INVERSE UNCERTAINTY QUANTIFICATION OF TRACE PHYSICAL MODEL PARAMETERS USING BAYESIAN ANALYSIS

BY

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THESIS

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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 based on Maximum Likelihood Estimation (MLE), Bayesian Maximum A Priori (MAP), and Markov Chain Monte Carlo (MCMC) 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, MAP and MCMC algorithm, with a particular focus on the subcooled boiling model. 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 system conditions. In this thesis, the steady-state cross-sectional averaged void fraction distribution from BFBT experiments is used as the input for inverse uncertainty algorithm, and the selected physical model's Probability Distribution Function (PDF) is the desired output quantity.

ACKNOWLEDGMENTS

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1 Introduction

1.1 Best-estimate and uncertainty analysis

U.S. NRC (Nuclear Regulatory Committee) advocated Best-Estimate calculations for the understanding of Emergency Core Cooling System (ECCS) performance during reactor transients (U.S. NRC, 1989). The term "best-estimate" is used to indicate the attempt to predict realistic thermal-hydraulics response of a reactor system. In terms of modeling thermal-hydraulics transient problem, the NRC has developed and assessed several advanced best-estimate code, including TRACE and RELAP5 (U.S. NRC, 2010; U.S. NRC, 2001). These codes predict the major phenomena observed over a broad range of thermal-hydraulics and fuel tests, such as Loss Of Coolant Accident (LOCA) and Reflooding, and could be used to perform best-estimate calculations of Emergency Core Cooling System (ECCS) performance.

The conservative approach provides a bound to the prediction by considering extreme (bounding) conditions. In a best-estimate calculation the model results should predict the mean of experimental data. In addition, a best-estimate calculation 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. In other words, this requires the analysis of uncertainty of a best-estimate calculation.

Besides the specific requirements of a best-estimate calculation, analysis of uncertainty is also important for code verification and validation (V&V). V&V are usually defined as a primary means to assess the accuracy and reliability of simulations. Verification is separated into two different groups: code verification and solution verification. The code verification assesses the reliability of software code, while the solution verification deals with the numerical accuracy of the computational model. In comparison, validation is defined as assessment of the physical modeling accuracy of a computational simulation by comparing with experimental data. Conceptually, verification is the process that ensures that the physical models are correctly

solved by the computer code, while validation is the process that ensures that the physical models are suitable for predicting desired phenomena by comparison with experiment (U.S. NRC, 1989).

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 very 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 (Boyack, 1990). The uncertainties of code predictions should be provided along with these predictions, which require an uncertainty analysis of the code by propagation of input uncertainties to the output predictions.

Uncertainty is an estimation of scatter in a measurement or in a predicted (e.g. simulation) result, usually determined with a certain level of confidence (often 95%) (Jaynes, 2003). Considering a model's prediction of output results as a function of uncertain input parameters, propagation of uncertainty is the effect of the input uncertainties on the output results. In other words, this quantifies the variation of the outputs due to the variation (range and distribution) of input parameters. For example, for a variable measured in an experiment, the uncertainty due to measurement limitations (limited number of measurements, instrument precision, etc.) will propagate to the outputs.

Sources of uncertainty may include (Kennedy, 2001):
- parameter uncertainty/variability, which comes from the input parameters to the computer model; either the exact value of the input parameters is unknown or there is variability in the input parameters.
- model discrepancy, which comes from the lack of knowledge of the true physics behind the phenomena. In this thesis, a framework based on Bayesian analysis is used to quantify the uncertainty of physical models.
- numerical uncertainty, which comes from numerical errors and numerical approximations, such as truncation error, runoff error, interpolation error, etc.
- experimental uncertainty, which comes from variability of experimental measurement.

Uncertainty is usually separated into two types:

- statistical uncertainty, which is due to the fact that the unknowns are different each time we measure. Usually, statistical uncertainty is capable of being estimated using probability distribution.
- systematic uncertainty, which is due to the fact that there are things that we do not know.

Despite a variety of sources of uncertainty, this thesis focuses on quantifying the model discrepancy (physical model uncertainty) and their statistical uncertainties.

Uncertainty Analysis (UA) aims to quantify the overall uncertainty associated with the output as a result of uncertainties in the input parameters (Neykov, 2006). There are basically two parts in an uncertainty analysis: quantifying the overall uncertainties in outputs and quantifying the uncertainties in the input parameters. The first part, called Forward Uncertainty Propagation (Kennedy, 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 (Kennedy, 2001) is a process of estimating the discrepancy between the experiment and mathematical model or estimating the values of unknown (input) parameters in the model given experimental measurements of a system and computer simulation results. Generally speaking, the inverse part is much more difficult than the forward part and sometimes it is ill-posed, meaning there might not exist a unique solution for the inverse problem. In this thesis, we are focusing on the inverse uncertainty quantification, and the forward uncertainty propagation will be used to validate the framework and solution of the inverse problem.

Many methods are available for both forward and inverse problems. For the forward uncertainty propagation, common methods (Lee, 2009), include Monte Carlo simulations (Mooney, 1997), perturbation methods, polynomial chaos expansion (PCE), first-order reliability method (FORM), and full factorial numerical integration (FFNI). For inverse uncertainty quantification, common methods include likelihood-based methods such as Maximum-Likelihood Estimation (MLE) (Scholz, 1985) and Bayesian-based methods (Gelman, 2014), such as Maximum A Posteriori (MAP) and Markov Chain Monte Carlo (MCMC) (Gilks, 2005).

In this thesis, the Monte Carlo sampling simulations will be used for the forward problems and a framework based on Bayesian analysis (MAP, MCMC) will be derived for the inverse problem. Since the concept of likelihood is directly related to Bayesian analysis, a likelihood-based method (MLE) will also be used for a consistency comparison with Bayesian-based methods (MAP, MCMC). These methods will be demonstrated by estimating uncertainties in the physical models used in TRACE code, such as interfacial drag coefficient, interfacial heat transfer coefficient, etc.

1.2 Two-phase two-fluid model description

In the process of forward uncertainty propagation, possible input parameters may include (Kennedy, 2001):

- 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 fuel rod diameter, the cladding thickness, flow area, etc.
- Physical model parameters used in the code, such as single-phase and two-phase heat transfer coefficients, interfacial and wall friction coefficients, void drift model parameters, etc.

The uncertainties and related Probability Density Functions (PDF) of BICs and geometry are usually determined by the experimental team, manufacturing tolerances or sometimes are suggested by researchers based on experience. With such information, forward uncertainty propagation could be done with the help of uncertainty analysis packages, such as DAKOTA (Giunta, 2007). However, PDFs for the physical models are the most important and the most difficult to obtain. This is because the physical models closure relations are usually implemented as empirical correlations directly in the computational code and are not directly available to the code user for manipulation.

Two-Phase Two-Fluid (TPTF) model (Ishii, 2010) is used in several advanced reactor thermal-hydraulics codes, including TRACE, RELAP5 and COBRA. The main difficulty in solving a two-phase flow problem comes from our lack of understanding and modeling of the

interaction mechanism at the interface between two phases. A number of correlations are used in modeling the interfacial transfer mechanism (especially the interfacial momentum transfer) and uncertainties in these correlations propagate to uncertainties in TPTF model predictions.

The conservation equations and the main correlations used in a TPTF model are described below. TRACE uses the simplified conservation equations (Ishii, 2010), (U.S. NRC, 2010),

Conservation of mass,

$$\frac{\partial(\alpha_g\rho_g)}{\partial t} + \nabla \cdot (\alpha_g\rho_g\vec{v}_g) = \Gamma_g \tag{1}$$

$$\frac{\partial(\alpha_l\rho_l)}{\partial t} + \nabla \cdot (\alpha_l\rho_l\vec{v}_l) = \Gamma_l \tag{2}$$

conservation of momentum,

$$\frac{\partial(\alpha_g\rho_g\vec{v}_g)}{\partial t} + \nabla \cdot (\alpha_g\rho_g\vec{v}_g\vec{v}_g) = -\alpha_g\nabla P_g + \alpha_g\rho_g\vec{g} - \vec{f}_i + \vec{f}_{wg} + \Gamma_g\vec{V}_i \tag{3}$$

$$\frac{\partial(\alpha_l\rho_l\vec{v}_l)}{\partial t} + \nabla \cdot (\alpha_l\rho_l\vec{v}_l\vec{v}_l) = -\alpha_l\nabla P_l + \alpha_l\rho_l\vec{g} + \vec{f}_i + \vec{f}_{wl} + \Gamma_l\vec{V}_i \tag{4}$$

conservation of energy,

$$\frac{\partial[\alpha_g\rho_g\left(e_g+\frac{v_g^2}{2}\right)]}{\partial t} + \nabla \cdot [\alpha_g\rho_g(e_g + \frac{P}{\rho_g} + \frac{v_g^2}{2})\vec{v}_g)] = q_{ig} + q_{wg} + q_{dg} + \alpha_g\rho_g\vec{g} \cdot \vec{v}_g +$$

$$\Gamma_g h_v' + (-\vec{f}_i + \vec{f}_{wg}) \cdot \vec{V}_g \tag{5}$$

$$\frac{\partial[\alpha_l\rho_l\left(e_l+\frac{v_l^2}{2}\right)]}{\partial t} + \nabla \cdot [\alpha_l\rho_l(e_l + \frac{P}{\rho_l} + \frac{v_l^2}{2})\vec{v}_l)] = q_{il} + q_{wl} + q_{wsat} + q_{dl} + \alpha_l\rho_l\vec{g} \cdot$$

$$\vec{v}_l + \Gamma_l h_l' + (\vec{f}_i + \vec{f}_{wl}) \cdot \vec{V}_l \tag{6}$$

where, the subscript (g, l) denotes gas and liquid phase.

- α_g, α_l : gas/liquid phase volume fraction, $\alpha = \alpha_g$ is void fraction.
- ρ_g, ρ_l : gas/liquid phase density.
- $\vec{v}_g, \vec{v}_l$: gas/liquid phase velocity.
- P : pressure.
- e_g, e_l : gas/liquid phase internal energy.
- $\vec{g}$: gravity.
- $\vec{f}_i$: the force per unit volume due to shear at the phase interface.
- $\vec{f}_{wg}, \vec{f}_{wl}$:the wall shear force per unit volume acting on the gas/liquid phase.

- $\vec{V_i}$: the flow velocity at the phase interface.
- q_{ig}, q_{il} : the phase interface to gas/liquid heat transfer flux.
- q_{wg}, q_{wl} : the wall to gas/liquid heat transfer flux.
- q_{dg}, q_{dl} : the power deposited directly to the gas/liquid phase.
- q_{wsat} : the wall to liquid heat flux that goes directly to boiling.
- h'_v, h'_l : the vapor/liquid enthalpy.

Closure is obtained for these equations using normal thermodynamic relations and correlations for phase change, heat source and force terms. The forces terms in momentum equations are cast into the following forms using the correlations for friction coefficients (U.S. NRC, 2010). For example,

$$\vec{f_i} = C_i(\vec{v}_g - \vec{v}_l)|\vec{v}_g - \vec{v}_l| \tag{7}$$

$$\vec{f}_{wg} = -C_{wg}\vec{v}_g|\vec{v}_g| \tag{8}$$

Where, C_i is the interfacial drag coefficient, C_{wg} is the gas phase wall drag coefficient.

The heat transfer flux terms in the energy equations are formed with Newton's law and the correlations for heat transfer coefficients (U.S. NRC, 2010). For example,

$$q_{wg} = h_{wg}a_w(T_w - T_g) \tag{9}$$

$$q_{ig} = h_{ig}a_i(T_{sv} - T_g) \tag{10}$$

Where, a_w is the heated surface area per volume of fluid and a_i is the interfacial area per unit volume. h_{wg} is the heat transfer coefficient (HTC) for wall to gas phase. h_{ig} is the interfacial HTC at the gas interface. (T_g, T_w, T_{sv}) are the temperature of gas, wall and saturated vapor. Similar forms exist for other heat transfer fluxes.

Closure relationships used to define these drag coefficients and heat transfer coefficients are provided with TRACE code (U.S. NRC, 2010). Four coefficients are mainly analyzed in this thesis: Single phase liquid to wall HTC, Subcooled boiling HTC, Wall drag coefficient and Interfacial drag (bubbly/slug Rod Bundle-Bestion) coefficient. As an example, let's take a look at the Interfacial drag (bubbly/slug Rod Bundle-Bestion) coefficient. It is modeled as,

$$C_i = \frac{\alpha_g(1-\alpha_g)^3 g\Delta\rho}{\bar{v}_{g,j}^2}\left(\frac{1-C_0\langle\alpha_g\rangle}{1-\langle\alpha_g\rangle}\bar{v}_g - C_0\bar{v}_l\right)^2 / |v_g - v_l|^2 \tag{11}$$

Where, $\Delta\rho$ is the density difference between liquid and gas phases, $\langle*\rangle$ denotes area averaged

properties. $\bar{v}_{g,j}$ and C_0 are drift flux velocity and the distribution parameter. For a rod bundle, $\bar{v}_{g,j}$ and C_0 are modeled as,

$$\bar{v}_{g,j} = 0.188\sqrt{g\Delta\rho D_h/\rho_g} \tag{12}$$

$$C_0 = 1.0 \tag{13}$$

Where, D_h is the hydraulic diameter.

Details about the modeling of other coefficients in TRACE are covered in the TRACE theory manual (U.S. NRC, 2010). Note that uncertainties in Eq. (11-13) will propagate to the uncertainties of the interfacial drag coefficient. It is the uncertainty of these coefficients that is important in uncertainty analysis and is the focus of this thesis.

When these correlations were originally developed, their accuracy and reliability was studied with particular experiments (Ishii, 1977) (Kaichiro, 1984) (Zuber, 1965). However, once these correlations were implemented in a thermal-hydraulics code (e.g. RELAP5, TRACE) and used for different physical systems, the accuracy and uncertainties information of these correlations was no longer known to the code user. Therefore, further work to quantify the accuracy and the uncertainties of the input physical models (correlations) is of critical need, which is the objective of this thesis.

A valid experiment benchmark is necessary for both the forward uncertainty propagation and inverse uncertainty quantification. One of the most valuable and publicly 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 full-scale BWR fuel assembly (Neykov, 2006). This thesis uses the BFBT benchmark to conduct uncertainty analysis of the thermal-hydraulics code system TRACE.

1.3   Organization of the thesis

The organization of this thesis is as follows:

Chapter 1: Introduction.

This chapter introduces the requirements of uncertainty quantification in current Best-Estimate calculations and available uncertainty quantification concepts and methods. Because the main simulation tool used in this thesis is TRACE, the Two-Phase Two-Fluid model used in reactor thermal-hydraulics codes is also described.

Chapter 2: Theory of parameter estimation.

In this chapter, Maximum Likelihood Estimation (MLE), Maximum A Posteriori (MAP) and Markov Chain Monte Carlo (MCMC) are derived in detail.

Chapter 3: Numerical tests.

In this chapter, the previously derived algorithms are applied to three sets of synthetic numerical data for verification.

Chapter 4: Application to BFBT benchmark.

