UNCERTAINTY QUANTIFICATION OF TRACE WALL HEAT TRANSFER MODELING IN SUBCOOLED BOILING USING BFBT EXPERIMENTS

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ABSTRACT

Forward quantification of uncertainties in code responses require knowledge of input model parameter uncertainties. Nuclear thermal-hydraulics codes such as RELAP5 and TRACE do not provide any information on physical model parameter uncertainties. A framework was developed to quantify input model parameter uncertainties using Maximum Likelihood Estimate (MLE) and Expectation-Maximization (E-M) algorithm for physical models using relevant experimental data.

The objective of the present work is to perform the sensitivity analysis of the code input (physical model) parameters in TRACE and calculate their uncertainties using an MLE algorithm, with a particular focus on the subcooled boiling model. In this paper, the OECD/NEA BWR full-size fine-mesh bundle test (BFBT) data will be used to quantify selected physical model uncertainty of the TRACE code. The BFBT is based on a multi-rod assembly with measured data available for single or two-phase pressure drop, axial and radial void fraction distributions, and critical power for a wide range of systems conditions. In this study, the steady-state cross-sectional averaged void fraction distribution from BFBT experiments is used as the input for MLE algorithm, and selected physical model Probability Distribution Function (PDF) is the desired output quantity.

KEYWORDS
Uncertainty Quantification, BFBT, MLE, TRACE, Subcooled boiling

1. INTRODUCTION

The current design and licensing of a nuclear reactor system rely on modeling the system with a best-estimate code system, such as TRACE [1, 2], for modeling thermal-hydraulics phenomenon inside the reactor core. The reliability of predictions of the system codes is closely related to the validation of their physical models. For example, the accuracy of void fraction prediction in a Boiling Water Reactor (BWR) is important, because void fraction has a significant effect on the reactivity, pressure drop, critical heat flux and many other phenomena which are relevant for safety margin evaluation [3]. The uncertainties of code predictions should be provided along with these predictions, which require an uncertainty analysis (UA) of the code by propagation of input uncertainties to the output predictions.

Uncertainty analysis (UA) aims to quantify the overall uncertainty associated with the response as a result of uncertainties in the input model parameters [4, 5]. A valid experiment benchmark is critical to the UA process. One of the most valuable publically available databases for the thermal-hydraulics modeling of BWR channels is the OECD/NEA BWR Full-size Fine-mesh Bundle Test (BFBT) benchmark, which includes sub-channel void fraction measurements in a representative BWR fuel assembly [4, 5]. In this paper, the BFBT benchmark is used to conduct uncertainty analysis of the thermal-hydraulics code system TRACE.

In the process of UA, possible input model parameters may include [5]:

- Boundary and Initial Conditions (BICs), such as mass flow rate, inlet fluid temperature (or inlet sub-cooling), system pressure and power (or outlet quality)
- Geometry, such as heated rod diameter, the cladding thickness, etc.
- Physical model parameters used in the code, such as single-phase and two-phase heat transfer coefficients, interfacial drag coefficients, void drift model parameters, etc.

The uncertainties and related Probability Density Function (PDF) of BICs and geometry are usually determined by the experimental team, manufacturing tolerances or sometimes suggested by researchers based on experience. With these uncertainties information, UA could be done with the help of UA packages, such as SUSA and DAKOTA [6, 7]. However, PDFs for the physical models are the most important and the most difficult to obtain. The physical models closure relations are implemented as empirical correlations. When the correlations were originally developed, their accuracy and reliability was studied with a particular experiment [8, 9]. However, once these correlations were implemented in a thermal-hydraulics code and used for different physical systems, the accuracy and uncertainties information of these correlations was no longer known to a code user. Further work to quantify the accuracy and the uncertainties of the input physical models correlations is necessary.

The objective of this paper is to quantify the uncertainties of two input model parameters [1](single-phase liquid to wall Heat Transfer Coefficient (HTC) and subcooled boiling HTC) used in TRACE using the Maximum Likelihood Estimate (MLE) algorithm [10, 11] and the steady-state sub-channel void fraction data from the BFBT benchmark. After the quantification of physical model uncertainty (inverse uncertainty quantification), the obtained physical model probability distribution functions (PDFs) are used to conduct an uncertainty analysis with TRACE code (forward uncertainty quantification).

