



Inverse uncertainty quantification of trace physical model parameters using BFBT benchmark data



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ABSTRACT

Forward quantification of simulation (code) response uncertainties requires knowledge of physical model parameter uncertainties. Nuclear thermal-hydraulics codes, such as RELAP5 and TRACE, do not provide any information on uncertainties of physical model parameters. A framework is developed to quantify uncertainties of physical model parameters using Maximum Likelihood Estimation (MLE), Bayesian Maximum A Priori (MAP), and Markov Chain Monte Carlo (MCMC) algorithms.

The objective of the present work is to perform the sensitivity analysis of the physical model parameters in code TRACE and calculate their uncertainties using MLE, MAP, and MCMC algorithms. The OECD/NEA BWR Full-size fine-mesh Bundle Test (BFBT) data is used to quantify uncertainty of selected physical models of 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 system conditions. In this work, the steady-state cross-sectional averaged void fraction distribution is used as the input data for inverse uncertainty quantification (IUQ) algorithms, and the selected physical model's probability distribution function (PDF) is the desired output quantity.

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1. Introduction

The U.S. Nuclear Regulatory Committee (NRC) advocates best-estimate calculations (D Auria et al., 2006) for the understanding of Emergency Core Cooling System (ECCS) performance during reactor transients. The term “best-estimate” is used to indicate the attempt to predict realistic thermal-hydraulics response of a reactor system. The conservative approach provides a bound to the prediction by considering extreme (bounding) conditions. In a best-estimate calculation, the calculation should predict the mean of experimental data and should consider the effects of all important variables whenever possible. If some variables are not possible or practical to consider in a phenomenon, the effect of omitting these variables should be provided in the form of computational uncertainty.

NRC has developed and assessed several advanced best-estimate codes for simulating thermal-hydraulics transient problems, including TRACE (Bajorek, 2008) and RELAP5 (United States Nuclear Regulatory Commission, 2002). These codes predict the major phenomena observed over a broad range of thermal-hydraulics and fuel tests, for example Loss Of Coolant Accident

(LOCA), and can be used to perform best-estimate calculations of ECCS performance. 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 is important for safety margin evaluation, because void fraction has a significant effect on the reactivity, pressure drop, critical heat flux, and other phenomena. Void fraction is determined by various physical models, such as drag models and heat transfer models. Part of the uncertainty in void fraction prediction is propagated from the uncertainties in these physical models.

Uncertainty analysis (UA) aims to quantify the overall uncertainty associated with the output as a result of uncertainties in the input parameters (Neykov, 2006; Gajev et al., 2014). There are essentially two parts in an uncertainty analysis. The first part, called Forward Uncertainty Quantification (FUQ) (Kennedy and O'Hagan, 2001), is the process of quantifying uncertainties in outputs. It focuses on the influence of the parametric (input) variability on the outputs. The second part, called inverse uncertainty quantification (IUQ) (Kennedy and O'Hagan, 2001), is a process of estimating the values of unknown (input) parameters given experimental measurements of a system and computer simulation results. IUQ is usually ill-posed (Shrestha and Kozłowski, 2015), because a unique solution might not exist. Common methods for FUQ problems include Monte Carlo simulation, perturbation

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method, and spectral expansion method (Lee and Chen, 2009; Robert and Casella, 2013; Mooney, 1997). Common methods for inverse problems include Maximum-Likelihood Estimation (MLE), Maximum A Posteriori (MAP), and Markov Chain Monte Carlo (MCMC) (Shrestha and Kozłowski, 2015; Gelman et al., 2014; McLachlan and Krishnan, 2007; Gilks, 2005).

The uncertainties of boundary conditions, initial conditions, and geometry are usually determined by the experimental team, manufacturing tolerances, or sometimes are suggested by researchers based on experience. With such information, FUQ can be done using uncertainty analysis packages, such as DAKOTA (Giunta et al., 2007) or RAVEN (Rabiti, 2012). However, uncertainties of physical models are the most important and are difficult to obtain. This is because the physical models closure relations are usually implemented as empirical correlations directly in computational code and are not available to the code user for manipulation. When these correlations were originally developed, their accuracy and reliability was studied with particular experiments (Ishii, 1977; Ishii and Hibiki, 2010; Kaichiro and Ishii, 1984; Zuber and Findlay, 1965). However, once these correlations were implemented in thermal-hydraulics codes (e.g. RELAP5 and TRACE) and used for different physical systems, the accuracy and uncertainty information of these correlations was no longer known to the code user. Therefore, quantifying the accuracy and the uncertainties of the physical models (correlations) is of critical need, which is the objective of this work.

The rest of this paper is organized as follows. In Section 2 we will develop a framework based on Bayes' theorem to quantify uncertainties in physical model parameters. Two algorithms, MAP and MCMC, are developed. In Section 3 we will apply the MAP and MCMC algorithms to BFBT benchmark data for assessing uncertainties in subcooled boiling heat transfer coefficient and interfacial drag (bubbly/slug) coefficient. In Section 4 we will summarize the current methods and discuss potential extension.

