A New Uncertainty Evaluation Method for SFP Criticality Calculation

Kazuya Yamaji, Tetsuya Sugimura, Yasuhiro Harada, Daisuke Sato, Shinya Kosaka

Mitsubishi Heavy Industries, Ltd.: Wadasakicho1-1-1, Hyogo-ku, Kobe, Japan, 652-8585
kazuya_yamaji@mhi.co.jp, tetsuya_sugimura@mhi.co.jp, yasuhiro_harada@mhi.co.jp, d_sato@mhi.co.jp, shinya_kosaka@mhi.co.jp

INTRODUCTION

A new uncertainty evaluation method for spent fuel pit (SFP) criticality calculation is proposed. The "uncertainty" here includes a mean value of differences of effective neutron multiplication factor (k-effective) between reference and calculation values, and a square root of its pooled variance.

In the conventional uncertainty evaluation method, uncertainty of the SFP criticality calculation are evaluated with the criticality experiment benchmarks, i.e. comparing the calculation results of k-effective using criticality calculation code with the criticality measurements obtained from several criticality experiments. We have selected the appropriate criticality experiments in the similar conditions to the target SFP, such as fuel composition, moderator density, structure material, fuel rod pitch, and energy of the average lethargy causing fission (EALF). Since the number of applicable criticality experiments is limited, the uncertainty tends to be large due to the statistical penalty. In addition, the uncertainty may vary depending on the selection of experiments.

In order to refine and reduce the k-effective uncertainty for the SFP criticality calculation, we propose a new evaluation method which expands the number of benchmark critical experiments by taking uncertainty propagation to the target SFP into account.

The uncertainty propagation we developed is obtained from sensitivity coefficients of k-effective with respect to microscopic cross-sections and the C_k value [1] based on the generalized perturbation theory (GPT).[2]

In this paper, we propose the new uncertainty evaluation method and its validity. The new method has some new approaches to consider the uncertainty propagation from criticality experiment benchmarks to the target SFP condition.

UNCERTAINTY EVALUATION METHOD

Conventional Method

From the comparison of k-effective between criticality experiments and calculations, a mean value of differences of k-effective and a square root of its pooled variance are defined as Equations (1) and (2), respectively:

$$1-\overline{k_{eff}} = 1-\sum_{n=1}^{N}\frac{1}{\sigma_n^2}k_{eff,n}\Bigg/\sum_{n=1}^{N}\frac{1}{\sigma_n^2}, \tag{1}$$

$$\Delta k_{eff} = U\times\left[\left\{\frac{1}{N-1}\sum_{n=1}^{N}\frac{1}{\sigma_n^2}\left(k_{eff,n}-\overline{k_{eff}}\right)^2+1\right\}\Bigg/\frac{1}{N}\sum_{n=1}^{N}\frac{1}{\sigma_n^2}\right]^{1/2}, \tag{2}$$

where $k_{eff,n}$ denotes calculated k-effective for criticality experiment n, and σ_n is obtained from

$$\sigma_n = \sqrt{\sigma_{calc,n}^2+\sigma_{\exp,n}^2}\,. \tag{3}$$

If measurement k-effective $k_{eff,n}^{\exp}$ is sub-criticality or over criticality, $k_{eff,n}$ is normalized as $k_{eff,n}/k_{eff,n}^{\exp}$. Criticality experiments are selected to cover criticality calculation conditions in the SFP. When the total number of criticality experiments N is increased, singles-side lower tolerance factor with 95% confidential $\times$ 95% probability U [3] (the statistical penalty) is also reduced. The above calculation procedure is exactly consistent with Ref.4.

New Method

Theoretical uncertainty propagation approach from criticality experiments to SFP

In the new method, the uncertainty is obtained from extended criticality experiment benchmarks considering uncertainty propagation to the target SFP condition. The derivation of the new method is described as below.

