible values of X_i. We define the total variance (taken over all input factors) of Y as Var(Y). Then the first order sensitivity coefficient, or Sobol' indices is defined as:

$$S_i = \frac{\text{Var}_{(X_i)}\left\{\mathbb{E}_{(\mathbf{X}_{\sim i})}(Y|X_i)\right\}}{\text{Var}(Y)} \tag{3}$$

S_i is also called the main effect and it quantifies the variability in Y that is caused by uncertainty in X_i alone. Furthermore, from the law of total variation:

$$\mathbb{E}_{(X_i)}\left\{\text{Var}_{(\mathbf{X}_{\sim i})}(Y|X_i)\right\} = \text{Var}(Y) - \text{Var}_{(X_i)}\left\{\mathbb{E}_{(\mathbf{X}_{\sim i})}(Y|X_i)\right\} \tag{4}$$

It follows that $\text{Var}_{(X_i)}\left\{\mathbb{E}_{(\mathbf{X}_{\sim i})}(Y|X_i)\right\}$ must be between 0 and Var(Y), indicating that $0 \leq S_i \leq 1$. If we flip $\mathbf{X}_{\sim i}$ and X_i in Equation 4, we get:

$$\mathbb{E}_{(\mathbf{X}_{\sim i})}\left\{\text{Var}_{(X_i)}(Y|\mathbf{X}_{\sim i})\right\} = \text{Var}(Y) - \text{Var}_{(\mathbf{X}_{\sim i})}\left\{\mathbb{E}_{(X_i)}(Y|\mathbf{X}_{\sim i})\right\} \tag{5}$$

Another kind of sensitivity indice naturally forms as:

$$T_i = \frac{\mathbb{E}_{(\mathbf{X}_{\sim i})}\left\{\text{Var}_{(X_i)}(Y|\mathbf{X}_{\sim i})\right\}}{\text{Var}(Y)} = 1 - \frac{\text{Var}_{(\mathbf{X}_{\sim i})}\left\{\mathbb{E}_{(X_i)}(Y|\mathbf{X}_{\sim i})\right\}}{\text{Var}(Y)} \tag{6}$$

Since $\text{Var}_{(X_i)}\left\{\mathbb{E}_{(\mathbf{X}_{\sim i})}(Y|X_i)\right\}/\text{Var}(Y)$ can be understood as the first order sensitivity indice of $\mathbf{X}_{\sim i}$, the expression 1 −

$\text{Var}_{(\mathbf{X}_{\sim i})}\{\mathbb{E}_{(X_i)}(Y|\mathbf{X}_{\sim i})\}/\text{Var}(Y)$ is the portion of total variance that is contributed from all input combinations that include X_i. Therefore, T_i measures the total effect and it is called total sensitivity indice. T_i includes first order effects of X_i and higher order effects of X_i by interaction with other input factors, so it is always larger than the main effect S_i.

The formulation can also be derived from Sobol' decomposition, also called variance decomposition [1] [7]. For independent input factors, the Sobol' indice satisfies the following relation:

$$\sum_{1\le i\le d} S_i + \sum_{1\le i<j\le d} S_{ij} + \sum_{1\le i<j<k\le d} S_{ijk} + \ldots + S_{1,2,\ldots,d} = 1 \quad (7)$$

There are 2^d sensitivity indices in total. Sobol' indices with multiple subscripts are called interaction terms. The total sensitivity indice T_i's for a given input factor X_i is the sum of all terms in the above relation that contain the subscript (i). For example, with $d = 3$, we will have $T_1 = S_1 + S_{12} + S_{13} + S_{123}$. As the number of indices grows exponentially with the dimension, it is impractical to compute all the sensitivity indices. The main and total effects are usually sufficient to identify the significant input factors (this is reasonable, as the sum of all the main effects will normally be close to 1), while the second-order interaction effects are only considered occasionally.

2. Methods to Calculate Sobol' indices

As we can see, Sobol' indice is a measure of how variance (or uncertainty) in output can be apportioned to each random input parameters, which a very straightforward measure of sensitivity analysis. Sobol' indice has gained wide interest and several methods have been developed to calculate it [5] [6] [8] [9]. Monte Carlo or Quasi Monte Carlo use brute-force sampling methods but they are hardly applicable for computationally prohibitive models. The minimum number of samples required is usually on the order of hundreds to thousands for sufficient accuracy. Therefore, Monte Carlo sampling is generally not recommended unless the model only takes a few seconds or less to run.