2. Theory of parameter estimation

The parameter estimation algorithms are derived in Bayesian analysis framework. The Bayes' theorem, which relates the prior distribution, likelihood function, and posterior distribution, is the basis of the framework. A prior distribution of a random variable is the probability distribution that expresses our experience about the quantity before we observe some evidence; the likelihood of a random variable is the probability of an event happens; a posterior distribution of a random variable is the probability distribution that expresses our knowledge based on observed evidence and prior experience. Let X be the interested parameter, such as the heat transfer coefficient, and consider X being a continuous random variable. Let $f(x; \vec{\theta})$ be the probability distribution function, where $\vec{\theta}$ is a parameter vector, such as the mean and variance. We need to formulate a problem such that $\vec{\theta}$ contains uncertainty information (e.g. mean and variance) for the random variable X (e.g. physical model parameter). The prior distribution, likelihood, and posterior distribution is denoted as $\pi(\vec{\theta})$, $L(\vec{\theta}|x)$, and $\pi(\vec{\theta}|x)$ respectively.

The likelihood is expressed as,

$$L(\vec{\theta}|x) = f(x; \vec{\theta}) \quad (1)$$

The prior distribution, likelihood, and posterior distribution are related by Bayes' theorem as,

$$\pi(\vec{\theta}|x) = \frac{L(\vec{\theta}|x)\pi(\vec{\theta})}{\int L(\vec{\theta}|x)\pi(\vec{\theta})d\vec{\theta}} \equiv K(x)L(\vec{\theta}|x)\pi(\vec{\theta}) \quad (2)$$

where, $K(x) = \frac{1}{\int L(\vec{\theta}|x)\pi(\vec{\theta})d\vec{\theta}}$ is the integration constant, which in practice is often difficult to obtain.

In this paper, X represents the physical model parameters of interest. Ideally, we would like to observe them directly; however, it is impossible to directly measure the physical model coefficients in practice. The output quantities that we can observe/calculate in an experiment/calculation are temperature, power, void fraction, and pressure drop. These output quantities are deterministic functions of the physical model parameters and contain the statistical information of the physical model parameters. We need to formulate our algorithms in such a way that we can estimate the parameter vector of the physical model parameter (denoted as $\vec{\theta}$) based on observable output quantities (denoted as Y), such as void fraction. Table 1 shows the notation of variables that are used in this paper.

Consider $\vec{Y}$ being a function of vector $\vec{X}$,

$$\vec{Y} = Y(\vec{X}) \quad (3)$$

If we assume $\vec{Y}$ is a linear function of $\vec{X}$, then when $\vec{X}$ is slightly perturbed around nominal value,

$$\vec{Y} = \vec{Y}_0 + \mathbf{A}\vec{X} \quad (4)$$

where $\mathbf{A}$ is the sensitivity coefficient matrix, defined as $\mathbf{A} \equiv \frac{\partial \vec{Y}}{\partial \vec{X}}$.

In the following derivation, the subscript i denotes the i^{th} experiment. For example, $\vec{Y}_i$ denotes the output from the i^{th} experiment. For the vector $\vec{X}$ or $\vec{Y}_i$, a further subscript j denotes the j^{th} element of the vector. For example, X_j denotes the j^{th} physical model parameter and Y_{ij} denotes the j^{th} output variable of the i^{th} experiment.

If one considers the random error of an experimental measurement, Eq. (4) becomes,

$$\vec{Y}_i = \vec{Y}_{0,i} + \mathbf{A}_i\vec{X} + \vec{E}_i \quad (5)$$

Note that for each measurement, the variables $\vec{Y}_{0,i}$, $\mathbf{A}_i$, $\vec{E}_i$ are different because the experimental conditions are different. In this work, the random error is assumed to be mean-zero and does not depend on either $\vec{X}$ or $\vec{Y}$.

We assume $\vec{X}$ follows a joint Gaussian distribution with mean and covariance ($\vec{\mu}_x$, Σ_x). Because Eq. (5) is linear, $\vec{Y}_i$ also follows a joint Gaussian distribution and has the following properties.

$$\vec{\mu}_{y,i} = \vec{Y}_{0,i} + \mathbf{A}_i\vec{\mu}_x \quad (6)$$

$$\Sigma_{y,i} = \mathbf{A}_i\Sigma_x\mathbf{A}_i^T + \Sigma_{e,i} \quad (7)$$

$$f_i(\vec{y}; \vec{\theta}) = (2\pi)^{-\frac{d_y}{2}} |\Sigma_{y,i}|^{-\frac{1}{2}} \exp \left[-\frac{1}{2} (\vec{y} - \vec{\mu}_{y,i})^T \Sigma_{y,i}^{-1} (\vec{y} - \vec{\mu}_{y,i}) \right] \quad (8)$$

where, d_y is the dimension of $\vec{Y}_i$. Note that Eq. (8) requires $\Sigma_{y,i}$ to be non-singular. In practice, this condition is satisfied by using appropriately selected measurement data.

Table 1
Variable notation used in this paper.

Variables	Meaning
$\vec{\theta}$	Parameter vector of the physical model parameter, such as mean and variance
$\vec{X}$	Physical model parameter
$\vec{Y}$	Output from experimental measurement
$\vec{Y}_0$	Output from code prediction
$\vec{E}$	Random error of experimental measurement
$\mathbf{A}$	Sensitivity coefficient matrix
$\vec{\mu}_x, \Sigma_x$	Mean and covariance matrix of physical model parameter
$\vec{\mu}_y, \Sigma_y$	Mean and covariance matrix of output
$\vec{\mu}_e, \Sigma_e$	Mean and covariance matrix of random error of experimental measurement

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