By using GPT, the sensitivity coefficient matrix of k-effective (k) with respect to cross-sections α_m in criticality experiments (EXP) and SFP is given by

$$\mathbf{S}_j = \begin{pmatrix}\dfrac{\partial k_j/k_j}{\partial\alpha_1/\alpha_1} & \cdots & \dfrac{\partial k_j/k_j}{\partial\alpha_m/\alpha_m} & \cdots & \dfrac{\partial k_j/k_j}{\partial\alpha_M/\alpha_M}\end{pmatrix}\quad (j=SFP, EXP) \tag{4}$$

Where α_m denotes not only cross-sections but also other nuclear constants such as fission spectrum and the number of released neutrons by fission ν.

The covariance matrix of cross-section set is defined as

$$\mathbf{W} = \begin{pmatrix}\dfrac{\langle\delta\alpha_1,\delta\alpha_1\rangle}{\alpha_1\alpha_1} & \cdots & \dfrac{\langle\delta\alpha_1,\delta\alpha_m\rangle}{\alpha_1\alpha_m} & \cdots & \dfrac{\langle\delta\alpha_1,\delta\alpha_M\rangle}{\alpha_1\alpha_M}\\ \vdots & \ddots & & & \vdots\\ \dfrac{\langle\delta\alpha_m,\delta\alpha_1\rangle}{\alpha_m\alpha_1} & & \dfrac{\langle\delta\alpha_m,\delta\alpha_m\rangle}{\alpha_m\alpha_m} & & \dfrac{\langle\delta\alpha_m,\delta\alpha_M\rangle}{\alpha_m\alpha_M}\\ \vdots & & & \ddots & \vdots\\ \dfrac{\langle\delta\alpha_M,\delta\alpha_1\rangle}{\alpha_M\alpha_1} & \cdots & \dfrac{\langle\delta\alpha_M,\delta\alpha_m\rangle}{\alpha_M\alpha_m} & \cdots & \dfrac{\langle\delta\alpha_M,\delta\alpha_{M\cdots}\rangle}{\alpha_M\alpha_M}\end{pmatrix}, \tag{5}$$

where the matrix element of $\mathbf{W}$ is correlation coefficient between α_m and $\alpha_{m'}$.

We define a new inner product between sensitivity coefficients in the M-dimensional space spanned by $\dfrac{\partial k/k}{\partial \alpha_m/\alpha_m}$ (m=1~M) as illustrated in Fig.1. The space is assumed to be filled with the correlation coefficient matrix $\mathbf{W}$. For criticality experiments and SFP, the inner products of $\mathbf{S}_j$ are defined as follows:

$$\left(\mathbf{S}_j,\mathbf{S}_j\right)_W = \mathbf{S}_j\mathbf{W}\mathbf{S}_j^T = \left\|\Delta\mathbf{k}_j\right\|^2 \quad \left(j = SFP, EXP\right), \tag{6}$$

$$\left(\mathbf{S}_{SFP},\mathbf{S}_{EXP}\right)_W = \mathbf{S}_{SFP}\mathbf{W}\mathbf{S}_{EXP}^T, \tag{7}$$

where the superscript T denotes transposition.
When the number of sensitivity coefficient elements is less than 3 or equal to 3, the inner products of $\mathbf{S}_{SFP}$ and $\mathbf{S}_{EXP}$ can be easily imaged from Fig. 1 and derived as

$$\left(\mathbf{S}_{SFP},\mathbf{S}_{EXP}\right)_W = \mathbf{S}_{SFP}\mathbf{W}\mathbf{S}_{EXP}^T = \left\|\Delta\mathbf{k}_{SFP}\right\|\left\|\Delta\mathbf{k}_{EXP}\right\|\cos\theta, \tag{8}$$

where θ corresponds to an angle formed by $\mathbf{S}_{SFP}$ and $\mathbf{S}_{EXP}$.

