

Application of Bayesian optimal experimental design to reduce parameter uncertainty in the fracture boundary of a fuel cladding tube under LOCA conditions

Takafumi Narukawa^{a, b*}, Akira Yamaguchi^a, Sunghyon Jang^a, and Masaki Amaya^b

^aThe University of Tokyo, Tokyo, Japan

^bJapan Atomic Energy Agency, Ibaraki, Japan

Abstract: The reduction of epistemic uncertainty for safety-related events that rarely occur or require high experimental costs is a key concern for researchers worldwide. In this study, we develop a new framework to effectively reduce parameter uncertainty, which is one of the epistemic uncertainties, by using the Bayesian optimal experimental design. In the experimental design, we used a decision theory that minimizes the Bayes generalization loss. For this purpose, we used the functional variance, which is a component of widely applicable information criterion, as a decision criterion for selecting informative data points. Then, we conducted a case study to apply the proposed framework to reduce the parameter uncertainty in the fracture boundary of a non-irradiated, pre-hydrated Zircaloy-4 cladding tube specimen under loss-of-coolant accident (LOCA) conditions. The results of our case study proved that the proposed framework greatly reduced the Bayes generalization loss with minimal sample size compared with the case in which experimental data were randomly obtained. Thus, the proposed framework is useful for effectively reducing the parameter uncertainty of safety-related events that rarely occur or require high experimental costs.

Keywords: Bayesian optimal experimental design, parameter uncertainty reduction, Zircaloy-4 cladding tube, fracture boundary, LOCA.

1. INTRODUCTION

The reduction of epistemic uncertainty [1] for safety-related events that rarely occur or require high experimental costs (hereinafter called "rare or costly events") has been an area of key concern. Epistemic uncertainty is defined as the uncertainty that arises from a lack of knowledge about the system and is thus a property of the analysts performing the study [1, 2]. The importance of reducing epistemic uncertainty is seen in the field of nuclear engineering when performing reliability research for studying fuel behavior under accident conditions. One major concern is the reduction of epistemic uncertainty in the fracture boundary of the high-burnup fuel cladding tube during a loss-of-coolant accident (LOCA). It is expensive to conduct experiments using a high-burnup fuel cladding tube specimen; therefore, only a limited number of experiments can be conducted [3].

In this situation, the approach of the optimal experimental design has a potential benefit. The optimal experimental design is a method for obtaining informative data points. By using the optimal experimental design method, we can effectively reduce the parameter uncertainty, which is one of the epistemic uncertainties [2, 4]. In the field of statistics, several methods have been proposed for developing an optimal experimental design for obtaining informative data points. For instance, optimal experimental designs have been developed based on the minimization of a loss function [5] or "alphabetic optimality" [6]. Certain studies have used the optimal experimental design methods for reliability engineering [7, 8]. These approaches rely on the information matrix of parameters. Thus, all parameters in a model receive equal attention, regardless of their influence on the value of the response variable [5, 9].

* Corresponding author, narukawa.takafumi@jaea.go.jp

Instead of using the information matrix, Paass et al. proposed an approach that minimized the loss function in a Bayesian decision framework [5]: they used a square loss function and proposed an optimal experimental design based on the analytical minimization of the loss function. In the field of nuclear engineering, Yamaguchi et al. proposed an epistemic uncertainty reduction method that maximized the expectation value of the logarithmic likelihood [10]. This approach is also considered to be an optimal experimental design approach that intends to minimize a loss function.

In general, a sample size is always limited when we model rare or costly events based on experiments. In this situation, it is valuable to consider the approach proposed by Paass [5], that is, a Bayesian approach using the Markov chain Monte Carlo (MCMC) method. This is because the approach can approximate posterior distributions very well using enough MCMC samples, even when the sample size is limited.

A small sample size may also result in overfitting. To avoid the overfitting, it is important to use a loss function that evaluates the prediction accuracy for obtaining the subsequent data points. Here, a Bayes generalization loss [11] is considered suitable because it is a measure of the predictive power of a model. However, the Bayes generalization loss cannot be calculated without knowing a true distribution. Watanabe developed a widely applicable information criterion (WAIC), the expectation value of which is asymptotically equal to the average Bayes generalization loss in both regular and singular models [11]. Using WAIC, we can obtain an estimate of the Bayes generalization loss with a posterior distribution. Watanabe mentioned that the WAIC could be used to design experiments [12].