The approach chosen here utilizes Polynomial Chaos Expansion (PCE) [2] [10]. PCE is a method that expands the model outputs with respect to orthogonal polynomials in the random model inputs [11]. Based on the orthogonality nature of the polynomials used to construct PCE, the variance caused by each input factor and their interactions with others are very easy to calculate, which makes the computation of Sobol' indices very straightforward. The detailed derivation of such calculation is outside the scope of this paper. It is suggested for the reader to find more implementation details in [2] [10], which demonstrates the process to compute the Sobol' indices analytically as a post-processing of the PCE coefficients. In the present work, the DAKOTA package [12] is used to calculate Sobol' indices based on PCE.

Another efficient option is to use the Kriging surrogate model. Surrogate model is an approximation of the input/output relation of a compututer code/model. It is also called metamodel, response surface or emulator. The Kriging surrogate models are built from a limited number of runs of the full model at specially selected values of the input parameters (the so-called experimental design) and a learning algorithm. The Kriging surrogate models can predict the responses at untried input locations with desired accuracy but with much smaller computational cost. Detailed introduction of of Kriging model and related issues are provided in a companion paper [13]. In this paper we focus on using the Kriging surrogate model for calculating the Sobol' indices, and the Sobol' indices computed using PCE will serve as a reference solution.

III. TRACE AND BFBT BENCHMARK

TRACE [14] has been designed to perform best-estimate analyses of loss-of-coolant accidents (LOCAs), operational transients, and other accident scenarios in pressurized light-water reactors (PWRs) and boiling light-water reactors (BWRs). It can also model phenomena occurring in experimental facilities designed to simulate transients in reactor systems. TRACE version 5.0 Patch 4 includes options for user access to 36 physical model parameters from the input file. For forward uncertainty propagation, the users are free to perturb these parameters by addition or multiplication according to their personal or expert judgment. The aim of this paper is to identify the significant ones among these 36 physical model parameters for the BFBT benchmark void fraction simulation.

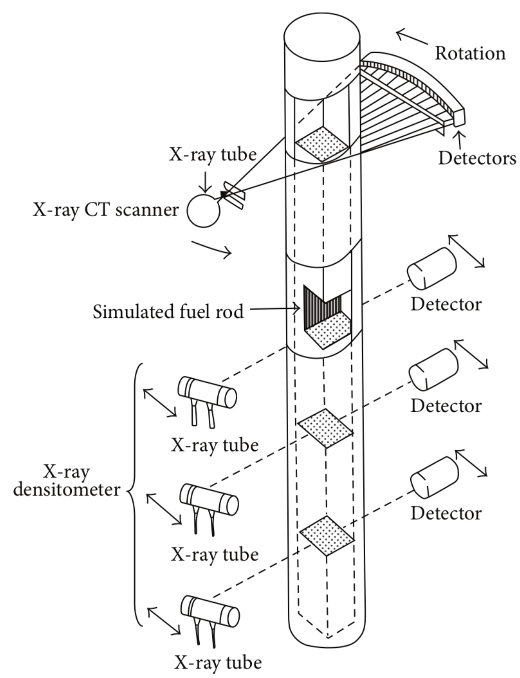

Fig. 1: BFBT benchmark void fraction measurement structure.

The international OECD/NRC BWR Full-size Fine-Mesh Bundle Tests (BFBT) [15] benchmark, based on the Nuclear Power Engineering Corporation (NUPEC) database, was created to encourage advancement in sub-channel analysis of two-phase flow in rod bundles, which has great relevance to the nuclear reactor safety evaluation. In the frame of the BFBT test program, single- and two-phase pressure losses, void fraction, and critical power tests were performed for steady-state and transient conditions.

The facility is full-scale BWR assembly, with measurement performed under typical reactor power and high-pressure, high-temperature fluid conditions found in BWRs. The full-scale fuel assembly inside the pressure vessel corresponds to the General Electric 8 by 8 assembly rod design, where each rod is electrically heated to simulate an actual reactor fuel rod. The heated length of the bundle corresponds to 3.7 m. Five different types of bundle assembly design with different combinations of geometries and power shapes were tested in the void distribution experiments.

Two types of void distribution measurement systems were employed: an X-ray computer tomography (CT) scanner and an X-ray densitometer (DEN). Under steady-state conditions, fine mesh void distributions were measured using the X-ray CT scanner located 50 mm above the heated length (i.e. at the assembly outlet). The X-ray densitometer measurements were performed at three different axial elevations from the bottom (i.e. 682 mm, 1706 mm and 2730 mm) under both steady-state and transient conditions. For each of the four different axial locations, the cross-sectional averaged void fraction was also measured. Figure 1 shows the void fraction measurement facility and locations. The void fraction data will be used in the current study, and they will be referred to respectively from lower to upper positions as VoidF1, VoidF2, VoidF3 and VoidF4 in the following. In this work the Sobol indices w.r.t. all these four output responses will be computed. The benchmark contains 392 steady-state void distribution test cases. For the current study, it is not practical to use all the test cases. We randomly selected the test case 4101-84 from assembly type 4. Table I shows the process conditions and void fraction measurements from this test case.