In this chapter, the previously derived algorithms are applied to BFBT benchmark data to estimate the probability distribution of two physical model parameters. The estimation results are then validated by forward uncertainty TRACE calculations using estimated distribution of model parameters.

Chapter 5: Discussion

In this chapter, the valuable features of MLE, MAP and MCMC algorithms are discussed.

Chapter 6: Conclusion

In this chapter, the main analysis and derivation conducted in this work is summarized.

Chapter 7: Future Work

In this chapter, some issues and limitations of MLE, MAP and MCMC algorithms and possible future work are addressed.

2   Theory of parameter estimation

In this chapter, the theory behind the estimation of parameters of interest using Bayesian Analysis is described in detail.

2.1   Notation and definitions

Before the derivation of algorithms, let us start with the clarification of several important terms. Let X be the output quantity of interest (such as the void fraction in a thermal-hydraulics experiment). Consider X be 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 of a random variable. It is the $\vec{\theta}$ that we usually need to estimate.

Here are the most important definitions that will be used through the thesis,

- *Expectation (or mean).* The expectation of a continuous random variable is defined as,

$$E(X) = \int xf(x; \vec{\theta})dx \tag{14}$$

  where we usually denote $E(X)$ as $\bar{X}$.

- *Variance.* The variance of a random variable is defined as,

$$\mathrm{Var}(X) = E((X - \bar{X})^2) \tag{15}$$

- *Covariance.* The covariance between two random variables is defined as,

$$\mathrm{Cov}(X, Y) = E((X - \bar{X})(Y - \bar{Y})) \tag{16}$$

- *Covariance Matrix.* If X, Y is replace with random vectors $\vec{X}, \vec{Y}$, respectively, the covariance matrix is defined as,

$$\mathrm{Cov}(\vec{X}, \vec{Y}) = E((\vec{X} - E(\vec{X}))(\vec{Y} - E(\vec{Y}))^T) \tag{17}$$

  where the superscript T is the transpose operator.

- *Conditional Expectation.* The conditional expectation represents the expectation value of a random variable X given the value of another random variable Y, and is denoted as $E(X|Y)$.

- *Minimum Mean Square Error (MMSE) estimator*. If we are trying to estimate the conditional expectation of random variable X using the given the observed value of

random variable Y, a MMSE estimator $\hat{X}$ minimizes the expectation value of the square of the error, that is

$$\hat{X} = g(Y), \quad g(Y) \quad \text{minimizes} \quad \mathrm{E}((X - g(Y))^2) \tag{18}$$

where, $g(Y)$ is a function of random variable Y. Probability theory shows that it is $\mathrm{E}(X|Y)$ that minimizes $\mathrm{E}((X - g(Y))^2)$ and is the MMSE estimator.

- *Linear MMSE estimator.* If we constrain our search for $g(Y)$ in a linear function space, meaning $g(Y) = aY + b$, we get the so called linear MMSE estimator, denoted as $\widehat{\mathrm{E}}(X|Y)$,

$$\hat{X} = \widehat{\mathrm{E}}(X|Y) = \mathrm{cov}(X,Y)\mathrm{cov}(Y,Y)^{-1}(Y - \bar{Y}) + \bar{X} \tag{19}$$

where, $\widehat{E}(X|Y)$ is an approximation to $E(X|Y)$, and

$$\mathrm{E}((X - \widehat{\mathrm{E}}(X|Y))^2) \geq \mathrm{E}((X - \mathrm{E}(X|Y))^2) \tag{20}$$

note that the equal sign happens when X and Y are jointly Gaussian random variables/vector.

- *Prior distribution.* In Bayesian statistical inference, a prior distribution of a random variable is the probability distribution that expresses our belief or experience about the quantity before we observe some evidence. For example, we might have some information (PDF) about the parameter vector $\vec{\theta}$, denoted as a prior distribution $\pi(\vec{\theta})$.

- *Likelihood function.* A likelihood function is a function of the parameters, such as $\vec{\theta}$, of a statistical model and depends on the observed output x. Mathematically, the likelihood of a parameter vector $\vec{\theta}$ given observed output x is defined as the probability of these x happen given $\vec{\theta}$,

$$L(\vec{\theta}|x) = f(x; \vec{\theta}) \tag{21}$$

- *Posterior distribution.* In Bayesian statistical inference, a posterior distribution of a random variable is the distribution of this random variable conditioned on observed evidence or output, it relates both the prior information $\pi(\vec{\theta})$ and the likelihood $L(\vec{\theta}|x)$. Mathematically, the posterior distribution, denoted as $\pi(\vec{\theta}|x)$, is calculated using Bayesian's theorem,

$$\pi(\vec{\theta}|x) = \frac{L(\vec{\theta}|x)\pi(\vec{\theta})}{\int L(\vec{\theta}|x)\pi(\vec{\theta}))d\vec{\theta}} \equiv K(x)L(\vec{\theta}|x)\pi(\vec{\theta}) \tag{22}$$

- *Markov process and stationary distribution.* A Markov process is a random process X if

X is given at present, the future and the past of X are independent. If a Markov process is aperiodic and irreducible, there exists a stationary distribution that the process will converge to, starting from any initial state (Gilks, 2005). Mathematically,

$$\vec{\pi}_{k+1} = \vec{\pi}_k \mathbf{P} \tag{23}$$

$$\lim_{k \to \infty} \vec{\pi}_k = \vec{\pi}_\infty, \quad \forall \vec{\pi}_0 \tag{24}$$

where, $\vec{\pi}_k, \vec{\pi}_\infty$ denotes the distribution at state k and stationary distribution, $\mathbf{P}$ is the probability transition matrix selected for different problems.

The goal of this thesis, given the observed output quantities x (e.g. void fraction), is to estimate the parameter vector $\vec{\theta}$ (e.g. input model uncertainty) based on our prior knowledge about $\vec{\theta}$.

2.2   Prior distribution

Based on our prior knowledge about the parameter vector $\vec{\theta}$, different prior distributions $\pi(\vec{\theta})$ might be chosen, including primarily non-informative prior distribution, conjugate prior distribution, reference prior, etc. This thesis will focus mainly on non-informative and conjugate prior distribution.

Non-informative prior: a non-informative prior distribution is applied when we have no prior knowledge/preference about $\vec{\theta}$. Conceptually, we might say that since we have no prior preference about $\vec{\theta}$, the probability distribution of $\vec{\theta}$ is "even" everywhere.

For different forms of $f(x; \vec{\theta})$, the prior distribution might belong to a location parameter family or a scale parameter family (Gelman, 2014),

- *Location parameter.* A parameter θ belongs to a location parameter family if $f(x; \theta)$ has the form of $\phi(x - \theta)$. For example, in a normal distribution $N(\mu, \sigma^2)$, the mean value μ is a location parameter, change in μ does not affect the shape of the distribution function. A prior distribution for location parameters is,

$$\pi(\theta) \equiv 1 \tag{25}$$

- *Scale parameter.* A parameter θ belongs to a scale parameter family if $f(x; \theta)$ has the

form of $\theta^{-1}\phi(\frac{x}{\theta})$. For example, in a normal distribution $N(\mu, \sigma^2)$, the standard deviation σ is a scale parameter. A prior distribution for scale parameters is,

$$\pi(\theta) \equiv \frac{1}{\theta}, (\theta > 0) \tag{26}$$

Conjugate prior: a conjugate prior distribution is applied if we expect the posterior distribution to have same form as the prior distribution. Recall Eq. (22); to get the posterior distribution $\pi(\vec{\theta}|x)$, a multi-dimensional integration is required to obtain $K(x)$. However, it is usually very difficult or not possible to do the integration analytically. If a conjugate prior distribution is used, we can easily obtain the posterior distribution by replacing $K(x)$ with the appropriate function since we know the family that the posterior distribution belongs to.

For example, if X follows a normal distribution $N(\mu, \sigma^2)$ and $\vec{\theta} = (\mu, \sigma^2)$, a conjugate prior distribution for $\vec{\theta}$ is available,

- If σ^2 is known, the conjugate prior distribution for μ is a normal distribution $N(\beta, \tau^2)$,

$$\pi(\mu) = \frac{1}{\sqrt{2\pi}\tau} \exp(-\frac{(\mu-\beta)^2}{2\tau^2}) \tag{27}$$

where, β, τ^2 are known hyperparameters associated with the prior information.

- If μ is known, the conjugate prior distribution for σ^2 is an inverse-gamma distribution $\Gamma^{-1}(r/2, \lambda/2)$,

$$\pi(\sigma^2) = \Gamma^{-1}(r/2, \lambda/2) = \frac{(\lambda/2)^{r/2}}{\Gamma(r/2)}(\sigma^2)^{-(r/2+1)}\exp(-\frac{\lambda}{2\sigma^2}) \tag{28}$$

where, r, λ are known hyperparameters associated with the prior information.

- If both μ and σ^2 are unknown, the conjugate prior distribution for (μ, σ^2) is normal-inverse gamma distribution,

$$\pi_1(\mu|\sigma^2) = N(\beta, \sigma^2/k) \tag{29}$$
$$\pi_2(\sigma^2) = \Gamma^{-1}(r/2, \lambda/2) \tag{30}$$

where, k is a known hyperparameter. The joint distribution of (μ, σ^2) is,

$$\pi(\mu, \sigma^2) = \pi_1(\mu|\sigma^2)\pi_2(\sigma^2) \propto (\sigma^2)^{-[(r+1)/2+1]}\exp\{-\frac{1}{2\sigma^2}[k(\mu-\beta)^2 + \lambda]\} \tag{31}$$

Conceptually, if we are to use a conjugate prior distribution, our prior knowledge about the parameter $\vec{\theta}$ is the prior distribution family and hyperparameter set $(\beta, \tau^2$ or $k, r, \lambda)$.

General prior: for a specific problem, we might need a more general prior distribution than a non-informative or conjugate prior distribution. For example, if we know that the parameter θ is only physical on an interval $[a, b]$ and we have no other information, we might want to use a uniform distribution in the interval; if we know that the parameter θ is always positive and is most likely to be small, we might want to use a gamma/inverse-gamma or a lognormal prior distribution. A general prior distribution adds difficulty to the overall analysis and parameter estimation, but the estimation is likely to be more reasonable.

2.3 Posterior distribution

2.3.1 Posterior distribution: general form

Once we know the form of $f(x; \vec{\theta})$ and the observed value x, we can calculate the posterior distribution. Here, we assume X follows a normal distribution.

Let $\vec{X} = (X^1, X^2, \dots, X^j, \dots, X^J)$ be a random vector of dimension J, where X^j's are independent random variables and X^j follows a distribution $f^j(x^j; \vec{\theta}^j)$. Since X^j's are independent random variables, the joint distribution of $\vec{X}$ is,

$$F(\vec{x}|\vec{\theta}) = \prod_{j=1}^{J} f^j(x^j; \vec{\theta}^j) \tag{32}$$

where, $\vec{x} = (x^1, x^2, \dots, x^j, \dots, x^J)$ and $\vec{\theta} = (\vec{\theta}^1, \vec{\theta}^2, \dots, \vec{\theta}^j, \dots, \vec{\theta}^J)$ are the output vector (e.g. void fraction) and parameter vector (e.g. input model uncertainty), respectively.

Let $\mathbf{x} = (\vec{x}_1, \vec{x}_2, \dots, \vec{x}_i, \dots, \vec{x}_N)$ be N observed samples/outputs of random vector $\vec{X}$ and $\vec{x}_i$'s are independent to each other. Then, by definition the likelihood function is,

$$L(\vec{\theta}|\mathbf{x}) = \prod_{i=1}^{N} F(\vec{x}_i; \vec{\theta}) = \prod_{i=1}^{N} \prod_{j=1}^{J} f^j(x_i^j; \vec{\theta}^j) \tag{33}$$

Note that Eq. (33) is a general representation of likelihood function for J random variables with each random variable have N observed samples.

If we assume $\vec{\theta}$ has a prior distribution $\pi(\theta)$, then we have the posterior distribution represented as,

$$\pi(\vec{\theta}|\mathbf{x}) = K(\mathbf{x})\pi(\vec{\theta})L(\vec{\theta}|\mathbf{x}) = K(\mathbf{x})\pi(\vec{\theta}) \prod_{i=1}^{N} \prod_{j=1}^{J} f^j(x_i^j; \vec{\theta}^j) \qquad (34)$$

where, $K(\mathbf{x})$ is the integration constant defined in Eq. (22) and $\pi(\vec{\theta})$ is the prior distribution.

2.3.2 Posterior distribution: normal form

For most cases we are dealing with normal distributions, meaning X^j follows normal distribution. X^j's are assumed to be independent, therefore $\vec{X}$ has a joint Gaussian distribution, denoted as $f_{JG}(\vec{x}; \vec{\theta})$,

$$f_{JG}(\vec{x}; \vec{\theta}) = \prod_{j=1}^{J} \frac{1}{\sqrt{2\pi}\sigma^j} \exp[-\frac{(x^j - \mu^j)^2}{2(\sigma^j)^2}] \qquad (35)$$

where, $\vec{\theta} = ([\mu^1, \sigma^1], ..., [\mu^J, \sigma^J])$.

The specific likelihood function is,

$$L(\vec{\theta}|\mathbf{x}) = \prod_{i=1}^{N} f_{JG}(\vec{x}_i; \vec{\theta}) = \prod_{i=1}^{N} \prod_{j=1}^{J} \frac{1}{\sqrt{2\pi}\sigma^j} \exp[-\frac{(x_i^j - \mu^j)^2}{2(\sigma^j)^2}] \qquad (36)$$

Now we have a specific representation of the posterior distribution defined in Eq. (22), it is,

$$\pi(\vec{\theta}|\mathbf{x}) = K(\mathbf{x})\pi(\vec{\theta})L(\vec{\theta}|\mathbf{x}) = K(\mathbf{x})\pi(\vec{\theta}) \prod_{i=1}^{N} \prod_{j=1}^{J} \frac{1}{\sqrt{2\pi}\sigma^j} \exp[-\frac{(x_i^j - \mu^j)^2}{2(\sigma^j)^2}]$$

$$(37)$$

At this point, if given the observed samples x_i^j and prior knowledge $\pi(\vec{\theta})$, we are ready to estimate the parameter vector $\vec{\theta}$ which is closely related to the uncertainties of our random variable of interest $\vec{X}$.

However, recall that the goal of this thesis is to estimate the uncertainties of physical model parameters used in TRACE, such as drag coefficient and heat transfer coefficient. This raises two important questions related to the above derivation. What are the random variables X that represent the physical model parameters? What are the observed quantities x in reality?

Since the physical model coefficients are our random variables of interest, it is clear that X^j should represent these physical model coefficients. Ideally, we would like to observe the value of these physical model coefficients, meaning x_i^j, in each specific experiment or calculation. In practice, it is impossible to directly measure the physical model coefficients. A further step is necessary to relate observable quantities to physical model coefficients (X^j).

2.3.3   Application implementation

The output quantity that we can observe/calculate in an experiment/calculation is temperature, void fraction and pressure drop. Mathematically, these output quantities are a deterministic function of the physical model coefficients, which means that *the output quantities contain the same statistical information as the physical model coefficients in certain conditions*. The necessary conditions are described below.

