ARTICLE

Estimation of sensitivity coefficients of core characteristics based on reduced order modeling using sensitivity matrix of assembly characteristics

Ryota Katano[a*†], Tomohiro Endo[a], Akio Yamamoto[a], Mohammad Abdo[b], and Hany Abdel-Khalik[c]

[a] *Nagoya University, Furo-cho, Chikusa-ku, Aichi 464-8603, Japan*

[b] *North Carolina State University, Raleigh, NC 27695, USA*

[c] *Purdue University, West Lafayette, IN 47906, USA*

Acknowledgements

We sincerely appreciate Nuclear Fuel Industries, Ltd. and Nuclear Engineering, Ltd. for their technical supports to the use of CASMO-4 code, SIMULATE-3 code, and perturbation of cross section library. This work was supported in part by JSPS KAKENHI, Grant-in-Aid for Scientific Research (C) (24561040, 16K06956).

We propose an estimation method of sensitivity coefficients of core neutronics parameters based on a multi-level reduced order modeling approach. The idea is to use lower-level models to identify the dominant input parameter variations, constrained to the so-called active subspace, which are employed to determine the sensitivity coefficients of the core neutronic parameters. In our implementation, the lower-level model is represented by 2D assembly calculations, which are employed in the preparation of the few-group cross-sections for core-wide calculations. The active subspace basis is estimated using the singular value decomposition of sensitivity matrices of assembly neutronics parameters. In numerical

*Corresponding author. Email: katano.ryota@jaea.go.jp

† Present address: Research Group for Nuclear Transmutation System, Japan Atomic Energy Agency, 2-4 Shirakata, Tokai-mura, Ibaraki 319-1195, Japan

verification calculation, sensitivity coefficients of core characteristics for a typical three-loop PWR equilibrium-cycle are estimated using the proposed method and the direct method. Comparison of these two results shows that the proposed method well reproduces the results obtained by the direct method with lower calculation costs. Through the verification calculations, applicability of the proposed method to practical light water reactor analysis is confirmed.

Keywords; reduced order modeling; sensitivity coefficient; active subspace, assembly calculation; light water reactor; numerical analysis

1. Introduction

For safe and efficient operation of nuclear reactors, it is important to quantify and reduce the uncertainty of core neutronics parameters predicted by numerical core analysis. The sensitivity coefficients of the core neutronics to cross section data are used for uncertainty quantification based on error propagation, cross section adjustment method, and a method to identify nuclear data for which further improvements are required to reduce uncertainties of target integral neutronics parameters [1-3]. Therefore, it is important to evaluate the sensitivity coefficients of core neutronics parameters in core analysis.

There are two conventional sensitivity estimation methods, i.e., the forward-based approach and the adjoint-based approach. The forward-based approach, which requires a perturbed calculation for each input parameter, can utilizes existing core analysis codes without major modifications. However, this approach would be impractical due to the large number of input parameters (e.g., fine-group microscopic cross sections). For this reason, the adjoint-based approach i.e., generalized perturbation theory (GPT) and depletion perturbation theory (DPT) are utilized to reduce the calculation costs [4, 5]. In their ideal application to the evaluation of first-order derivatives, a single adjoint model evaluation is required for every

response of interest, and independently of the number of model parameters. This property makes adjoint-based methods the most efficient when few responses are required and only first-order variations are the most dominant. In practice, however, the application of the adjoint-based approach to light water reactor (LWR) analysis is difficult due to complexity and non-linear effects in core analysis, e.g., lattice-core two-step calculation, non-linear effect represented by thermal-hydraulics feedback, and the large number of core responses. Thus, an efficient estimation method for sensitivity coefficients without the adjoint-based approach is highly desirable.

To address these challenges, reduced order modeling (ROM)-based methods have been investigated by previous works to reduce the computational burden of sensitivity coefficients evaluations when neither forward nor adjoint-based methods is found practical [6-11]. The idea is to perform a physics-based reduction of the input parameter space and/or the response space. The reduction implies that not all input parameter variations are important, i.e., they do not contribute to the evaluation of sensitivity coefficients. Unlike traditional screening approaches, which eliminates parameters that are considered unimportant based on expert judgement or a one-at-a-time sensitivity analysis, ROM employs the physics model to identify the important parameter variations using range finding algorithm.

In our current implementation, we focus on the use of singular value decomposition (SVD) as a range finding algorithm. SVD identifies an active subspace (AS) in the input parameter space, whose size is much smaller than the dimension of the input parameter space. With this, the cost of forward-based sensitivity coefficient evaluation can be significantly reduced. The premise here is that all parameter variations that are orthogonal to the AS produce negligible variations in the responses of interest, i.e., core neutronic parameters.

Earlier work has explored the ROM application to core neutronics calculations. For example, researchers have shown that the size of the AS for assembly and core-wide calculations is extremely small [8,12]. Abdo, et. al., [9-11] has employed a multi-level ROM

(M_LROM) approach to approximate the AS using a lower-level model. In this work, we employ a similar approach, where AS is constructed using the sensitivity coefficients of the assembly calculations to identify the dominant parameter variations for core-wide calculations. The errors resulting from this approximation have been bounded by rigorous metrics in earlier work [13]. Instead of repeating these results, we employ a numerical verification test to assess the quality of the approximated AS.

In our implementation, the AS will be determined by executing assembly calculations only once in advance of core calculations. Once determined, the AS can be reused for various cores loaded with the assemblies that are employed to obtain the AS. If new assembly designs are introduced, one can expand the AS by appending the sensitivity coefficients to the AS basis. In earlier work, Abdo [13] has shown that this idea could be helpful in determining the minimum number of assembly calculations required to properly cover the AS.

In Section 2, outline of ROM and AS in estimation of sensitivity coefficients is described. In Section 3, theory of the proposed method to obtain an AS basis using assembly calculations is discussed. Decomposition of a core sensitivity matrix by assembly sensitivity matrices and the application of assembly calculations with coarse calculation condition are described. In Section 4, comparison of the results of present and direct methods are provided. Finally, concluding remarks are summarized in Section 5.

2. Reduced order modeling of input parameters

Firstly, let us consider N input parameters $\sigma_1, \sigma_2, \cdots, \sigma_N$ and M core neutronics parameters $R_1, R_2, \cdots R_M$ (which are calculated using $\sigma_1, \sigma_2, \cdots, \sigma_N$). Variation of i-th neutronics parameters ΔR_i due to the perturbation of input parameters ($\Delta\sigma_1, \Delta\sigma_2, \cdots, \Delta\sigma_N$) is approximately expressed as follows based on the first order approximation of the Taylor expansion:

$$\Delta R_i = \sum_{j=1}^{N} G_{ij} \Delta \sigma_j \,, \tag{1}$$

where G_{ij} is a sensitivity coefficients of R_i to σ_j ($\equiv \partial R_i / \partial \sigma_j$). The matrix expression of Equation (1) is given by:

$$\Delta \vec{R} = \mathbf{G} \Delta \vec{\sigma} \,, \tag{2}$$

where vectors $\Delta \vec{\sigma}$ and $\Delta \vec{R}$, and matrix **G** are defined as follows:

$$\Delta \vec{\sigma} = \left(\Delta \sigma_1, \Delta \sigma_2, \cdots, \Delta \sigma_N \right)^T, \tag{3}$$

$$\Delta \vec{R} = \left(\Delta R_1, \Delta R_2, \cdots, \Delta R_M \right)^T, \tag{4}$$

$$\mathbf{G} = \begin{pmatrix} dR_1 / d\vec{\sigma} \\ \vdots \\ dR_M / d\vec{\sigma} \end{pmatrix}, \tag{5}$$

$$dR_i / d\vec{\sigma} = \left(\frac{\partial R_i}{\partial \sigma_1}, \cdots, \frac{\partial R_i}{\partial \sigma_N} \right). \tag{6}$$

It is noted that $\Delta \vec{\sigma}$ is an *N*-dimensional column vector, $\Delta \vec{R}$ is an *M*-dimensional column vector, **G** is an *M*-by-*N* matrix, and $dR_i / d\vec{\sigma}$ is an *N*-dimensional row vector.