2. BFBT BENCHMARK

The international BFBT benchmark is a valuable benchmark for the sub-channel analysis of two-phase flow in BWR rod bundles. This benchmark is specified such that it can be used to compare numerical predictions of system, sub-channel or CFD void distribution and critical powers to full-scale experimental data on a prototypical BWR rod bundle. The void distribution and critical power has been measured in the BFBT facility in a multi-rod assembly with a typical BWR reactor power and fluid conditions. The facility is able to simulate the high-pressure, high-temperature fluid conditions found in BWRs. An electrically-heated rod bundle has been used to simulate a full-scale BWR fuel assembly [4].

There are two types of void distribution measurement systems: an X-ray CT scanner and an X-ray densitometer. 3 X-ray densitometers (DEN #3, #2 and #1) are located at 3 axial elevations shown in Figure 1. The X-ray CT scanner is located 50 mm above the heated length. Both transient and steady-state void fractions are measured [4]. The measurement systems' name is also used to denote the different axial elevations in this paper.

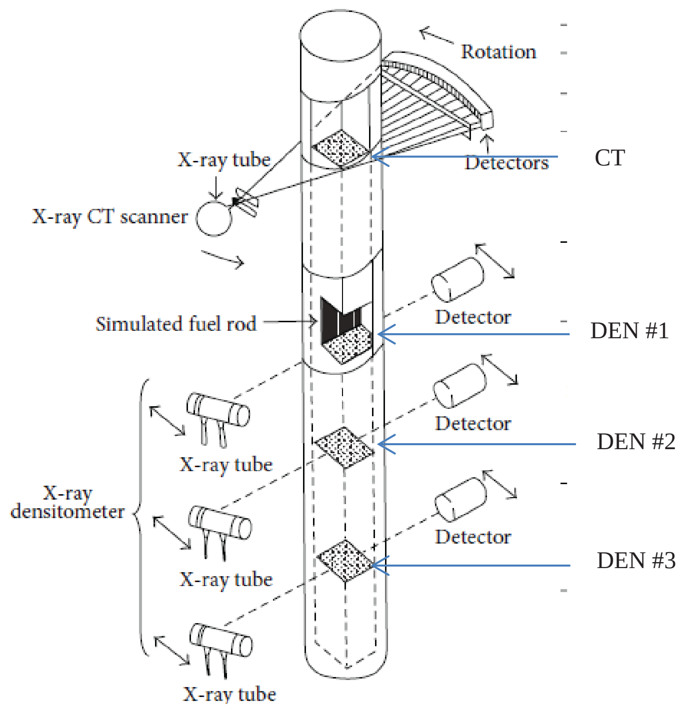

Figure 1. Void fraction measurement: 4 axial elevations are denoted by the measurement systems name DEN #3, DEN #2, DEN #1 and CT

Five different types of bundle assembly design were tested in the void distribution experiments. Only test assembly type 4 steady-state void fraction measurements are used in this paper. Test assembly type 4 is 8x8 fuel bundle with large water rod at the bundle center. The main features of test assembly type 4 are shown in Table I [4].

Table I. Geometry and power shape of test assembly type 4

Item	Data
Test assembly type	4
Simulated fuel assembly type	High burn-up 8 x 8
Number of heated rods	60
Heated rods outer diameter (mm)	12.3
Heated rods pitch (mm)	16.2
Axial heated length (mm)	3708
Number of water rods	1
Water rods outer diameter (mm)	34.0
Channel box inner width (mm)	132.5
Channel box corner radius (mm)	8.0
In channel flow area (mm^2)	9463
Spacer type	Ferrule
Number of spacers	7
Spacer pressure loss coefficients	1.2
Spacer location (mm)	455, 967, 1479, 1991, 2503, 3051, 3527 (distance from bottom of heated length to spacer bottom face)
Radial power shape	Simulation pattern for beginning of operation
Axial power shape	Uniform

3. WORK FLOW AND METHODOLOGY

3.1 Work flow

As suggested in BFBT benchmark [4, 5], analysis in this research was performed in three steps:

1) **Step 1:** this step is a standard type of accuracy analysis where the overall predictions are compared to the experimental data. Assembly type 4 data is used in this step. Experimental cases of various geometry and experimental conditions of assembly type 4 are modeled in detail in TRACE and the cross sectional averaged void fractions are obtained from TRACE results. Then results from TRACE predictions are compared with experimental measurement for analyzing the accuracy of TRACE predictions.
2) **Step 2:** this step aims to quantify the uncertainty of two modeling parameters used in TRACE, single-phase liquid to wall HTC and subcooled boiling HTC. A Sensitivity Analysis (SA) is performed for these two parameters to provide the necessary input data for the MLE algorithm. The sensitivity analysis is conducted by perturbing these two parameters a small value and then calculating the sensitivity coefficient of the void fraction to these parameters. After the sensitivity analysis, the obtained sensitivity coefficient will be used as input to MLE algorithm. Then, the probability distribution functions (PDFs) of selected physical models are calculated with MLE algorithm. This step is the inverse uncertainty quantification.
3) **Step 3:** this step is the uncertainty analysis to obtain uncertainties of TRACE predictions by using the PDFs calculated in Step 2. These two selected parameters will be sampled form the PDFs calculated in step 2 and the samples will be used as input to TRACE model for forward uncertainty quantification. Finally, the uncertainty of TRACE predictions will be obtained and analyzed.

3.2 Methodology

The MLE algorithm [10, 11] requires the input data set (p, $R^{code}, R^{exp}, \frac{\partial R}{\partial p}$). p denotes the multiplier used for adjusting an input model parameter (in this case, physical model); R^{code} and R^{exp} are the response of interest (in this case, void fraction) from predictions and experimental measurement, respectively; the derivative $\frac{\partial R}{\partial p}$ represents the effect of the parameter p on the response of interest, also called sensitivity coefficient. $\frac{\partial R}{\partial p}$ is calculated numerically by finite-difference of perturbed TRACE simulations.

The relation between the response (in this case, void fraction) and the input model parameter (in this case, selected physical models) is assumed to be linear,

$$R(p) = R_0 + \frac{\partial R}{\partial p}(p - p_0) \tag{1}$$

where, $p_0 = 1$ represent the input model parameter value originally used by TRACE and R_0 is the prediction if $p_0 = 1$ is used. This linearity assumption will be investigated in the SA step before $\frac{\partial R}{\partial p}$ is estimated.

The input model parameter is assumed to follows a normal distribution,

$$p \sim N(\mu, \sigma^2) \tag{2}$$

where, mean value (μ) and variance (σ^2) are the variables of interest that we have no prior information. Estimation of (μ, σ^2) is based on a series of observations, which in this case are the void fraction measurements. The MLE algorithm tries to find the (μ, σ^2) such that it maximizes the likelihood that the observations will occur. Practically, the Expectation-Maximization (E-M) iterative scheme is applied to the MLE algorithm. Detailed description and derivation of MLE and E-M scheme are referred to [9, 10].

Following the inverse uncertainty quantification step (estimation of PDFs for the selected input model parameters), each selected input model parameter is sampled randomly from their distribution and these sampled parameters are implemented in TRACE for new simulation (forward uncertainty quantification). Now, these responses bring the information about uncertainties of TRACE predictions.

Figure 2 is a schematic showing of the work flow.