Let Y denote experimentally observable output quantity, such as temperature, void fraction and pressure drop. Y should be a deterministic function the physical model coefficient X, which gives,

$$Y = Y(X) \tag{38}$$

The statement that Y contains the same information as X means: if we have observed samples **y**, the following conditional distribution equation is correct under certain conditions,

$$\pi(\vec{\theta}|x) = \pi(\vec{\theta}|y) \tag{39}$$

The necessary condition is that the function $Y(X)$ is invertible.

Now, let's consider the multi-variable case, meaning Y is a function of vector $\vec{X}$,

$$Y = Y(\vec{X}) \tag{40}$$

where, following the previous notation, $\vec{X}$ is a J-dimensional vector.

First let's consider a simple case $J = 2$ and then generalize the result to other dimension,

$$Y^1 = Y^1(X^1, X^2) \tag{41}$$

and let's assume Y^1 is a linear function of $\vec{X}$,

$$Y^1 = Y_0^1 + a_{1,1}(X^1 - x_0^1) + a_{1,2}(X^2 - x_0^2) \tag{42}$$

where, $a_{1,1}, a_{1,2}$ are used to denote the sensitivity coefficient of Y with respect to X^1, X^2, that

is $a_{1,j} = \frac{\partial Y^1}{\partial X^j}$. x_0^1, x_0^2 are nominal values of X^1, X^2, respectively. It is clear that the assumption

shown in Eq. (42) can be derived from Taylor series expansion. Since x_0^1, x_0^2 are known

constants and $a_{1,1}, a_{1,2}$ are also known constants (obtained from sensitivity analysis), to

simplify the notation let's absorb x_0^1, x_0^2 into constant Y_0^1, Eq. (42) simplifies to,

$$Y^1 = Y_0^1 + a_{1,1}X^1 + a_{1,2}X^2 \tag{43}$$

Note that Y^1 alone contains less information than X^1, X^2. In other words, it is not possible to

invert Y^1 to obtain X^1, X^2. There are two ways to solve this problem, described in the

following two sections, 2.3.3.1 and 2.3.3.2.

2.3.3.1   MLE 1: multiple output variables

A possible solution is to have another random variable Y^2 that is also a deterministic function

of X^1, X^2. Following the same assumption as Y^1, Y^2 it simplifies to,

$$Y^2 = Y_0^2 + a_{2,1}X^1 + a_{2,2}X^2 \tag{44}$$

Then, the condition to invert Y becomes,

$$\det\mathbf{A} = \det \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \neq 0 \tag{45}$$

where $\mathbf{A}$ is the sensitivity coefficient matrix. The condition shown in Eq. (45) means the

sensitivity coefficient matrix is invertible.

This is easier to generalize after rewriting Eqs. (43) and (44) in a matrix form,

$$\vec{Y} = \vec{Y}_0 + \mathbf{A}\vec{X} \tag{46}$$

where, $\vec{Y} = (Y^1, Y^2)^{\mathrm{T}}$ and $\vec{Y}_0 = (Y_0^1, Y_0^2)^{\mathrm{T}}$.

Before continuing the derivation, it is useful to clarify Y^1 and Y^2. As said earlier, Y^1 and Y^2

are output quantities (observables) in a thermal-hydraulic experiment, such as temperature, void

fraction or pressure drop. The choice of Y^1 and Y^2 is not unique, but the condition shown in

Eq. (45) has to be satisfied and will be the main constraint in selecting Y^1 and Y^2 when the

inverse uncertainty algorithm is applied to a practical thermal-hydraulics problem.

Since $\vec{Y}$ contains the same information as $\vec{X}$, we have,

$$\pi(\vec{\theta}|\vec{x}) = \pi(\vec{\theta}|\vec{y}) \tag{47}$$

Because each component of $\vec{X}$ follows a Gaussian distribution and each component of $\vec{Y}$ is a linear combination of $\vec{X}$, $\vec{Y}$ follows a jointly Gaussian distribution. The following are the statistical properties of $\vec{Y}$,

$$\vec{\mu}_x = \mathrm{E}(\vec{X}) = \begin{pmatrix} \mu^1 \\ \mu^2 \end{pmatrix} \tag{48}$$

$$\vec{\mu}_y = \mathrm{E}(\vec{Y}) = \begin{pmatrix} Y_0^1 + a_{1,1}\mu^1 + a_{1,2}\mu^2 \\ Y_0^2 + a_{2,1}\mu^1 + a_{2,2}\mu^2 \end{pmatrix} \tag{49}$$

$$\mathbf{\Sigma}_x = \mathrm{cov}(\vec{X}, \vec{X}) = \begin{pmatrix} (\sigma^1)^2 & 0 \\ 0 & (\sigma^2)^2 \end{pmatrix} \tag{50}$$

$$\mathbf{\Sigma}_y = \mathrm{cov}(\vec{Y}, \vec{Y}) = \begin{pmatrix} (a_{1,1})^2(\sigma^1)^2 + (a_{1,2})^2(\sigma^2)^2 & a_{1,1}a_{2,1}(\sigma^1)^2 + a_{1,2}a_{2,2}(\sigma^2)^2 \\ a_{1,1}a_{2,1}(\sigma^1)^2 + a_{1,2}a_{2,2}(\sigma^2)^2 & (a_{2,1})^2(\sigma^1)^2 + (a_{2,2})^2(\sigma^2)^2 \end{pmatrix} \tag{51}$$

Note that Y^1 and Y^2 are usually not independent.

Now we rewrite Eq. (48) – Eq. (51) into a matrix form as,

$$\vec{\mu}_y = \vec{Y}_0 + \mathbf{A}\vec{\mu}_x \tag{52}$$

$$\mathbf{\Sigma}_y = \mathbf{A}\mathbf{\Sigma}_x\mathbf{A}^{\mathrm{T}} \tag{53}$$

and the joint distribution of $\vec{Y}$ is,

$$f(\vec{y}; \vec{\theta}) = \frac{1}{2\pi}|\mathbf{\Sigma}_y|^{-\frac{1}{2}}\exp[-\frac{1}{2}(\vec{y} - \vec{\mu}_y)^{\mathrm{T}}\mathbf{\Sigma}_y^{-1}(\vec{y} - \vec{\mu}_y)] \tag{54}$$

To clarify, Table 1 gives a practical meaning of the most important variables.

Table 1 Practical meaning of important variables

Variables	Meaning
$\vec{X}$	input model parameter random variable
$\vec{Y}$	output random variable from experimental measurement
$\vec{Y}_0$	output random variable from code prediction
$\vec{E}$	random error of experimental measurement
$\mathbf{A}$	sensitivity coefficient matrix
$\vec{\mu}_x, \mathbf{\Sigma}_x$	mean and covariance matrix of input model parameter random variable
$\vec{\mu}_y, \mathbf{\Sigma}_y$	mean and covariance matrix of output random variable
$\vec{\mu}_e, \mathbf{\Sigma}_e$	mean and covariance matrix of random error of experimental measurement

Two additional considerations have to be made for completeness,

- Random error: in the previous derivation, random error of an experimental measurement is ignored. The random error is usually assumed to be mean-zero and does not depend on $\vec{X}$ or $\vec{Y}$.

- For different observed sample i, the sensitivity coefficient matrix and other quantities might be different. This is modified in the following equations by consistently adding the subscript i to relevant quantities.

The previous equations now become,

$$\vec{Y}_i = \vec{Y}_{0,i} + \mathbf{A}_i\vec{X} + \vec{E}_i \tag{55}$$

$$\vec{\mu}_{y,i} = \vec{Y}_{0,i} + \mathbf{A}_i\vec{\mu}_x \tag{56}$$

$$\mathbf{\Sigma}_{y,i} = \mathbf{A}_i\mathbf{\Sigma}_x\mathbf{A}_i^{\mathrm{T}} + \mathbf{\Sigma}_{e,i} \tag{57}$$

$$f_i(\vec{y};\vec{\theta}) = \frac{1}{2\pi}|\mathbf{\Sigma}_{y,i}|^{-\frac{1}{2}}\exp[-\frac{1}{2}(\vec{y} - \vec{\mu}_{y,i})^{\mathrm{T}}\mathbf{\Sigma}_{y,i}^{-1}(\vec{y} - \vec{\mu}_{y,i})] \tag{58}$$

If there are N sets of observed samples, the posterior distribution can be written as a function of $\mathbf{y}$. The assumption is that $\vec{Y}_i$'s are independent to each other,

$$L_1(\vec{\theta}|\mathbf{y}) = \prod_{i=1}^{N} \frac{1}{2\pi}|\mathbf{\Sigma}_{y,i}|^{-\frac{1}{2}}\exp[-\frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}}\mathbf{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})] \tag{59}$$

$$\pi_1(\vec{\theta}|\mathbf{y}) = K(\mathbf{y})\pi(\vec{\theta}) \prod_{i=1}^{N} \frac{1}{2\pi}|\mathbf{\Sigma}_{y,i}|^{-\frac{1}{2}}\exp[-\frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}}\mathbf{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})] \tag{60}$$

The subscript 1 in the likelihood function and posterior distribution denotes **MLE 1**, the subscript i is used to denote i'th observed sample, while the superscript j is used to denote

j'th variable.

Eqs. (59) and (60) are the starting point for the following MLE, MAP and MCMC estimates.

2.3.3.2 MLE 2: assumption of independence between output variables

Though a single Y^1 has less information than X^1, X^2, we usually have more than one observed value of Y^1, that is we have $Y_1^1, Y_2^1, \cdots, Y_N^1$. These Y_i^1's contain enough information for estimating X^1, X^2. The issue is that Y_i^1's are correlated with each other and it is difficult to obtain their joint distribution. In order to proceed, Y_i^1's *are assumed to be independent of each other*. Without confusion, let's drop the superscript and denote the output variables as $Y_1, Y_2, \cdots, Y_i, \cdots, Y_N$, then,

$$Y_i = Y_{0,i} + \vec{A}_i \vec{X} + E_i \tag{61}$$

$$\mu_{y,i} = Y_{0,i} + \vec{A}_i \mu_x \tag{62}$$

$$\Sigma_{y,i} = \vec{A}_i \Sigma_x \vec{A}_i^T + \Sigma_{e,i} \tag{63}$$

$$f_i(\vec{y}; \vec{\theta}) = \frac{1}{\sqrt{2\pi\Sigma_{y,i}}} \exp[-\frac{(y_i - \mu_{y,i})^2}{2\Sigma_{y,i}}] \tag{64}$$

Note that the difference between Eqs. (55) – (58) and Eqs. (61) – (64) is that $\vec{A}_i$ is now a vector.

The posterior distribution can be written as,

$$L_2(\vec{\theta}|\mathbf{y}) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\Sigma_{y,i}}} \exp[-\frac{(y_i - \mu_{y,i})^2}{2\Sigma_{y,i}}] \tag{65}$$

$$\pi_2(\vec{\theta}|\mathbf{y}) = K(\mathbf{y})\pi(\vec{\theta}) \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\Sigma_{y,i}}} \exp[-\frac{(y_i - \mu_{y,i})^2}{2\Sigma_{y,i}}] \tag{66}$$

The subscript 2 in the likelihood function and posterior distribution denotes **MLE 2**.

2.3.3.3 Difference between MLE 1 and MLE 2

Though Eqs. (59) (60) and Eqs. (65) (66) have similar form, they are not identical because of the additional assumption used to obtain Eqs. (65) (66). The difference is whether we deal with **multiple** output variables (**MLE 1**) or **single** output variable (**MLE 2**). If we need to estimate J model parameters, we need to provide J output variables for solution of **MLE 1** and a single output variable for solution of **MLE 2**. The **MLE 1** provides a chance to estimate the correlation

between different input model parameters. The capabilities and limitations of each model are discussed when these two solutions are applied to numerical data.

2.4 Maximum Likelihood Estimation and Expectation-Maximization algorithm

We will derive solution algorithm for MLE with **MLE 1** Eq. (59) and then generalize the results to **MLE 2** by replacing vectors and matrixes with scalars and vectors, respectively.

The idea behind MLE is to maximize the likelihood function to solve for the parameter vector $\vec{\theta}$. Though direction maximization could be done using for example Newton's method, an Expectation-Maximization (E-M) algorithm (Malachlan, 2007) (Shrestha, 2015) is usually applied to maximize the likelihood function. There are 2 steps in E-M algorithm,

- Maximization. Assuming the covariance matrix $\mathbf{\Sigma}_x$ is known, $\vec{u}_x$ could be solved by maximize the likelihood function.

$$\vec{u}_{x,\text{new}} = \max_{\vec{u}_x} L_1(\vec{\theta}|\mathbf{y}) \tag{67}$$

- Expectation. Once the $\vec{u}_x$ is obtained, the covariance matrix $\mathbf{\Sigma}_x$ can be updated using conditional expectation.

$$\mathbf{\Sigma}_{x,\text{new}} = \mathrm{E}[(\vec{X} - \vec{u}_{x,\text{new}})(\vec{X} - \vec{u}_{x,\text{new}})^{\mathrm{T}}|\mathbf{y}] \tag{68}$$

The reason that E-M algorithm works is that the likelihood is guaranteed to increase.

Since maximizing the logarithm of the likelihood function is the same as maximizing the likelihood function itself, it is easier to proceed with maximizing the logarithm of the likelihood function, called log-likelihood,

$$\log L_1(\vec{\theta}|\mathbf{y}) = \sum_{i=1}^{N} [-\frac{1}{2}\log|\mathbf{\Sigma}_{y,i}| - \log 2\pi - \frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}}\mathbf{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})] \tag{69}$$

2.4.1 Maximization step

Note that the log-likelihood in Eq. (69) is a quadratic function of $\vec{\mu}_x$ due to the particular properties of Gaussian distribution. By taking a derivative of the log-likelihood with respect to

$\vec{\mu}_x$ and setting it equal be zero, we get a system of linear equations for solving $\vec{\mu}_x$,

$$\frac{\partial \log L_1(\vec{\theta}|\mathbf{y})}{\partial \vec{\mu}_x} = 0 \tag{70}$$

which gives,

$$\mathbf{M}_L \vec{\mu}_x = \vec{B}_L \tag{71}$$

where,

$$\mathbf{M}_L = \begin{pmatrix} \sum_{i=1}^{N} (a_{1,1,i}, a_{2,1,i}) \boldsymbol{\Sigma}_{y,i}^{-1} (a_{1,1,i}, a_{2,1,i})^{\mathrm{T}} & \sum_{i=1}^{N} (a_{1,1,i}, a_{2,1,i}) \boldsymbol{\Sigma}_{y,i}^{-1} (a_{1,2,i}, a_{2,2,i})^{\mathrm{T}} \\ \sum_{i=1}^{N} (a_{1,2,i}, a_{2,2,i}) \boldsymbol{\Sigma}_{y,i}^{-1} (a_{1,1,i}, a_{2,1,i})^{\mathrm{T}} & \sum_{i=1}^{N} (a_{1,2,i}, a_{2,2,i}) \boldsymbol{\Sigma}_{y,i}^{-1} (a_{1,2,i}, a_{2,2,i})^{\mathrm{T}} \end{pmatrix} \tag{72}$$

$$\vec{B}_L = \begin{pmatrix} \sum_{i=1}^{N} (a_{1,1,i}, a_{2,1,i}) \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{y}_{0,i}) \\ \sum_{i=1}^{N} (a_{1,1,i}, a_{2,1,i}) \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{y}_{0,i}) \end{pmatrix} \tag{73}$$

In the matrix form,

$$\mathbf{M}_L = \sum_{i=1}^{N} \mathbf{A}_i^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} \mathbf{A}_i \tag{74}$$

$$\vec{B}_L = \sum_{i=1}^{N} \mathbf{A}_i^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{y}_{0,i}) \tag{75}$$

An update to $\vec{\mu}_x$ is obtained by solving Eq. (71).