In this study, we developed a new framework to reduce the parameter uncertainty in modeling rare or costly events using the Bayesian optimal experimental design. In the experimental design, we used a decision theory, which minimizes the Bayes generalization loss. For this purpose, the functional variance, which is one of the components of WAIC, was used as a decision criterion for selecting informative data points. Also, we applied the framework to reduce the parameter uncertainty in the fracture boundary of a non-irradiated, pre-hydrated Zircaloy-4 cladding tube specimen under LOCA conditions.

In **Section 2**, we summarize a Bayesian decision theory referring to [5] and an approach of Bayesian optimal experimental design using the functional variance. Then, in **Section 3**, we propose a framework for reducing parameter uncertainty using the Bayesian optimal experimental design. In **Section 4**, we perform a numerical demonstration to show the applicability of the proposed framework to reduce the parameter uncertainty in the context of nuclear engineering. The last section concludes this paper.

2. BAYESIAN OPTIMAL EXPERIMENTAL DESIGN USING FUNCTIONAL VARIANCE

2.1. Bayesian Decision Theory

Let \mathbb{R}^N be an N -dimensional Euclidian space, $q(y)$ be a true probability distribution of a scalar output value y , n be the sample size, and $Y^n = (y_1, y_2, \dots, y_n)$ be a sequence of \mathbb{R}^N -valued random variables that are independently subject to $q(y)dy$. The set of input values x and parameters ω are denoted as $X \subset \mathbb{R}^M$ and $W \subset \mathbb{R}^d$, respectively, where \mathbb{R}^M and \mathbb{R}^d are an M -dimensional Euclidian space and a d -dimensional Euclidian space, respectively. The corresponding parametric model is described as $p(y|\mathbf{x}, \boldsymbol{\omega})$, where \mathbf{x} is an input vector and $\boldsymbol{\omega}$ is a vector of parameters. In the Bayesian decision theory, an action a whose result depends on the unknown output y is performed based on the data $\mathbf{D} = (\mathbf{X}^n, Y^n)$, where $\mathbf{X}^n = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$, $\mathbf{x}_i = (x_{1i}, x_{2i}, \dots, x_{ji})$, $i = 1, 2, \dots, n$, and $j \in \mathbb{N}$, and a vector of input data \mathbf{x} . The loss function $L(y, a) \in [0, \infty)$ is defined as the loss if y is the true value and if we have taken the action $a \in A$, where A is a design space. In the Bayesian decision theory, the action \hat{a} that minimizes the

loss function is selected based on the data \mathbf{D} and the input data \mathbf{x} as follows:

$$\begin{aligned}\hat{a}(\mathbf{x}, \mathbf{D}) &= \arg \min_{a \in A} \iint L(y, a) p(y|\mathbf{x}, \mathbf{D}) p(\mathbf{x}) d\mathbf{x} dy, \\ &= \arg \min_{a \in A} \iiint L(y, a) p(y|\mathbf{x}, \boldsymbol{\omega}) p(\mathbf{x}) p(\boldsymbol{\omega}|\mathbf{D}) d\boldsymbol{\omega} d\mathbf{x} dy,\end{aligned}\quad (1)$$

where $\hat{a}(\mathbf{x}, \mathbf{D})$ is a decision function, $p(\mathbf{x})$ is a distribution of future inputs, which is assumed to be a uniform distribution in this study, and $p(\boldsymbol{\omega}|\mathbf{D})$ is a joint posterior distribution of $\boldsymbol{\omega}$ given \mathbf{D} .