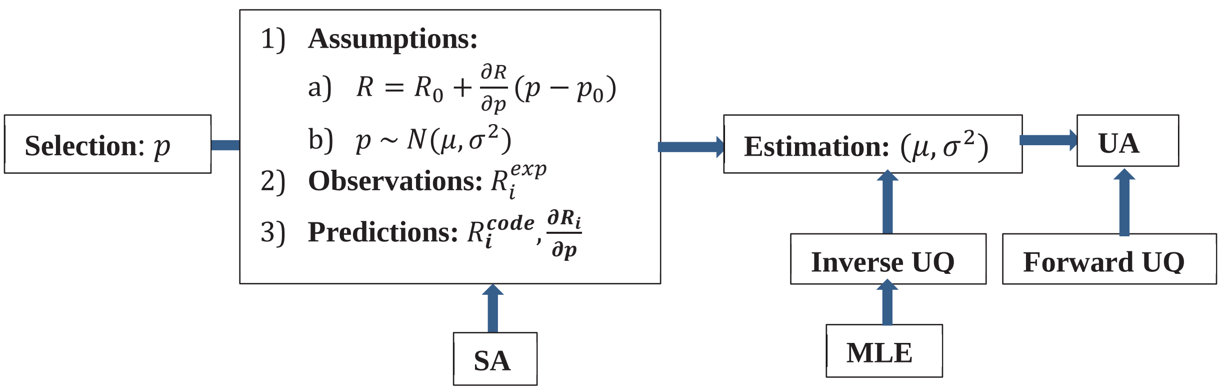

Figure 2. Schematic view of the work flow

4. RESULTS

4.1 Step 1: Accuracy Analysis

The accuracy analysis aims to compare the TRACE predictions with experimental measurement. 35 of 86 test cases of assembly type 4 are selected, cross-sectional average void fraction at 4 axial elevations are obtained using TRACE. Each case has different thermal-hydraulics conditions (pressure, inlet temperature, flow rate and power). The variation in experimental conditions used in this work is shown in Table II,

Table II. Variation of experimental conditions

Parameters	Variations
Pressure (MPa)	3.9 - 8.7
Inlet temperature (°C)	238 - 292
Inlet subcooling (kJ/kg)	50. - 56.
Flow rate (t/h)	10. - 70.
Power (MW)	0.62 - 7.3
Exit quality (%)	8 - 25
Exit void fraction (%)	45 - 90

Comparison between the predicted and measured void fraction at 4 axial elevations (DEN #3, DEN #2, DEN #1 and CT) is shown in Figure 3. TRACE gives an overall good trend prediction. For the lowest and highest axial elevations (DEN #3 and CT), TRACE predictions are close to the measurement. However, predictions in the middle elevations (DEN #2 and DEN #1) tend to under-estimate the void fraction, with an absolute difference of about 5-10%. Both measurement and TRACE uncertainties contribute to the difference.

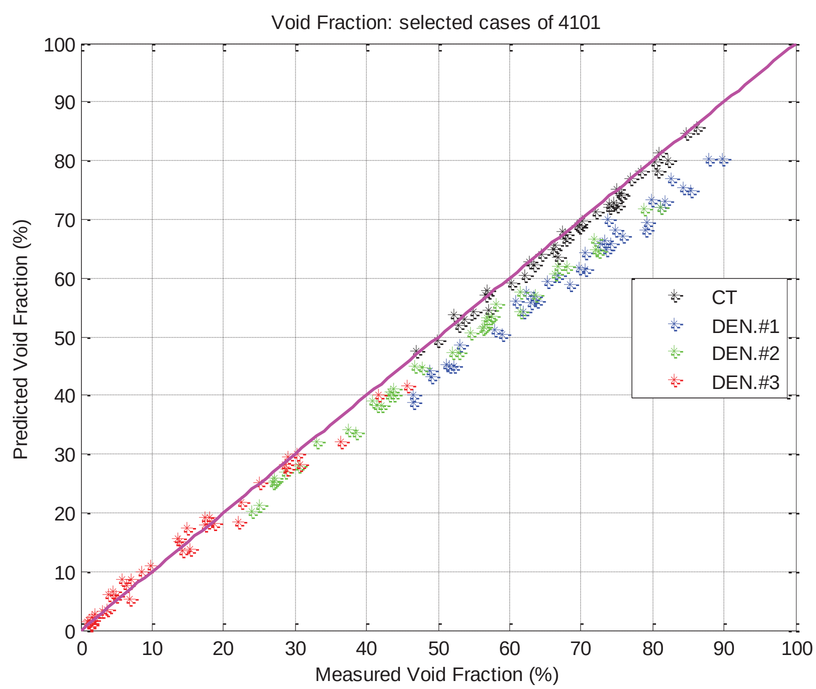

Figure 3. Comparison between TRACE predictions and experimental measurement on void fraction in test assembly 4

4.2 Step 2: Inverse Uncertainty Quantification

In this paper we are interested in quantifying the uncertainty of the single phase liquid to wall and subcooled boiling HTC model. The flow is in a single phase regime when the wall temperature is below the conditions necessary for the Onset of Nucleate Boiling (ONB); the flow changes to a subcooled nucleate boiling regime when the condition for ONB is satisfied but the bulk liquid temperature is subcooled. When the bulk liquid temperature reaches saturation, other bulk boiling mechanisms begin to prevails, such as slug flow or annular flow [1, 9]. This means that only the void fraction data measured at lower elevation (X-ray densitometer DEN #3) is valuable in this step. It was confirmed that the sensitivity coefficient for single-phase liquid to wall and subcooled boiling HTC at higher elevations (DEN #2, DEN #1 and CT) is trivial ($\frac{\partial R}{\partial p} \sim 0$) and thus it is not suitable for inverse uncertainty quantification.