2.4.2 Expectation step

Since the mean vector $\vec{\mu}_x$ has been updated, the expectation step updates the covariance matrix of X conditioned on the observed output Y,

$$(\sigma^j)^2_{\text{new}} = \mathrm{E}[(X^j - \mu^j)^2 | \vec{Y}_i] \tag{76}$$

$$= \mathrm{E}[(X^j - \hat{X}^j + \hat{X}^j - \mu^j)^2 | \vec{Y}_i]$$

$$= \mathrm{E}[(X^j - \hat{X}^j)^2 | \vec{Y}_i] + \mathrm{E}[(\hat{X}^j - \mu^j)^2 | \vec{Y}_i] + \mathrm{E}[(X^j - \hat{X}^j)(\hat{X}^j - \mu^j) | \vec{Y}_i]$$

where, $\hat{X}^j$ is the linear MMSE of X^j conditioned on $\vec{Y}_i$.

Using the properties of linear MMSE, we have,

$$\hat{X}^j = \mathrm{cov}[X^j, \vec{Y}_i] \mathrm{cov}[\vec{Y}_i, \vec{Y}_i]^{-1} (\vec{Y}_i - \vec{\mu}_{y,i}) + \mu^j \tag{77}$$

$$\mathrm{E}[(X^j - \hat{X}^j)^2 | \vec{Y}_i] = \mathrm{cov}[X^j, X^j] - \mathrm{cov}[X^j, \vec{Y}_i] \mathrm{cov}[\vec{Y}_i, \vec{Y}_i]^{-1} \mathrm{cov}[\vec{Y}_i, X^j] \tag{78}$$

$$\mathrm{E}[(\hat{X}^j - \mu^j)^2 | \vec{Y}_i] = \{\mathrm{cov}[X^j, \vec{Y}_i] \mathrm{cov}[\vec{Y}_i, \vec{Y}_i]^{-1} (\vec{Y}_i - \vec{\mu}_{y,i})\}^2 \tag{79}$$

$$\mathrm{E}[(X^j - \hat{X}^j)(\hat{X}^j - \mu^j) | \vec{Y}_i] = 0 \tag{80}$$

Using the above substitutions, we get,

$$(\sigma^j)^2_{new} = (\sigma^j)^2_{old} - \text{cov}[X^j, \vec{Y_i}]\text{cov}[\vec{Y_i}, \vec{Y_i}]^{-1}\text{cov}[\vec{Y_i}, X^j] + \{\text{cov}[X^j, \vec{Y_i}]\text{cov}[\vec{Y_i}, \vec{Y_i}]^{-1}(\vec{Y_i} - \vec{\mu}_{y,i})\}^2 \tag{81}$$

Since we have N sets of observed output, the effect of each set could be added to the update of the covariance matrix by a simple average,

$$(\sigma^j)^2_{new} = (\sigma^j)^2_{old}$$
$$+\frac{1}{N}\sum_{i=1}^{N}\left(-\text{cov}[X^j, \vec{Y_i}]\text{cov}[\vec{Y_i}, \vec{Y_i}]^{-1}\text{cov}[\vec{Y_i}, X^j] + \{\text{cov}[X^j, \vec{Y_i}]\text{cov}[\vec{Y_i}, \vec{Y_i}]^{-1}(\vec{Y_i} - \vec{\mu}_{y,i})\}^2\right) \tag{82}$$

With the help of two new covariance matrixes, Eq. (82) could be written in a matrix form,

$$\mathbf{\Sigma}_{xy,i} = \text{cov}(\vec{X}, \vec{Y_i}) = \mathbf{A}_i\mathbf{\Sigma}_x \tag{83}$$

$$\mathbf{d\Sigma}_x = \sum_{i=1}^{N}\left(-\mathbf{\Sigma}_{xy,i}^T\mathbf{\Sigma}_{y,i}^{-1}\mathbf{\Sigma}_{xy,i} + [\mathbf{\Sigma}_{xy,i}^T\mathbf{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})][\mathbf{\Sigma}_{xy,i}^T\mathbf{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})]^T\right) \tag{84}$$

$$\mathbf{\Sigma}_{x,new} = \mathbf{\Sigma}_{x,old} + \frac{1}{N}\text{diag}(\mathbf{d\Sigma}_x) \tag{85}$$

Algorithm 1 shows the MLE algorithm.

Algorithm 1 MLE (E-M) algorithm

---

1. Read data. $\mathbf{A}_i, \vec{Y}_i, \vec{Y}_{0,i}$.
2. Initialize matrix. $\boldsymbol{\Sigma}_x, \boldsymbol{\Sigma}_{y,i}, \boldsymbol{\Sigma}_{e,i}, \boldsymbol{\Sigma}_{xy,i}$.
3. Initialize vector. $\vec{\mu}_x, \vec{\mu}_{y,i}$
4. For $k = 1: \text{IterK}$
5.   Initialize $\mathbf{M}, \vec{B}$
6.   **Maximization Step**
7.   For $i = 1: N$
8. $\boldsymbol{\Sigma}_{y,i} = \mathbf{A}_i \boldsymbol{\Sigma}_x \mathbf{A}_i^{\mathrm{T}} + \boldsymbol{\Sigma}_{e,i}$
9. $\mathbf{M} = \mathbf{M} + \mathbf{A}_i^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} \mathbf{A}_i$
10. $\vec{B} = \vec{B} + \mathbf{A}_i^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{y}_{0,i})$
11. $\vec{\mu}_x = \mathbf{M}^{-1} \vec{B}$
12.   **Expectation Step**
13.   For $i = 1: N$
14. $\vec{\mu}_{y,i} = \vec{y}_{0,i} + \mathbf{A}_i \vec{\mu}_x$
15. $\boldsymbol{\Sigma}_{y,i} = \mathbf{A}_i \boldsymbol{\Sigma}_x \mathbf{A}_i^{\mathrm{T}} + \boldsymbol{\Sigma}_{e,i}$
16. $\boldsymbol{\Sigma}_{xy,i} = \mathbf{A}_i \boldsymbol{\Sigma}_x$
17. $\mathbf{d}\boldsymbol{\Sigma}_x =$
            $\mathbf{d}\boldsymbol{\Sigma}_x - \boldsymbol{\Sigma}_{xy,i}^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} \boldsymbol{\Sigma}_{xy,i} + [\boldsymbol{\Sigma}_{xy,i}^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})][\boldsymbol{\Sigma}_{xy,i}^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})]^{\mathrm{T}}$
18. $\boldsymbol{\Sigma}_x = \boldsymbol{\Sigma}_x + \frac{1}{N} \text{diag}(\mathbf{d}\boldsymbol{\Sigma}_x)$

Note that since X^j's are assumed to be independent, the covariance matrix is only updated on the diagonal element. However, if we have prior knowledge that these model parameters $\vec{X}$ are correlated, this algorithm provides an opportunity to estimate the correlation terms in covariance matrix. We will discuss the correlation term in details when the algorithm is applied to a numerical experiment.

As for **MLE 2**, the algorithm could be easily obtained by replacing the covariance matrix and sensitivity matrix with vectors and replacing vectors with scalars.

2.5   Maximum A Posterior (MAP) algorithm

The main idea behind MAP is to maximize the posterior distribution for solving the parameter vector $\vec{\theta}$. The difference between the likelihood function and the posterior distribution is the prior distribution $\pi(\vec{\theta})$ and a constant $K(\mathbf{y})$. Using the concept of Expectation-Maximization, the MAP solution algorithm is derived in a similar way, by adding the effect of the prior distribution.

Let $\mathbf{M}_\pi, \vec{B}_\pi$ be the coefficient matrix and source vector due to the effect of prior distribution, respectively. $\mathbf{M}_\pi, \vec{B}_\pi$ could be obtained by differentiating the logarithm of prior distribution. For example, if the normal-inverse gamma prior distribution is used, $\mathbf{M}_\pi, \vec{B}_\pi$ will be used in the maximization step for solving $\vec{\mu}_x$ as,

$$\mathbf{M}_\pi = \text{diag}(\frac{k^1}{(\sigma^1)^2}, \cdots, \frac{k^j}{(\sigma^j)^2}, \cdots, \frac{k^J}{(\sigma^J)^2}) \tag{86}$$

$$\vec{B}_\pi = [\frac{k^1 \beta^1}{(\sigma^1)^2}, \cdots, \frac{k^j \beta^j}{(\sigma^j)^2}, \cdots, \frac{k^J \beta^J}{(\sigma^J)^2}]^\text{T} \tag{87}$$

Using these correction terms, the MAP's version of the coefficient matrix and source vector for solving $\vec{\mu}_x$ becomes,

$$\mathbf{M}_p = \mathbf{M}_L + \mathbf{M}_\pi \tag{88}$$

$$\vec{B}_p = \vec{B}_L + \vec{B}_\pi \tag{89}$$

where, the subscript p denotes posterior distribution. Then the MAP algorithm is shown in Algorithm 2.

Algorithm 2 MAP (E-M) algorithm

1. Read data. $\mathbf{A}_i, \vec{Y}_i, \vec{Y}_{0,i}$.
2. Initialize matrix. $\mathbf{\Sigma}_x, \mathbf{\Sigma}_{y,i}, \mathbf{\Sigma}_{e,i}, \mathbf{\Sigma}_{xy,i}$.
3. Initialize vector. $\vec{\mu}_x, \vec{\mu}_{y,i}$
4. Choose a prior distribution.
5. For $k = 1:\text{IterK}$
6.   Initialize $\mathbf{M}, \mathbf{M}_\pi, \vec{B}, \vec{B}_\pi$
7.   **Maximization Step**
8.   For $i = 1:N$
9. $\mathbf{\Sigma}_{y,i} = \mathbf{A}_i \mathbf{\Sigma}_x \mathbf{A}_i^{\mathrm{T}} + \mathbf{\Sigma}_{e,i}$
10. $\mathbf{M} = \mathbf{M} + \mathbf{A}_i^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} \mathbf{A}_i$
11. $\vec{B} = \vec{B} + \mathbf{A}_i^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{y}_{0,i})$
12. $\mathbf{M} = \mathbf{M} + \mathbf{M}_\pi$
13. $\vec{B} = \vec{B} + \vec{B}_\pi$
14. $\vec{\mu}_x = \mathbf{M}^{-1} \vec{B}$
15.   **Expectation Step**
16.   For $i = 1:N$
17. $\vec{\mu}_{y,i} = \vec{y}_{0,i} + \mathbf{A}_i \vec{\mu}_x$
18. $\mathbf{\Sigma}_{y,i} = \mathbf{A}_i \mathbf{\Sigma}_x \mathbf{A}_i^{\mathrm{T}} + \mathbf{\Sigma}_{e,i}$
19. $\mathbf{\Sigma}_{xy,i} = \mathbf{A}_i \mathbf{\Sigma}_x$
20. $\mathbf{d\Sigma}_x =$
            $\mathbf{d\Sigma}_x - \mathbf{\Sigma}_{xy,i}^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} \mathbf{\Sigma}_{xy,i} + [\mathbf{\Sigma}_{xy,i}^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})][\mathbf{\Sigma}_{xy,i}^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})]^{\mathrm{T}}$
21. $\mathbf{\Sigma}_x = \mathbf{\Sigma}_x + \frac{1}{N} \text{diag}(\mathbf{d\Sigma}_x)$

2.6 Markov Chain Monte Carlo (MCMC)

Recall that the MLE and MAP algorithms developed thus far are based on the particular properties of the normal distribution, the conjugate distribution and the linearity assumption. If any of these conditions are not satisfied, the application of MLE and MAP would be difficult because we would not be able to obtain an explicit analytical form of the likelihood function and posterior distribution. The MCMC process solves this problem.

Recall that the posterior distribution $\pi(\vec{\theta}|\mathbf{y})$ can be generalized as the following form,

$$\pi(\vec{\theta}|\mathbf{y}) = K(\mathbf{y})\pi(\vec{\theta})L(\vec{\theta}|\mathbf{y}) \tag{90}$$

However, difficulties exist in calculating $K(\mathbf{y})$, $\pi(\vec{\theta})$ and $L(\vec{\theta}|\mathbf{y})$ when the distribution of Y and the posterior distribution is general:

- $L(\vec{\theta}|\mathbf{y})$. Recall that in the derivation of MLE and MAP, X is assumed to follow a

Gaussian distribution and thus Y also follows a Gaussian distribution with an additional linearity assumption. If these assumptions are not satisfied, analytical maximization of the likelihood function becomes impossible.

- $\pi(\vec{\theta})$. In the previous derivation, $\pi(\theta)$ is differentiable in real space R or positive real space R^+ to ensure that the analytical differentiation is possible. However, in practice the parameter vector might only be physical on a certain interval. For example, in estimating a model parameter (e.g. subcooled boiling heat transfer coefficient), we have prior knowledge that the correct value of this model parameter should be close to the nominal value used in the code and should always be positive, but this prior knowledge is difficult to be considered in MLE and MAP algorithm.

- $K(\mathbf{y})$. Unless a conjugate prior distribution is used, which depends on the distribution family of X, the constant $K(\mathbf{y})$ is obtained with a multi-dimensional integration as given in Eq. (22). This integration is both analytically and numerically difficult.

These difficulties can be overcome using MCMC process. The idea behind MCMC is to sample the posterior distribution without knowledge of the explicit form of the posterior distribution. This sampling is implemented by using an iterative Monte Carlo sampling, which usually forms a Markov Chain. We need to devise an aperiodic and irreducible Markov Chain that converges to the posterior distribution of interest, that is to devise the probability transition matrix $\mathbf{P}$.

Many sampling methods exist, such as Metropolis-Hastings sampling, Gibbs sampling and other advanced methods (Gilks, 2005). Among these methods, Metropolis-Hastings sampling (Chib, 1995) has the least requirements on the posterior distribution and will be used in this thesis.

Metropolis-Hastings algorithm

Let's start with a posterior distribution $\pi(\theta|\mathbf{y})$ which only has a scalar parameter θ. In order to proceed, a proposal distribution $g(\xi|\theta_k)$ is needed, where ξ is a dummy variable used to denote a random process. This proposal distribution gives the rule of how the Markov Chain proceeds given a current state θ_k. The Metropolis-Hastings algorithm proceeds in three main steps:

1. Sample a proposal variable ξ from $g(\xi|\theta_k)$.

2. Calculate the acceptance probability.

$$r(\xi, \theta_k) = \min\{1, \frac{\pi(\xi|\mathbf{y})g(\theta_k|\xi)}{\pi(\theta_k|\mathbf{y})g(\xi|\theta_k)}\} \qquad (91)$$

3. Accept $(\theta_{k+1} = \xi)$ or drop $(\theta_{k+1} = \theta_k)$ with probability $r(\xi, \theta_k)$.

The following **Algorithm 3** shows these steps.