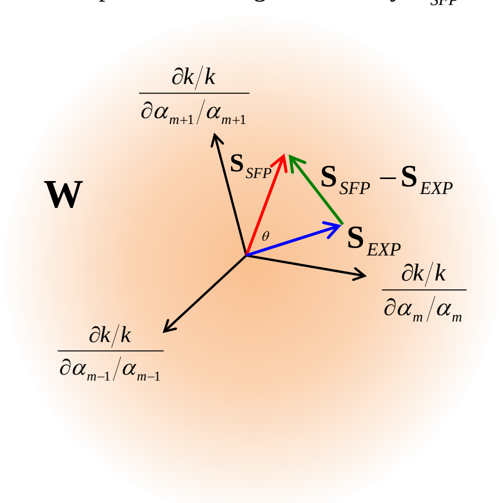

Fig. 1. Relationship between $\mathbf{S}_{EXP}$ and $\mathbf{S}_{SFP}$ in M-dimensional space spanned by sensitivity coefficient elements.

The C_k value, which denotes the similarity between the criticality experiment and the SFP, is defined by

$$C_k = \frac{\left(\mathbf{S}_{SFP},\mathbf{S}_{EXP}\right)_W}{\sqrt{\left(\mathbf{S}_{SFP},\mathbf{S}_{SFP}\right)_W}\sqrt{\left(\mathbf{S}_{EXP},\mathbf{S}_{EXP}\right)_W}}. \tag{9}$$

The following equation is also obtained from the same definition as Equation (6),

$$\begin{aligned}&\left(\mathbf{S}_{SFP}-\mathbf{S}_{EXP},\mathbf{S}_{SFP}-\mathbf{S}_{EXP}\right)_W\\ &=\left(\mathbf{S}_{SFP}-\mathbf{S}_{EXP}\right)\mathbf{W}\left(\mathbf{S}_{SFP}-\mathbf{S}_{EXP}\right)^T\\ &=\left\|\Delta\mathbf{k}_{SFP}-\Delta\mathbf{k}_{EXP}\right\|^2 \le \left\|\Delta\mathbf{k}_{SFP}\right\|^2+\left\|\Delta\mathbf{k}_{EXP}\right\|^2\end{aligned}. \tag{10}$$

By using the cosine theorem in Fig.1 and Equations (6), (7), (9) and (10), the following equation can be derived,

$$\begin{aligned}&\left\|\Delta\mathbf{k}_{SFP}-\Delta\mathbf{k}_{EXP}\right\|^2\\ &=\left\|\Delta\mathbf{k}_{SFP}\right\|^2+\left\|\Delta\mathbf{k}_{EXP}\right\|^2-2\left(\mathbf{S}_{SFP},\mathbf{S}_{EXP}\right)_W\\ &=\left\|\Delta\mathbf{k}_{SFP}\right\|^2+\left\|\Delta\mathbf{k}_{EXP}\right\|^2-2C_k\left\|\Delta\mathbf{k}_{SFP}\right\|\left\|\Delta\mathbf{k}_{EXP}\right\|\end{aligned}. \tag{11}$$

From Equation (11), the propagated uncertainty from the extended criticality experiments to the target SFP condition can be derived as

$$\begin{aligned}\sigma_{repre} &= \left\|\Delta\mathbf{k}_{SFP}-\Delta\mathbf{k}_{EXP}\right\|\\ &=\sqrt{\left\|\Delta\mathbf{k}_{SFP}\right\|^2+\left\|\Delta\mathbf{k}_{EXP}\right\|^2-2C_k\left\|\Delta\mathbf{k}_{SFP}\right\|\left\|\Delta\mathbf{k}_{EXP}\right\|}\end{aligned}. \tag{12}$$

The propagated uncertainty means k-effective penalty so as to apply a mean value of differences of k-effective and a square root of its pooled variance obtained from the extended criticality experiment benchmarks to the target SFP. By considering σ_{repre}, Equation (3) can be rewritten as

$$\sigma_n = \sqrt{\sigma_{calc,n}^2+\sigma_{\exp,n}^2+\sigma_{repre,n}^2}. \tag{13}$$

By using Equation (13) instead of Equation (3), the $1-\overline{k_{eff}}$ and Δk_{eff} values are evaluated with the same procedure as the conventional method.

In the conventional method, the weight of criticality experiment results is independent of the similarity between the criticality experiment and the SFP system. In the new method, the similarity is considered and the weight of higher similarity experiments is larger than that of lower similarity experiments.