IV. RESULTS AND ANALYSIS

1. Centered Parameter Study

Before computing the Sobol' indices, it has to be mentioned that not all of the 36 physical model parameters are active during the simulation of BFBT benchamrk. Many of the closure models are not relevant to the BFBT benchmark and will not be called by TRACE. For example, stratified flow (parameter P1003 and P1007) and reflooding (parameter P1034 and P1035) do not occur in the BFBT benchmark experiment. Also, PCE suffers from the so called "curse of dimensionality", which means that the computational cost increases exponentially with the input dimension. We need to remove some parameters through a preliminary reduction study. This preliminary selection was done by centered parameter study, in which each physical model parameter was perturbed a few steps around the nominal value (which is 1.0) one-by-one. DAKOTA [12] was used here to perturb each parameter 20 steps above and below nominal values with a step size of 0.05. The void fraction variance was calculated for each parameter. As expected, most of the variances are 0 or very close to 0. Ultimately, only 8 parameters produce variances larger than 10^{-3} for at least one of the output parameters VoidF1, VoidF2, VoidF3 and VoidF4. These 8 parameters are shown in Table II.

2. Global Sensitivity Analysis with Monte Carlo Sampling

After selecting the 8 potential significant parameters, we performed Monte Carlo sampling to calculate the correlation coefficients (PCC and SRCC) to see if they will provide consistant results with Sobol' indices. All the 8 physical model parameters are assumed to follow uniform distributions over the range of $[0, 5]$. The assumption is quite arbitrary and is not the focus of the current research as long as we use the same prior distributions for all the semsitivity study that are to be compared. We generated 1000 Monte Carlo samples of the input parameters and ran TRACE accordingly. Figure 2 shows the PCC and SRCC between each input parameters and each responses. A larger value (close to 1.0 or -1.0) means this parameter is significant to the corresponding output. Positive correlation coefficients means that the output values increases together with the input factor and vise versa.

3. Global Sensitivity Analysis with Sobol' indices Computed by Polynomial Choas Expansion

We omitted the technical details used to calculate Sobol' indices by PCE. The main and total effect sensitivity indices are reported by DAKOTA [12] using sparse polynomial chaos. We performed a convergence study to ensure that the order of orthogonal polynomials is high enough to produce accurate results. The interested readers are recommeded to refer to DAKOTA user manual [12] for more details. Table 3 shows the main and total effect Sobol' indices calculated using PCE.

By looking at Table 2 and Table 3 together, several major conclusions can be drawn as below:

1. P1009, P1013 and P1023 have negligible Sobol' indices and their PCC and SRCC are also very small, indicating that void fraction is not sensitive to those parameters.
2. P1029 is only important for VoidF4.
3. The sensitivity ranking for each of the parameters is mostly consistent between Sobol' indices and PCC/SRCC.
4. Sobol' indices are a better measure of sensitivity than correlation coefficients, as they directly represent the part of output variance that can be attributed to each parameter. PCC/SRCC cannot consistently reflect this relative importance as good as Sobol' indices. For example, Sobol' indices show that only P1022 and P1028 are important for VoidF3, while PCC/SRCC show that P1008 and P1012 should be included, too.

Taking into account the details of each parameter, the observed sensitivity ranking can be explained as below:

1. The significance of P1008 (single phase liquid to wall heat transfer coefficient) decreases to almost zero at higher elevations. This is because single-phase liquid exists only in the lower elevations of the bundle.
2. Similarly, P1012 (subcooled boiling HTC) is only important at lower elevations because this is where subcooled boiling occurs.

TABLE I: Process conditions and void fraction data for the selected cases of assembly 4 in the BFBT benchmark

Test ID	Pressure (MPa)	Flow rate (t/h)	Inlet subcooling (kJ/kg)	Power (MW)	VoidF1 (%)	VoidF2 (%)	VoidF3 (%)	VoidF4 (%)
4101-84	8.680	54.66	53.2	3.35	3.80	37.4	57.9	60.2

TABLE II: List of 8 selected physical model parameters selected after centered parameter study

Parameter	Description
P1008	Single phase liquid to wall heat transfer coefficient
P1009	Single phase vapor to wall heat transfer coefficient
P1012	Subcooled boiling heat transfer coefficient
P1013	Nucleate boiling heat transfer coefficient
P1022	Wall drag coefficient
P1023	Form loss coefficient
P1028	Interfacial drag (bubbly/slug Rod Bundle - Bestion) coefficient
P1029	Interfacial drag (bubbly/slug Vessel) coefficient