The aim of the optimal experimental design is to select a new observation $\tilde{\mathbf{x}}$ in such a way that the information obtained from $\tilde{\mathbf{x}}$ will be maximized. Together with its still unknown y value, $\tilde{\mathbf{x}}$ defines a new observation $(\tilde{\mathbf{x}}, \tilde{y})$ and the new data $\mathbf{D} \cup (\tilde{\mathbf{x}}, \tilde{y})$. The action $\hat{a}(\mathbf{x}, \tilde{\mathbf{D}}_{\tilde{\mathbf{x}}, \tilde{y}})$ that minimizes the loss function is selected based on the data $\tilde{\mathbf{D}}_{\tilde{\mathbf{x}}, \tilde{y}} = \mathbf{D} \cup (\tilde{\mathbf{x}}, \tilde{y})$ and the input data \mathbf{x} as follows:

$$\begin{aligned}\hat{a}(\mathbf{x}, \tilde{\mathbf{D}}_{\tilde{\mathbf{x}}, \tilde{y}}) &= \arg \min_{a \in A} \iint L(\tilde{\mathbf{x}}, \tilde{y}, \mathbf{x}) p(\mathbf{x}) p(\tilde{y}|\tilde{\mathbf{x}}, \mathbf{D}) d\tilde{y} d\mathbf{x}, \\ &= \arg \min_{a \in A} \iiint L(y, a) p(y|\mathbf{x}, \tilde{\mathbf{D}}_{\tilde{\mathbf{x}}, \tilde{y}}) p(\mathbf{x}) p(\tilde{y}|\tilde{\mathbf{x}}, \mathbf{D}) d\tilde{y} d\mathbf{x} dy.\end{aligned}\quad (2)$$

2.2. Decision Criterion Based on Functional Variance

For optimal experimental design, it is important to select a loss function that appropriately describes the goals of a given experiment [13]. We focus on the parameter uncertainty reduction of rare or costly events. Therefore, we use the Bayesian generalization loss [11], which is a measure of the prediction accuracy, as a loss function. In the rest of this section, we summarize the decision criterion based on the functional variance that minimizes the Bayesian generalization loss.

The expectation values over Y^n and the posterior distribution of $\boldsymbol{\omega}$ are denoted by $\mathbb{E}[\cdot]$ and $\mathbb{E}_{\boldsymbol{\omega}}[\cdot]$, respectively. Here, the predictive distribution $p^*(y)$ and the entropy S are given as follows:

$$p^*(y) = \mathbb{E}_{\boldsymbol{\omega}}[p(y|\mathbf{x}, \boldsymbol{\omega})], \quad (3)$$

$$S = - \int q(y) \log q(y) dy, \quad (4)$$

where \log is the natural logarithm. The Bayes generalization loss is defined as follows:

$$G_n = - \int q(y) \log p^*(y) dy. \quad (5)$$

Then,

$$G_n = S + \int q(y) \log \frac{q(y)}{p^*(y)} dy. \quad (6)$$

The second term on the right side of equation (6) is the Kullback–Leibler (KL) distance [14] of the true and the predictive distributions. Therefore, when the value of G_n is smaller, $p^*(y)$ provides a better prediction of $q(y)$. However, G_n cannot be calculated without knowing the true distribution $q(y)$. Here, WAIC is defined as follows using the training loss T_n and the functional variance $V_{\boldsymbol{\omega}}[\log p(y_i|\mathbf{x}_i, \boldsymbol{\omega})]$ which can be calculated using data and a model [11]:

$$WAIC = T_n + \frac{1}{n} \sum_{i=1}^n V_{\boldsymbol{\omega}}[\log p(y_i|\mathbf{x}_i, \boldsymbol{\omega})], \quad (7)$$

$$T_n = -\frac{1}{n} \sum_{i=1}^n \log p^*(y_i|\mathbf{x}_i, \boldsymbol{\omega}), \quad (8)$$