Adjustment approach of cross-section covariance to be consistent with experiment results

K-effective measurements $k_{EXP}^{\exp}$ in the criticality experiments have experiment uncertainties. Our criticality calculations employ the multi-group Monte-Carlo code. In our criticality calculations, calculation results k_{EXP}^{calc} include the uncertainties of cross-sections (covariance of nuclear data) $\sqrt{\mathbf{S}_{EXP}\mathbf{W}\mathbf{S}_{EXP}^T}$, the uncertainty of transport calculation modeling such as energy-group condensation σ_{model} and statistical error of the Monte-Carlo code σ_{calc}. The total calculation uncertainty can be written as

$$\sigma_{calc}^{tatal} = \sqrt{\mathbf{S}_{EXP}\mathbf{W}\mathbf{S}_{EXP}^T+\sigma_{model}^2+\sigma_{calc}^2}. \tag{14}$$

In Equation (14), the uncertainty of cross-section is larger than that of transport calculation modeling in the Monte-Carlo code. Therefore, we assume that calculation uncertainties are mainly caused by the uncertainties of nuclear cross-sections except the statistical error of the Monte-Carlo code and the uncertainty of transport calculation modeling is negligible. Equation (14) is rewritten as

$$\sigma_{calc}^{total} \approx \sqrt{\mathbf{S}_{EXP}\mathbf{W}\mathbf{S}_{EXP}^{T} + \sigma_{calc}^{2}} \; . \qquad (15)$$

In this discussion, experiment and calculation results are assumed to be normally distributed with their uncertainties.

In actual calculations, the calculation uncertainties are not necessarily consistent with the experiment results. Figures 2 and 3 show the examples of inconsistency between calculation and experiment uncertainties,

$$\left|k_{EXP}^{\exp} - k_{EXP}^{calc}\right| + \sigma_{\exp} \neq \sqrt{\mathbf{S}_{EXP}\mathbf{W}\mathbf{S}_{EXP}^{T} + \sigma_{calc}^{2}} \; . \qquad (16)$$

Figures 2 and 3 indicate underestimation and overestimation of nuclear cross-section uncertainty, respectively.

In order for the calculation uncertainties to be consistent with the experiment results as illustrated in Fig.4 and to capture the effect of σ_{model}, the uncertainties of nuclear cross-section are adjusted as

$$\left|k_{EXP}^{\exp} - k_{EXP}^{calc}\right| + \sigma_{\exp} = \sqrt{\mu \times \mathbf{S}_{EXP}\mathbf{W}\mathbf{S}_{EXP}^{T} + \sigma_{calc}^{2}} \; . \qquad (17)$$

The adjustment factor μ in Equation (17) can be derived as

$$\mu = \frac{\left(\left|k_{EXP}^{\exp} - k_{EXP}^{calc}\right| + \sigma_{\exp}\right)^{2} - \sigma_{calc}^{2}}{\mathbf{S}_{EXP}\mathbf{W}\mathbf{S}_{EXP}^{T}} \; , \qquad (18)$$

and the cross-section covariance matrix **W** used in the new method is adjusted to $\mu\mathbf{W}$. Then σ_{repre} in Equation (12) can be rewritten as

$$\tilde{\sigma}_{repre} = \mu \times \sigma_{repre} \; . \qquad (19)$$

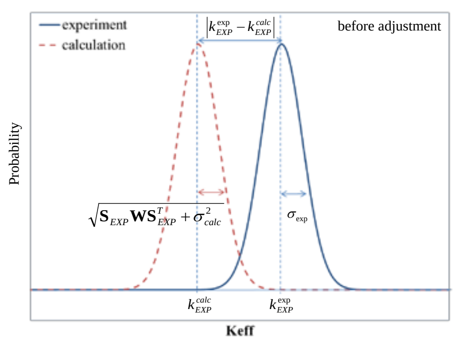

Fig. 2 Underestimation of calculation uncertainty.