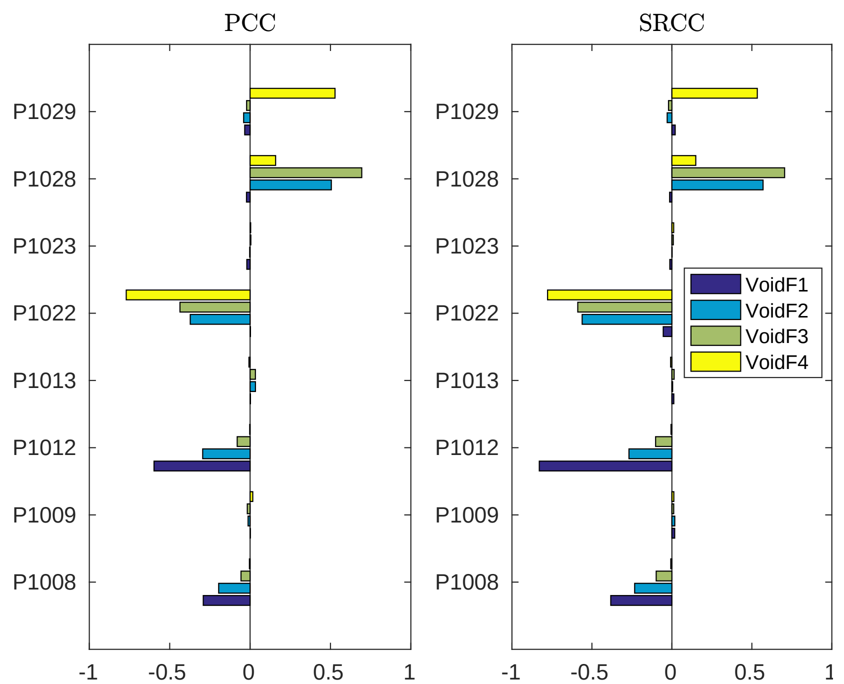

Fig. 2: PCC and SRCC for 8 physical model parameters.

3. P1022 (wall drag coefficient) increases at higher elevations.

4. P1028 (interfacial drag bundle coefficient) dominates at intermediate locations.

4. Build and Validate the Kriging Surrogate Model

In this section, the process of building and validating the Kriging surrogate models will be presented. The theory and related issues and solution of construction and validation are provided in a companion paper [13]. First we generated traing samples of different sizes (20 -200) with Latin Hypercube Sampling (LHS) [16]. We then ran TRACE at these design sites to generate void fraction values, which will be used to train the Kriging surrogate models. Matern covariance kernel and constant trend functions are chosen, and Maximum Likelihood Estimation (MLE) is used to estimate the hyper-parameters. The 1000 Monte Carlo samples generated to calculate the PCC/SRCC were used to validate the surrogate models (note that Cross Validation is also a popular option for metamodel validation). The validation is performed based on the accuracy of the metamodel's capability to predict the responses at samples other than the training sites. The predictivity coefficient Q_2 is usually used to evaluate the fitted Kriging surrogate model:

$$Q_2 = 1 - \frac{\sum_{i=1}^{N_{\text{val}}} \left(Y_i - \hat{Y}_i\right)}{\sum_{i=1}^{N_{\text{val}}} \left(\bar{Y} - Y_i\right)} \tag{8}$$

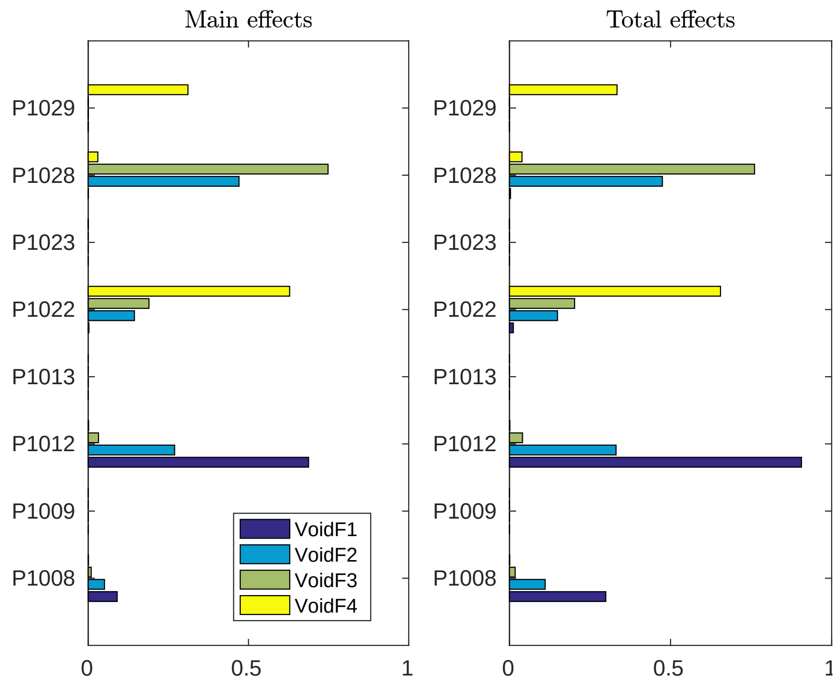

Fig. 3: Sobol' indices (main and total effects) for 8 physical model parameters.