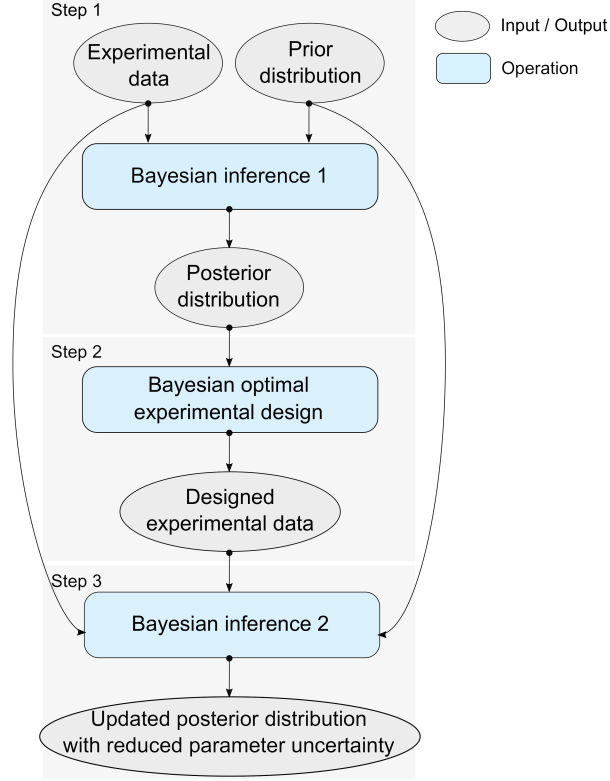


Figure 1: Illustration of the proposed parameter uncertainty reduction framework.

$$V_{\omega}[\log p(y_i|\mathbf{x}_i, \boldsymbol{\omega})] = \mathbb{E}_{\omega}[(\log p(y_i|\mathbf{x}_i, \boldsymbol{\omega}))^2] - \mathbb{E}_{\omega}[\log p(y_i|\mathbf{x}_i, \boldsymbol{\omega})]^2. \quad (9)$$

WAIC has the following relationship with G_n :

$$\mathbb{E}[G_n] = \mathbb{E}[WAIC] + O\left(\frac{1}{n^2}\right). \quad (10)$$

From equation (10), it is clear that the expectation value of WAIC is asymptotically equal to that of the Bayes generalization loss. Thus, WAIC can be used as a loss function and the minimization of WAIC makes it possible to select the informative data points.

For selecting the data points that minimize WAIC, we focus on using the functional variance, which is one of the components of WAIC. As shown in equation (9), the functional variance shows the sensitivity of each data point to the posterior distribution of the estimated parameters. Therefore, WAIC can be effectively reduced by acquiring data points with a large functional variance. Thus, to select data points that maximize the functional variance, we use the following decision criterion:

$$\hat{\mathbf{x}}(\mathbf{x}, \tilde{\mathbf{D}}_{\tilde{\mathbf{x}}, \tilde{\mathbf{y}}}) = \arg \max_{\tilde{\mathbf{x}} \in A} V_{\omega}[\log p(\tilde{\mathbf{y}}|\tilde{\mathbf{x}}, \boldsymbol{\omega})]. \quad (11)$$

Using this method, we can design experiments if a posterior distribution is created only once.

3. PARAMETER UNCERTAINTY REDUCTION FRAMEWORK

Our proposed framework to reduce parameter uncertainty in a model is summarized in **Figure 1**. The proposed framework consists of three steps. In step 1, a Bayesian inference [15] is performed using already obtained experimental data and a prior distribution, and a posterior distribution of parameters is

obtained. In step 2, the experimental design is conducted via equation (11) using the posterior distribution. Finally, in step 3, a Bayesian inference is conducted using the following equation for the prior distribution, the already obtained experimental data, and the designed experimental data:

$$p_{post}(\boldsymbol{\omega}|\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*) \propto L(\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*|\boldsymbol{\omega})p_{prior}(\boldsymbol{\omega}), \quad (12)$$

where $\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*$ is the designed experimental data including the already obtained experimental data; $p_{post}(\boldsymbol{\omega}|\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*)$ is the joint posterior distribution of $\boldsymbol{\omega}$ given $\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*$; $L(\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*|\boldsymbol{\omega})$ is the likelihood of $\tilde{\mathbf{D}}_{\tilde{\mathbf{x}},\tilde{\mathbf{y}}}^*$; and $p_{prior}(\boldsymbol{\omega})$ is the joint prior distribution of $\boldsymbol{\omega}$. As a result of step 3, the posterior distribution of parameters is updated and the parameter uncertainty is reduced effectively .