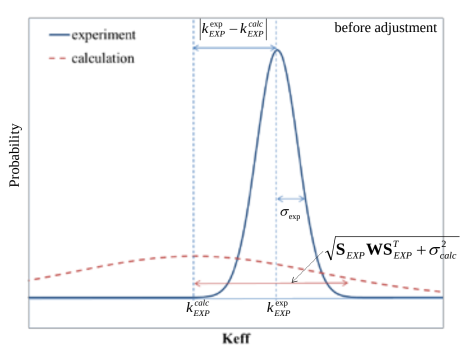

Fig. 3 Overestimation of calculation uncertainty.

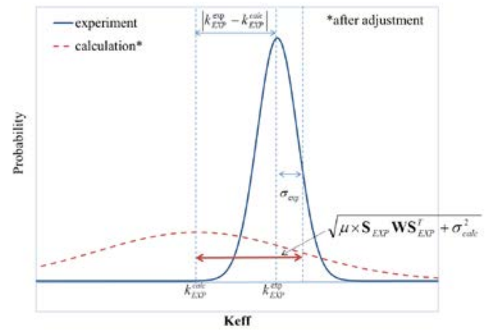

Fig. 4 Adjustment of calculation uncertainty.

VALIDATIONS

We validated the new uncertainty evaluation method from the following viewpoints.

(i) K-effective considering uncertainties evaluated by the new method can represent measurement results corresponding to the SFP within experiment uncertainties.

(ii) The new method can reduce the k-effective uncertainty for the SFP criticality calculations in comparison with the conventional method.

We applied the SCALE 6.0 code system [5] to the criticality safety design analysis of SFPs. In the validations, SCALE6.0 is used for k-effective and sensitivity coefficient calculation. In SCALE6.0, the 238-group cross-section library based on ENDF/B-VII.0 and the Monte-Carlo transport module KENO-VI are used. Sensitivity coefficients are calculated by TSUNAMI-3D. Criticality experiments used for the uncertainty evaluation are obtained from the international handbook of evaluated criticality safety benchmark project (ICSBEP). [6]

Prediction of k-effective considering calculation uncertainties in experiments corresponding to the SFP

For the validation of the new method, we should confirm that k-effective considering uncertainties evaluated by the new method can represent measurements in the SFP. The most straightforward approach is actual comparison of k-effective between measurement and calculation results in the target SFP. However, we can hardly obtain the measured k-effective in the actual SFPs.

Instead of the actual target SFPs, we selected one criticality experiment as the “pseudo SFP” from the N benchmark problems in the ICSBEP. The uncertainties are evaluated by benchmarks using other N-1 criticality experiments from the ICSBEP. In this validation, we used 210 benchmarks (N=210). A comparison of k-effective between experiments and calculations considering uncertainties in the pseudo SFPs is summarized in Fig.5 as the validation results. In this validation, k-effective considering calculation uncertainties is conservatively defined as

$$\tilde{k}_{SFP}^{calc} = k_{SFP}^{calc} + \left(1-\overline{k_{eff}}\right) + \sqrt{\Delta k_{eff}^2 + (2\sigma_{calc})^2} \; . \quad (20)$$

As shown in Fig.5, the calculation results with uncertainties can represent the experiment results within experiment uncertainties. There are no results that underestimate experiment k-effectives beyond experiment uncertainties. The square root of this pooled variance ($\sqrt{\Delta k_{eff}^2 + (2\sigma_{calc})^2}$) is conservatively used as positive k-effective bias in Equation 20 and most of the calculation results are above the upper bound of the experiment uncertainty. We confirmed that the new method works well.

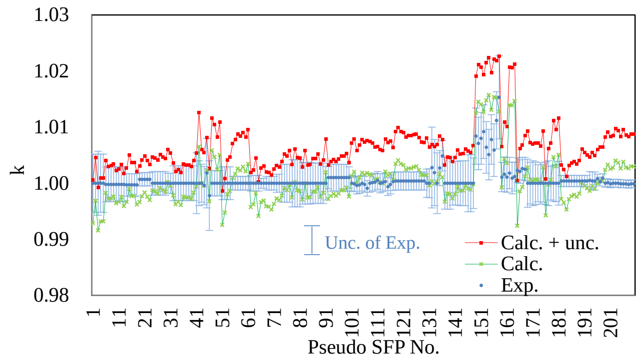

Fig. 5 Comparison of k-effective between experiments and calculation results by using the new method in the pseudo SFP systems.