The *j*-th column vector $\vec{G}_j$ of the matrix **G** can be obtained by the direct perturbation method (using forward calculations) as follows:

$$\vec{G}_j = \frac{\vec{R}\left(\vec{\sigma} + \Delta \sigma_j \vec{e}_j \right) - \vec{R}\left(\vec{\sigma} \right)}{\Delta \sigma_j}, \tag{7}$$

where the scalar $\Delta \sigma_j$ is the amount of variation for the *j*-th input parameter and the vector $\vec{e}_j$ is the unit vector whose j-th element is 1 and all the other elements are zero. In the direct approach, the matrix **G** is obtained by evaluation of the Equation (7) for all input parameters. Thus, the required number of forward calculations to estimate the sensitivity coefficients is proportional to the number of input parameters.

Next, SVD of the matrix **G** is performed as follows [14]:

$$\mathbf{G} = \mathbf{U}\mathbf{D}\mathbf{V}^T \,, \tag{8}$$

where,

U : *M*-by-*M* unitary matrix,

V : *N*-by-*N* unitary matrix,

D : *M*-by-*N* diagonal matrix with singular values ($d_1 \geq d_2 \geq \cdots \geq d_M \geq 0$).

Furthermore, the smaller singular values than *r*-th largest singular value are neglected as follows:

$$d_1 \geq \cdots \geq d_r > d_{r+1} \approx \cdots \approx d_M \approx 0 . \tag{9}$$

Assuming Equation (9), Equation (8) is rewritten as follows:

$$\mathbf{G} = \mathbf{U}_r \mathbf{D}_r \mathbf{V}_r^T , \tag{10}$$

where,

$\mathbf{U}_r$: *M*-by-*r* unitary matrix,

$\mathbf{V}_r$: *N*-by-*r* unitary matrix,

$\mathbf{D}_r$: *r*-by-*r* diagonal matrix which have *r* singular values $d_1 \geq d_2 \geq \cdots \geq d_r > 0$ as diagonal elements.

Therefore, when Equation (9) is established, the matrix **G** can be decomposed with the appropriate *N*-dimensional orthonormal vectors as follows:

$$\mathbf{G} = \mathbf{F}\mathbf{V}_r^T , \tag{11}$$

where, the matrix **F** is *M*-by-*r* matrix and $\mathbf{V}_r^T \mathbf{V}_r = \mathbf{I}_{r\times r}$ (*r*-by-*r* identity matrix). It is noted that the columns of $\mathbf{V}_r$ are the subspace basis spanned by the row vectors of **G**. By substituting Equation (11) into Equation (2), the following expression are obtained:

$$\Delta\vec{R} = \mathbf{F}\mathbf{V}_r^T \Delta\vec{\sigma} . \tag{12}$$

By transforming variation of input parameters as $\Delta\vec{\sigma} = \mathbf{V}_r \Delta\vec{\alpha}$, the following expression can be derived since $\mathbf{V}_r^T \mathbf{V}_r = \mathbf{I}_{r\times r}$:

$$\Delta\vec{R} = \mathbf{F}\Delta\vec{\alpha} , \tag{13}$$

where the vector $\Delta\vec{\alpha}$ is an *r*-dimensional vector whose elements are expansion coefficients of $\Delta\vec{\sigma}$. As obvious from Equation (13), the *j*-th column vector $\vec{F}_j$ of the matrix **F** can be

obtained by varying only the *j*-th element of $\Delta\vec{\alpha}$. In such case, the variation of input parameters is expressed as $\Delta\vec{\sigma} = \Delta\alpha_j \vec{v}_j$ (the vector $\vec{v}_j$ is the *j*-th column vector of the matrix $\mathbf{V}_r$), thus $\vec{F}_j$ is obtained as follows:

$$\vec{F}_j \approx \frac{\vec{R}\left(\vec{\sigma} + \Delta\alpha_j \vec{v}_j\right) - \vec{R}\left(\vec{\sigma}\right)}{\Delta\alpha_j}, \tag{14}$$

where the scalar $\Delta\alpha_j$ is the amount of variation for the *j*-th element of $\Delta\vec{\alpha}$.

The number of column of matrix **F** is *r*. Therefore, matrix **F** is obtained by *r* forward calculations. Then, matrix **G** is obtained by Equation (11). Consequently, matrix **G** is obtained by *r* forward calculations using the orthonormal expansion. Namely, the degree of freedom (DOF) of the input parameters for sensitivity estimation is reduced from *N* (i.e., the original dimension) to *r* (i.e., the dimension of the subspace spanned by orthonormal column basis $\mathbf{V}_r$). The ROM is achieved by expansion of the input parameters in such a subspace spanned by the columns of $\mathbf{V}_r$. and the columns $\mathbf{V}_r$ is an AS basis in the proposed method. When $r << N$, required number of core calculations can be drastically reduced.

3. Utilization of assembly calculation

3.1. Decomposition of Sensitivity matrix of core characteristics

The simplest method to obtain an AS basis corresponding to core neutronics parameters is utilization of the core sensitivity matrix: SVD is performed to the core sensitivity matrix, then AS basis is obtained as the columns of $\mathbf{V}_r$. The AS basis obtained by this method can accurately reproduce the relation of Equation (11). However, this method is meaningless since this method requires the core sensitivity matrix, which is the target matrix. Therefore, an M_LROM approach is used to obtain an AS basis using the sensitivity matrix of the assembly neutronics parameters.

Firstly, it is assumed that the variation of the core neutronics parameters is caused by the variation of the assembly neutronics parameters, e.g., the homogenized multi-group

macroscopic corss sections. When a core calculation is performed using the macroscopic cross sections obtained by assembly calculations, this assumption is considered to be natural and straightforward. With this assumption, the sensitivity coefficients can be expanded by L assembly neutronics parameters Σ_k as follows:

$$\frac{\partial R_i}{\partial \sigma_j} = \sum_{k=1}^{L} \frac{\partial R_i}{\partial \Sigma_k} \frac{\partial \Sigma_k}{\partial \sigma_j}, \tag{15}$$

and the matrix expression of Equation (15) is:

$$\mathbf{G} = \mathbf{G}_1 \mathbf{G}_2, \tag{16}$$

where $\mathbf{G}_1$ and $\mathbf{G}_2$ are the sensitivity matrix of the core neutronics parameters to the assembly neutronics parameters ($\equiv \partial R_i / \partial \Sigma_k$) and the sensitivity matrix of the assembly neutronics parameters to the input parameters ($\equiv \partial \Sigma_k / \partial \sigma_j$), respectively. $\mathbf{G}_2$ can be obtained by the assembly calculations. After the evaluation of $\mathbf{G}_2$, the SVD is performed as follows:

$$\mathbf{G}_2 = \mathbf{U}_r \mathbf{D}_r \mathbf{V}_r^T. \tag{17}$$

When Equation (9) holds true for the singular values of $\mathbf{G}_2$, then $\mathbf{U}_r$, $\mathbf{V}_r$, and $\mathbf{D}_r$ become an L-by-r unitary matrix, an N-by-r unitary matrix, and an r-by-r diagonal matrix, respectively. Then, the Equation (16) is rewritten as follows:

$$\mathbf{G} = \mathbf{G}_1 \mathbf{U}_r \mathbf{D}_r \mathbf{V}_r^T. \tag{18}$$

The matrix $\mathbf{G}_1 \mathbf{U}_r \mathbf{D}_r$ is an M-by-r matrix and $\mathbf{V}_r$ is an N-by-r matrix whose columns are orthonormal basis. These are corresponding to the matrices $\mathbf{F}$ and $\mathbf{V}_r$ in the Equation (11). In forward calculations, N assembly calculations are required to obtain $\mathbf{G}_2$ and an AS basis is constructed using Equation (17). Then r core analysis (i.e., r assembly calculations + r core calculations) are required to estimation of the sensitivity matrix of core neutronics parameters using the obtained AS basis from assembly calculation results. Namely, in this approach, $N + r$ assembly calculations and r core calculations are required to estimate the sensitivity matrix of the parameters of a certain core. This implies that the required

number of core calculations is reduced from N to r. The decomposition of Equation (16) would hold true for the cores if the same set of assemblies are loaded. Thus, once the $\mathbf{G}_2$ is obtained, the calculation cost to estimate core sensitivity matrix would be reduced for cores loaded with same fuel assemblies.