4. NUMERICAL DEMONSTRATION

4.1. Fracture Probability Estimation Model of a Fuel Cladding Tube

We demonstrate the applicability of the proposed framework for reducing parameter uncertainty in the context of nuclear engineering. In this numerical demonstration, we conducted the Bayesian optimal experimental design using a fracture probability estimation model of a fuel cladding tube that was developed in our previous study [16]. The fracture probability estimation model was developed to provide an estimate of the fracture probability of a non-irradiated, pre-hydrated Zircaloy-4 cladding tube specimen under LOCA conditions. This non-irradiated, pre-hydrated Zircaloy-4 cladding tube specimen is used as a surrogate specimen for a high burnup fuel cladding tube specimen. This is because the amount of oxidation and the initial hydrogen concentration are the main contributors to the fuel fracture boundary [17]. Although the pre-hydrated cladding tube specimen is used as a surrogate specimen for the high-burnup fuel cladding tube specimen, it still requires high experimental costs to conduct experiments using the pre-hydrated cladding tube specimen. Therefore, using the optimal experimental design, we obtained informative data points and effectively reduced the parameter uncertainty in the model with minimal data acquisition.

The fracture probability estimation model was developed using a generalized linear model and the experimental data of the fracture or non-fracture of the cladding tube specimen, which were obtained by integral thermal shock tests [16]. The experimental data were converted into binary data: fracture = 1 and non-fracture = 0. Here, we define a true distribution for the binary data as follows:

$$Y_i \sim \text{Bernoulli}(P_{true}(Y_i = 1|\mathbf{X}_i)), \quad (13)$$

$$P_{true}(Y_i = 1|\mathbf{X}_i) = \Phi(10 + 7\log(X_{1i}) + 20\log(\frac{X_{2i}}{10^4} + \gamma_{true})), \quad (14)$$

$$\gamma_{true} = 1, \quad (15)$$

where Y_i is a binary response variable for the i th observation concerning the fracture or the non-fracture of the cladding tube specimen; $P_{true}(Y_i = 1|\mathbf{X}_i)$ is the probability that $Y_i = 1$ given \mathbf{X}_i ; \mathbf{X}_i is the vector of explanatory variables for the i th observation; Φ is the cumulative distribution function of the standard normal distribution; and X_{1i} and X_{2i} are explanatory variables of the equivalent cladding reacted (ECR) in (-) and the initial hydrogen concentration in weight parts per million (wppm) for the i th observation, respectively.

The model is defined as

$$Y_i \sim \text{Bernoulli}(P_{pred}(Y_i = 1|\mathbf{X}_i)), \quad (16)$$

$$P_{pred}(Y_i = 1|\mathbf{X}_i) = \Phi(\beta_0 + \beta_1 \log(X_{1i}) + \beta_2 \log(\frac{X_{2i}}{10^4} + \gamma_{pred})), \quad (17)$$

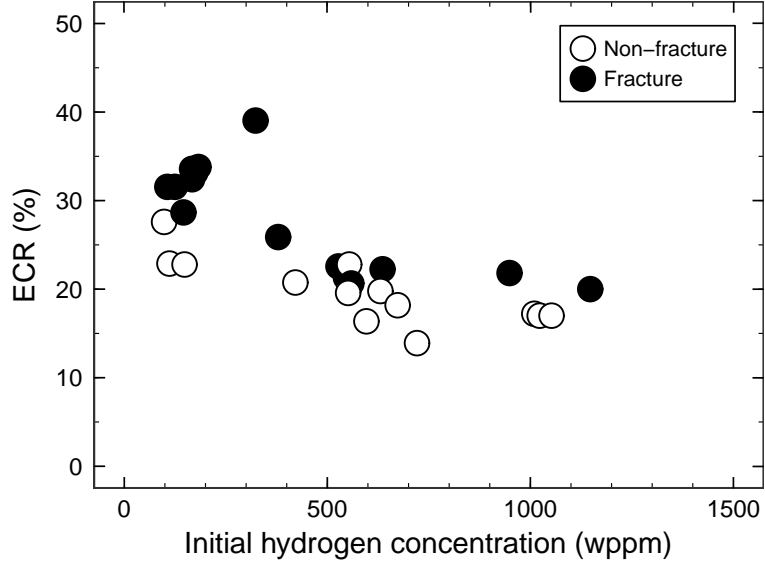


Figure 2: Experimental data generated from the true distribution.

