Inverse Uncertainty Quantification of TRACE Physical Model Parameters Using BFBT Benchmark with Investigation of Measurement Bias

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INTRODUCTION

The best estimate plus uncertainty (BEPU) methodology has the potential to replace conservative approach, based on an expert judgment with statistical techniques that provide an estimate and its uncertainty. Development of best estimate thermal-hydraulics codes lead to improved agreement of code prediction with experimental results, nevertheless some discrepancies exist. Besides measurement uncertainties, those discrepancies can be caused by model assumptions, numerical error, nodalisation or improper boundary or initial conditions.

The biggest challenge is the assessment of uncertainty for influential code parameters. For example, physical model parameters that are used in closure relations in thermal-hydraulic codes, such as RELAP5 or TRACE are not provided with corresponding uncertainties. Inverse uncertainty quantification (IUQ) can be used to evaluate those uncertainties with the use of experimental data [1][2]. Additionally, this analysis can be used to calibrate model parameters.

Most of the work in IUQ, models random error of an experiment as zero mean additive Gaussian noise [1][2]. Nevertheless, this assumption is very restrictive and is not met in case of biased measurement. The calibrated values of model parameters and estimated uncertainty will be then biased and not applicable for a wide range of experimental results, i.e. results not used for calibration. Following work presents a method of identifying experimental bias in IUQ analysis.

The IUQ methodology with Bayesian framework will be applied to steady-state void fraction measurement from Nuclear Power Engineering Center (NUPEC) BWR Full-size Fine-mesh Bundle Test (BFBT) Benchmark [3] for assessment of uncertainty in physical model parameters in TRACE code. Through the analysis, it can be shown that if the error term is not modeled correctly, the calibrated model parameters will not improve code prediction for independent measurement, i.e. measurement without bias. Which leads to a conclusion that the measurement error was incorrectly modeled in calibration analysis. This method can be also applied to identify the bias in the measurement.

BFBT Benchmark

NUPEC BWR Full-size Fine-mesh Bundle Test Benchmark consist of steady-state and transients measurements of void fraction and critical power and was used for multiple code validation efforts. In this study only steady-state void fraction measurement was used. Void fraction was reported in 4 locations along the test section. Three lower measurements are performed with the use of densitometers and are called from the bottom of the test section DEN#3 at 682mm, DEN#2 at 1706mm, DEN#1 at 2730mm. Fourth measurement location is equipped with CT scanner at elevation of 3708mm.

Unlike CT scanner which was rotating during the experiment, densitometers remained stationary throughout the data collection process. Pencil type beam was shot between rods of the bundle and effectively not the whole area of the channel was scanned. Void fraction is distributed non-uniformly in the channel and for that reason measurement is biased. For bubbly flow, voids are concentrated near walls and measurement between fuel rods will under predict the cross sectional average. For slug flow, voids are concentrated in the center and measurement of the densitometer over-predicts cross sectional average [4].

The correction factors were developed for the densitometer measurements to account for bias in the experiment [5], the correction was applied to the void fraction measurement between 0.2 and 0.9. The void fraction CT scanner results were used as a reference to develop the correction formula. Resulting formula is presented in Eqn. 1, for void fraction in percent. The constant c depends on the assembly type: $c = 1.231$ for assemblies $0-3$ and $c = 1.167$ for assemble 4, due to difference in geometries.

$$\alpha_{corrected} = \frac{\alpha_{measured}}{-0.001\alpha_{measured} + c} \quad (1)$$

Physical model parameters

The physical model parameters are used for closure relations in codes such as TRACE or RELAP5. TRACE code allows the user to perturb 36 physical model parameters from the input file, through multiplication factor, with value of 1.0 indicating nominal value (i.e. no perturbation). The code results with multiplication factor of 1.0 will be considered as the default value, multiplication factors that are calibrated using the data will be referred to as the calibrated values. Different models and hence different physical model parameters are of interest, depending on the physical problem. Sensitivity analysis will be used to identify important parameters. Sensitivity coefficients for the most important physical model parameters for void fraction prediction, are presented in Table I [6]. Sensitivity coefficient is defined in Eqn. 2, where Y denotes void fraction and X physical model parameter.

$$s_c = \frac{\Delta Y}{\Delta X}\frac{X}{Y}100\% \quad (2)$$

Parameter estimation

The estimation of the parameter uncertainty will follow methodology presented in [2], where IUQ is done within Bayesian framework. Posterior distribution is related to prior and a likelihood through Bayes theorem, see Eqn. 3.