Algorithm 3 Metropolis-Hastings algorithm: 1-D

1. Initialize θ_0.
2. Choose the proposal distribution.
3. For $k = 0$: IterK
4.   Sample a proposal variable ξ from $g(\xi|\theta_k)$.
5.   Calculate the accept probability. $r = \min\{1, \frac{\pi(\xi|\mathbf{y})g(\theta_k|\xi)}{\pi(\theta_k|\mathbf{y})g(\xi|\theta_k)}\}$
6.   Sample a uniformly distributed random variable η in $[0,1]$.
7.   If $(\eta < r)$, $\theta_{k+1} = \xi$; else continue.

The algorithm could be different for different forms of posterior distribution and choice of proposal distribution. If the proposal distribution were close to the posterior distribution, the algorithm would be more efficient because more proposed random variables would be accepted.

For multi-dimensional parameter vector $\vec{\theta}$, $\vec{\theta}$ can be sampled element by element using the Metropolis-Hastings algorithm:

1. Sample a proposal variable ξ_m from $g_m(\xi|\theta_{k,m})$.

2. Update the proposal element ξ_m to the mth element of parameter vector $\vec{\theta}_k$ as $\vec{\xi}$,

$$\vec{\xi} = (\theta_{k,1}, \theta_{k,2}, \cdots, \xi_m, \theta_{k,m+1}, \cdots) \qquad (92)$$

3. Calculate the acceptance probability.

$$r(\vec{\xi}, \vec{\theta}_k) = \min\{1, \frac{\pi(\vec{\xi}|\mathbf{y})g_m(\theta_{k,m}|\xi_m)}{\pi(\vec{\theta}_k|\mathbf{y})g_m(\xi_m|\theta_{k,m})}\} \qquad (93)$$

4. Accept $(\theta_{k+1,m} = \xi_m)$ or drop $(\theta_{k+1,m} = \theta_{k,m})$ with probability $r(\vec{\xi}, \vec{\theta}_k)$.

The multi-dimensional version of the sampling algorithm is shown in the following **Algorithm 4**.

Algorithm 4 Metropolis-Hastings algorithm: Multi-dimensional

1. Initialize $\vec{\theta}_0$.
2. Choose the proposal distribution.
3. For $k = 0$: IterK
4.   For $m = 1$: M
5.   Sample a proposal variable ξ_m from $g_m(\xi|\theta_{k,m})$.
6.   Update the mth element of $\vec{\theta}_k$ with ξ_m as $\vec{\tilde{\xi}}$.
7.   Calculate the accept probability. $r = \min\{1, \frac{\pi(\vec{\tilde{\xi}}|\mathbf{y})g_m(\theta_{k,m}|\xi_m)}{\pi(\vec{\theta}_k|\mathbf{y})g_m(\xi_m|\theta_{k,m})}\}$
8.   Sample a uniformly distributed random variable η in $[0,1]$.
9.   If $(\eta < r)$, $\theta_{k+1,m} = \xi_m$; else continue.

2.7 Summary of Chapter 2

In this chapter, detailed derivation is provided for the Maximum Likelihood Estimation (MLE), Maximum A Posterior (MAP) method and Expectation-Maximization (E-M) algorithms. In addition, the concept of Markov Chain Monte Carlo (MCMC) and the Metropolis-Hastings sampling method for MCMC is provided.

Variations on these algorithms include different methods of processing output variables (single or multiple), output correlations (independent or correlated) and prior distributions (none, conjugate, non-informative or uniform). A summary of possible variations and their capabilities are listed in Table 2.

Table 2 Summary of various algorithms

Algorithms	Output variables	Output Correlation	Prior distribution
MLE 1a	multiple	independent	N/A
MLE 1b	multiple	correlated	N/A
MLE 2	single	independent	N/A
MAP 1	multiple	correlated	conjugate
MAP 2	single	independent	conjugate
MCMC 1	multiple	independent	non-informative
MCMC 2	multiple	independent	conjugate
MCMC 3	multiple	independent	uniform

In the following Chapters, we will test these algorithms with numerical data (with known solution) and then apply them to an experimental benchmark (without known solution).

3   Numerical tests

Before the algorithms are applied to an experimental benchmark data, we will first test the three algorithms (MLE, MAP, MCMC) with a set of numerical data.

3.1   Numerical data

Recall from Table 1, a numerical data set $(\vec{Y}_i, \vec{Y}_{0,i}, \mathbf{A}_i, \vec{E}_i)$ is needed as input to the algorithm. The input random variable $\vec{X}$ is to be estimated. For the numerical test the distribution of $\vec{X}$ is known. Then, $(\vec{Y}_i, \vec{Y}_{0,i}, \mathbf{A}_i, \vec{E}_i)$ will be generated randomly and related to $\vec{X}$. Table 3 summarizes how the data are generated.

Table 3 Creation of data for the numerical test of MLE, MAP, MCMC

Variables	Meaning	Data
$\vec{X}$	input model parameter	sampled from $(\vec{\mu}_x, \mathbf{\Sigma}_x)$
$\vec{E}_i$	error from experiment measurement	sampled uniformly from $\varepsilon_0 * [-0.5, 0.5]$
$\mathbf{\Sigma}_{e,i}$	covariance matrix of error	$1/12 * \varepsilon_0^2 * \mathbf{I}$
$\mathbf{A}_i$	sensitivity coefficient matrix	sampled uniformly from $a_0 * [-0.5, 0.5]$
$\vec{Y}_{0,i}$	output from code prediction	sampled uniformly from $y_0 * [-0.5, 0.5]$
$\vec{Y}_i$	output from experiment measurement	$\vec{Y}_i = \vec{Y}_{0,i} + \mathbf{A}_i \vec{X}_i + \vec{E}_i$

In Table 3, ε_0, a_0, y_0 are used to denote the intensity of these random variables. By adjusting ε_0, a_0, y_0 and $\vec{\mu}_x, \mathbf{\Sigma}_x$, various numerical data can be produced. For testing purposes, three primarily set of data are created using the parameters shown in Table 4.

Table 4 Numerical data sets

Variables	DATA-I	DATA-II	DATA-III
$\vec{X}$	Independent Gaussian	Correlated Gaussian	Independent Uniform
$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0
Correlation	0.0	0.5	0.0
ε_0	2.0	2.0	2.0
a_0	5.0	5.0	5.0
y_0	10.0	10.0	10.0
(N,J)	(100,2)	(100,2)	(100,2)

As shown in Table 4, **DATA-I** and **DATA-II** are created using jointly Gaussian distributions without and with correlation, respectively; **DATA-III** is created using an independent uniform distribution, which should be difficult to estimate using both MLE and MAP algorithm. Note that the ratio of ε_0 to y_0 represents the relative error of the measurement, which could be freely adjusted.

3.2   MLE test results

After applying the MLE algorithm to the three sets of data, the statistical properties of the input data *X* are estimated (Table 5). All iterations were started with a zero mean vector and identity covariance matrix.

Table 5 Comparison of estimated solutions from different MLE algorithms

Algorithm	Variables	DATA-I	DATA-II	DATA-III
Exact	$\vec{X}$	Independent Gaussian	Correlated Gaussian	Independent Uniform
	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0
	correlation	0.0	0.5	0.0
MLE 1a	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.27 $\pm$ 2.07 1.60 $\pm$ 3.87	-2.28 $\pm$ 2.05 1.41 $\pm$ 4.05	-1.87 $\pm$ 2.10 2.06 $\pm$ 4.04
	correlation	N/A	N/A	N/A
MLE 1b	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.27 $\pm$ 2.07 1.60 $\pm$ 3.87	-2.28 $\pm$ 2.07 1.41 $\pm$ 4.09	-1.86 $\pm$ 2.10 2.06 $\pm$ 4.04
	correlation	0.03	0.57	-0.03
MLE 2	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.14 $\pm$ 1.73 1.47 $\pm$ 4.20	-2.17 $\pm$ 1.66 1.17 $\pm$ 4.22	-1.70 $\pm$ 2.12 2.23 $\pm$ 4.10
	correlation	N/A	N/A	N/A

Figure 1 shows how the likelihood function converges with the E-M iterations for DATA-II, the convergence profile is similar for other data set. Figure 2 shows the comparison between estimated solutions of different data sets and algorithms. Based on the likelihood convergence profile and the estimate results comparison, the following statements can be made,

- *The likelihood function.* Regardless of different solution algorithms and different data sets, the likelihood function is increasing monotonically with the E-M iteration. This is desired behavior because we want to maximize the likelihood function, which verifies the reliability of the algorithms. For the data sets used, the likelihood function converges to a maximum after about 20 E-M iterations, the number of iterations depends on specific data.

- *The mean value estimation.* Regardless of different solution algorithms and different data sets, the mean values are estimated consistently close to the exact solution (-2.0, 2.0). The deficiency in the estimation of different solution algorithm comes from the random error (ε_0) and the limited number of data (N).

- *The covariance matrix estimation.* Regardless of different solution algorithms and different data sets, the variances are estimated close to the exact variances (4.0, 16.0). However, the estimation of **MLE 1a, 1b** is better than the estimation of **MLE 2**. Besides, **MLE 1a, 2** are not capable of estimating the correlation terms, while **MLE 1b** finds the correlation terms very well. The **MLE 1b** is better compared with **MLE 1a**.

- *The random error.* For the purpose of this study the correct (exact) covariance matrix of the error is used when the algorithms are applied to the data. If the information about the error is incorrect or not known, the estimation of the covariance matrix ($\boldsymbol{\Sigma}_x$) of input model parameters will be worse.
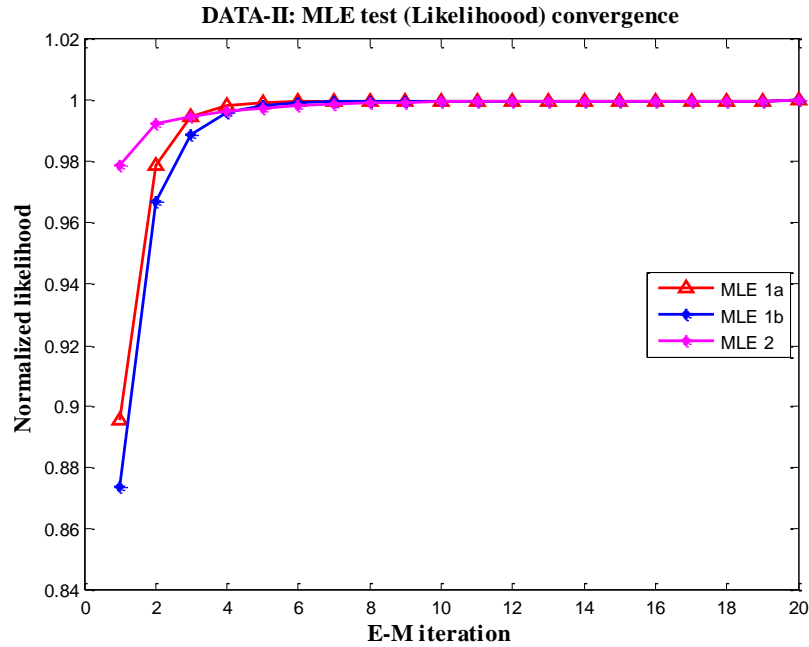
Figure 1 Likelihood function convergence of DATA-II: MLE test
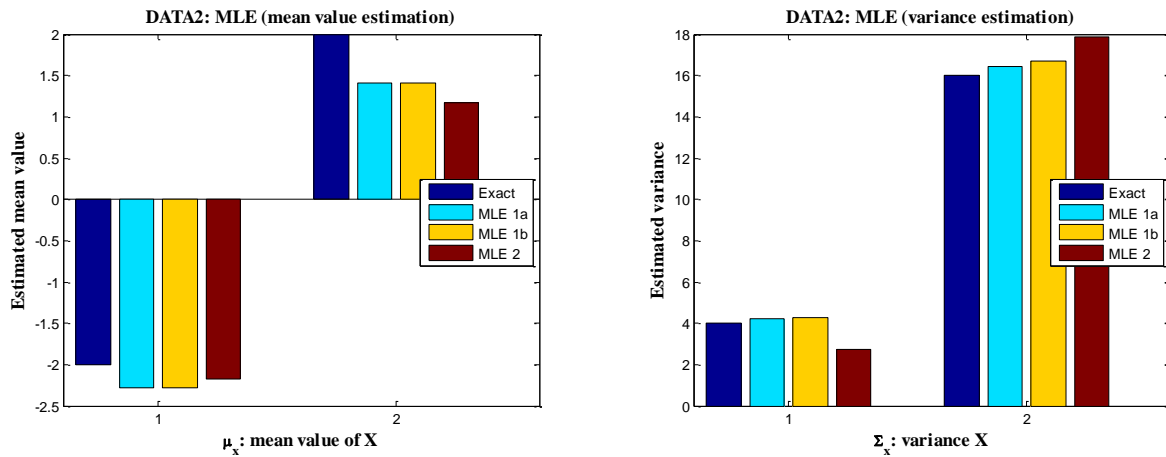

Figure 2 Comparison between estimated solutions of different algorithms with DATA-II

3.3   MAP test results

3.3.1   Prior distribution

As mentioned earlier, a conjugate prior distribution is chosen for the MAP algorithm. Since $\vec{X}$ is assumed to be jointly Gaussian distribution, the prior distribution is chosen to be normal-inverse gamma distribution,

$$\pi(\vec{\theta}) \propto \prod_{j=1}^{J} [(\sigma^j)^2]^{-[(r^j+1)/2+1]} \exp\{-\frac{1}{2(\sigma^j)^2}[k^j(\mu^j - \beta^j)^2 + \lambda^j]\} \qquad (94)$$

Our prior knowledge is indicated by the hyperparameters $(r^j, k^j, \beta^j, \lambda^j)$. For example, β^j and $\frac{\lambda^j}{r^j-2}$ is our prior knowledge of the expected value of μ^j and $(\sigma^j)^2$. Usually r^j is chosen to be 3, thus λ^j is the expectation value of $(\sigma^j)^2$. Table 6 gives the values of the hyperparameters used in the following MAP calculations.

Table 6 Hyperparameter values used in MAP estimates

Variables	Meaning	Value
$\vec{r}$	shape factor of normal-inverse gamma distribution	$(3,3)^{\mathrm{T}}$
$\vec{k}$	shape factor of normal-inverse gamma distribution	$(1.0, 1.0)^{\mathrm{T}}$
$\vec{\beta}$	expectation value of prior $\vec{\mu}$	$(-2.0, 2.0)^{\mathrm{T}}$
$\vec{\lambda}$	expectation value of prior $\vec{\sigma}^2$	$(4.0, 16.0)^{\mathrm{T}}$

Note that exact value of the mean and variance of $\vec{X}$ is used for $\vec{\beta}$ and $\vec{\lambda}$.