$$\gamma_{pred} = 1, \quad (18)$$

where $P_{pred}(Y_i = 1 | \mathbf{X}_i)$ is the probability that $Y_i = 1$ when \mathbf{X}_i is given, and β_0 , β_1 , and β_2 are unknown coefficients to be estimated. These unknown coefficients are estimated using Bayesian inference with the following marginal prior distributions [16]:

$$p_{prior}(\beta_0) \sim Normal(7.59, 2.10), \quad (19)$$

$$p_{prior}(\beta_1) \sim Normal(6.67, 1.84), \quad (20)$$

$$p_{prior}(\beta_2) \sim Normal(0, 100). \quad (21)$$

4.2. Bayesian Optimal Experimental Design and Parameter Uncertainty Reduction

We performed the Bayesian optimal experimental design over a design space that consisted of 816 discrete data points: ECR ranged from 0% to 50% in increments of 1%, and the initial hydrogen concentration ranged from 0 to 1500 wppm in increments of 100 wppm.

Let us assume that experimental data generated from the true distribution are initially provided as shown in **Figure 2**. Using these data, we performed Bayesian inference 1 in step 1 of **Figure 1** and obtained a joint posterior distribution of the unknown coefficients, that is, β_0 , β_1 , and β_2 . The joint posterior distribution of the coefficients was approximated by numerical simulation using the MCMC algorithm. In particular, the No-U-Turn sampler (NUTS) [18], an adaptive form of the Hamiltonian Monte Carlo sampling for MCMC samplers, was used in this study. We performed the numerical simulations using Stan, a probabilistic programming language [19, 20], via the rstan package version 2.15.1 [21, 22], for the R language version 3.3.1 [23]. For the MCMC sampling for the joint posterior distribution, a total of 27,000 iterations were run for four chains, and the first 2,000 iterations of each chain were discarded as *warm-up* iterations [15]. The thinning interval of the chains was set to 1. Thus, the total number of iterations was 10^5 .

Then, we calculated the functional variance using equation (11) over the design space and obtained the designed experimental data in descending order of functional variance. Here, we changed the number

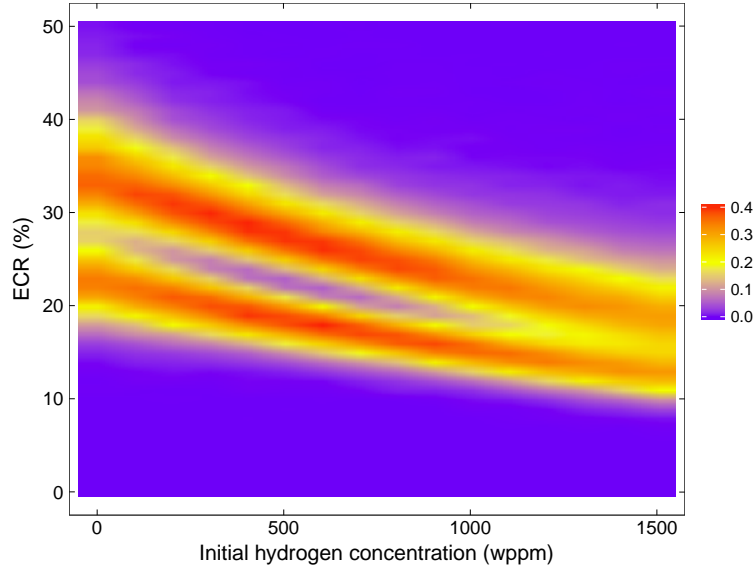


Figure 3: Calculated functional variance over the design space.

of observations of the designed experimental data from 1 to 200. Furthermore, we performed Bayesian inference 2 in step 3 of **Figure 1** using both the designed experimental data and the experimental data shown in **Figure 2**. The same MCMC method as the Bayesian inference 1 in step 1 of **Figure 1** was used for the Bayesian inference 2. The total number of iterations was 20,000 for this Bayesian inference. As a result, we obtained an updated parameter distribution with reduced parameter uncertainty.