where N_{val} is the size of the validation set (in this case 1000). Y_i denotes TRACE simulation outputs of the validation set and $\bar{Y}$ is their empirical mean. $\hat{Y}_i$ represents the prediction from Kriging surrogate model. In the current research we simulate the validation samples sets using Kriging surrogate models built from training samples of different sizes (from 20 to 200), and then compare their accuracy according to the Q_2 value. In practical situations, a metamodel with a predictivity greater than 0.7 is often considered as a good approximation of the full model [17].

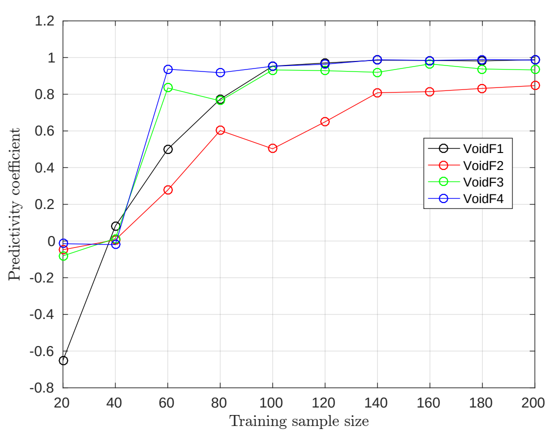

Fig. 4: Predictivity coefficient with the training sample size

Figure 4 shows the evolution of predictivity coefficient for four response values with different training sizes. As expected, the Q_2 values are approaching 1.0 by adding more training samples. We can also learn that to get a satisfactory predictivity coefficient (above 0.7), we need at least 140 training samples.

In the following we will use Kriging surrogate model built with 140 training samples and further validate its capability to predict the void fractions compared with direct TRACE simulation.

The primary assumption of Kriging surrogate model is that the response of the computer model under consideration is a sample path of an underlying Gaussian random field. It indicates that the output responses at different samples follow joint Gaussian distributions. Kriging surrogate model can not only provide the response prediction, but also the Mean Squared Error (MSE, or variance) of its prediction. The differences between TRACE simulation and Kriging surrogate model prediction are called residuals. And by dividing the residuals by the corresponding standard deviations of the prediction we get the standardized residuals. By assumption the standardized residuals follow the standard normal distribution. Therefore, 99.7% of all the standardized residuals are expected to fall within $[-3, 3]$.

Figure 5 shows the comaprisons of VoidF1 - VoidF4 from TRACE simulations and Kriging surrogate model predictions. Most of the points fall close to the diagonal line. Figure 6 shows the values of all the 1000 standardized resiudals for each void fraction output. It can be seen that for all the four void fraction responses, less that 0.3% of the standardized residuals fall above 3 or below -3. The standardized residuals for VoidF1 have the most points that are not lying within [-3, 3].

Figure 7 shows the Q-Q plot of the standardized residuals. If they do follow normal distributions, The Q-Q plots should fall closely to a straight line. This is true for VoidF2, VoidF3 and VoidF4. But many points for VoidF1 deviate from the straight line. This is because that VoidF1 often has small

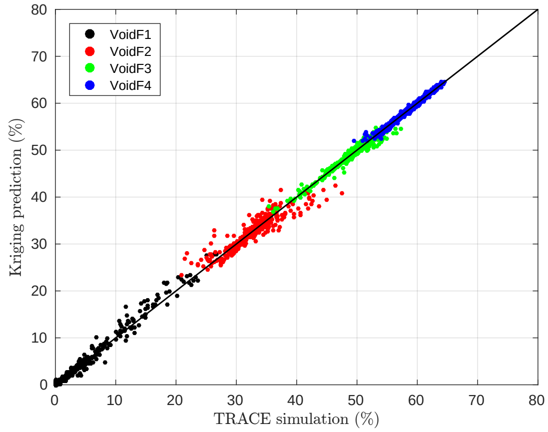

Fig. 5: Comparison of void fractions from TRACE simulation and Kriging surrogate model prediction

values (close to 0), which makes the relative error much larger.