3.3.2 Estimation results

Using the hyperparameters given in Table 6, the MAP algorithm is applied to the data sets and the estimation results are shown in Table 7.

Table 7 Comparison of estimated solutions with different MAP algorithms

Algorithm	Variables	DATA-I	DATA-II	DATA-III
	$\vec{X}$	Independent Gaussian	Correlated Gaussian	Independent Uniform
Exact	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0
	Correlation	0.0	0.5	0.0
MAP 1	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.26 $\pm$ 2.04 1.61 $\pm$ 3.81	-2.27 $\pm$ 2.04 1.42 $\pm$ 4.03	-1.86 $\pm$ 2.07 2.06 $\pm$ 3.98
	Correlation	0.03	0.58	-0.03
MAP 2	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.14 $\pm$ 1.71 1.47 $\pm$ 4.13	-2.17 $\pm$ 1.63 1.17 $\pm$ 4.16	-1.71 $\pm$ 2.09 2.23 $\pm$ 4.04
	Correlation	N/A	N/A	N/A

The results show that the estimation results from MAP algorithm are close to the exact solution.

MAP 2 results have larger error on the estimation than **MAP 1**, just like what was observed with the MLE algorithm.

3.4   MCMC test results

As was described in Section 2.6, MCMC algorithm requires a prior distribution, likelihood function and a proposal distribution.

3.4.1   Proposal distribution

The proposal distribution affects the efficiency of the sampling scheme, which means that if the proposal distribution is close to the posterior distribution, the sampling scheme is more efficient because more sampled data will be accepted. However, for the purpose of this thesis, the efficiency of the sampling scheme is not the goal. To simplify the problem, the proposal distribution is chosen to be a Gaussian distribution,

$$g(\xi|\theta_k) \sim N(\theta_k, \sigma^2) \tag{95}$$

where σ^2 is the variance data sampled at the previous step. This proposal distribution is also called the independent proposal distribution, because

$$\frac{g(\theta_k|\xi)}{g(\xi|\theta_k)} = 1 \tag{96}$$

3.4.2   Prior distribution

Three types of prior distribution mentioned in Section 2.2 are tested, including **non-informative prior**, **conjugate prior** and **general prior**. Table 8 summarizes the prior distributions used in this thesis.

Table 8 Prior distribution used in MCMC test

Algorithms	Prior type	Prior distribution
MCMC 1	**Non-informative**	$\pi(\vec{\theta}) = \prod_{j=1}^{J} \frac{1}{(\sigma^j)^2}$
MCMC 2	**Conjugate**	$\pi(\vec{\theta}) \propto \prod_{j=1}^{J} [(\sigma^j)^2]^{-[(r^j+1)/2+1]} \exp\{-\frac{1}{2(\sigma^j)^2}[k^j(\mu^j - \beta^j)^2 + \lambda^j]\}$
MCMC 3	**Uniform**	θ_k distribute uniformly in $[a_k, b_k]$

The conjugate prior distribution is chosen to be the same as the prior distribution used in the MAP algorithm. For general prior distribution, a multi-variable uniform distribution is chosen. A

uniform distribution is chosen due to the fact that we might have a prior knowledge that the model parameters of interest only exist in a certain interval. In this MCMC test, because the exact mean values are $(-2.0, 2.0)$ and variances are $(4.0, 16.0)$, $[a_k, b_k]$ is chosen to be $[-4.0, 4.0]$ and $[0, 36]$, respectively.

3.4.3 Test results

Presently, the correlation between elements of $\vec{X}$ is not estimated in MCMC algorithm. The following figures and table gives the sampling results. The number of samplings in each case is 20000.

Figure 3 shows an example of the sampled distribution of $\vec{\mu}_x$ and Σ_x using uniform prior distribution. Table 9 shows the estimation results obtained from the sampled distribution. The sample average of the sampled $\vec{\mu}_x$ and Σ_x is used as the estimation of $\vec{\mu}_x$ and Σ_x, respectively. Though the sampled distributions are different using different prior distribution, the estimation results are close to the exact solution. This is because the data are created with exact (known) distribution and sufficient data points ($N = 100$ in this case) are used in the estimation. This means that if enough data points are available, the prior distribution has little effect on the estimation. This is also true for the MAP estimation.
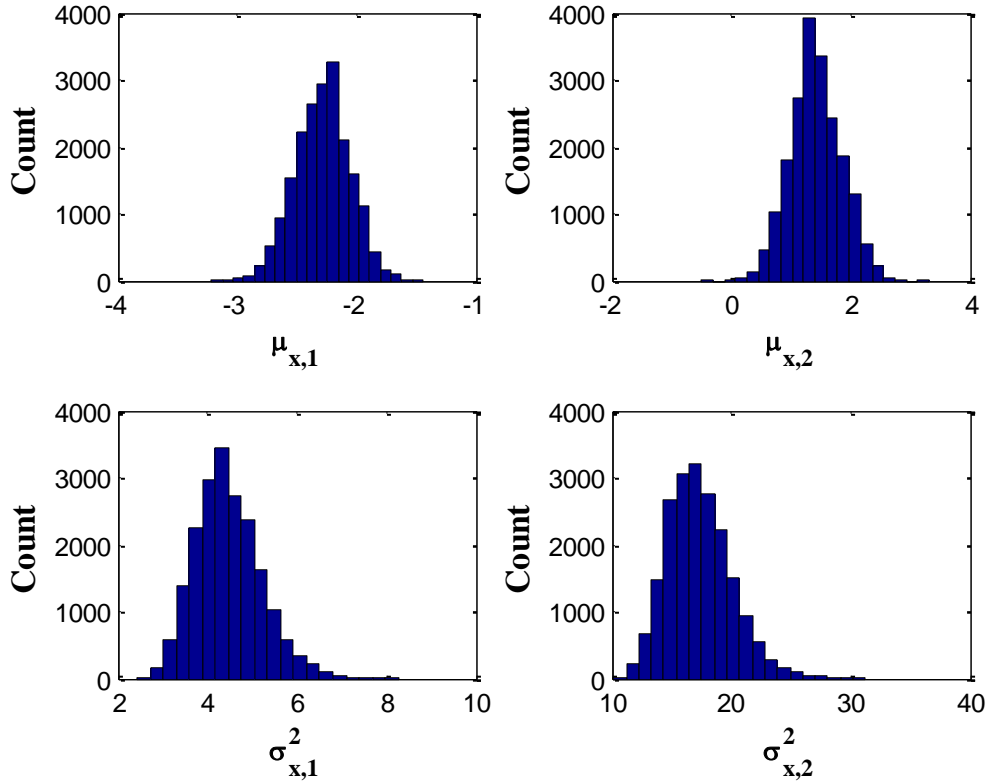
Figure 3 Sampled distribution of θ using uniform prior distribution for DATA-II

Table 9 Comparison between estimated solutions with different MCMC algorithms

Algorithm	Variables	DATA-I	DATA-II	DATA-III
	$\vec{X}$	Independent Gaussian	Correlated Gaussian	Independent Uniform
Exact	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0	-2.0 ± 2.0 2.0 ± 4.0
	correlation	0.0	0.5	0.0
MCMC 1	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.26 $\pm$ 2.11 1.58 $\pm$ 3.92	-2.29 $\pm$ 2.08 1.41 $\pm$ 4.12	-1.5 $\pm$ 2.14 2.08 $\pm$ 4.09
	correlation	N/A	N/A	N/A
MCMC 2	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.26 $\pm$ 2.07 1.60 $\pm$ 3.87	-2.28 $\pm$ 2.04 1.41 $\pm$ 4.05	-1.86 $\pm$ 2.10 2.04 $\pm$ 4.04
	correlation	N/A	N/A	N/A
MCMC 3	$\vec{\mu}_x \pm \vec{\sigma}_x$	-2.26 $\pm$ 2.13 1.60 $\pm$ 3.97	-2.28 $\pm$ 2.11 1.43 $\pm$ 4.17	-1.88 $\pm$ 2.17 2.06 $\pm$ 4.15
	correlation	N/A	N/A	N/A

3.5 Summary of Chapter 3

In this chapter, three data sets with different distribution were created for testing purposes. The data sets were created to be as practical and comprehensive as possible by considering different distribution types, correlation between variables and the error (or noise) found in real data. These data points were then used in testing MLE, MAP and MCMC algorithms.

For these data sets, estimations by all three types of algorithm (MLE, MAP and MCMC)were reasonably close to the exact solution, however some algorithms may have larger differences between the exact and estimated solution. For example, MLE, MAP **1a, 2** and MCMC algorithms are not capable of estimating the correlation between variables, whereas MCMC is capable of estimating a general prior distribution, which is very useful when the algorithm is applied to practical data.

In terms of the estimation results, no significant difference was observed between different algorithms, because sufficient data points were used. In other words, prior knowledge is not the most significant criterion if the number of data points is large enough.

4 Application to BFBT benchmark

One of the most valuable publicly 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 (Neykov, 2006). In this chapter, the BFBT benchmark data will be used to conduct inverse uncertainty quantification of physical model parameters in the thermal-hydraulics code system TRACE, using methods developed in previous Chapters. Then, the results will be validated by a forward uncertainty propagation analysis using the probability density functions obtained from the inverse uncertainty quantification.

This Chapter is organized to follow the order of performed the analysis:
- Section 4.1: Description of BFBT benchmark.
- Section 4.2: Accuracy analysis (AA) of TRACE prediction.
- Section 4.3: Sensitivity analysis (SA) (Gajev, 2014) of model parameters.
- Section 4.4: Validation of linearity assumption.
- Section 4.5: Inverse uncertainty quantification (IUQ) with MLE, MAP and MCMC.
- Section 4.6: Validation of MLE, MAP and MCMC results.
- Section 4.7: Summary of the Chapter.

4.1 Description of BFBT benchmark

The 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 power 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 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 was used to simulate a full-scale BWR fuel assembly (Neykov, 2006).

There are two types of void distribution measurement systems: an X-ray CT scanner and an X-ray densitometer shown in Figure 4. Three X-ray densitometers (DEN #3, #2 and #1) are located at three axial elevations within the heated section. The X-ray CT scanner is located 50 mm above the heated section. Under steady-state conditions, fine mesh void distributions were measured using the X-ray CT scanner. The X-ray densitometer measurements were performed at three axial elevations. In the BFBT benchmark data library, the measured fine mesh void distributions were also processed to give the cross-sectional averaged void fraction, which is used in this thesis for comparison with TRACE predictions. Both transient and steady-state void fractions were measured (Neykov, 2006), but only steady-state measurements are used in this thesis.
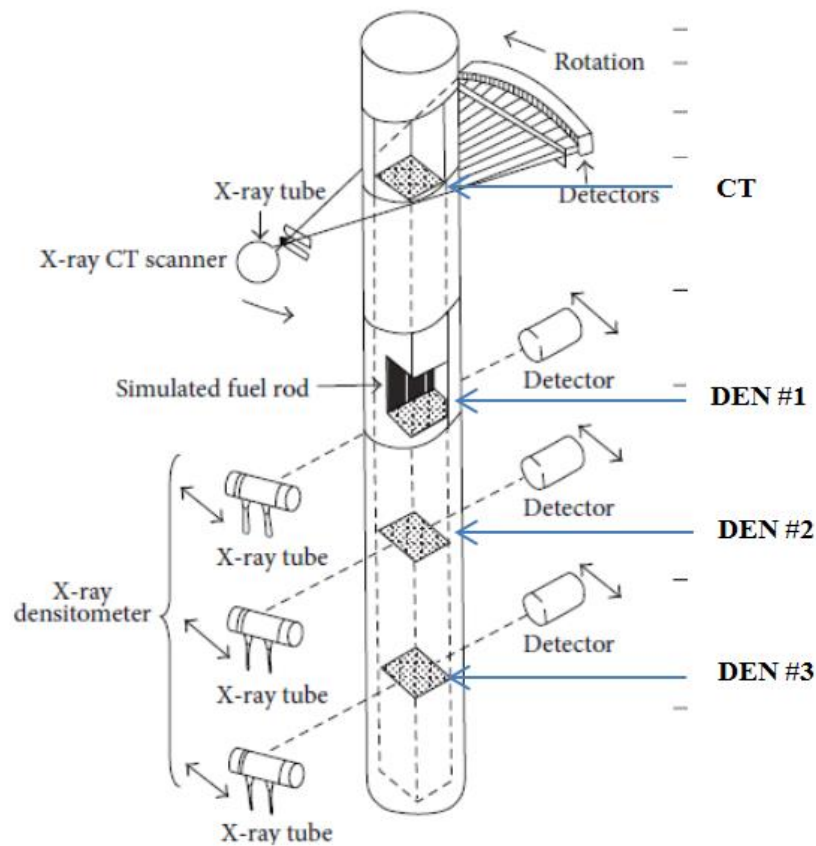

Figure 4 Void fraction measurement, 4 axial elevations are denoted by the measurement systems' name: DEN #3, DEN #2, DEN # 1 and CT

Two types of BWR assemblies are simulated in the BFBT test facility, a current (contemporary to the experiment) 8×8 fuel bundle and an 8×8 high burn-up bundle. There are five

different bundle geometry and power profile combinations that were tested in the void distribution experiments. Figure 5 summarizes the assembly types (identified as Type 0 through Type 4) used in the void distribution measurements.
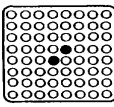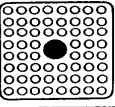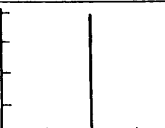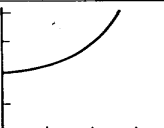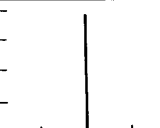
Test assembly No.	0	1	2	3	4
Fuel Type	Current use 8×8				High burnup 8×8
Planar power profile	Uniform	Simulated design profile	Simulated design profile	Simulated design profile	Simulated design profile
Axial power profile	Uniform	Cosine	Half-cosine	Inlet peak	Uniform
Heated length	Full	Full	Half	Full	Full
Axial powe distribution Axial └─► Power					

Figure 5 Test assembly and radial power distribution used for the void distribution measurements (Neykov, 2006)

4.2   Accuracy analysis of TRACE prediction

The accuracy analysis aims to compare the TRACE predictions with experimental measurement. Five types of assembly bundles are modeled in TRACE to predict the cross-section averaged void fraction. TRACE void fraction predictions are obtained at four axial elevations (corresponding to DEN#3, DEN#2, DEN#1 and CT) and compared with the experimental measurement data. Each case has different thermal-hydraulic conditions (pressure, inlet temperature, flow rate and power). The range of experimental conditions used in this work is shown in Table 10. The void fraction comparison is shown in Figure 6.