For evaluating the effectiveness of our proposed framework, we calculated the Bayes generalization loss using the updated parameter distribution. The Bayes generalization loss was calculated using the R language as described by Matsuura [24].

4.3. Results and Discussion

Figure 3 shows calculated functional variances over the design space. The calculated functional variance is high near the observed experimental data.

Figure 4 shows the relationship between the Bayes generalization loss calculated over the design space and the number of observations of the experimental data. To illustrate the effectiveness of the proposed framework for parameter uncertainty reduction of the fracture probability estimation model, the Bayes generalization loss for a random experiment is also shown in this figure. Here, the random experiment indicates that the experimental data to be obtained are not designed, but are randomly generated from the design space. Dots and error bars in this figure show the means and the standard deviations of 100 independent experiments. As shown in this figure, when the optimal experimental design is performed, the Bayes generalization loss converges rapidly with an increasing number of observations of the experimental data. Therefore, the proposed framework is useful for effectively reducing the parameter uncertainty of a model.

As shown in **Figure 4**, even if a large number of designed experimental data are acquired, the generalization loss does not converge to the entropy S . Thus, the model used in this demonstration cannot accurately represent the true distribution. This implies that the model needs to be improved. In our proposed methodology, we selected data points with a high functional variance. We may apply this method sequentially along with the model selection. This simultaneous optimization of sampling and

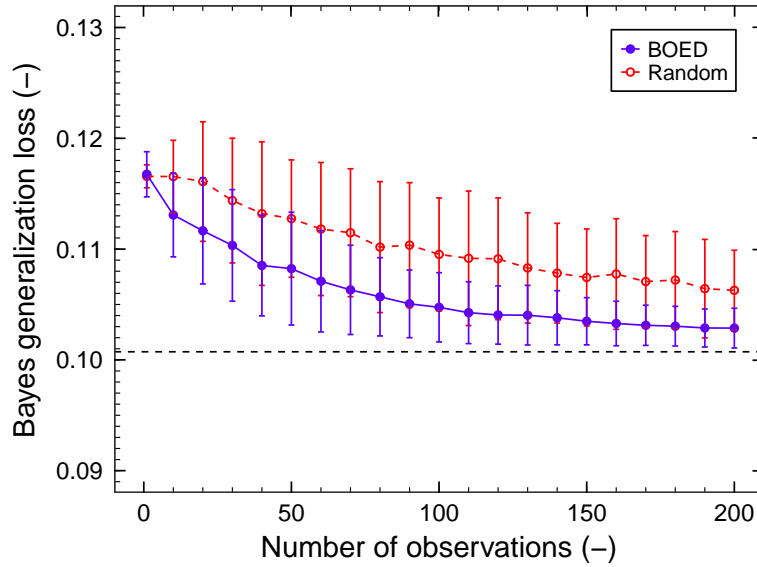


Figure 4: The relationship between the Bayes generalization loss and the number of observations of the experimental data. BOED is the case of the proposed framework using the Bayesian optimal experimental design and Random is the case of the random experiment. The black dashed line shows the entropy S .

model is seen in an active learning framework [5]. We plan to conduct further studies to implement this active learning framework for reducing epistemic uncertainties, namely, the parameter, model, and completeness uncertainties.

5. CONCLUSION

We developed a new framework to reduce parameter uncertainty in a model using the Bayesian optimal experimental design. In the experimental design, we used the functional variance, which is one of the components of WAIC, as a decision criterion for selecting informative data points. Also, using a case study, we applied the framework to reduce parameter uncertainty in the fracture boundary of a non-irradiated, pre-hydrated Zircaloy-4 cladding tube specimen under LOCA conditions. The results of the case study proved that the proposed framework greatly reduced the Bayes generalization loss with minimal sample size compared with the case in which the experimental data were randomly obtained. Thus, the proposed framework is useful for effectively reducing parameter uncertainty of safety-related events that rarely occur or require high experimental costs .

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