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Proposal and applicability of estimated criticality lower-limit multiplication factor using the bootstrap method

Takuto Hayashi[a*], Tomohiro Endo[a], and Akio Yamamoto[a]

[a] *Department of Applied Energy, Graduate School of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8603, Japan*

Abstract

To judge whether an application system is a subcritical state or not based on numerical results of the effective neutron multiplication factor k_{eff}, an evaluation method of the estimated criticality lower-limit multiplication factor (ECLLMF) using the bootstrap method is newly proposed. By utilizing numerical results of k_{eff} for critical benchmark-problems that are selected depending on neutronic similarity to the application system, the ECLLMF should be carefully and conservatively estimated based on uncertainties of k_{eff} due to a criticality safety analysis code, experimental uncertainty, and covariance matrix of the nuclear data library. Furthermore, the frequency distribution of k_{eff} for these problems does not necessarily obey an ideal normal distribution. Using a resampling technique called 'bootstrap method,' the proposed method can reasonably estimate the ECLLMF considering the uncertainties and nuclear data-induced correlation between each critical benchmark-problem without the assumption of normality. To investigate the applicability of the proposed method, the approach-to-criticality experiment was carried out at the Kyoto University Critical Assembly (KUCA). Comparison of numerical results of k_{eff} and the ECLLMF using the bootstrap method indicated that the proposed method was able to judge an actual subcritical core as subcritical state.

*Corresponding author. Email: t-hayashi@fermi.energy.nagoya-u.ac.jp

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1. Introduction

Criticality safety control is important to prevent criticality accidents at facilities and equipment that handle nuclear fuel materials. The criticality safety analysis is carried out by predicting the effective neutron multiplication factor k_{eff} via numerical calculations. Evaluation of the adequate safety margin depending on the uncertainty is necessary because numerical results of k_{eff} include uncertainties due to statistical uncertainty of continuous energy Monte Carlo calculation, experimental uncertainty, and covariance matrix of nuclear data. Then, the subcritical judgment criterion is set based on the safety margin.

An example of the subcritical judgment criterion is the estimated criticality lower-limit multiplication factor (ECLLMF) using the assumption of normality for uncertainties [1]. The ECLLMF using the assumption of normality is analytically evaluated using the statistical property of the non-central Student's *t*-distribution [2]. This method evaluates the ECLLMF by assuming the normal distribution even if an actual frequency distribution of k_{eff} does not obey the normal distribution. In addition, this method cannot consider the calculational, experimental, and nuclear data-induced uncertainties of k_{eff}, and the correlation between the application and critical benchmark systems.

To solve the above-mentioned problems, the evaluation method of ECLLMF using the bootstrap method [3],[4] is newly proposed in the present paper. The bootstrap method does not require the assumption of normality by resampling the k_{eff} that are calculated for selected critical benchmark-problems. Therefore, the proposed method can reasonably evaluate the ECLLMF considering the actual frequency distribution of k_{eff}. Our previous study clarifies

that the ECLLMF using the proposed method is almost equal to that with the assumption of normality when the frequency distribution of k_{eff} obeys the normal distribution [5]. The effects of skewness and kurtosis of the frequency distribution of k_{eff} on the ECLLMF are also investigated [5]. As in the same manner of the Whisper-1.1 code [6], the evaluation method of the ECLLMF using the bootstrap method is considered the uncertainties of k_{eff} and the nuclear data-induced correlation between the application system and critical benchmark-problems [7],[8]. Although the numerical verifications are carried out in our previous study, the proposed method is not applied to an actual experimental system. Therefore, applicability of the proposed method to an actual system has not been clarified.

The purpose of the present paper is the investigation about the applicability of the ECLLMF using the bootstrap method to an actual experimental system. To achieve this purpose, the approach-to-criticality experiment at Kyoto University Critical Assembly (KUCA)-C core was numerically analysed. Namely, we aimed to validate whether the proposed method was able to judge an actual subcritical core as subcritical state by comparing numerical results of k_{eff} with the ECLLMF using the bootstrap method.

Subsequent sections of the paper are structured as follows. In Section 2, the theory of the ECLLMF using the bootstrap method is explained. The experimental and calculational conditions, and results are described in Section 3. Finally, Section 4 presents the concluding remarks.

2. Theory

2.1. Estimated Criticality Lower-Limit Multiplication Factor

In this section, the theoretical concept of the ECLLMF is briefly explained. The ECLLMF is the upper subcritical limit, which is a criterion of effective neutron multiplication factor that can be treated as subcritical state in consideration of calculational uncertainties. The evaluation process of ECLLMF consists of the following two procedures: One is calculations for similar

critical benchmark-problems, and the other is statistical processing for the calculated values of k_{eff} selected from the critical benchmark-problems.

Let us consider an application system for criticality safety analysis, and collect critical systems strongly-correlated with the application system. Using a criticality safety analysis code such as the continuous energy Monte Carlo code MCNP6.2 [9], effective neutron multiplication factors k_{eff} are evaluated for the application and collected critical systems. Note that the calculated values of k_{eff} for critical systems are not necessarily equal to unity because of calculational uncertainty (*e.g.*, statistical uncertainty of the Monte Carlo code), experimental uncertainty (*e.g.*, fabrication tolerance), and nuclear data-induced uncertainty. Then, the calculated value of k_{eff} for the application system (hereafter denoted as k_A) can be regarded as a sample belonging to a population distribution of collected critical systems. For example, let us assume that the population distribution follows the normal distribution with population mean μ and variance σ^2. Generally, the supercritical and subcritical probabilities are p and $(1-p)$ when $k_A = \mu - \alpha_p \sigma$ corresponds to the lower $100p$th percentile of the population distribution, where p is the supercritical probability, and $-\alpha_p$ is the lower $100p$th percentile of the standard normal distribution. Namely, if the population distribution is exactly known as the normal distribution $\mathcal{N}(\mu, \sigma^2)$, the ECLLMF can be estimated by $\mu - \alpha_p \sigma$ so that the supercritical probability is equal to p.