The proposed method assumes that the sensitivity matrix of core neutronics parameters can be decomposed as Equation (16). When Equation (16) holds true, Equation (18), which is obtained by the decomposition of the sensitivity matrix of the assembly neutronics parameters, is equivalent to Equation (11). Namely, the AS basis for the assembly neutronics parameters is equivalent to that of the core neutronics parameters in such a case. However, by the assembly calculations, various assembly neutronics parameters would be obtained for various state points (e.g., burnup points, void fraction, fuel temperature). Validity and accuracy of Equation (16) would significantly depends on the choice of assembly neutronics parameters (Σ). Thus, Σ should be carefully chosen to make Equation (16) valid.

3.2. Application of approximate assembly calculation

As mentioned in the previous section, the number of assembly calculations is not reduced in the ROM-approach using the sensitivity matrix of the assembly neutronics parameters; $N + r$ assembly calculations are still necessary. The assembly neutronics parameters are tabulated for various conditions (state-points) e.g., burnup, fuel temperature, moderator temperature, void fraction, boron concentration, and control rod insertion/removal. When type of branch calculations is increased and/or the fine state points are taken into account, the calculation cost of the assembly calculations would be increased. In a typical LWR core analysis, calculation cost of the assembly calculations is not negligible, thus the approach proposed in the previous section would not significantly improve the efficiency of sensitivity estimation of the core neutronics parameters.

Thus, in this study, we use an AS estimation method using approximate values $\tilde{\Sigma}$ of assembly neutronics parameters obtained by approximate assembly calculations employing the coarse tabulation condition (e.g., coarse burnup steps) instead of the neutronics parameters evaluated with the original fine conditions [15].

Figure 1 shows image of burnup dependence of the assembly neutronics parameters. In Figure 1, the solid line and the dotted line represent the assembly neutronics parameters obtained with non-perturbed input parameters and perturbed input parameters, respectively. In addition, the solid arrow and dotted arrow represent the direction and amount of the perturbation at the fine and coarse burnup point, respectively. Each arrow corresponds to the sensitivity vector (i.e., the row vector of the sensitivity matrix) of the assembly neutronics parameters to the input parameters, though Figure 1 is a two-dimensional plot in which the axis of input parameters is not explicitly shown. The basis of the subspace spanned by these sensitivity vectors corresponds to $\mathbf{V}_r$ in Equation (11). When the width of the coarse burnup points is appropriately small, assembly neutronics parameters linearly varies between two adjacent coarse burnup points. Namely, the assembly neutronics parameters at the fine burnup points can be estimated by the linear combination of those at the coarse burnup points. Therefore, the sensitivity vectors of the assembly neutronics parameters at the fine burnup points are given by the linear combination of those at coarse burnup points. Consequently, the subspace $\mathbf{V}_c$ spanned by the sensitivity vectors at coarse burnup points is approximately equivalent to the subspace $\mathbf{V}_f$ spanned by the sensitivity vectors at fine burnup points.

There are two approaches to estimate sensitivity coefficients at coarse state points. In the first approach, fine state-point condition (fine burnup step) is used for assembly calculations and then parts of the calculation results are picked up as the results of coarse state-point. In this case, computation time for assembly calculation cannot be reduced. In the second approach, coarse state point (coarse burnup point) is directly used in assembly calculation. In the second approach, computation time can be reduced. However, utilization of

coarse step degrades assembly calculation results. Thus when the second approach is used, equivalence of these two approaches should be confirmed. In Reference 15, it is shown that the sensitivity vector obtained by approximate assembly calculations with coarse burnup steps can well reproduce that obtained by assembly calculation with fine burnup steps for UO_2- fuel and MOX fuel assemblies. Thus, in a typical LWR core analysis, the subspace $\mathbf{V}_{\tilde{c}}$ spanned by the sensitivity vectors obtained by the approximate assembly calculation with coarse burnup steps (the second approach) is approximately equivalent to the subspace $\mathbf{V}_c$ obtained the first approach. Namely, $\mathbf{V}_{\tilde{c}}$ can approximate $\mathbf{V}_f$ as well as $\mathbf{V}_c$. In this study, we propose a method using the basis of subspace $\mathbf{V}_{\tilde{c}}$ as an AS basis, which is obtained from the sensitivity matrix $\tilde{\mathbf{G}}_2$ based on the approximate assembly neutronics parameters with coarse calculation condition.

The required number of forward calculations to obtain $\tilde{\mathbf{G}}_2$ still remains *N*. However, due to less number of state points, number of neutron transport calculation, burnup calculation, and the effective cross section calculation in approximate assembly calculations will be reduced. Thus, the calculation cost to obtain an AS basis will be reduced by employing the approximate assembly calculations.

3.3. Accuracy of sensitivity vector

The proposed method utilizes the following assumptions to construct an AS basis for ROM:

- The core sensitivity matrix can be decomposed using the assembly sensitivity matrix as shown in Equation (16).
- Equation (9) holds true about the singular values of the assembly sensitivity matrix.
- The assembly neutronics parameters at fine state points can be given by the linear combination of those of coarse state points.

- The sensitivity matrix of approximate assembly neutronics parameters obtained with coarse burnup steps can well reproduce that of the assembly neutronics parameters obtained with original fine burnup steps.

Namely, the sensitivity matrix of core neutronics parameters obtained by the proposed method includes some approximations.

For practical application, user should determine the number of AS dimensions required to obtain the target accuracy or estimate approximation error by the user specified number of AS dimensions. Thus, in this paper, the accuracy of approximation versus number of AS dimensions r is quantitatively evaluated. The relative difference norm of the row vectors of the sensitivity matrix of core neutronics parameters to the reference values obtained by the direct method is defined as follows:

$$e_r = \frac{\left\| \vec{g}_r - \vec{g}_{ref} \right\|_2}{\left\| \vec{g}_{ref} \right\|_2}, \tag{19}$$

where, r is number of dimensions of AS, $\vec{g}_r$ and $\vec{g}_{ref}$ are the row vectors of sensitivity matrix obtained by the proposed and the direct methods, respectively. When the sensitivity matrix obtained by the proposed method is equal to that obtained by the direct method, the relative difference norm given by Equation (19) will be zero.