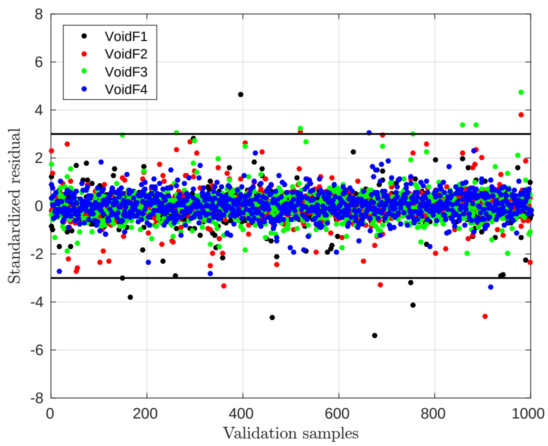

Fig. 6: Standardized redisuals of void fraction predictions

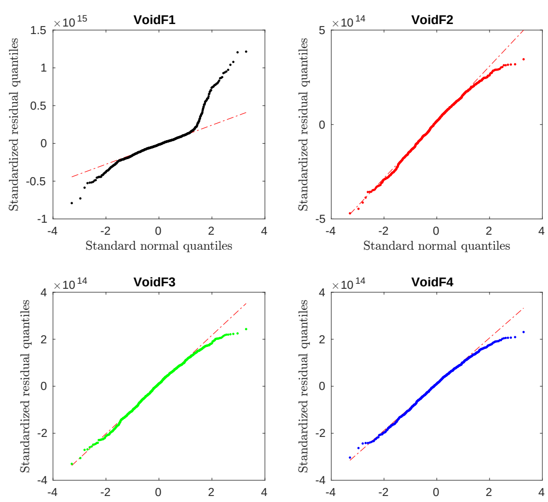

Fig. 7: Q-Q plot of the standardized residuals

Now the Kriging surrogate model built with 140 training samples has been successfully validated. Note that the Kriging surrogate model can be evaluated in a extremely short time. For example, in our case the Kriging surrogate model can be evaluated about 250 times in 1 second, making it practical to calculate the Sobol' indices by sampling the Kriging surrogate model.

5. Global Sensitivity Analysis using Kriging Surrogate Model

To calculate the Sobol' indices, we used the "D_3" Monte Carlo sampling method recommended in [9]. The total computational cost of such method is $N(2d + 2)$ where d is the input dimension and N is the number of samples. Usually N is expected to be at least 1000 which means that for the currently problem of dimension 8 we wound need 18,000 TRACE model evaluations. This is only practical by using some cheap surrogate models. Figure 8 and Figure 9 show the convergence of the main and total effect Sobol' indices by using different sample sizes N. We can see that the Sobol' indices are converging to certain equilibrium values when enough samples are used.

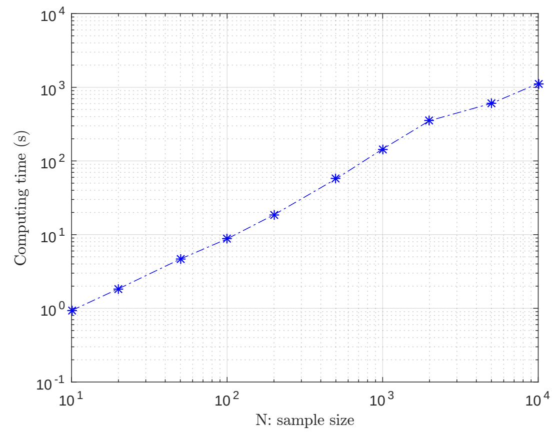

Fig. 10: Computing cost of evaluating Sobol' indices using Kriging surrogate model

Figure 10 shows the computing time required to evaluate the Sobol' indices using Kriging surrogate models. Even with $N = 10000$ (180,000 model evaluations), it only takes about 1100 seconds to run th Kriging surrogate model with one processor, which would otherwise take about 2000 hours (each TRACE simulation takes 40 seconds) to run TRACE directly with the same processor.

6. Compare Sobol' indices from Kriging Surrogate Model and Polynomial Choas Expansion

Now that we have converged values of the main and total effect Sobol' indices, we can compare them with Sobol' indices computed using PCE. Figure 11 and Figure 12 show the comparison of the main and total effects respectively. It can be seen that the sensitivity indices from two different approaches are close to each other, except for some small differences for VodiF2. However, PCE takes about 1121 TRACE evaluations even with sparse polynomials while Kriging surrogate model only needs 140. Furthermore, when we have larger input di-