Note that, the true population distribution is unknown in an actual situation and does not necessarily follow the normal distribution. Thus, instead of using μ and σ, the ECLLMF has to be estimated by utilizing these sample estimates, *i.e.*, the sample mean $\bar{k}$ and unbiased sample variance s^2, respectively. However, if $k_A = \bar{k} - \alpha_p s$, the supercritical probability is not equal to p due to statistical uncertainties of the estimators $\bar{k}$ and s. Consequently, a margin value α is determined based on the following probabilistic relationship:

$$\Pr\left(\bar{k} - \alpha s \leq k_p\right) = \gamma, \tag{1}$$

where $\Pr(x \leq y)$ means the probability satisfying $x \leq y$, k_p corresponds to the lower

$100p$th percentile for the cumulative frequency of collected critical systems, and γ is the confidence level. Equation 1 indicates that the probability satisfying $\bar{k} - \alpha s \leq k_p$ is γ. If the distribution can be approximated by a normal distribution, α can be analytically estimated based on the statistical property of the non-central Student's *t*-distribution. When the sample size of collected critical systems is small, the estimated α value becomes larger than α_p as a result of the low precision of the sample mean and standard deviation. As the sample size becomes sufficiently large, the estimated α saturates α_p because the sample mean and standard deviation agree with the population mean and standard deviation, respectively.

2.2. Bootstrap Method

In this section, an evaluation method for ECLLMF using the bootstrap method [3],[4] is newly proposed and the numerical calculation procedure is explained. In general, the bootstrap method enables us to numerically estimate histogram, variance, and confidence interval for an estimator (*e.g.*, mean, variance, median) by a large number of resamples from original data. If the sample size of the original data is N, N-times sampling with replacement is carried out to produce a resample. In other words, the bootstrap method generates virtual resamples by duplicate sampling based on the empirical distribution inferred from the histogram of original data.

In the proposed method, the margin value α is estimated by generating a large number of resamples from the original data of k_{eff}, which are calculated for selected critical benchmark-problems. Resampling k_{eff} of critical benchmark-problem with strong correlation to the application system would be better than resampling from the original data of k_{eff} with the same weights. Thus, the weighted resampling method [10] is utilized with weights based on the nuclear data-induced correlation coefficient (also known as the representativity factor [11],[12]) between the application system and selected critical benchmark-problems. In addition, the frequency distribution of k_{eff} is assumed to be expressed by a Gaussian mixture model, where

each of k_{eff} values for the selected critical benchmark-problems follows a normal distribution to consider calculational, experimental, and nuclear data-induced uncertainties of k_{eff}.

Calculation procedures of the ECLLMF using the bootstrap method are summarized as follows:

1. Prepare an original dataset of N numerical results for selected critical benchmark-problems, $\mathbf{K} = \{k_1, k_2, \dots, k_N\}$. Note that the experimental k_{eff} values (hereafter denoted as k_{exp}) are not necessarily equal to unity because of the simplification of the benchmark model (*e.g.*, simplified geometry and neglected impurities). Thus, each element k_i in $\mathbf{K}$ is corrected by the bias between the experimental value $k_{\mathrm{exp},i}$ and unity:

$$k_i = k_{\mathrm{calc},i} - (k_{\mathrm{exp},i} - 1), \tag{2}$$

   where the subscript 'i' is the index for selected critical benchmark-problems and $k_{\mathrm{calc},i}$ is the numerical result of k_{eff} obtained by the Monte Carlo code in this study.
2. Prepare a dataset of N total uncertainties of k_i for selected critical benchmark-problems, $\mathbf{U} = \{u_1, u_2, \dots, u_N\}$. The estimation of total uncertainties $\mathbf{U}$ is explained in Sec. 2.3.
3. Select N 'bootstrap indexes $\boldsymbol{j} = \{j_1, j_2, \dots, j_N\}$' from the index ($1 \le i \le N$) of selected critical benchmark-problems by sampling with replacement. Let the weighting factor for each of selected critical benchmark-problems be w_i, which is evaluated as described Sec. 2.4. The normalized weighting factor w_i is used as the probability to select for the corresponding index i. This procedure corresponds to the intensively resampling from highly correlated critical benchmark-problems.
4. Select a set of k_j and u_j corresponding the bootstrap index j from $\mathbf{K}$ and $\mathbf{U}$, then add a perturbed uncertainty zu_j to k_j (hereafter denoted as $x_j^* = k_j + zu_j$), where the subscript j means an element in the vector of bootstrap indexes $\boldsymbol{j}$ and z is a standard normal random number and superscript '$*$' means the bootstrap sample.