The proposed method utilizes only forward calculations. Namely, the finite difference approximation is applied to evaluate the sensitivity coefficients. Therefore, due to the non-linear effect and numerical round off error, discretization error is inevitably included in the estimated sensitivity coefficients. Thus, it is difficult to identify the source of relative difference given by the Equation (19), i.e., the AS expansion or the finite difference approximation. In order to clarify this point, the relative difference norm given by Equation (20) is defined as the theoretical value:

$$e_{theory,r} = \frac{\left\| \left(\mathbf{I} - \mathbf{V}_r \mathbf{V}_r{}^T \right) \vec{g}_{ref} \right\|_2}{\left\| \vec{g}_{ref} \right\|_2}. \quad (20)$$

The numerator of the right hand side of Equation (20) represents the magnitude of orthogonal components of the reference sensitivity vector to AS. Namely, Equation (20) gives the accuracy of the proposed method without the non-linear effects and the numerical round off error. In verification calculation in this paper, the approximation accuracy is discussed with Equations (19) and (20), though the reference values of the sensitivity vectors are evaluated with the direct method.

3.4. Procedure of sensitivity matrix estimation with proposed method

In this chapter, utilization of the sensitivity matrix of the approximate assembly neutronics parameters to obtain AS is described. The procedure of the proposed method to estimate the sensitivity matrix of core neutronics parameters is summarized as follows:

1). The sensitivity matrix $\tilde{\mathbf{G}}_2$ of the approximate assembly neutronics parameters $\tilde{\Sigma}$ is evaluated with *N* (= the number of input parameters) forward assembly calculations with coarse condition.

2). SVD of $\tilde{\mathbf{G}}_2$ performed as Equation (17) and *r*-dimensional AS basis $\mathbf{V}_r$ is obtained by truncating small singular values.

3). The input parameters are expanded in the AS basis as $\Delta\vec{\sigma} = \mathbf{V}_r \Delta\vec{\alpha}$ and the sensitivity matrix **F** to the expansion coefficients is evaluated by Equation (14) with *r* forward assembly and core calculations.

4). The sensitivity matrix of the core neutronics parameters is reconstructed by Equation (11).

4. Numerical verification

To verify the validity of proposed method, the proposed method and the direct method are applied to a typical 3-loop PWR equilibrium core analysis. In this section, the conditions and results of the verification calculation are described.

4.1. Calculation conditions

The CASMO-4/SIMULATE-3 code system is used in this verification calculation [16, 17]. 5040 cross sections in L-library, which is a cross section library of CASMO-4, are taken into account as input parameters (N = 5040): These are the 70 group cross sections for 4 reactions (capture, fission, scattering, and average number of neutrons per fission ν) of 18 heavy nuclides (U-234, 235, 236, 238, Np-237, Pu-238, 239, 240, 241, 242, Am-241, 242, 243, Cm-242, 243, 244, 245 and 246), i.e., $5040 = 18 \times 4 \times 70$. The input parameters are listed in Table. 1.

The target core is a typical 3-loop equilibrium PWR core and the sensitivity coefficients of the target core parameters are estimated. In CASMO-4/SIMULATE-3 calculations, the calculation conditions comparable to those of the typical design calculation are used and the thermal-hydraulic feedback effects are explicitly taken into account.

The fuel pin arrangement, specifications of the fuel assembly and fuel pin loaded into target core are shown in Figure 2, Tables 2 and 3. Figures 3 and 4 show the fuel loading pattern and the assembly average burnup distribution of the target core at beginning of cycle (BOC), respectively. The cycle burnup is 15 GWd/t. The target core neutronics parameters are the critical boron concentration at end of cycle (EOC) and the relative assembly power of the fuel assembly filled by hatched lines in Figure 4 (0.0 GWd/t assembly at 5-th row and 2-th column). This assembly has highest relative power at EOC with the non-perturbed calculation.

The approximate assembly calculations for UO_2 fuel and UO_2-Gd_2O_3 fuel (Gd fuel), which loaded into the target core, are performed and the sensitivity matrix of the approximate assembly neutronics parameters to input parameters is evaluated. Each approximate assembly calculation is performed with 600 ppm boron concentration, 900 K fuel temperature, and 581 K moderator temperature. For UO_2 fuel assembly, the burnup calculation is performed from 0.0 to 70.0 GWd/t with 6 coarse burnup steps (i.e., 0.0, 0.1, 1.0, 5.0, 35.0, 70.0 GWd/t). For Gd fuel assembly, the burnup calculations is performed from 0.0 to 70.0 GWd/t with 52 steps (i.e., 0.0, 0.1, increments by 0.5 from 0.5 to 24.0, 35.0, 70.0 GWd/t). The tabulated points for branch calculations are set as follows:

- Boron concentration : 0.0, 1200.0, 2400.0 ppm
- Fuel temperature : 556 K
- Moderator temperature : 556 K

For branch calculation, 6 coarse burnup steps used in UO_2 fuel assembly are chosen both for the UO_2 and Gd fuel assemblies. Namely, the number of tabulated points for UO_2 and Gd fuel assemblies are 42 (= 6 + (3 + 1 + 1 + 1) × 6) and 88 (= 52 + (3 + 1 + 1 + 1) × 6), respectively. It is noted that the typical number of tabulated points for UO_2 and Gd fuel assembly are 400 and 600, respectively. The calculation cost to obtain an AS basis is reduced to (42 + 88) / (400 + 600) ≈ 13% by the utilization of the approximate assembly calculations.

As the approximate neutronics parameters $\tilde{\Sigma}$, various parameters obtained by assembly calculations can be used. In the present study, homogenized macroscopic 2-group cross sections (diffusion coefficient, capture, fission, production, removal, ν) at each state points are used. The total number of $\tilde{\Sigma}$ is 1300 (1300 = (42 UO_2 burnup steps + 88 Gd burnup steps) × 5 reactions × 2 groups) and $\tilde{\mathbf{G}}_2$, which is the sensitivity matrix of $\tilde{\Sigma}$, is the 1300-by-5040 matrix. 100080 (= 5040 times per assembly × 2 assemblies) forward

assembly calculations are performed to obtain $\tilde{\mathbf{G}}_2$ with 10 % perturbation for each cross section listed in Table 1.

After SVD of $\tilde{\mathbf{G}}_2$, the first *r* right singular vectors of $\tilde{\mathbf{G}}_2$, which correspond to the *r* largest singular values, are used as the AS basis $\mathbf{V}_r$. The perturbation is given to the expansion coefficients of input parameters (70 group microscopic cross sections) with expansion in the AS basis to estimate sensitivity coefficients of core neutronics parameters. The amount of perturbation to the expansion coefficients is decided as the relative norm of the perturbation vector to input parameters is 0.1, i.e., approximately 10% perturbation. It is noted that the sensitivity matrix of the core neutronics parameters to the expansion coefficients (e.g., the matrix **F** in Equation (11)) is obtained with assembly calculations using not coarse tabulated points but typical tabulated points (i.e., 400 points for UO_2 and 600 points for Gd). The relative difference norm of the sensitivity vectors obtained by the proposed method to those obtained by the direct method is evaluated with Equations (19) and (20) at the AS dimension of r = 1, 5, 10, 20, 50, 100 and 200.

The reference values of relative sensitivity coefficients are obtained by the direct method with 5040 set of assembly and core calculations with 50 % perturbation for each input parameters (70 group microscopic cross sections) by Equation (7). As mentioned later, 10 % perturbation in direct method would be too small and large numerical round off error may arise for some cross sections. Thus, 50 % perturbation is used to obtain reference values instead of 10 % which is given to obtain $\tilde{\mathbf{G}}_2$, i.e., larger perturbation is adopted to obtain accurate sensitivity coefficients as the reference values.