TABLE I: Sensitivity coefficients for the most influential physical model parameters in void fraction determination [6]

Parameter	DEN#3	DEN#2	DEN#1	CT
Single phase liquid to wall heat transfer	-4.22	-0.36	-0.20	-0.03
Subcooled boiling heat transfer	-10.77	-0.38	-0.20	-0.03
Wall drag	-0.63	-1.28	-1.66	-2.97
Interfacial drag (bubbly/slug rod bundle-Bestion)	0.73	1.94	2.25	0.93

$$\pi(\boldsymbol{\theta}|y) = \frac{L(\boldsymbol{\theta}|y)\pi(\boldsymbol{\theta})}{\int L(\boldsymbol{\theta}|y)\pi(\boldsymbol{\theta})d\boldsymbol{\theta}} \quad (3)$$

In the formula $\pi(\boldsymbol{\theta}|x)$ is the posterior, $L(\boldsymbol{\theta}|y)$ is the likelihood and $\pi(\boldsymbol{\theta})$ is the prior. The integral is the normalizing constant which is difficult to compute in case of high dimensional space. To avoid the need of computing the normalizing constant, the Markov Chain Monte Carlo (MCMC) with Metropolis-Hastings algorithm was used to draw samples from posterior probability distribution [7].

Due to the computational cost associated with uncertainty quantification using MCMC algorithm, evaluation of original model is not practical. Convergence of MCMC requires code executions for each experiment at the order of $O(10^5 - 10^6)$, to decrease computational cost a surrogate model was created for each experiment. Model based on Gaussian Process (GP) related void fraction to four physical model parameters presented in Table I. This type of regression is commonly used in statistics as an interpolation method. Interpolated values are modeled by a Gaussian random process [8]. The Gaussian Process surrogate model was created for each set of experimental conditions with the use of scikit-learn package for Python [8].

Likelihood function is chosen based on the relation between observed quantity and model perdition. Most commonly represented as additive zero mean, Gaussian noise $y = G(\theta) + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$. The likelihood function becomes:

$$L(\boldsymbol{\theta}|y) = \frac{1}{(2\pi)^{N/2}\sigma^N} exp\Big[-\sum_{i=1}^{N} \frac{[y_i^m - y_i^c]^2}{2\sigma^2}\Big] \quad (4)$$

Resulting posterior distribution can be then used for calibration of model parameters.

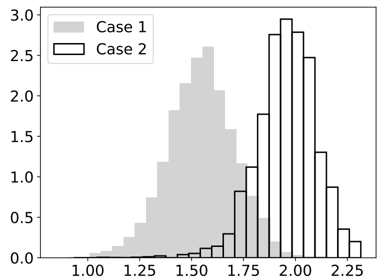
RESULTS

The IUQ was performed twice, using corrected and uncorrected void fraction measurement data. Case 1 (c1) corresponds to corrected void fraction measurements, Case 2 (c2) corresponds to original (biased) void fraction measurements. Following nomenclature is used for physical model parameters: p_1 - Single phase liquid to wall heat transfer, p_2 - Subcooled boiling heat transfer, p_3 -Wall drag, p_4 - Interfacial drag (bubbly/slug rod bundle-Bestion). Available experimental test conditions were divided into calibration and validation sets. The calibration was performed with all 86 assembly 4 experiments using only measurement of the densitometer, i.e. DEN#1, DEN#2, DEN#3. CT scanner measurements were not used in the calibration. CT scanner measurements are unbiased and more accurate than densitometer measurement. CT scanner measurements and densitometer measurements performed with assemblies $0-3$ were used for validation. Measurement uncertainty was set to 0.02, as suggested in the benchmark specifications for CT scanner. Densitometer measurement uncertainty was not reported.