Table 10 Variation of experimental conditions (Neykov, 2006)

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

Figure 6 shows a comparison between the predicted and measured void fraction at four axial elevations (DEN #3, DEN #2, DEN #1 and CT). Overall TRACE captures correct trend. In general, TRACE predictions for the lowest and highest axial elevations (DEN #3 and CT) are close to the measurement. However, TRACE 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.
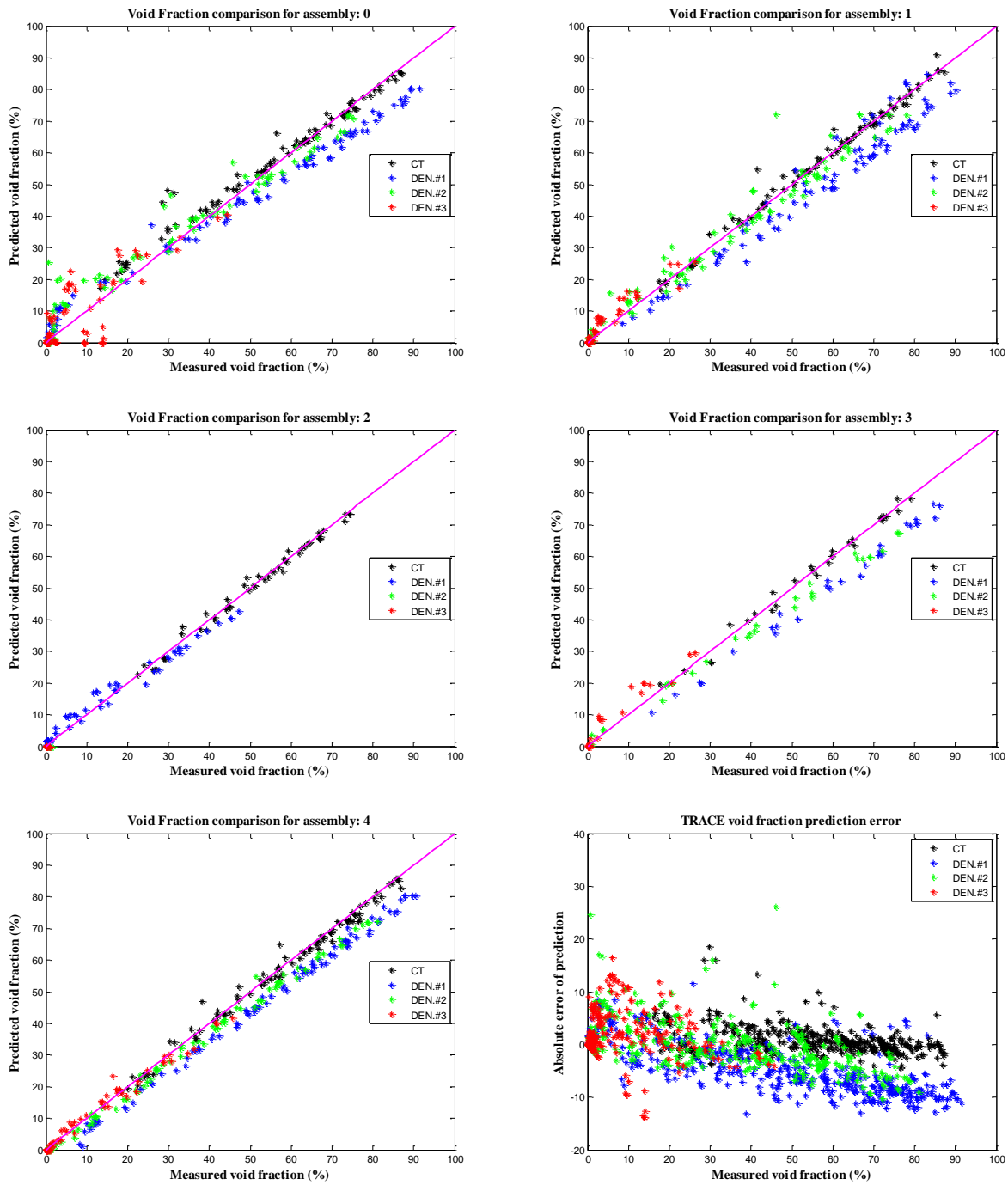
Figure 6 Comparison of TRACE and measurement void fraction

4.3   Sensitivity analysis of model parameters

Many parameters contribute to the uncertainties in TRACE prediction. The focus of this thesis is the internal physical model parameters used in TRACE. TRACE (version 5.0 Patch 4) includes options for uncertainty quantification by allowing the adjustment of 36 physical model parameters from the input file. Following a sensitivity analysis of all 36 physical models, Table 11 (Hu, 2015) shows four parameters that are the most important (most sensitive) for void fraction prediction. Sensitivity analysis shows that other physical model parameters, such as liquid to interface bubbly-slug heat transfer coefficient and nucleate boiling heat transfer coefficient, have little to no effect on void fraction prediction. These coefficients are not shown in Table 11.

Table 11 Sensitivity coefficients † for Test assembly 4 at 4 axial locations (U.S. NRC, 2010)

Parameters	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

†: Sensitivity coefficient $= \frac{\Delta Y}{\Delta X} \frac{X}{Y} * 100\%$

Table 11 shows an example of the calculated sensitivity coefficients. In the table, a positive/negative sensitivity coefficient means that the predicted void fraction increases/decreases with the parameters. From the sensitivity coefficient, we see that different coefficients dominate at different locations. The sensitivity of single-phase liquid to wall heat transfer coefficient decreases greatly at higher axial positions, because the single-phase liquid exists primarily in the lower regions. Similarly, the subcooled boiling heat transfer is only dominant in lower positions where subcooled boiling would occur. However, the drag force tends to dominate in higher positions, thus the sensitivity is larger there. The sensitivity coefficients are different for different thermal-hydraulic conditions and assembly geometry. These four physical models are observed to be important for all BFBT cases. The sensitivity coefficients are necessary for the sensitivity coefficient matrix (**A**) for MLE, MAP and MCMC algorithm.

4.4 Validation of linearity assumption

Thus far, we have prepared necessary data for inverse uncertainty quantification by performing accuracy analysis ($\vec{Y}, \vec{Y}_0$) and sensitivity analysis (**A**). However, the inverse uncertainty quantification using MLE, MAP and MCMC relies on the linear assumption made in Eq. (42). It is very important to validate this assumption prior to application.

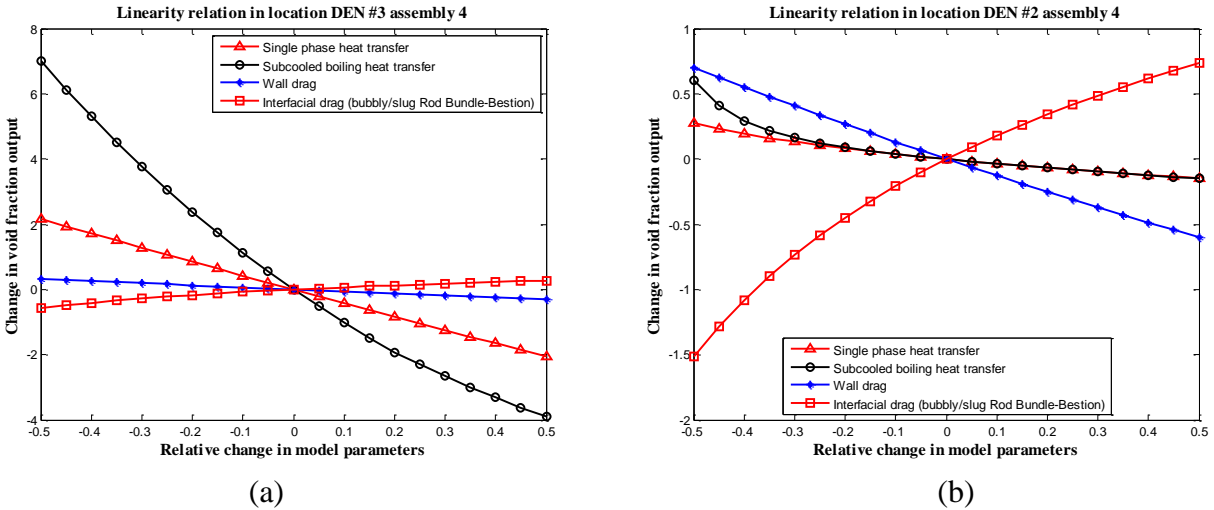(a)   (b)

Figure 7 Validation of linearity assumption for physical model parameters

Figure 7 shows the relation between the predicted void fraction and the four model parameters: single-phase heat transfer coefficient, subcooled boiling heat transfer coefficient, wall drag coefficient and interfacial drag (bubbly/slug Rod Bundle-Bestion) for one case. Figure 7(a) shows that for void fraction prediction at the lowest axial position (**DEN #3**), the linearity assumption is valid for a ± 0.5 variation of model parameters. Figure 7(b) shows that for void fraction prediction at the middle of heated section (**DEN #2**), the linearity assumption is valid for a smaller variation of model parameters. The results are qualitatively similar for other axial locations and other test cases. For this work, we use the model parameter variation of [-0.5, 0.5] as the range where the linearity assumption is valid.

4.5 Inverse uncertainty quantification with MLE, MAP and MCMC

Before we can apply the MLE, MAP and MCMC algorithm, we also need information for the random error of the experimental measurement. In this work, we assume the experimental error is uniformly distributed on [-5, 5].

Many data sets could be used for the inverse uncertainty quantification algorithm. For the purpose of this thesis, we use the data from Test assembly 4 axial location **DEN #3**. Two model parameters, subcooled boiling heat transfer coefficient and interfacial drag (bubbly/slug Rod Bundle-Bestion), are chosen as the $\vec{X}$ random variables because they have the largest sensitivity coefficients.

4.5.1 Criterion for selecting test cases

Some cases in the BFBT benchmark are invalid for inverse uncertainty quantification calculation, and there are two main reasons why. One reason is that the measured void fraction is obviously wrong, in some cases being less than 0 or larger than 1. The other reason is that the sensitivity coefficient is too small, which makes the sensitivity coefficient matrix (**A**) close to singular. Three criteria are implemented to select appropriate test cases:

1. The measured void fraction should be positive.
2. The predicted void fraction should be positive.
3. The absolute value of the sensitivity coefficient should be larger than a pre-set tolerance (0.1 in this work).

4.5.2 Inverse uncertainty quantification results with MLE

We apply the MLE algorithm with the data obtained in the previous sections. The results are listed in Table 12.

Table 12 Estimated distribution of two model parameters with MLE

Algorithms	Subcooled boiling HTC	Interfacial drag(bubbly/slug)	Correlation
MLE 1a	1.15 ± 0.05	1.70 ± 0.15	N/A
MLE 1b	1.15 ± 0.05	1.70 ± 0.17	0.31
MLE 2	1.17 ± 1.36	1.76 ± 0.49	N/A

Three MLE algorithms give consistent results for the mean value of the model parameters, but the algorithm **MLE 2** gives a significantly higher variance. The mean value is a translation parameter estimated by the maximization step and has little dependence on the variance estimation. The algorithm **MLE 2** gives a larger variance because of the independence assumption between the output variables. Another observation is that the correlation calculated by **MLE 1b** shows that these two model parameters are loosely and positively correlated.

4.5.3 Inverse uncertainty quantification results with MAP

The application of MAP algorithm requires that we provide the hyperparameters of the conjugate prior distribution, which have to be estimated by some prior knowledge. The results from MLE estimation is a good choice if the MAP algorithm is applied to different data. If the same data are used, we should provide some prior knowledge.

Table 13 shows the assumption of the conjugate prior distribution. Because we do not have prior information on the expectation value of prior $\vec{\mu}$ and $\vec{\sigma}^2$, they are both assumed to be 1.0. A mean value of 1.0 means the model parameters should not be adjusted. This is a critical limitation for the application of MAP algorithm.

Table 13 Value of prior distribution hyperparameters used in MAP application

Variables	Meaning	Value
$\vec{r}$	shape factor of normal-inverse gamma distribution	$(3,3)^{\text{T}}$
$\vec{k}$	shape factor of normal-inverse gamma distribution	$(1.0,1.0)^{\text{T}}$
$\vec{\beta}$	expectation value of prior $\vec{\mu}$	$(1.0,1.0)^{\text{T}}$
$\vec{\lambda}$	expectation value of prior $\vec{\sigma}^2$	$(1.0,1.0)^{\text{T}}$

The MAP results are shown in Table 14. We see that because of our prior information, the estimated mean value of the two model parameters is closer to 1.0 compared with MLE estimation . In addition, the estimated correlation is smaller, because the two model parameters are independent in prior distribution. If different prior distribution is used, the estimation results will change. For example, based on accuracy analysis in Section 4.2, we might be able to qualitatively estimate what the prior distribution should be and then choose more appropriate prior distribution.

Table 14 Estimated distribution of two model parameters with MAP

Algorithms	Subcooled boiling HTC	Interfacial drag(bubbly/slug)	Correlation
MAP 1	1.06 ± 0.21	1.24 ± 0.46	0.16
MAP 2	1.08 ± 1.23	1.31 ± 0.49	N/A

4.5.4 Inverse uncertainty quantification results with MCMC

The application of MCMC algorithm requires a prior distribution. The prior distributions used in this work for **MCMC 1, 2, 3** are listed in Table 15.

Table 15 Prior distribution used in MCMC application

Algorithms	Prior type	Prior distribution
MCMC 1	Non-informative	$\frac{1}{(\sigma^1)^2(\sigma^2)^2}$
MCMC 2	Conjugate	the same as Table 13
MCMC 3	Uniform	$\vec{\mu} \in [0.5,1.5] \times [0.5,1.5],\ \vec{\sigma}^2 \in [0.,1.0] \times [0.,1.0]$

The results of MCMC estimation are listed in Table 16. The main observations are:

- For **MCMC 1**, the estimation results are close to MLE estimation, which is expected because we add little information than the MLE by adding the non-informative prior distribution.

- For **MCMC 2**, the estimation results are close to the MAP 1 estimation, because these two algorithms use the same posterior distribution.

- For **MCMC 3**, the estimation results are limited to a range where the linearity assumption is valid. Test on **MCMC 3** with a larger interval, for example $\vec{\mu} \in [0.,2.0] \times [0.,2.0]$, the estimation results becomes closer to MLE estimation, because we add less limitation/information to the prior distribution.

Table 16 Estimated distribution of two model parameters with MCMC

Algorithms	Subcooled boiling HTC	Interfacial drag(bubbly/slug)	Correlation
MCMC 1	1.15 ± 0.05	1.69 ± 0.21	N/A
MCMC 2	1.11 ± 0.29	1.46 ± 0.52	N/A
MCMC 3	1.11 ± 0.12	1.32 ± 0.50	N/A

4.6 Validation of MLE, MAP and MCMC results

In Section 4.5, we obtained physical model uncertainty estimates with different algorithms. However, we do not know if these uncertainty estimates are valid. In this section, we are going to validate these estimation results by performing forward uncertainty propagation using BFBT benchmark data that was not used in Section 4.5 for the physical model uncertainty estimates. A Monte Carlo sampling-based uncertainty propagation method is used: we sample the model parameters according to their estimated distributions, perform TRACE calculations and process the uncertainties of TRACE predictions.

There are 8 estimation results in Section 4.5, from which we selected two bounding results to perform the forward uncertainty propagation calculation: results from **MLE 1a** (Table 12) and **MCMC 3** (Table 16).The physical model uncertainty estimates presented in Section 4.5 were obtained with data obtained from axial location (**DEN #3**) of Test assembly 4. To validate the results with forward uncertainty propagation, we are going to perform new TRACE calculations for different axial locations.