4.2. Results

Firstly, the results of the sensitivity coefficients of boron concentration at EOC are shown. Figure 5 shows the relative sensitivity coefficients obtained by the proposed method with r = 200 and reference values of those obtained by the direct method. The horizontal axis

represents the cross section ID listed in Table 1. Figure 5 shows that the magnitude and sign of the sensitivity coefficients of boron concentration at EOC are well reproduced with 200 (<< 5040) calculations. In addition, Figure 6 shows the comparison between the relative sensitivity coefficients obtained by the proposed method and those obtained by the direct method. In Figure 6, the horizontal axis and vertical axis represent the relative sensitivity coefficients of the boron concentration at EOC obtained by the direct method and the proposed method, respectively. As shown in Figure 6, the values obtained by the proposed method reproduce the reference values as the dimension of AS increases. These results show that the matrix decomposition in Equation (16) is valid because core calculations are performed with the homogenized cross sections obtained by the assembly neutronics parameters. Figure 7 shows the relative difference norm of the sensitivity coefficients of boron concentration at EOC versus the number of AS dimension. In Figure 7, “Experiment” and “Theory” represent the relative difference norms given by Equations (19) and (20), respectively. As shown in Figure 7, both the relative difference norms of “Experiment” and “Theory” are decreased as the AS dimension increases in the range of $r < 50$. The relative difference of “Theory” is reduced to 2 % at $r = 200$. On the other hand, the relative difference norm of “Experiment” is 7 %, which larger than that of “Theory”. This is caused by the finite difference approximation in the proposed method. In the same way, the results of the relative sensitivity coefficients of the relative assembly power are shown in from Figure 8 to Figure 10. As shown in Figures 8 and 9, the magnitude and sign of the sensitivity coefficients of the relative assembly power obtained by the proposed method well reproduce those of reference. Namely, the proposed method can be applied to not only boron concentration but also relative assembly power.

The proposed method does not require dedicated calculations such as generalized adjoint calculation for each neutronics parameters. The proposed method can simultaneously estimate the sensitivity coefficients for various neutronics parameters with lower calculation

cost. In addition, burnup, thermal-hydraulic feedback effect, and refueling are explicitly taken into account in this verification calculation. Even in such a situation, the proposed method works well although application of the adjoint-approach would be difficult.

As shown in Figure 10, the relative difference norm of “Experiment” tends to increase in the range of $r > 20$ and is about 10 %, which is larger than that of “Theory”. This is caused by the finite difference approximation for the estimation of sensitivity coefficients of the relative assembly power. Figure 11 shows that the relative sensitivity coefficients of relative assembly power obtained by the direct method with 10 % perturbation for input parameters. Compared to the Figure 8 (a), some sensitivity coefficients, e.g., Np-237 capture (ID: 1120 ~ 1190), seem to contain noise. Since 10 % perturbation is smaller than 50 %, which is used to obtain the reference values, and the effect of the numerical round off error would be larger. This is same as for the expansion coefficients in the proposed method. Especially for larger r, the sensitivity coefficients of the assembly neutronics parameters to the expansion coefficients becomes smaller, thus the perturbation of the core neutronics parameters to the expansion coefficients will be small. Therefore, tighter convergence criteria or larger perturbation is necessary to reduce the numerical round off error. In this verification calculation, magnitude of perturbation to each expansion coefficient is constant and is independent to the number of AS dimensions. Thus, the numerical round off error becomes significant as r is increased, consequently, the relative difference norm tends to increase as shown in Figure 10. Appropriate choice of magnitude of perturbation considering the non-linear effect and numerical round off error would be a future task.

5. Conclusion

We proposed a method to estimate the sensitivity coefficients of the core neutronics parameters based on the reduced order modeling (ROM) using the sensitivity matrix of assembly neutronics parameters obtained by approximate assembly calculations employing

the coarse state points. The proposed method assumes that the sensitivity matrix of the core neutronics parameters can be expressed by linear combination of the active subspace (AS) basis obtained from the sensitivity matrix of the assembly neutronics parameters. The proposed method obtains an AS basis by the singular value decomposition (SVD) of the sensitivity matrix of the approximate assembly neutronics parameters evaluated by forward calculations. The required number of the forward core calculations to estimate the sensitivity coefficients is reduced using the AS basis: The variation of the input parameters is expanded by the AS basis so that the degree of freedom of the input parameters is reduced from the number of the input parameters to the number of the AS dimensions. The proposed method utilizes only forward calculations and has potential to significantly reduce the calculation cost compared to the direct method. Thus, the proposed method can be a candidate for the practical estimation method of the sensitivity coefficients when the adjoint-approach is computationally impractical such as the case with LWR core analysis.

The proposed method is applied to a typical 3-loop PWR equilibrium core analysis. A total of 5040 input parameters i.e., the 70-group microscopic cross sections of the heavy nuclides are taken into account. Through the verification calculation, it is confirmed that the sensitivity coefficients of boron concentration and relative assembly power estimated by the proposed method can well reproduce those of the direct method. The verification results show that the proposed method can estimate the sensitivity coefficients of the various core neutronics parameters with less calculation cost even when the adjoint-approach is difficult to be applied.

The relative difference norm of “Experiment” of the sensitivity coefficients of relative assembly power tends to increase in the range of large r. This is caused by numerical round off error of the finite difference approximation; this problem is common to the forward sensitivity estimation. The appropriate amount of perturbation in the proposed method should be investigated in the future. In this work, the approximation accuracy of the proposed

method is discussed compared to the results of the direct method. However, in a practical application, the number of AS dimensions to achieve the target precision has to be estimated without the result of the direct method. Thus, an estimation method of the upper bound of the approximation error versus AS dimension such as Reference 13 should be applied.

References

[1] Iwamoto H, Nishihara K, Sugawara T, Tsujimoto K. Sensitivity and uncertainty analysis for an accelerator driven system with JENDL-4.0. J. Nucl. Sci. Technol. 2013 Jul; 50:856-862.

[2] Takeda T, Yoshimura Y. Prediction uncertainty evaluation methods to core performance parameters in large liquid-metal fast breeder reactor. Nucl. Sci. Eng. 1989 Oct; 103:257.

[3] Chiba G, Narabayashi T. Variance reduction factor of nuclear data for integral neutronics parameters. Nuclear Data Sheets. 2015 Jan; 123:62-67.

[4] Usachev L N. Perturbation theory for the breeding ratio and for other number ratios pertaining to various reactor processes. J. Nucl. Energy A/B. 1964 Oct; 18:571-583.

[5] Williams M. Development of depletion perturbation theory for coupled neutron/nuclide fields. Nucl. Sci. Eng. 1979 Apr; 70:20-36.

[6] Kennedy C, Rabiti C, Abdel-Khalik H. Generalized perturbation theory free sensitivity analysis for eigenvalue problems. Nucl. Technol. 2012 Aug; 179:169-179.

[7] Kennedy C, Abdel-Khalik H. Depletion GPT-free sensitivity analysis of the TMI reactor eigenvalue model. Proc. PHYSOR-2014; 2014 Sep 28-Oct 3; Kyoto (Japan). [CD-ROM].

[8] Bang Y, Abdel-Khalik H, Jessee M, Mertyurek U. Hybrid reduced order modeling for assembly calculations. Nucl. Eng. Des.. 2015 Dec; 295:661-666.

[9] Abdo M, Abdel-Khalik H. Development of multi-level reduced order modeling methodology. ANS Annual Meeting, 2015 Jun; 112:445-448.

[10] Abdo M, Abdel-Khalik H. Assessment of the validation domain of reduced order modeling. ANS winter meeting, 2015 Nov, 113:1212-1216.

[11] Abdo M, Abdel-Khalik H. Efficient active subspace identification via MLROM. Proc. PHYSOR-2016, 2016 May 1-5; Sun Valley (ID).

[12] Jessee M, Turinsky P, Abdel-Khalik H. Efficient subspace methods-based algorithms for performing sensitivity, uncertainty, and adaptive simulation of large-scale computational models. Nucl. Sci. Eng. 2008 Jul; 159:256-272.

