# Uncertainty Quantification of BWR Fuel Assembly Criticality with the Efficient Random Sampling Method Based on the Control Variates Method and Sensitivities

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#### 1. Introduction

In the field of nuclear reactor physics, relevant parameters and quantities are predicted through numerical calculations using the evaluated nuclear data. Since the evaluated nuclear data should include uncertainties, calculation results also should include uncertainties. Quantification of these nuclear datainduced uncertainties in the calculation results is important to reduce the design margin in current nuclear systems, to develop innovative nuclear systems, etc.

One method of estimating these uncertainties is the sampling method. This method obtains multiple samples of the concerned parameters and estimates the variance of these parameters from the samples. However, the estimated variance of the parameters should include statistical uncertainties due to the limited number of samples, and thus this method requires a large number of samples to make the statistical uncertainties sufficiently small. To solve this issue, the CV-S method, which combines the control variates (CV) method [1] and sensitivity, was devised as a method to efficiently estimate the variance with a small number of samples at Hokkaido University, and its usefulness has been demonstrated through our previous works [2-3]. In the present work, we attempt to further improve the CV-S method and apply it to the uncertainty quantification calculations for the infinite neutron multiplication factor of the BWR fuel assembly.

# 2. Theory and Methods

In this section, methods introduced to improve the CV-S method are described.

# 2.1 Combination of multiple mockup parameters

In the CV method, a mockup parameter, which has a large correlation to a concerned (target) parameter and whose statistics are known or can be easily evaluated, should be prepared in advance. In the CV-S method, not the mockup parameter itself but the same parameter which linearly depends on the fluctuation of the input nuclear data is used. This linear behavior of the mockup parameter is obtained by sensitivities of the mockup parameter with respect to the nuclear data. Hence, the statics of this mockup parameter can be easily calculated. The previous studies have used a single mockup parameter for estimation. In the present work, we propose to prepare multiple mockup parameters and combine them into one fictitious mockup parameter. If this combined mockup parameter has a stronger correlation to the target parameter than each mockup parameter, it is expected that the performance of the CV-S method can be enhanced.

In the present work, we propose to use the following combined mockup parameter  $k_m$  defined from a set of mockup parameters  $k_{m,i}$  as

$$k_m = \prod_j k_{m,j}^{a_j},$$

where  $a_j$  is a weight for the *j*th mockup parameter in the parameter combination. This idea is taken from the previous work done by Kugo et al. [4], and this work suggests to define the weight as

$$\boldsymbol{a} = \boldsymbol{\Sigma}_m^{-1} \boldsymbol{\sigma}_{t,m}$$

where  $\boldsymbol{a}$  is a column vector containing  $a_j$  at the *j*-th row,  $\boldsymbol{\Sigma}_m$  is a covariance matrix of mockup parameters, and  $\boldsymbol{\sigma}_{t,m}$  is a covariance column vector between a target parameter and mockup parameters. This equation is derived so as to minimize the prediction uncertainty of the extended bias factort mehod [4]. In the CV-S method, the covariance matrix  $\boldsymbol{\Sigma}_m$  is known in advance, but that estimated from the samples should be used to obtain the vector  $\boldsymbol{a}$ . It is easy to demonstrate that the rigorous values of  $\boldsymbol{a}$  is obtained if the covariance matrix and vector,  $\boldsymbol{\Sigma}_m$  and  $\boldsymbol{\sigma}_{t,m}$ , are estimated from the samples. Note that this is true only if the sample covariance matrix  $\boldsymbol{\Sigma}_m$  is non-singular.

#### 2.2 Use of the dimensionless parameters

In the conventional CV-S method, it is known that the efficiency is dependent on the statistics (mean values and variances) of the target and mockup parameters in addition to the correlation between them [2]. In order to solve this issue, we propose to use not the parameter values themselves but dimensionless parameters which are re-defined as the relative differences from the reference values, here the mean values.

Let us suppose that the target parameter  $k_t$  is expressed by the following equation:

$$k_t = \bar{k}_t \left( 1 + \sum_i \hat{S}_{t,i} Z_i + \sum_i \tilde{S}_{t,i} Z_i^2 + \cdots \right),$$

where  $\bar{k}_t$  is the mean value of  $k_t$ , and  $Z_i$  is the relative uncertainties (standard deviations) of the *i* th input

parameter (nuclear data).  $\hat{S}_{t,i}$  and  $\tilde{S}_{t,i}$  are the first- and second-order derivatives of the target parameter with respect to the *i*th input nuclear data.

This is transformed into the following equation of a relative difference from the mean value:

$$p_t = \frac{k_t - \bar{k}_t}{\bar{k}_t} = \sum_i \hat{S}_{t,i} Z_i + \sum_i \tilde{S}_{t,i} Z_i^2 + \cdots$$

With the same way, the *j*th dimensionless mockup parameter  $p_{m,j}$  can be defined as

$$p_{m,j} = \frac{k_{m,j} - \bar{k}_{m,j}}{\bar{k}_{m,j}} = \sum_i \hat{S}_{m,j,i} Z_i,$$

where  $\bar{k}_{m,j}$  is a mean value of  $k_{m,j}$  and the dimensionless combined mockup parameter  $p_m$  can be defined as

$$p_m = \frac{k_m - \bar{k}_m}{\bar{k}_m} = \sum_j a_j p_{m,j}.$$

We have confirmed that this operation allows us to exclude the influence of the statistics of the target and mockup parameters on the efficiency of the estimation in the CV-S calculations.

#### 3. Numerical Results

This section describes the problem specification and numerical results.