4.6.1 Validation of MLE results with Test assembly 4

The forward uncertainty propagation process includes the following steps:

1. Monte Carlo sampling: the selected model parameters are sampled according to their distribution.
2. TRACE input preparation: the model parameters are adjusted in TRACE input file based on sampled values.
3. TRACE calculation: void fraction is predicted at different axial locations.
4. Uncertainty information: the uncertainty information is derived from TRACE predictions.

Figure 8 shows a schematic view of the forward uncertainty propagation process. This process takes significant computational effort because thousands of TRACE calculations are required. However, the computation time can be reduced by performing TRACE calculations simultaneously.
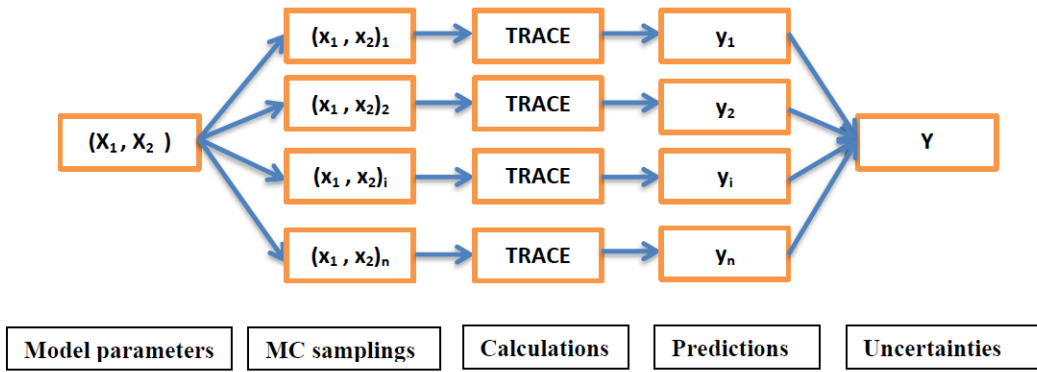
Figure 8 Schematic view of the forward uncertainty propagation process (Hu, 2015)
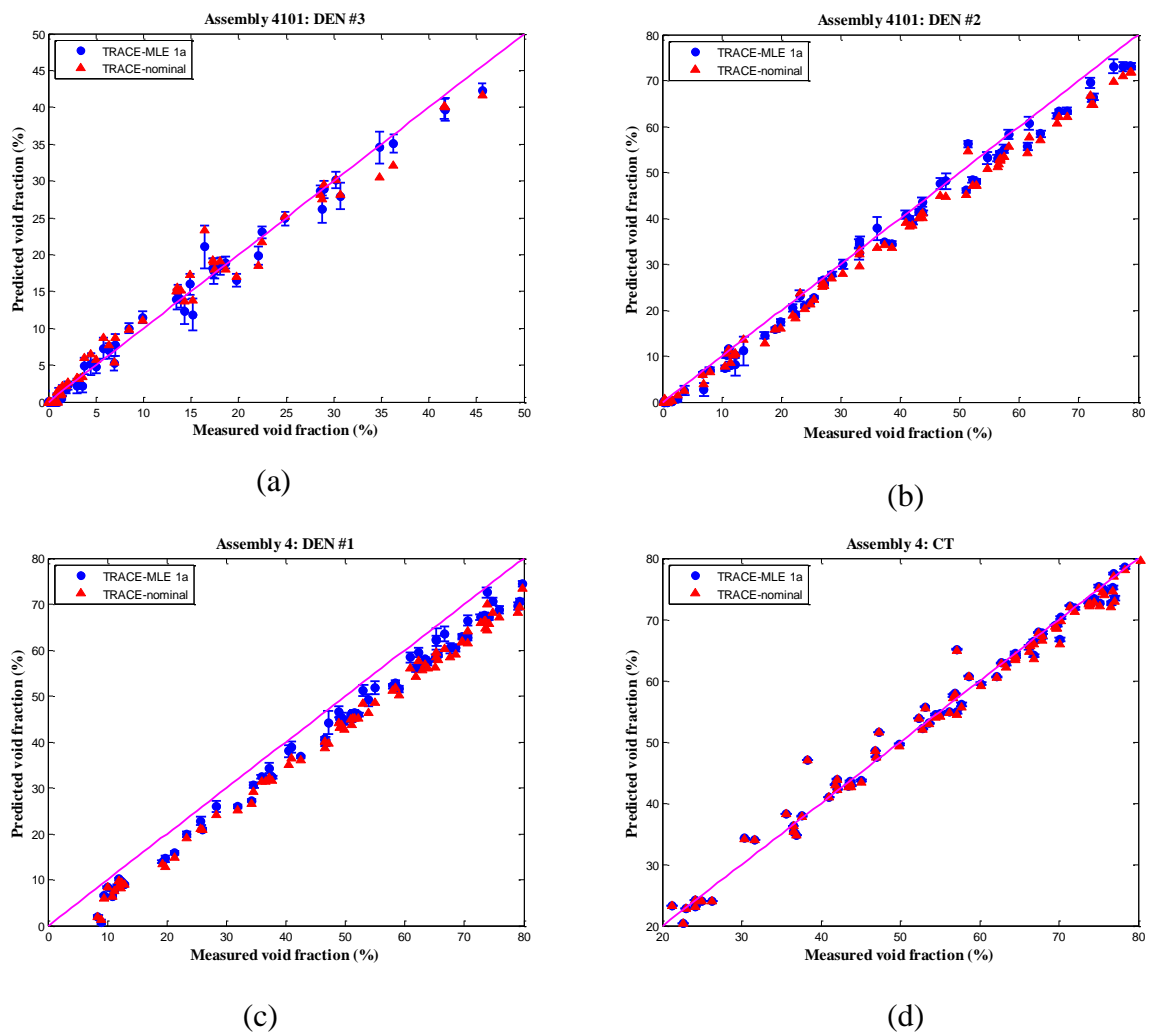

(a)

(b)

(c)

(d)

Figure 9 Comparison of TRACE predictions without and with uncertainty information of model parameters

Figure 9 shows the comparison of TRACE predictions without and with uncertainty information of model parameters. Based on the comparison, we find:

- **DEN #3**: The MLE estimation was performed using data from this position. The original TRACE predictions (TRACE-nominal) do not include uncertain model parameters, as TRACE underestimates the void fraction in some cases while overestimates the void fraction in other cases. The MLE algorithm tries to minimize the global error by adjusting the two model parameters. The new TRACE predictions (TRACE-MLE 1a) are closer to the measured data, see Figure 9(a).

- **DEN #2, 1**: Though MLE estimation does not use data in these two locations, the new TRACE predictions (TRACE-MLE 1a) are better than the original TRACE predictions (TRACE-nominal), see Figure 9(b), 9(c). It is possible to further improve the TRACE predictions at location **DEN #2, 1** by performing MLE estimation using data from these locations.

- **CT**: At this location, where the void fraction is considerably larger, the flow regime has typically developed into annular or mist flow. The two selected models, subcooled boiling heat transfer coefficient and interfacial drag (bubbly-slug), have little effect on the void fraction at this location. The new TRACE predictions (TRACE-MLE 1a) are essentially the same as the original predictions (TRACE-nominal), see Figure 9(d).

4.6.2   Validation of MLE result vs MCMC result

We validated the results from algorithm **MCMC 3** the same way as MLE1a in Section 4.6.1. Because the void fraction comparison is very similar to Figure 9, we compare the error distribution between TRACE-nominal, TRACE-MLE1a and TRACE-MCMC3, the comparison is shown in Figure 10.
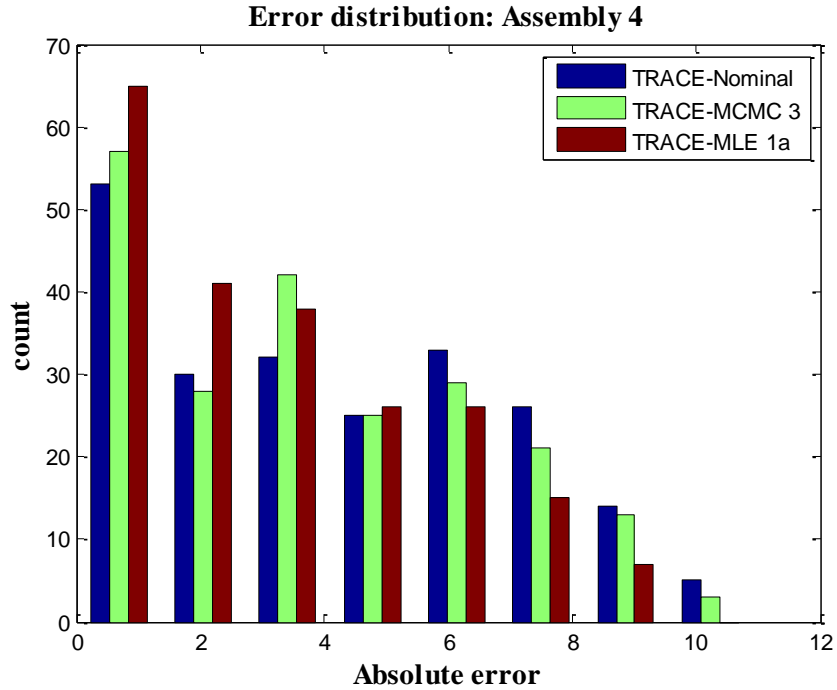
Error distribution: Assembly 4

Figure 10 Error distribution of TRACE calculation without and with uncertainty information in model parameters

Figure 10 shows that the TRACE-MLE1a and TRACE-MCMC3 prediction error is distributed more towards smaller error compared with TRACE predictions without uncertainty model parameters (TRACE-nominal). However, comparison of **MLE 1a** and **MCMC 3** shows that the **MLE 1a** results are more accurate than **MCMC 3** results. This is most likely due to using an inaccurate prior distribution.

4.7   Summary of Chapter 4

In this Chapter, we applied the MLE, MAP and MCMC algorithms to BFBT benchmark data and estimated the uncertainty distribution of two model parameters: subcooled boiling heat transfer coefficient and interfacial drag (bubbly/slug rod bundle) coefficient.

These algorithms tend to give various estimation results. This is expected especially for MAP and MCMC algorithms, because the assumption of the unknown prior distribution is difficult and vary. Despite the differences in these algorithms, we find that the estimation results are consistent. For example, if the prior distribution for MCMC algorithm is chosen to be uniform (1)

on the entire domain, the MLE and MCMC algorithms are mathematically identical; this is what we find from the comparison of MLE results with **MCMC 1** and **MCMC 3**.

After obtaining the uncertainty estimates, we validated the uncertainty estimates by applying the estimated distributions of model parameters to TRACE prediction. The new predictions succeed in reducing the void fraction prediction error, but it is not possible to eliminate all prediction error. We are only adjusting two model parameters, and there exists uncertainties in all model parameters.

This work shows the difficulty of choosing a proper prior distribution for Bayesian-based MAP and MCMC algorithms, which is the primary limitation of Bayesian-based methods. However, if we could obtain accurate prior information, the MAP and MCMC algorithms would be more powerful than MLE algorithm.

5　Discussion

There are several important features in the algorithms developed in this thesis. The first feature is the potential to apply the algorithm to estimate many physical models simultaneously. The algorithms developed in thesis are all generalized into matrix/vector form, which makes them valid for any number of input physical parameters and outputs. For example, we can estimate the uncertainties of three or more physical models at the same time provided with a consistent sensitivity coefficient matrix and output data. We tested the algorithms with only two input physical parameters because of the considerable computation load in calculating the sensitivity coefficients using TRACE. In addition, the algorithms could be implemented in any programming language very easily.

The second feature is that the MAP and MCMC algorithm considers prior information. Given the prior information and new experiment data, the MAP and MCMC algorithms are capable of updating our knowledge of the uncertainty in the models. The available prior information and single experiment data might not be enough to give the correct uncertainty information. However, this feature enables us update our knowledge whenever there is new experiment data.

The third feature is the capability of the MCMC algorithm in processing any form of prior information and different models. Compared with the MLE and MAP algorithm, the MCMC algorithm is capable of working with more general likelihood functions and prior distributions. For example, we could avoid the linearity assumption with more advanced MCMC algorithm and get a more accurate estimation. Future work on developing advanced MCMC algorithm would be valuable.

The fourth feature is the wide application field of these algorithms. These algorithms do not depend on any properties of experiment nor of modeling. Thus, the algorithms could be applied to many other problems. For example, the algorithm could be applied to estimate the uncertainties of cross section data used in a neutron transport problem.

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6   Conclusion

Uncertainty information of physical model parameters is important for the purposes of uncertainty quantification, such as best estimate plus uncertainty calculation. In this work, the MLE, MAP and MCMC algorithms based on Bayesian analysis are developed, tested and applied. Numerical tests with artificial data verified the implementation of these algorithms. The application of these algorithms to BFBT benchmark data shows the typical work flow for applying these algorithms. Also, the application to BFBT benchmark data validated these algorithms.

We applied the MLE, MAP and MCMC algorithms to BFBT benchmark data and estimated the uncertainty distribution of two model parameters: subcooled boiling heat transfer coefficient and interfacial drag (bubbly/slug rod bundle) coefficient. These algorithms tend to give various estimation results. This is expected especially for MAP and MCMC algorithms, because the assumption of the unknown prior distribution is difficult and vary. Despite the differences in these algorithms, we find that the estimation results are consistent.

After obtaining the uncertainty estimates, we validated the uncertainty estimates by applying the estimated distributions of model parameters to TRACE prediction. The new predictions succeed in reducing the void fraction prediction error, but it is not possible to eliminate all prediction error. We are only adjusting two model parameters, and there exists uncertainties in all model parameters. Application of the algorithms to other physical models and experimental data will be helpful for future work.

7 Future Work

These algorithms are capable of reducing prediction error and provide uncertainty information for further analysis. However, a few problems exist and needs future work.

Assumption: A lot of assumptions were made to derive the algorithms. Two main assumptions are an assumed Gaussian distribution of output variables and an assumed linearity relation between input model parameters and output variables. These assumptions are required to obtain an analytical form of likelihood function. However, the statistical information of these variables is not known. For a more general case, it might be not possible to get analytical form of likelihood function. There is a way to process more general case by calculating and maximizing the likelihood function numerically. The likelihood function could be calculated numerically using Monte Carlo integration and could be maximized using Newton's method. However, the numerical calculation is much more expensive and has convergence issues.

Uncertain parameters: In practical application, such as with TRACE, many uncertain parameters contribute to prediction error. In current algorithms, we are unable to account for other uncertain parameters except for selected model parameters, which means the validity of estimated results is not guaranteed.

Prior information: As evident, the prior information is critical in applying MAP and MCMC algorithm. Unless we are confident with our prior information, it is not reliable to apply the MAP and MCMC algorithm. An algorithm to initially estimate the prior information might be helpful, but the algorithm would not work on the same data as MLE, MAP and MCMC.

Experimental data: The validity of experimental data determines the validity of estimated results. For example, if obviously incorrect measurements exist, we would need to find and remove these data before applying the algorithms. The process of removing data negates the validity of estimation results. A standard algorithm in choosing data is necessary.

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