The inverse uncertainty quantification using MLE relies on the linear assumption made in Eq. (1). It is important to validate this assumption for each application. Figure 4 shows the relation between the predicted void fraction and the single phase liquid to wall HTC and the subcooled boiling HTC for one of the experiments. This figure shows that the linear assumption is valid in a rather wide range [0.5, 1.5] for the single phase liquid to wall model; however, the linearity assumption is valid in a smaller range [0.8, 1.2] for the subcooled boiling model.

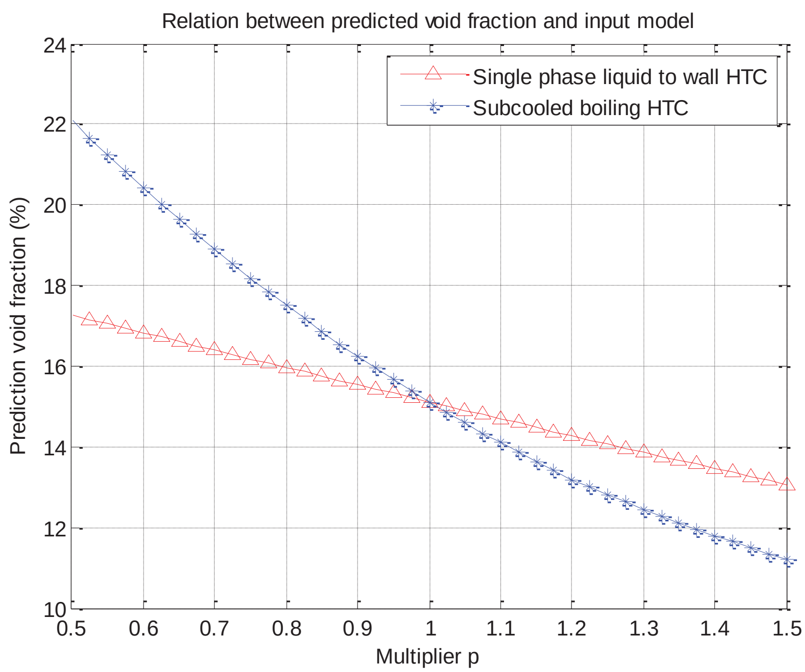

Figure 4. Linearity assumption validation. Case 4101-85 of assembly 4 is used

Based on the linear assumption, the sensitivity coefficient was calculated using a two-point central finite-difference method,

$$\frac{\partial R}{\partial p} = \frac{R(1+\varepsilon) - R(1-\varepsilon)}{2\varepsilon} \tag{3}$$

where $\varepsilon = 0.1$ was used.

Figure 5 shows the calculated sensitivity coefficients for all 35 test cases used in this work. The red-triangle data represent the derivative of the predicted void fraction with respect to the single-phase liquid to wall HTC, the blue-star data represent the derivative of the predicted void fraction with respect to the subcooled boiling HTC. The figure shows that the void fraction is more sensitive to the subcooled boiling model than the single-phase liquid to wall model. Both models have a negative correlation with the void fraction.

Now, the input data set ($p,\ R^{code}, R^{exp}, \frac{\partial R}{\partial p}$) for MLE algorithm is available. The PDFs for these two physical models are calculated and listed in Table III. The physical model PDFs are valuable for the forward uncertainty analysis, because they provide quantitative description of the TRACE code input model uncertainties. The result shows that subcooled boiling HTC lies in the range [0.988, 1.376] with a probability of about 0.95. The fact that the linear assumption works well in this range confirms validity of the calculated PDF. However, because the void fraction is less sensitive to the single-phase liquid to wall HTC, the calculated distribution is less reliable, which is shown by its large variance.