# 3.1 Problem specification

In this work, the uncertainty of the infinite neutron multiplication factor  $k_{\infty}$  of the BWR fuel assembly was estimated with the conventional random sampling method and the proposed CV-S method with the dimensionless combined mockup parameter. The target BWR fuel assembly is one prepared through the OECD/NEA burnup credit benchmark phase III-C [5]. The schematic diagram of this assembly is shown in Fig. 1. Mockup parameters are  $k_{\infty}$  of fuel pincells which compose the target fuel assembly. As shown in Fig. 1, five types of the UO<sub>2</sub> pellet with different uranium enrichment are loaded in this assembly, and thus the five fuel pincells were considered. Sensitivities of  $k_{\infty}$  at four different fuel burnups, 0, 15, 30, and 45 GWD/t, with respect to the nuclear data were calculated for each of these fuel pincell models with the depletion perturbation theory, and a set of the 20 mockup parameters were prepared. The nuclear data used in the calculations are JENDL-5, and the uncertainties of only the reaction cross sections of actinoids were taken into account. All the calculations were carried out with the deterministic reactor physics code CBZ [6].



Fig. 1. Schematic diagram of the target BWR fuel assembly

#### 3.2 Numerical results

We estimate the relative standard deviations of  $k_{\infty}$  of the target assembly at specific burnup. Thirty sets of nuclear data were randomly generated according to the covariance matrices, and 30 samples of the target and mockup parameters are obtained from these random nuclear data sets. This calculation was carried out 30 times with other random seeds, and the uncertainty (standard errors) of the estimation from 30 samples was also estimated.

First, the results of the uncertainty estimation of  $k_{\infty}$ at 6 GWD/t, where the highest estimation efficiency is observed with the CV-S method, are shown in Fig. 2. The relative standard deviation of  $k_{\infty}$  estimated with the conventional method is 0.00396 and its standard error is 0.00047. On the other hand, the CV-S method yields the estimated standard deviation of 0.00401 with the standard error of 0.00011. The standard deviation estimated by the CV-S method agrees with that with the conventional method within the statistical uncertainties, so this suggests that the estimation with the proposed CV-S method is unbiased and has the smaller standard error than the conventional method. Based on this result, the estimation results using 30 samples by the CV-S method is as accurate as those using about 600 samples by the conventional method.



Fig. 2. Relative standard deviation of  $k_{\infty}$  at 6 GWD/t

In the above calculations, the mockup parameters are based on the sensitivities of  $k_{\infty}$  of the pincell models with respect to the nuclear data. These sensitivities include the fuel burnup effect, which is contribution of the nuclear data to the nuclide number densities at the concerned fuel burnup. Existing reactor physics codes have capabilities of calculating sensitivities of the static parameters, but most of them cannot calculate the sensitivities including the burnup effect. Thus, we made the same calculations with the different mockup parameter set in which the fuel burnup effect is not taken into account. Figure 3 shows the results with the CV-S method using the sensitivities without the burnup effect. Compared with Fig. 2, the efficiency of the CV-S method becomes worse when the fuel burnup effect is not considered.



Fig. 3. Relative standard deviation of  $k_{\infty}$  at 6 GWD/t (without burnup effects)

Similar calculations were made for  $k_{\infty}$  at the beginning, middle, and end of the fuel burnup. The fuel burnup of 12 GWD/t was also concerned since this burnup corresponds to the Gd burn-out. The uncertainty reduction (UR), which is defined as a ratio of standard error of the CV-S estimation to that of the conventional method estimation, is shown in Table I. This table also shows the results obtained with the single mockup parameter, which gives the smallest UR. On all the target parameters, multiple use of the mockup parameters gives better results than the single use. Furthermore, UR obtained with the multiple parameters without the fuel burnup effect becomes large compared with UR with the burnup effect in all these cases.

Table I. Standard deviation estimated by various methods

	Uncertainty Reduction		
Burnup [GWD/t]	Single mockup	20 mockups	20 mockups
			(without burnup effect)
6	0.523	0.229	0.405
12	0.414	0.304	0.414
25	0.349	0.307	0.455
50	0.528	0.261	0.632

In the above calculations, the sample covariance matrix of the mockup parameters was used to determine

the proper weights and this treatment is theoretically reasonable as mentioned in the preceding section. The same calculations were carried out using the rigorous covariance matrix and the results are shown in Fig. 4. This result suggests that the use of the sample covariance matrix is preferred whereas the reason of the apparent bias is unclear at this moment.



Fig. 4. Relative standard deviation of  $k_{\infty}$  at 6 GWD/t (using rigorous covariance matrix)

# 3.3 Divergence of calculation results due to the rank deficiency of the mockup covariance matrix

Let the number of the mockup parameters and the number of samples M and N, respectively. The covariance matrix of the mockup parameters, whose size is  $M \times M$ , is generated from the N samples in the proposed procedure. Since the rank of the sample covariance matrix should be less than N, the convariance becomes rank deficient if N < Mmatrix or independence of the sample is not guaranteed in the set of the samples. In the present work, we have used 30 samples and 20 mockup parameters. When the number of samples is fixed 30, it is expected that the sample covariance matrix becomes close to be rank deficient if the number of mockup parameters is increased. To check this, we added 10 other mockup parameters, and did the same calculations for  $k_{\infty}$  at 6 GWD/t with different number of the mockup parameters. The results are shown in Fig. 5. As expected, when the number of mockup parameters is close to the number of samples, 30 in this case, the efficiency of the CV-S method deteriorates.



Fig. 5. Dependence of uncertainty reduction on the number of mockup parameters

## 3. Conclusions

In order to increase the efficiency of the CV-S method, we have proposed to use the dimensionless parameters and to introduce a fictitious mockup parameter which is combined from multiple mockup parameters. Through numerical calculations targeting the BWR fuel assembly, improvement in the prediction accuracy of the proposed CV-S method has been clearly demonstrated.

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