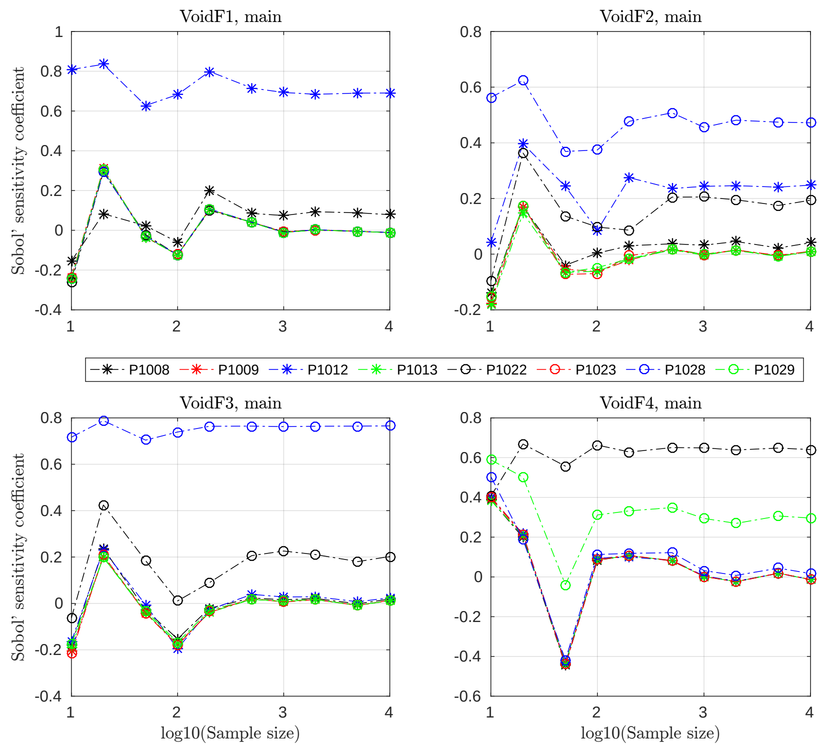

Fig. 8: Convergence of the main effect Sobol' indices calculated with Kriging surrogate model

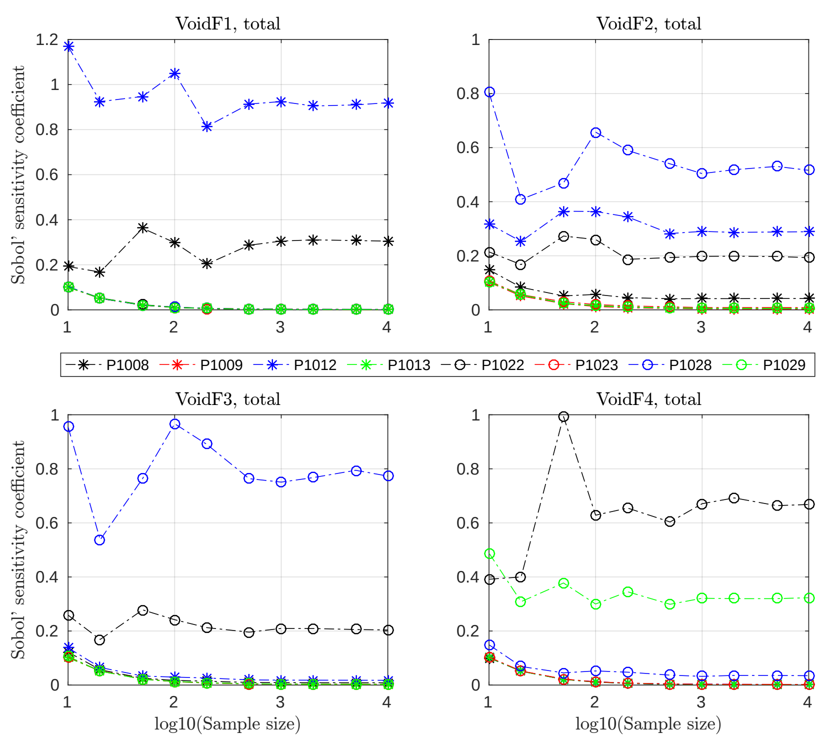

Fig. 9: Convergence of the total effect Sobol' indices calculated with Kriging surrogate model

mensions, the computational cost using PCE will increase much faster than using GP.

V. CONCLUSIONS

In this paper, we performed global sensitivity analysis of TRACE void fraction predictions w.r.t. its 8 physical model parameters based on the BFBT benchmark. Three methods are used: (1): correlation coefficients (PCC/SRCC) using Monte Carlo sampling (2): Sobol' indices using Polynomial Chaos Expansion (PCE) (3): Sobol' indices using Kriging surrogate models.

The sensitivity rankings are generally consistent between Sobol' indices and correlation coefficients. However, Sobol' indices can directly represent the part of output variance that can be attributed to each parameter. PCC/SRCC cannot consistently reflect this relative importance between different parameters as good as Sobol' indices.