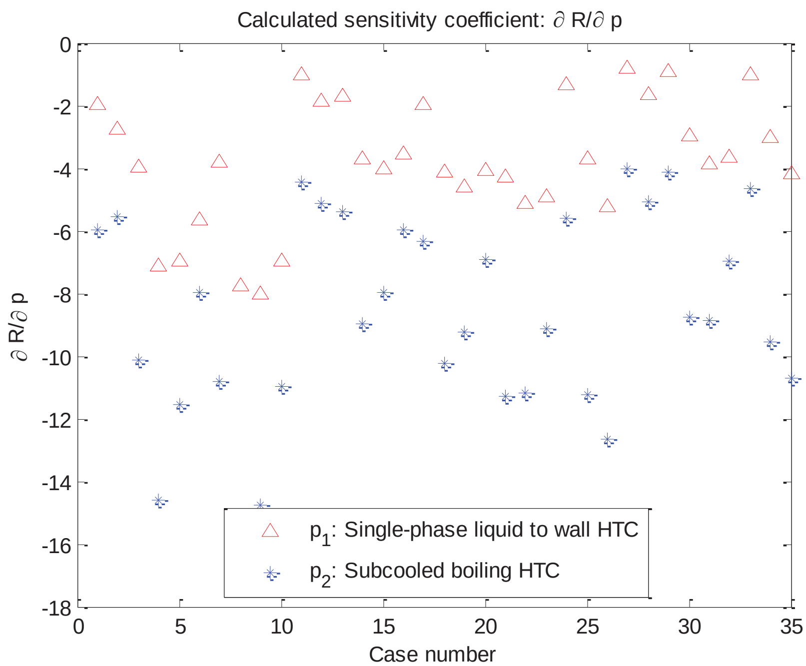

Figure 5. Sensitivity coefficients used in inverse uncertainty quantification, the response is cross-sectional average void fraction at the lowest elevation (DEN #3)

Table III. Probability density function of 2 input model parameters

Modeling Parameters	**PDF**	μ	σ
Single-phase liquid to wall HTC (p_1)	Normal	0.627	0.350
Subcooled boiling HTC (p_2)	Normal	1.182	0.097

4.3 Step 3: Forward Uncertainty Quantification

Following step 2, the estimated uncertainty distributions of two physical models are available for forward uncertainty analysis. 4 test cases (4101-17, 4101-44, 4101-66, and 4101-85) from test assembly 4 are selected to represent the typical experimental conditions. For each test case, a single-phase liquid to wall HTC and subcooled boiling HTC is sampled randomly from their distribution, then the sampled parameters are used for TRACE simulation and finally the resulting TRACE predictions are collected. The output (void fraction) distribution is shown in Figure 6. Though distributions of the output (void fraction) are not smooth due to the limited number of samples (200 samples in this work), Figure 6 gives a straightforward view of the uncertainty information of the void fraction, which is useful for further safety analysis. Because of the nonlinear relation between output and input model parameters, the distribution of output void fraction deviates from a normal distribution.