5. A set of the bootstrap sample $\mathbf{X}^{*b} = \{x_{j_1}^{*b}, x_{j_2}^{*b}, \dots, x_{j_N}^{*b}\}$ is repeatedly sampled ($b = 1,2, \dots, B$), where the superscript '$* b$' means the bth set of bootstrap sample, and B is the total number of bootstrap sampling. In the case of estimating the confidence interval using the bootstrap method, $B = 10^3$ is a typical number [4]. To estimate the ECLLMF, B is set to be a sufficiently large number ($B = 10^5$) so that statistical uncertainty caused by the bootstrap sampling would be less than statistical uncertainty of Monte Carlo calculation using the MCNP6.2 code. Consequently, B sets of bootstrap samples $\mathbf{X}^{*1}, \mathbf{X}^{*2}, \dots, \mathbf{X}^{*B}$ are provided.
6. For each set of bootstrap samples generated in procedure 5, bootstrap replicates of the sample mean $\hat{k}^{*b}$ and sample standard deviation $\hat{s}^{*b}$ are evaluated, respectively:

$$\hat{k}^{*b} = \frac{1}{N}\sum_{l=1}^{N} x_{j_l}^{*b}, \tag{3}$$

$$\hat{s}^{*b} = \sqrt{\frac{1}{N-1}\sum_{l=1}^{N}\left(x_{j_l}^{*b} - \hat{k}^{*b}\right)^2}. \tag{4}$$

where the hat '$\widehat{\ }$' means an estimator such as mean or standard deviation.

7. The lower $100p$th percentile for the cumulative frequency of the original dataset (k_p) is numerically evaluated based on the cumulative distribution function (CDF) of the Gaussian mixture model. The CDF is the weighted sum of the individual CDFs as follows:

$$F(x) = \frac{\sum_{i=1}^{N} w_i F_i(x)}{\sum_{i=1}^{N} w_i}, \tag{5}$$

$$F_i(x) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{x - k_i}{\sqrt{2u_i^2}}\right)\right], \tag{6}$$

where w_i and u_i are the weighting factor and total uncertainty for k_i corresponding to the i th critical benchmark-problem, respectively, and $\mathrm{erf}(x)$ means the error function. Based on Equations 5 and 6, k_p is calculated using the bisection method so as to satisfy $F(k_p) = p$, where the supercritical probability p is set to be 2.5% in this paper.

8. To evaluate the bootstrap histogram for $\bar{k} - \alpha s$, the following value of k_{sub}^{*b} is calculated using the bootstrap replicate of the sample mean $\hat{k}^{*b}$ and standard deviation $\hat{s}^{*b}$:

$$k_{\mathrm{sub}}^{*b} = \hat{k}^{*b} - \alpha \hat{s}^{*b}. \tag{7}$$

The bootstrap replicate of k_{sub}^{*b} are sorted in ascending order. Then, the γB th smallest value in the sorted k_{sub}^{*b} is denoted as $k_{\mathrm{sub}}^{*(\gamma B)}$. If the γB value is not an integer, $k_{\mathrm{sub}}^{*(\gamma B)}$ is obtained by linear interpolation between the two nearest neighbor values corresponding to integer values. The value of α is determined so that $k_{\mathrm{sub}}^{*(\gamma B)}$ is equal to k_p using the bisection method:

$$k_{\mathrm{sub}}^{*(\gamma B)} = k_p. \tag{8}$$

The confidence level γ is set to be 97.5% in this paper.

9. Finally, the ECLLMF using the bootstrap method k_{sub}^{*} is obtained by the expected value of B bootstrap replicates $k_{\mathrm{sub}}^{*1}, k_{\mathrm{sub}}^{*2}, \ldots, k_{\mathrm{sub}}^{*B}$:

$$k_{\mathrm{sub}}^{*} = \frac{1}{B} \sum_{b=1}^{B} k_{\mathrm{sub}}^{*b}. \tag{9}$$

2.3. Uncertainty Quantification for k_{eff}

In this section, the uncertainty quantification for the effective neutron multiplication factor k_{eff} is explained. To evaluate the ECLLMF, the proposed method assumes that the calculated k_i value for each of selected critical benchmark-problems has uncertainties due to the

following three causes: calculational uncertainty of the Monte Carlo code, experimental uncertainty in the benchmark-problem, and covariance data of nuclear data. The total uncertainty of k_i for the ith critical benchmark-problem is estimated by the square root for the sum of squares of calculational, experimental, and nuclear data-induced uncertainties:

$$u_i = \sqrt{u_{\mathrm{calc},i}^2 + u_{\mathrm{exp},i}^2 + u_{\mathrm{XS},i}^2}, \tag{10}$$

where $u_{\mathrm{calc},i}$ is the calculational uncertainty of the Monte Carlo code, $u_{\mathrm{exp},i}$ is the experimental uncertainty in the ith critical benchmark-problem, and $u_{\mathrm{XS},i}$ is a posterior nuclear data-induced uncertainty after applying the generalized linear least squares (GLLS) method [13].

The $k_{\mathrm{calc},i}$ value calculated by the Monte Carlo code is expected to approximately follow a normal distribution based on the central limit theorem. Thereby, the calculational uncertainty $u_{\mathrm{calc},i}$ is approximately obtained by the statistical uncertainty of k_{eff}-eigenvalue calculation using the Monte Carlo code. Since the Monte Carlo calculation can be regarded as a rigorous numerical method to solve the neutron transport equation, other analytical modeling uncertainties are assumed to be smaller than the calculational uncertainty. Namely, other analytical modeling uncertainties except for the statistical uncertainty of the Monte Carlo code are disregarded in this study. The experimental uncertainty $u_{\mathrm{exp},i}$ is provided along with the experimental value $k_{\mathrm{exp},i}$ in the benchmark problems such as ICSBEP [14]. As shown in Sec. 3.3, $u_{\mathrm{exp},i}$ is larger than $u_{\mathrm{calc},i}$ because sufficient number of active cycles is generally used in the Monte Carlo code to reduce the calculational uncertainty $u_{\mathrm{calc},i}$.