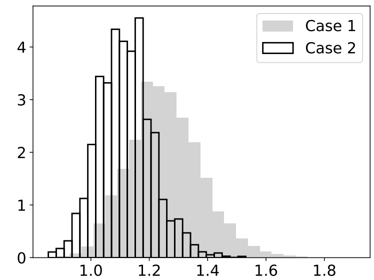
Marginal posterior distributions of the physical model parameters are presented in Figure 1. The posterior distributions can be approximated by the normal distribution, mean and standard deviation were computed, see Table II. Distributions for Cases 1 and 2 do not differ for parameter p_1 and p_2 (less then 30% relative change for p_1 and 10% for p_2) but are significantly different for p_3 and p_4 (97% for p_3 and 213% for p_4). Sensitivity analysis has shown that parameters p_1 and p_2 have higher sensitivity at lowest measurement location where void fraction is small, with most of the void fraction measurement below 20%. The correction formula was only applied to measurements of void fraction in a range between 20% and 90%, for that reason distributions p_1 and p_2 were not significantly affected by correction to void fraction. Contrary, parameters p_3 and p_4 were highly affected by application of correction formula because of higher sensitivity at higher void fractions. Distributions of the physical model parameters were then used to evaluate void fraction with the TRACE code. Figure 2 presents void fraction prediction of TRACE code with the default and the calibrated values of the physical model parameters for Case 1. Comparison to the experimental measurement is included.

Mean absolute error was calculated for both cases, presented in Table III. Void fraction was evaluated with TRACE code using default and calibrated physical model parameters. The TRACE prediction for all measurement location was improved using calibrated physical model parameters for Case 1. For Case 2 improvement in TRACE prediction is observed only for measurements preformed with densitometer. There is significant increase of error (81% relative change) for TRACE prediction for CT scanner measurement with the use of calibrated physical model parameters.

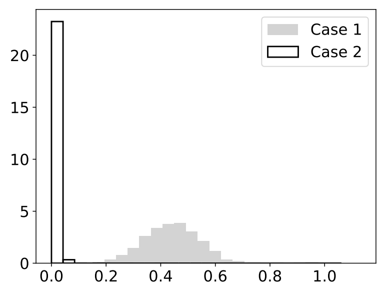
The CT scanner measurement was performed using different and more accurate technique without measurement bias. For that reason, it was treated as an benchmark test of the IUQ analysis and was considered to be independent from densitometer measurement, i.e. it was not subject to the measurement bias. The agreement of the TRACE prediction with the calibrated physical model parameter for Case 1 indicate that error term was modeled correctly, i.e. the assumption of additive zero mean normal error is valid. However, for Case 2 calibrated values of physical model parameters did not improve void fraction prediction for CT scanner. This analysis indicates that the parameters were partially calibrated to account for the



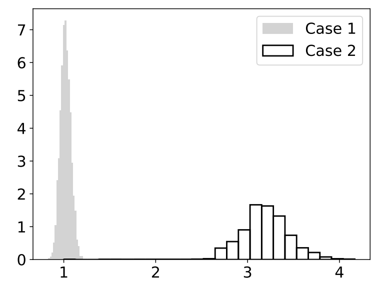
(a) Single phase liquid to wall heat transfer coefficient



(b) Subcooled boiling heat transfer coefficient

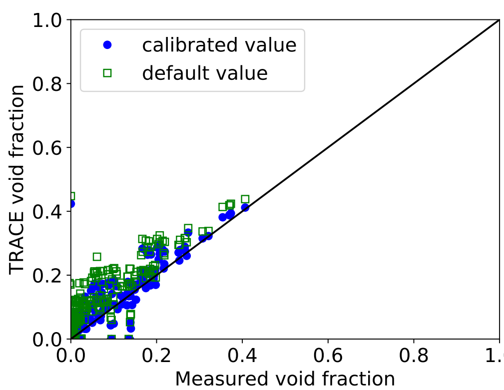


(c) Wall drag coefficient

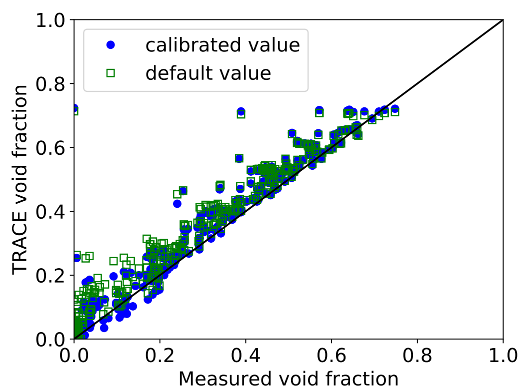


(d) Interfacial drag coefficient

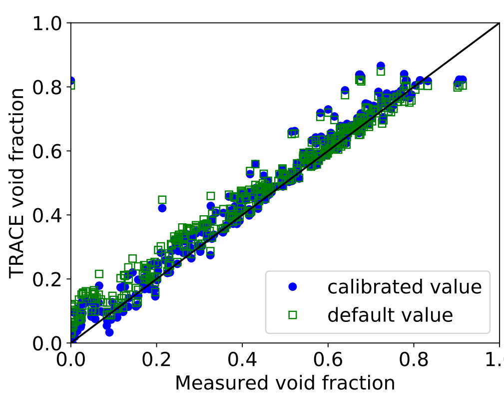
Fig. 1: Marginal posterior distribution of physical model parameters. Case1 with corrected void fraction, Case2 uncorrected void fraction.