[13] Abdo M. Multi-level reduced order modeling equipped with probabilistic error bounds. Ph D. Thesis, North Carolina State University, 2016.

[14] Golub G. Matrix Computations (3rd ed.). John Hopkins; 1996.

[15] Katano R, Yamamoto A, Endo T. Application of partially-converged solution of assembly calculation for core sensitivity analysis based on reduced order modeling. Trans. Am. Nucl. Soc, 2015, 113:1161-1164.

[16] Smith K, Rhodes J. CASMO-4 characteristics methods for two dimensional PWR and BWR core calculations. Trans. Am. Nucl. Soc, 2000, 83:322.

[17] Smith K, et al. SIMULATE-3 methodology. Studsvik/SOA-95/18; 1995.

Figure captions

Figure 1. Burnup dependence of assembly neutornics perameters with/without perturbations.

Figure 2. Geometry of fuel assemblies (1/8 configuration).

Figure 3. Core configuration (1/8 core).

Figure 4. Assembly average burnup distribution at beginning of cycle (BOC) (1/8 core, GWd/t).

Figure 5. Relative sensitivity coefficients of boron concentration at EOC.

Figure 6. Comparison of relative sensitivity coefficients of boron concentration at end of cycle (EOC). r indicates dimension of active subspace in the present method.

Figure 7. Active subspace (AS) dimension versus relative difference norm of relative sensitivity of boron concentration at EOC.

Figure 8. Relative sensitivity coefficients of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3).

Figure 9. Comparison of relative sensitivity coefficients of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3).

Figure 10. AS dimension versus relative difference norm of relative sensitivity of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3).

Figure 11. Relative sensitivity coefficients of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3) obtained by the direct method with 10% perturbation for input data.

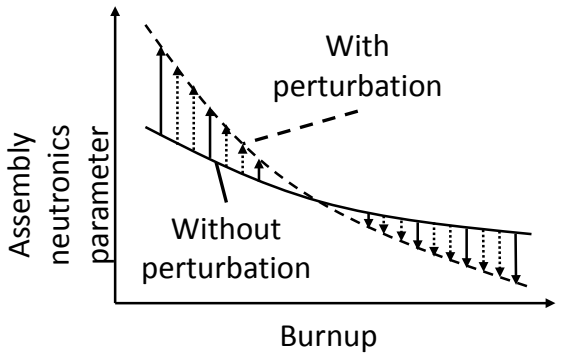


Figure 1. Burnup dependence of assembly neutornics parameters with/without perturbations.

R. Katano: Estimation of core sensitivity coefficients based on Reduced-Order Modeling using sensitivity matrix of assembly characteristics

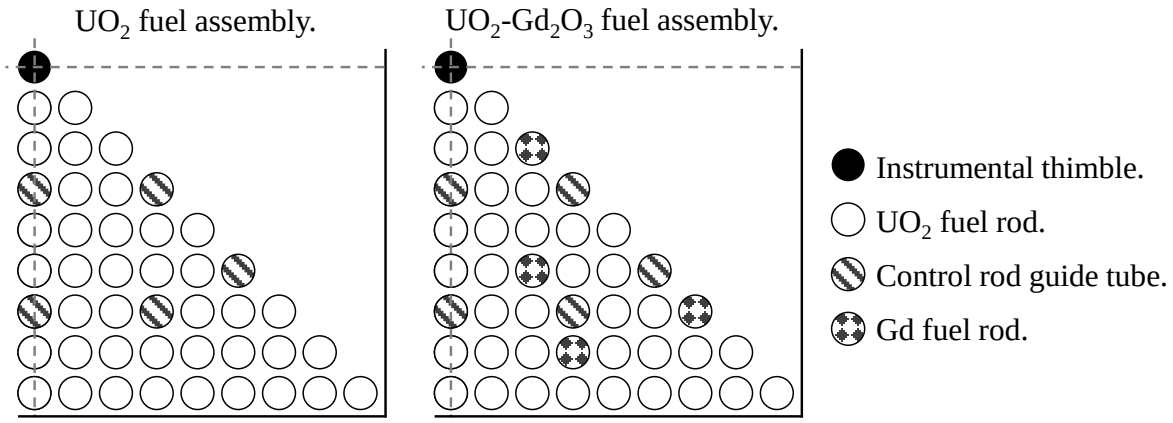


Figure 2. Geometry of fuel assemblies (1/8 configuration).

R. Katano: Estimation of core sensitivity coefficients based on Reduced-Order Modeling using sensitivity matrix of assembly characteristics

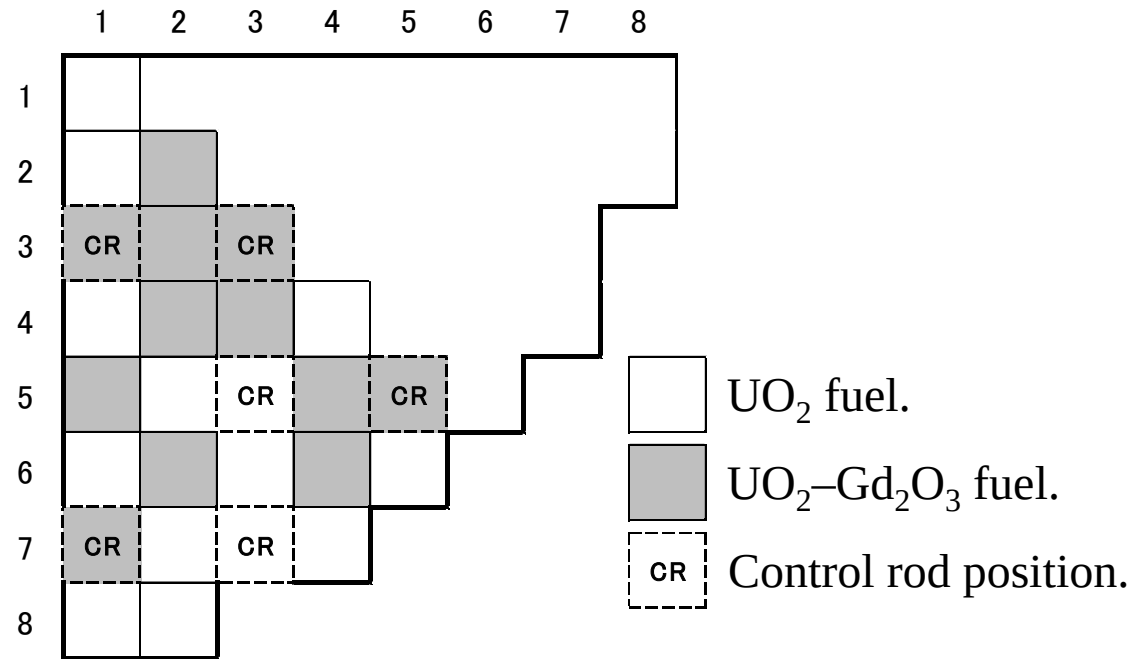


Figure 3. Core configuration (1/8 core).