As in the same methodology in the Whisper-1.1 code [6], rather than simply using a priori nuclear data-induced uncertainty, reducing the uncertainty through the data assimilation technique using critical benchmark-problems would be more reasonable evaluation of the $u_{\mathrm{XS},i}$ value. Namely, based on the GLLS method, the a posteriori nuclear data-induced covariance matrix $\boldsymbol{\Sigma}_{k'}$ is evaluated as:

$$\mathbf{\Sigma}_{k'} = \mathbf{S}_{k,\sigma}\mathbf{\Sigma}_{\sigma}\mathbf{S}_{k,\sigma}^{\top} - \mathbf{S}_{k,\sigma}\mathbf{\Sigma}_{\sigma}\mathbf{S}_{k,\sigma}^{\top}\left(\mathbf{S}_{k,\sigma}\mathbf{\Sigma}_{\sigma}\mathbf{S}_{k,\sigma}^{\top} + \mathbf{V}_{\text{exp}}\right)^{-1}\mathbf{S}_{k,\sigma}\mathbf{\Sigma}_{\sigma}\mathbf{S}_{k,\sigma}^{\top}, \tag{11}$$

$$\mathbf{S}_{k,\sigma} \equiv [\mathbf{S}_{k_1,\sigma} \quad \mathbf{S}_{k_2,\sigma} \quad \cdots \quad \mathbf{S}_{k_N,\sigma}]^{\top}, \tag{12}$$

$$\mathbf{V}_{\text{exp}} \equiv \text{diag}\left(u_{\text{exp},1}, u_{\text{exp},2}, \cdots, u_{\text{exp},N}\right), \tag{13}$$

where $\mathbf{\Sigma}_{\sigma}$ is a priori covariance data of nuclear data before applying the GLLS method; $\boldsymbol{S}_{k,\sigma}$ is the sensitivity matrix for $\{k_{\text{calc},1}, k_{\text{calc},2}, \ldots, k_{\text{calc},N}\}$; $\mathbf{V}_{\text{exp}}$ is the experimental variance matrix which is a diagonal matrix consisting of $\{u_{\text{exp},1}, u_{\text{exp},2}, \cdots, u_{\text{exp},N}\}$; and the superscripts '$\top$' and '$-1$' indicate transpose and inverse of the matrix, respectively. Finally, the square root of the diagonal elements of $\mathbf{\Sigma}_{k'}$ corresponds to the nuclear data-induced uncertainties $\{u_{\text{XS},1}, u_{\text{XS},2}, \cdots, u_{\text{XS},N}\}$ after applying the GLLS method. In this study, the GLLS calculation based on Equations (11)–(13) was carried out using the SCALE6.2.3/TSURFER module [15] with the sensitivity coefficient matrix $\boldsymbol{S}_{k,\sigma}$ evaluated by the iterated fission probability method of the MCNP6.2 code [16].

2.4. Selection and Weighting of Critical Benchmark-Problems

In this section, the selection method of critical benchmark-problems and the calculation method of their weighting factors are explained. Critical benchmark-problems should be carefully selected and resampled based on weighting factors representing the similarity of neutronic parameter such as k_{eff}. As in the same manner in the Whisper-1.1 code [6], the weighting factors are evaluated by the nuclear data-induced correlation (or representativity factor [11],[12]) between the application system and critical benchmark-problems.

The nuclear data-induced correlation coefficient $c_{k,i}$ between the application system k_A and the ith critical benchmark-problem $k_{\text{calc},i}$ are obtained using the sandwich formula with k_{eff}-sensitivity coefficient matrices and a covariance matrix of nuclear data $\mathbf{\Sigma}_{\sigma}$:

$$c_{k,i} = \frac{\text{cov}(k_A, k_{\text{calc},i})}{\sqrt{\text{var}(k_A)}\sqrt{\text{var}(k_{\text{calc},i})}}, \tag{14}$$

$$\mathrm{var}(k_A) = \mathbf{S}_{k_A,\sigma}\boldsymbol{\Sigma}_\sigma\mathbf{S}_{k_A,\sigma}^{\top}, \tag{15}$$

$$\mathrm{var}(k_{\mathrm{calc},i}) = \mathbf{S}_{k_i,\sigma}\boldsymbol{\Sigma}_\sigma\mathbf{S}_{k_i,\sigma}^{\top}, \tag{16}$$

$$\mathrm{cov}(k_A, k_{\mathrm{calc},i}) = \mathbf{S}_{k_A,\sigma}\boldsymbol{\Sigma}_\sigma\mathbf{S}_{k_i,\sigma}^{\top}, \tag{17}$$

where $\mathrm{var}(k_A)$ and $\mathrm{var}(k_{\mathrm{calc},i})$ are nuclear data-induced variances of k_A and $k_{\mathrm{calc},i}$; $\mathrm{cov}(k_A, k_{\mathrm{calc},i})$ is nuclear data-induced covariance between k_A and $k_{\mathrm{calc},i}$; $\mathbf{S}_{k_A,\sigma}$ and $\mathbf{S}_{k_i,\sigma}$ are k_{eff}-sensitivity coefficient matrices (or row vectors) of k_A and $k_{\mathrm{calc},i}$ with respect to nuclear data. As the value of $c_{k,i}$ is closer to unity, the variation in $k_{\mathrm{calc},i}$ caused by uncertainty of nuclear data is expected to have a more similar trend to that in k_A.