Finally, the Sobol' indices calculated using PCE and Kriging surrogate models are close to each other, but Kriging surrogate model takes much less computational cost. Moreover, it has the potentional to be more applicable when the input dimension gets larger. As a result, we recommend using Sobol' indices for global sensitivity analysis, which can identify significant input model parameters. When the computer model is expensive to run and the responses change smoothly with the input parameters, Kriging surrogate model can be used to efficiently compute the Sobol' indices at a much lower computational cost.

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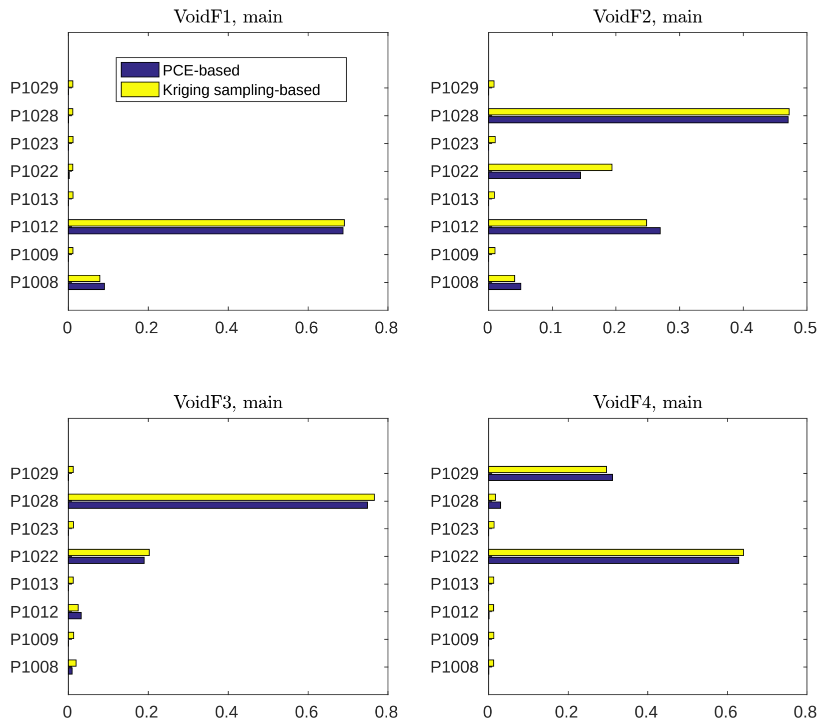

Fig. 11: Comparison of the main effect Sobol' indices from PCE and Kriging surrogate model

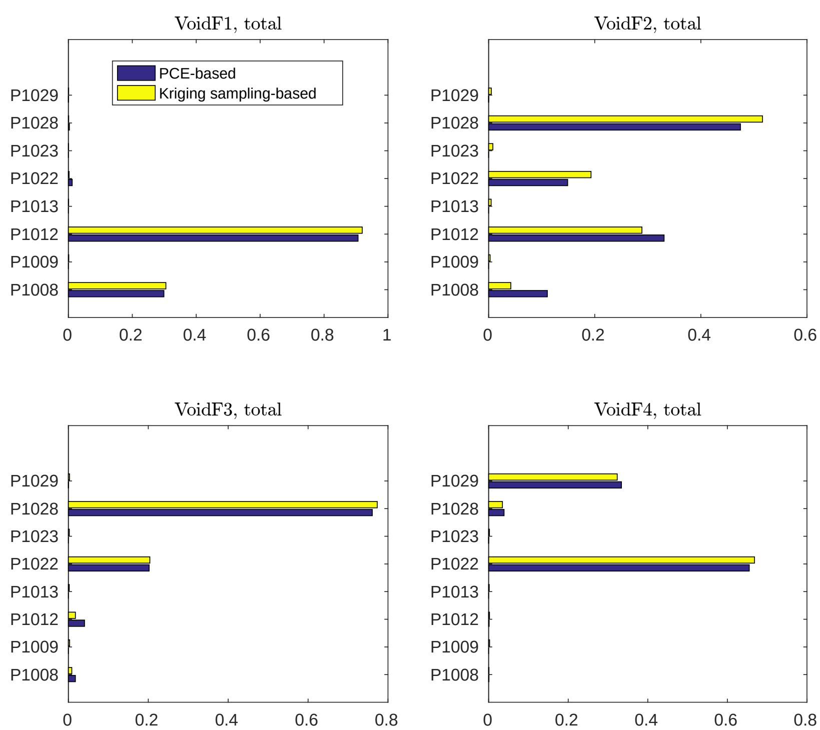

Fig. 12: Comparison of the total effect Sobol' indices from PCE and Kriging surrogate model