R. Katano: Estimation of core sensitivity coefficients based on Reduced-Order Modeling using sensitivity matrix of assembly characteristics

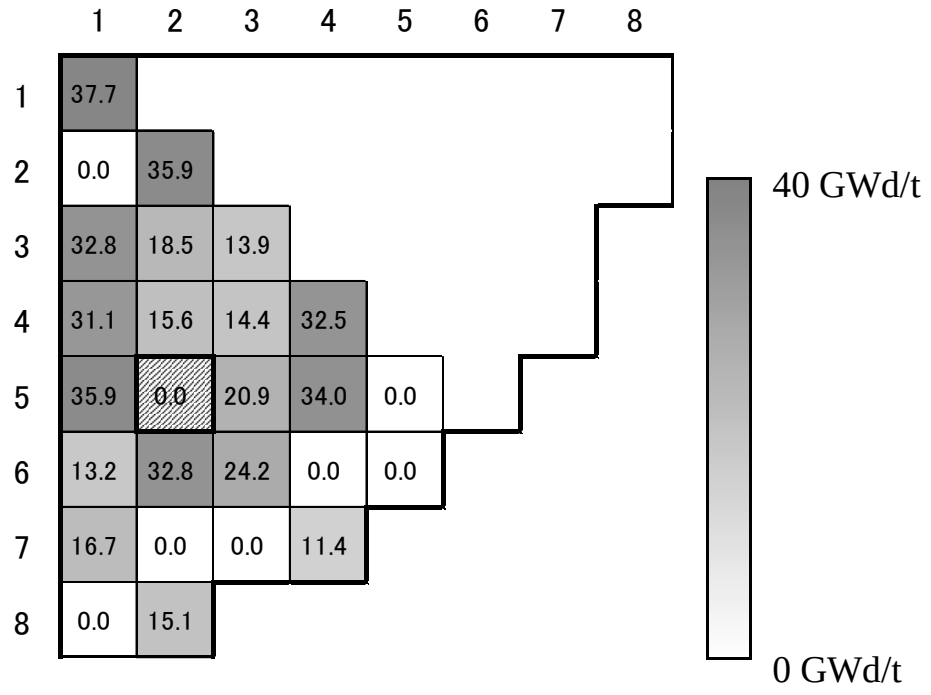
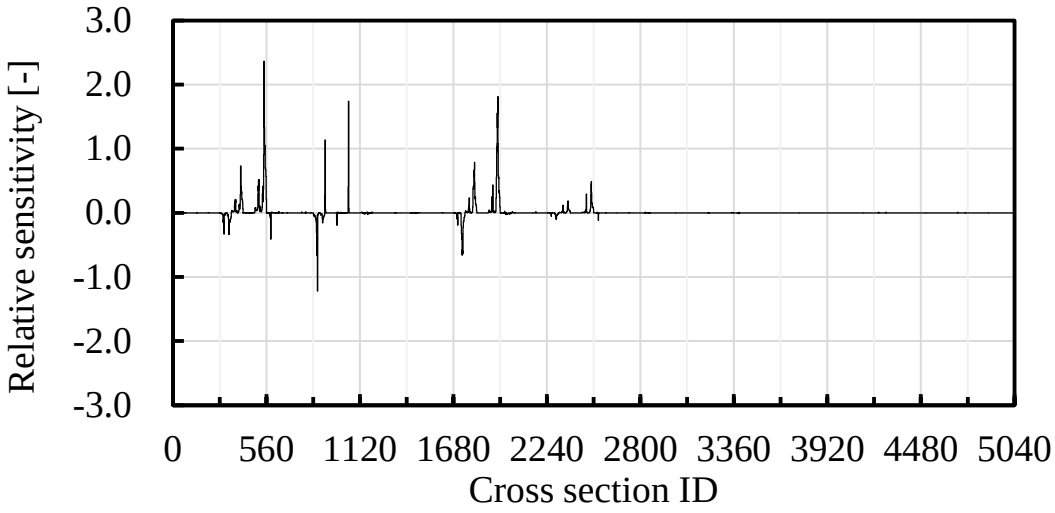
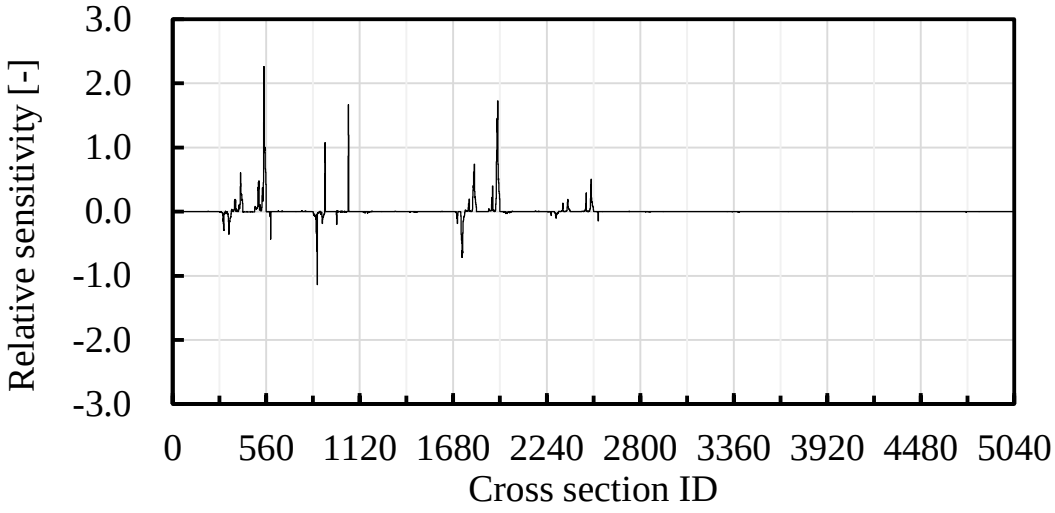


Figure 4. Assembly average burnup distribution at beginning of cycle (BOC) (1/8 core, GWd/t).

R. Katano: Estimation of core sensitivity coefficients based on Reduced-Order Modeling using sensitivity matrix of assembly characteristics