Using the evaluated correlation coefficient $c_{k,i}$, the weighting factor for the ith critical benchmark-problem is empirically evaluated by the following linear function:

$$w_i = \frac{c_{k,i} - c_{k,\mathrm{acc}}}{c_{k,\mathrm{max}} - c_{k,\mathrm{acc}}}, \tag{18}$$

where $c_{k,\mathrm{max}} = \max(c_{k,i})$ is the largest correlation coefficient among selected $c_{k,i}$, and $c_{k,\mathrm{acc}}$ is a threshold for the acceptable correlation coefficient. The $c_{k,\mathrm{acc}}$ value is determined so that the sum of w_i satisfies Equation (19) shown in later. If $c_{k,i} > c_{k,\mathrm{acc}}$, the ith critical benchmark-problem is selected for the evaluation of the ECLLMF. Here, the total number of selected critical benchmark-problems N is efficiently determined until the descending order-based sum of weighting factors w_i satisfies the following relationship [6]:

$$\sum_{i=1}^{N} w_i = w_{\mathrm{req}}, \tag{19}$$

$$w_{\mathrm{req}} = w_{\mathrm{min}} + w_{\mathrm{penalty}}(1 - c_{k,\mathrm{max}}), \tag{20}$$

where w_{req} means the required total weight, w_{min} is the minimum total number of selected critical benchmark-problems, and w_{penalty} is a penalty factor when the critical benchmark-problem is weakly correlated with the application system. For example, if an application system and critical benchmark-problems are completely dissimilar, *i.e.*, $c_{k,\mathrm{max}} = 0$, the total weight is

required by $(w_{\min} + w_{\text{penalty}})$. Referring to the default values of the Whisper-1.1 code [6], $w_{\min} = 25$ and $w_{\text{penalty}} = 100$ were used in this paper.

3. Application to KUCA Experiment

3.1. Experimental Conditions

At the Kyoto University Critical Assembly (KUCA) [17], the approach-to-criticality experiment was carried out in the C35G0 (4 rows) assembly. The core configuration and detector location are shown in **Figure 1**.

< Figure 1 >

The KUCA C-core is a light-water reflected and moderated core. The fuel used in the C-core is a plate-type fuel (93% enriched) made of U-Al alloy (thickness 0.5 mm) that is cladded with a thick aluminum layer (thickness 0.5 mm). The overall length, width, and thickness of the fuel plate are 600 mm, 62 mm, and 1.5 mm, respectively. The region containing uranium (U-Al alloy) is called fuel meat, of which length, width, and thickness are 570 mm, 52.8 mm, and 0.5 mm, respectively. Each fuel plate contains 8.89 g of ^{235}U. A fuel element is composed by inserting the fuel plates in an aluminum fuel frame (called C35G0). The maximum number of fuel plates and fuel pitch of the C35G0 frame are 40 and 3.49 mm, respectively. The fuel elements are loaded in a core tank (diameter 2 m and depth 2 m). The light-water is poured into the core tank to be used as the reflector and moderator for neutrons. Control rods (C1,C2,C3), safety rods (S4,S5,S6), Am-Be neutron source (N), fission chambers (1,2,3), BF_3 detectors (1,3), and ^{3}He detectors (2) are placed around the core. The safety rods are fully withdrawn during the experiment.

The approach-to-criticality experiment started from a base core configuration (hereafter denoted as step 0), where the number of fuel plates is less than critical mass to surely satisfy

the subcritical state. The number of critical fuel plates was step-by-step predicted using the inverse multiplication method [17]. In this study, each of the fuel loading patterns was denoted as steps 1–4. **Table 1** shows the number of fuel plates loaded in each fuel frame for steps 0–4. Finally, the criticality was achieved at step 4 without the start-up neutron source. Note that the excess reactivity was compensated by inserting the C3 control rod.

< Table 1 >

3.2. Calculational Conditions

Although the calculation model was based on the reference [17], a simplified model was used for some parts where detailed information was not available. The water density was estimated based on the actual water temperature of 297.55 K [18]. The k_{eff}-eigenvalue calculation of the application system and the critical benchmark-problems was carried out using the MCNP6.2 code [9] and cross-section library ENDF/B-VII.1 [19]. The total number of neutron histories was 50 million, *i.e.*, neutron history per cycle=100,000, active cycle=500, and inactive cycle=100. The critical benchmark-problems were selected from the ICSBEP database [14] using the Whisper-1.1 code [6]. The values of $c_{k,\mathrm{acc}}$ and $c_{k,\mathrm{max}}$ for the application system (step 4) were 0.8212 and 0.9011, respectively. The number of selected critical benchmark-problems was 97.

The GLLS calculation was carried out using the SCALE6.2.3/TSURFER module [15]. The 56 energy-group sensitivity coefficient matrix (or the sdf-formatted file which is utilized in the SCALE6.2.3 code) was evaluated by the iterated fission probability method of the MCNP6.2 code [16]. The sdf-formatted files were obtained by converting the MCNP6.2 output file using an in-house Python program. As the covariance matrix of nuclear data, the 56 energy-group covariance data (56groupcov7.1) provided along with the SCALE6.2.3 code was used.

The ECLLMF calculation was carried out using the programming language R for

statistical computing. The supercritical probability p and confidence level γ were 2.5% and 97.5%, respectively [1]. The total number of bootstrap sampling B was set to be 10^5. Since the fuel composition and H/U ratio were constant at steps 0–4, the fuel loading pattern at step 4 was utilized as a representative application system. The ECLLMF using the bootstrap method, k^*_{sub} was evaluated by the procedure as described in Sec. 2.2. To discuss the impact on ECLLMF by considering the actual frequency distribution of k_i, total uncertainty of k_i and nuclear data-induced correlation, the following four Cases of ECLLMFs were calculated:

A) ECLLMF based on the assumption of normality [1], where the frequency distribution of k_i was approximated by a normal distribution. Then, the margin value α was analytically evaluated using the statistical property of the non-central Student's *t*-distribution [2]. The ECLLMF in Case A was denoted as k_{sub}.