Comparison of $1-\overline{k_{eff}}$ *and* Δk_{eff} *between the conventional and new methods*

We compared $1-\overline{k_{eff}}$ and Δk_{eff} between the conventional and new methods as shown in Figs. 6 and 7. In the conventional method, the numbers of the criticality experiment benchmarks selected for uncertainty evaluations in the SFP loading UO_2 and MOX are 129 and 18, respectively. The results of new method depend on the pseudo SFP conditions. We confirmed that the new method can reduce a mean value of differences of k-effective and a square root of its pooled variance. In our actual criticality safety design, negative $1-\overline{k_{eff}}$ is conservatively set to zero.

CONCLUSIONS

We proposed a new uncertainty evaluation method using sensitivity analysis and confirmed that this method can well represent experiment results and reduce the k-effective uncertainty for the SFP criticality calculations.

NOMENCLATURE

m , m' = index of cross-section for energy group g, reaction type x, and nuclide k

M = the total number of cross-section type, summary of energy group, reaction type and nuclide

$\sigma_{calc,n}$ = statistical error (1σ) of the Monte-Carlo code for criticality experiment n

$\sigma_{exp,n}$ = experiment error for criticality experiment n

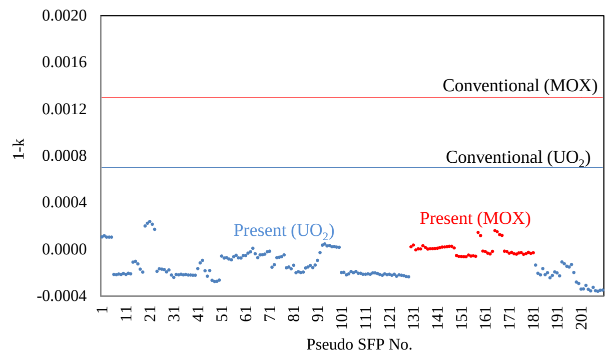

Fig. 6 Comparison of a mean value of k-effective differences between the conventional and new methods in the pseudo SFP systems.

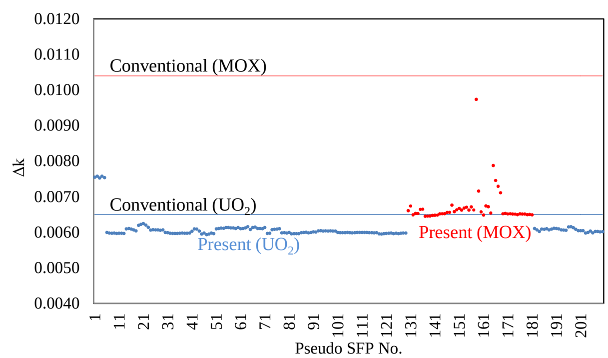

Fig. 7 Comparison of statistical error for a mean value of k-effective differences between the conventional and new methods in the pseudo SFP systems.

REFERENCES

1. B.L.BROADHEAD, et. al., "Sensitivity- and Uncertainty-based Criticality Safety Validation Techniques," *Nucl. Sci. Eng.*, **146** 340 (2004).
2. A. GANDINI, "A Generalized Perturbation Method for Bilinear Functionals of the Real and Adjoint Neutron Fluxes," *J. Nucl. Energy*, **21**, 755 (1967).
3. D. B. OWEN, "Factor For One-sided Tolerance Limits and for Variables Sampling Plans," SCR-607 (1963).
4. J. C. DEAN, et. al., "Guide for Validation of Nuclear Criticality Safety Calculational Methodology," NUREG/CR-6698 (2001).
5. "SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing and Evaluations," NUREG/CR-0200, Rev.6.
6. "International Handbook of Evaluated Criticality Safety Benchmark Experiments," September 2010, OECD/NEA (2010).