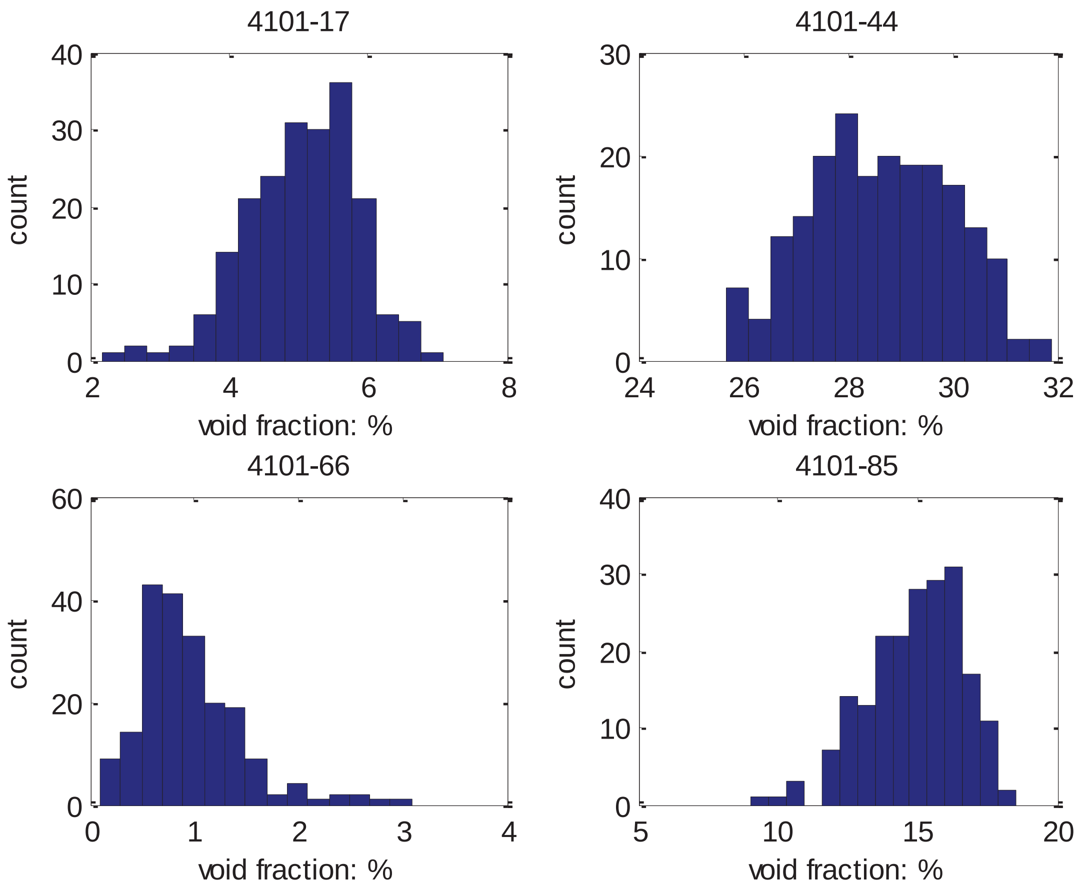

Figure 6. TRACE void fraction uncertainty distribution at the lowest elevation (DEN #3). Number of total samples is 200

The mean and variance of the output void fraction is critical to further analysis. Table IV shows the calculated mean and variance of void fraction predictions by TRACE. The sample mean and standard deviation of TRACE predictions is shown for each case. In Table IV, the second column is the measured void fraction of each case; the third and fourth columns are the mean and variance of 200 TRACE predictions samples as in Figure 6. Except for test number 4101-17, the adjusted TRACE predictions matches well with the experimental measurement. Besides, the uncertainty information of input model parameters are propagated to the output void fraction predictions.

Table IV. Uncertainties of TRACE void fraction predictions

Test No.	Measured (%)	TRACE	
		Mean (%)	**Standard deviation** (%)
4101-17	6.9	5.0	0.8
4101-44	28.6	28.6	1.4
4101-66	0.9	1.0	0.5
4101-85	13.9	14.8	1.7

5. CONCLUSIONS

In this paper, the steady-state void fraction measurement of the NUPEC BFBT benchmark is used to perform an uncertainty quantification study with TRACE code and MLE algorithm. The inverse uncertainty analysis was performed for two physical models, single-phase liquid to wall HTC and subcooled boiling HTC, using MLE algorithm to estimate their probability distribution function. Forward uncertainty analysis was then performed to show typical usage of the obtained physical model uncertainty information (PDF).

Though the obtained physical model uncertainty information (PDF) can be used for future uncertainty analysis, a few concerns should be noted. The main concern comes from the freedom of selecting experimental cases. Inverse parameter estimation is not a well-posed problem, and the MLE algorithm can give different results using different experimental responses. Another concern is due to the reliability of linearity assumption. Multiple calculations should be done to validate this assumption before the inverse uncertainty quantification. Finally, only two input model parameters are considered in this research, however there are many other parameters that contribute to the uncertainties of TRACE predictions. A more complicated uncertainty quantification method is necessary to include the effect of these parameters.

In this paper, the sensitivity of input model parameters is calculated locally using a two-point finite-difference approximation, as shown in Eq. (3). More advanced methods could be used in the future. Another improvement is to calculate the sensitivity and forward uncertainty using an UA packages, such as SUSA and DAKOTA [6, 7]. However, the inverse uncertainty to estimate input physical model PDF is a must, as demonstrated in this paper.

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