B) ECCLMF using the bootstrap method without the total uncertainty and correlation for each of selected critical benchmark-problems. Namely, the total uncertainty and weighting factor were set to be $u_i = 10^{-8}$ and $w_i = 1/N$, respectively. By compared with Case A, Case B aimed to discuss the impact of considering the actual frequency distribution on ECLLMF.

C) ECLLMF using the bootstrap method only with the total uncertainty that was estimated as described Sec. 2.3. The weighting factor was set to be $w_i = 1/N$ like Case B. Comparison between Cases B and C aimed to discuss the impact of considering the total uncertainty on ECLLMF.

D) ECCLMF using the bootstrap method with the total uncertainty and correlation that were estimated as described Secs. 2.3 and 2.4. Comparison between Cases C and D aimed to discuss the impact of considering the nuclear data-induced correlation (or the difference in weighting factor w_i) on ECLLMF.

By comparing numerical results of k_{eff} and the evaluated ECLLMF in Case D, the subcritical judgments were carried out for steps 0–4. If a numerical result of $k_A + 3u_A$ for each step was

smaller than the ECLLMF k^*_{sub}, the fuel loading pattern was judged as subcritical state, vice versa. Here, k_A and u_A are the numerical result of k_{eff} and the calculational uncertainty (1σ) calculated by the MCNP6.2 code for each of steps 0–4. The $k_A + 3u_A$ was utilized instead of k_A to consider the calculational uncertainty for the application system [20].

3.3. Results and Discussion

Figure 2(a) shows the variation of calculational uncertainty (*i.e.*, statistical uncertainty of the MCNP6.2 code) $u_{\text{calc},i}$, experimental uncertainty $u_{\text{exp},i}$, and nuclear data-induced uncertainty $u_{\text{XS},i}$ with respect to effective neutron multiplication factor k_i of the ith critical benchmark-problem. As shown in Figure 2(a), $u_{\text{exp},i}$ was larger than $u_{\text{calc},i}$ because sufficient number of active cycles (=500) was used in the MCNP6.2 calculation to reduce $u_{\text{calc},i}$. In addition, $u_{\text{exp},i}$ was larger than $u_{\text{XS},i}$ because the data assimilation by the SCALE6.2.3/TSURFER module was carried out for selected critical benchmark-problems to reduce $u_{\text{XS},i}$. Consequently, it was confirmed that the dominant contribution of total uncertainty u_i for each of selected critical benchmark-problems was the experimental uncertainty $u_{\text{exp},i}$.

Figure 2(b) shows the variation of the correlation coefficient $c_{k,i}$ with respect to effective neutron multiplication factor k_i of the ith critical benchmark-problem. As shown in Figure 2(b), the experiment of heu-comp-therm-002, of which the abbreviation is denoted as hct2, had the highest $c_{k,i}$ in the selected critical benchmark-problems. For the selected problems in this study, there was a weak positive correlation ($\sim$0.64) between k_i and $c_{k,i}$.

< Figure 2 >

Table 2 summarizes the results of ECLLMF calculations for Case A (assumption of normality), Case B (bootstrap method without total uncertainty and correlation), Case C

(bootstrap method only with total uncertainty), and Case D (bootstrap method with total uncertainty and correlation). Since the positive correlation between k_i and $c_{k,i}$ (Figure 2(b)) resulted in the higher weight w_i for the larger k_i, the weighted mean of k_i in Case D was larger than the sample means of k_i in Cases A–C. In addition, Cases C and D considered the total uncertainty for each of selected critical benchmark-problems. Thus, the standard deviations s in Cases C and D were larger than those in Cases A and B.

< Table 2 >

To discuss the margin values α and ECLLMFs, histograms of effective neutron multiplication factor k_{eff} for Cases A–D are presented in **Figure 3**. The solid and dotted lines show the means $\bar{k}$ and ECLLMFs in Cases A–D, respectively. The dashed line in Figure 3(a) shows the normal distribution $\mathcal{N}(\bar{k}, s^2)$, where $\bar{k}$ and s^2 are the sample mean and unbiased variance of k_i, respectively. Figure 3(b) shows the frequency distribution of k_i with the corresponding histogram of bootstrap replicates of k_{sub}^{*b}. Similarly, Figures 3(c) and 3(d) show the Gaussian mixture models for Cases C and D with the corresponding histograms of k_{sub}^{*b}.

The means $\bar{k}$ and standard deviations s in Cases A and B were the same because each k_i had same weighting factor in Case B. Conversely, the margin value α in Case B was smaller than that in Case A; thereby k_{sub}^{*} in Case B was approximately 0.71% larger than k_{sub} in Case A. The skewness and kurtosis of frequency distribution of k_i in Figure 3(b) were approximately $+0.44$ and -0.67, respectively. As discussed in our previous study [5], the positive skewness and negative kurtosis resulted in the decrease of the margin value α when the ECLLMF was estimated using the bootstrap method. Namely, the bootstrap method was able to reasonably evaluate the margin value α considering the actual frequency distribution of k_i, without the assumption of normality.

Comparison of Cases B and C indicates that the consideration of total uncertainty resulted in the larger variance of k_{sub}^{*b} in Case C (see Figure 3(b) and 3(c)). By increasing the variance of k_{sub}^{*b}, the margin value α in Case C was increased so that the probability of $k_{\mathrm{sub}}^{*b} \leq k_p$ equaled γ. Furthermore, the standard deviation s in Case C was larger than that in Case B. Thus, by considering the total uncertainty, the αs-value in Case C was approximately 1.6 times larger than Case B. As a result, k_{sub}^{*} in Case C was approximately 0.61% smaller than that in Case B. Consequently, it was confirmed that the consideration of total uncertainty of k_i was important to conservatively evaluate the ECCLMF.