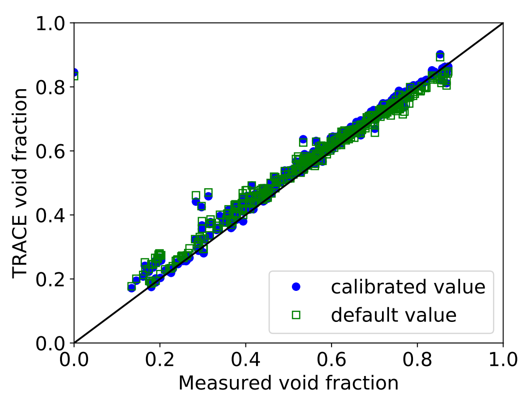
(a) DEN#3



(b) DEN#2



(c) DEN#1



(d) CT

Fig. 2: Void fraction comparison for TRACE code and measurement for corrected data with default and calibrated values of physical model parameters, Case 1.

TABLE II: Statistics for marginal probability distributions of physical model parameters, (μ - mean, σ - standard deviation c1, c2 - corrected and uncorrected void fraction).

Parameter	μ_{c1}	σ_{c1}	μ_{c2}	σ_{c2}	$\frac{\mu_{c2}-\mu_{c1}}{\mu_{c1}}$
Single phase liquid to wall heat transfer	1.54	0.17	1.96	0.14	0.27
Subcooled boiling heat transfer	1.25	0.12	1.12	0.09	-0.10
Wall drag	0.43	0.10	0.01	0.02	-0.98
Interfacial drag (bubbly/slug rod bundle-Bestion)	1.02	0.06	3.19	0.25	2.13

TABLE III: Mean absolute error (MAE) between TRACE prediction and experimental results, for validation experiments, using calibrated and default physical model parameters in TRACE. For Case 1 MAE is calculated with respect to corrected values of void fraction, for Case 2 the error is calculated with respect to uncorrected void fraction measurement.

	Default c1	Calibrated c1	Default c2	Calibrated c2
DEN#3	0.047	0.027	0.045	0.030
DEN#2	0.060	0.045	0.048	0.035
DEN#1	0.049	0.042	0.062	0.042
CT	0.026	0.024	0.026	0.047

bias in the experimental measurement and were not applicable to experiment with different error distribution. Through this analysis, bias in experimental data was identified.

CONCLUSIONS

Paper presented an inverse uncertainty quantification of physical model parameter in TRACE code. Influence of measurement bias on posterior probability distribution was investigated. The analysis has shown that misrepresentation of measurement uncertainty can cause calibration results not to be applicable for prediction outside the calibration range.

The main difficulty is the fact that if validation is performed with the data from the same experiment, i.e. using the same measurement technique and equipment, error misrepresentation will not be evident in the validation. Dividing experiments from the same facility or benchmark into calibration and validation sets is common practice while using IUQ. This can lead to significant errors in calibration as well as UQ.

The method to test the assumption of measurement error distribution, can be summarized in the following steps: (1) perform calibration of model parameters with Bayesian framework for data with unknown error distribution, assuming distribution for which the test is performed, (2) choose benchmark data with measurement error consistent with assumption used in step (1), (3) evaluate code prediction for benchmark data with default as well as calibrated model parameters, (4) calculate error in model prediction for default and calibrated model parameters, (5) if code prediction deteriorates, the assumed error distribution is invalid.

The method can be used to identify measurement bias, by performing IUQ with assumption of zero mean Gaussian noise. If the calibrated results do not improve the prediction, the measurement was biased. It is worth noting that the benchmark case with known distribution should be chosen carefully. The benchmark experiments should have comparable sensitivity for physical model parameters as the studied data and have similar experimental matrix.

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