The comparison between Cases C and D revealed that the consideration of the nuclear data-induced correlation affected on the mean $\bar{k}$ in Case D, *i.e.*, increase of $\bar{k}$ in the case of KUCA C-core. The reason for this is because k_i values with higher correlation coefficients (*i.e.*, higher weighting factors) are intensively resampled in the weighted bootstrap procedure. Although the consideration of correlation also affected s and α, the increase of αs was smaller than that of $\bar{k}$. As a result, k_{sub}^{*} in Case D was slightly (approximately 0.16%) larger than that in Case C. Note that whether the consideration of correlation results in conservative or non-conservative evaluation of ECLLMF is case-by-case, *i.e.,* depends on the shape change in the Gaussian mixture model. When the critical benchmark-problems with high correlation coefficients $c_{k,i}$ were selected like this study, the consideration of the nuclear data-induced correlation had the smaller impact on ECLLMF than that of the total uncertainty of k_i. Overall, it was confirmed that the consideration of the actual frequency distribution of k_i had the largest impact on ECLLMF.

< Figure 3 >

Table 3 shows the results of MCNP6.2 calculations and subcritical judgment. As shown in Table 3, the k_A value became larger as the number of fuel plates increased. By comparing

$k_A + 3u_A$ with the ECLLMF using the bootstrap method with total uncertainty and correlation (0.98874 in Case D), step 0 was judged as subcritical state. Namely, it was confirmed that the proposed method was able to judge the actual subcritical core as subcritical state. Note that actual steps 1–3 were subcritical states, although the numerical predictions for these steps were not judged as subcritical states based on the safety margin of the ECLLMF. The C/E-value was approximately 1.008 in the critical state (step 4), *i.e.*, the present MCNP6.2 results seemed to be overestimated by approximately 800 pcm compared with the actual experimental results. The bias of C/E-value was probably caused by the uncertainties of the calculation model and fuel composition. As a future work, further uncertainty quantification of calculation model and fuel composition for the KUCA C-core is necessary.

< Table 3 >

4. Conclusion

In the present paper, the evaluation method of ECLLMF using the bootstrap method was newly proposed. The proposed method can reasonably evaluate the ECLLMF by resampling k_{eff} of selected critical benchmark-problems, without the assumption of normality. The total uncertainty for each of selected critical benchmark-problems is estimated by the square root for the sum of squares of calculational, experimental, and nuclear data-induced uncertainties. Then, the frequency distribution of k_{eff} is expressed by a Gaussian mixture model, where the nuclear data-induced correlation coefficient is utilized for the weighting factors to consider the nuclear data-induced correlation between the application system and selected critical benchmark-problems.

To investigate the applicability of the ECLLMF using the bootstrap method, the approach-to-criticality experiment at KUCA-C core was numerically analysed. The bootstrap method was able to evaluate the ECLLMF considering the actual frequency distribution of k_{eff}, which had

the largest impact on ECLLMF. Furthermore, the bootstrap method also enabled to consider the total uncertainty and the nuclear data-induced correlation of k_{eff}. The consideration of total uncertainty was important to conservatively evaluate the ECCLMF by the larger margin value α and standard deviation s. Consequently, it was confirmed that the proposed method was able to judge the actual subcritical core as subcritical state. Thus, the applicability of the ECLLMF using the bootstrap method was demonstrated for the subcritical core in the actual experiment.

Future tasks are the application of the proposed method to evaluate the ECLLMF of fuel debris in the Fukushima Daiichi nuclear power plants, and the comparison with the upper subcritical limit evaluated by the Whisper-1.1 code [6].

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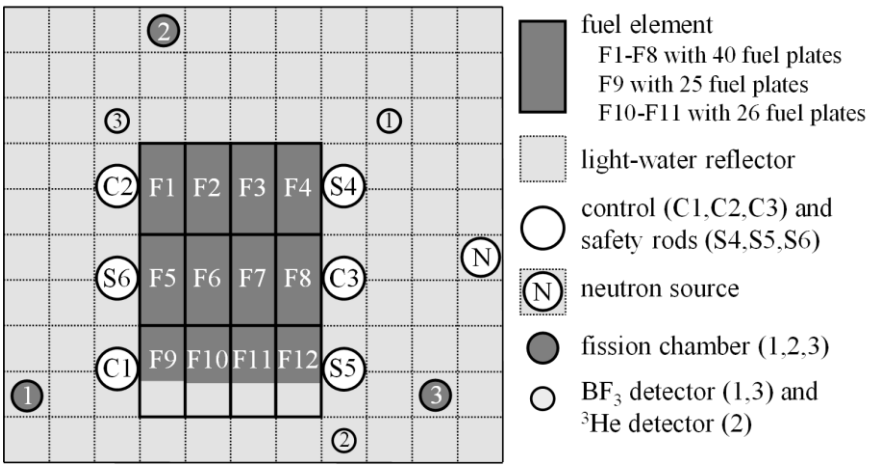
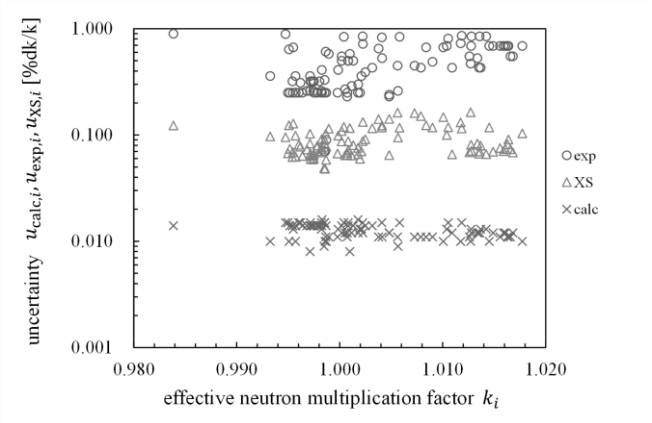
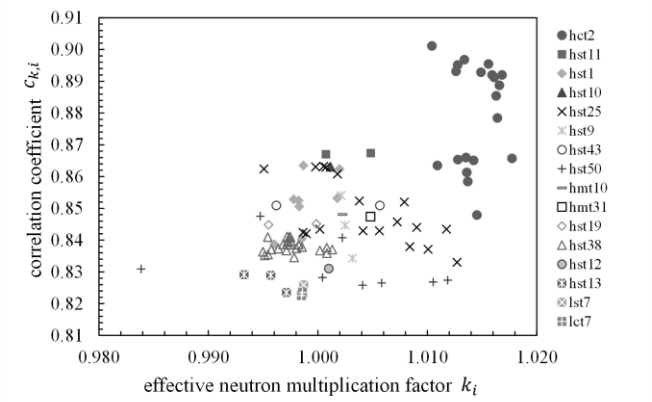


Figure 1. Horizontal view of the core configuration and detector location (step 4).



(a) calculational, experimental, and nuclear data-induced uncertainties



(b) correlation coefficient

Figure 2. Variation of (a) calculational, experimental, and nuclear data-induced uncertainties and (b) correlation coefficient with respect to effective neutron multiplication factor.

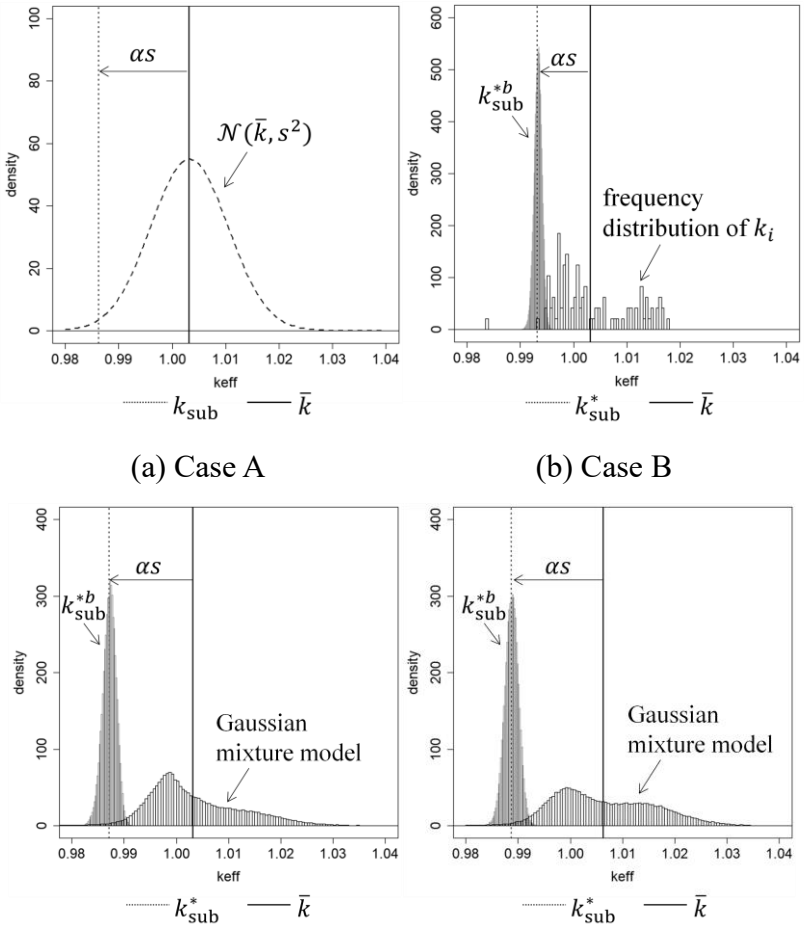


Figure 3. Histograms of effective neutron multiplication factor.

Table 1. Fuel loading patterns and control rods positions.

Step	Number of fuel plates in each frame			Total number	Control rods position	
	F1-F8	F9	F10-12	of fuel plates	C1,C2	C3
0	40	13	13	372	U.L.	U.L.
1	40	18	18	392	U.L.	U.L.
2	40	22	22	408	U.L.	U.L.
3	40	24	24	416	U.L.	U.L.
4	40	25	26	423	U.L.	466.84 mm

U.L.: Upper limit (fully withdrawn), 650.00 mm.

Table 2. Results of ECLLMF calculation.

	Case A	Case B	Case C	Case D
$\bar{k}$	1.00323	1.00323	1.00323	1.00637
s	0.007252	0.007252	0.008868	0.009429
α	2.3486	1.3760	1.8122	1.8692
αs	0.01703	0.00998	0.01607	0.01762
ECLLMF	0.98620	0.99325	0.98716	0.98874

A: assumption of normality, B: bootstrap method without total uncertainty and correlation,

C: bootstrap method only with total uncertainty,

D: bootstrap method with total uncertainty and correlation.

Table 3. Results of MCNP6.2 calculation and subcritical judgment.

Step	Total number of fuel plates	k_A	u_A	$k_A + 3u_A$	Subcritical judgment
0	372	0.98011	0.00012	0.98047	true
1	392	0.99241	0.00012	0.99277	false
2	408	1.00154	0.00012	1.00190	false
3	416	1.00562	0.00013	1.00601	false
4	423	1.00829	0.00012	1.00865	false

true: $k_A + 3u_A < k^*_{\mathrm{sub}}$, false: $k_A + 3u_A \geq k^*_{\mathrm{sub}}$.