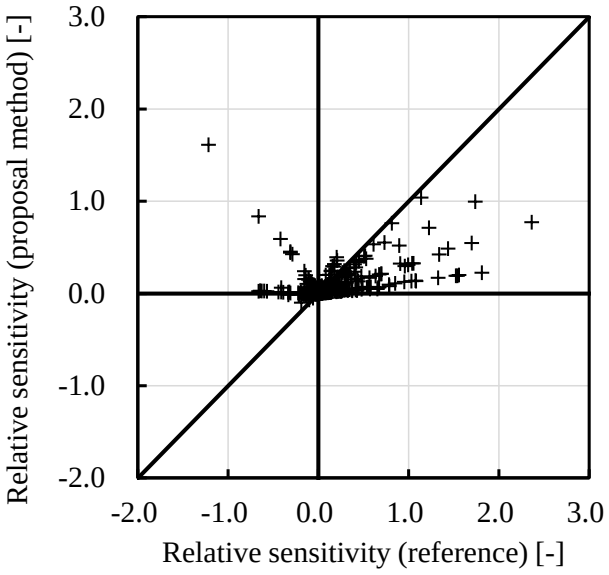


(a) Reference

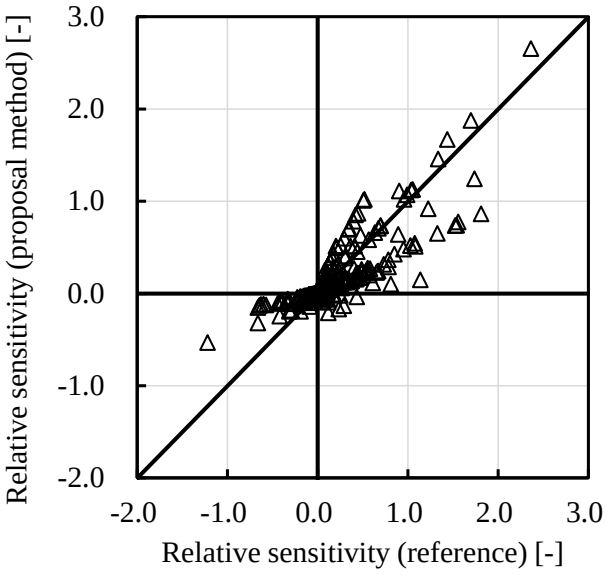


(b) Proposed method: r = 200

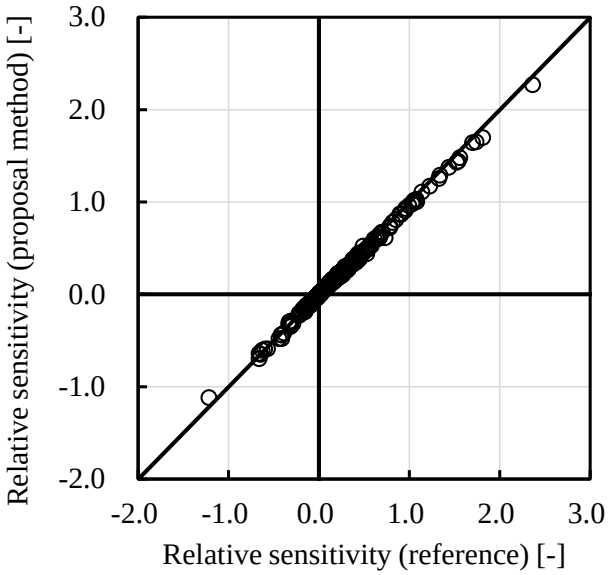
Figure 5. Relative sensitivity coefficients of boron concentration at EOC.



(a) r = 1



(b) r = 5



(c) r = 20

Figure 6. Comparison of relative sensitivity coefficients of boron concentration at end of cycle (EOC). r indicates dimension of active subspace in the present method.

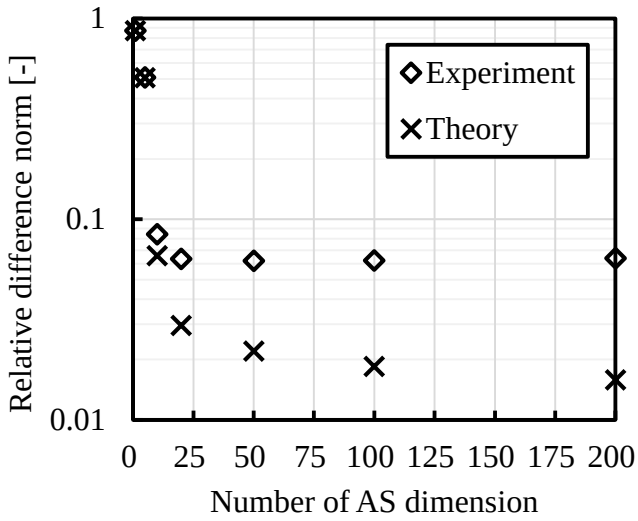
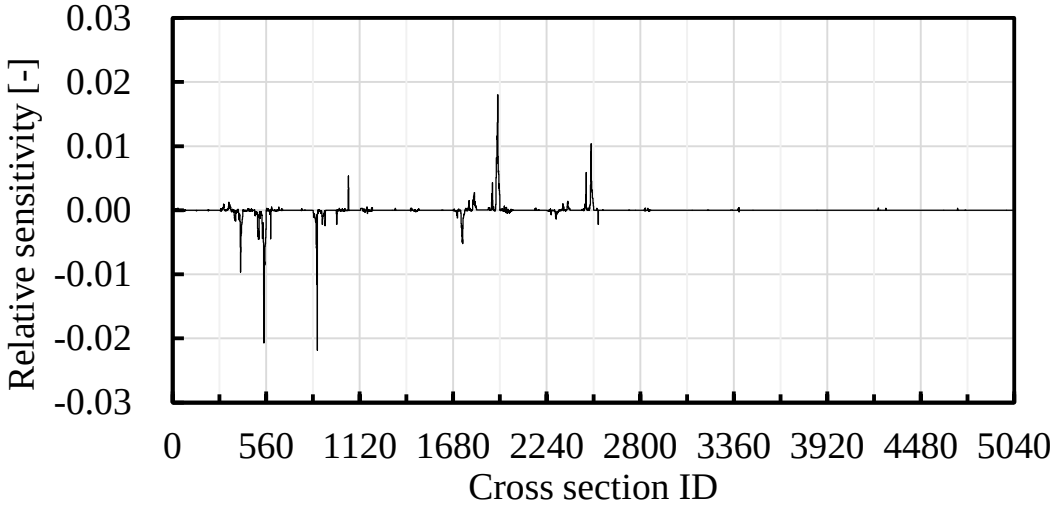
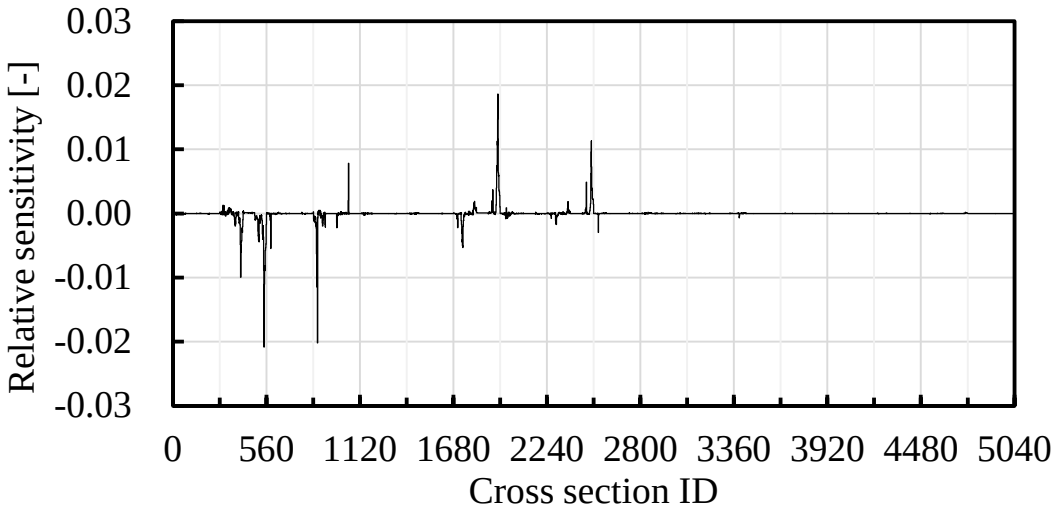


Figure 7. Active subspace (AS) dimension versus relative difference norm of relative sensitivity of boron concentration at EOC.

R. Katano: Estimation of core sensitivity coefficients based on Reduced-Order Modeling using sensitivity matrix of assembly characteristics

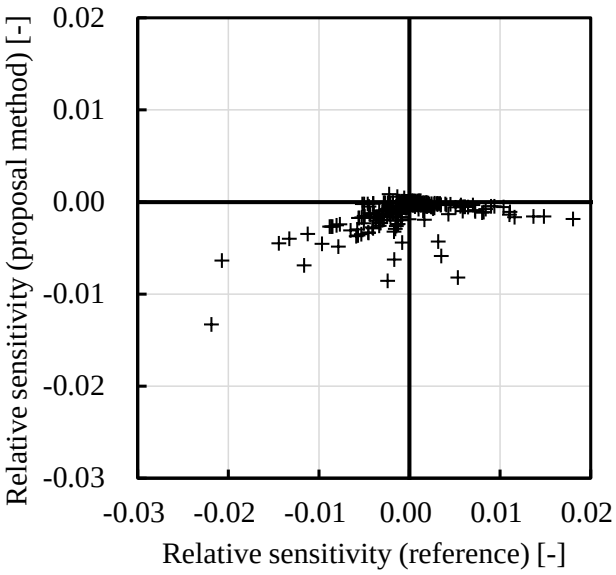


(a) Reference

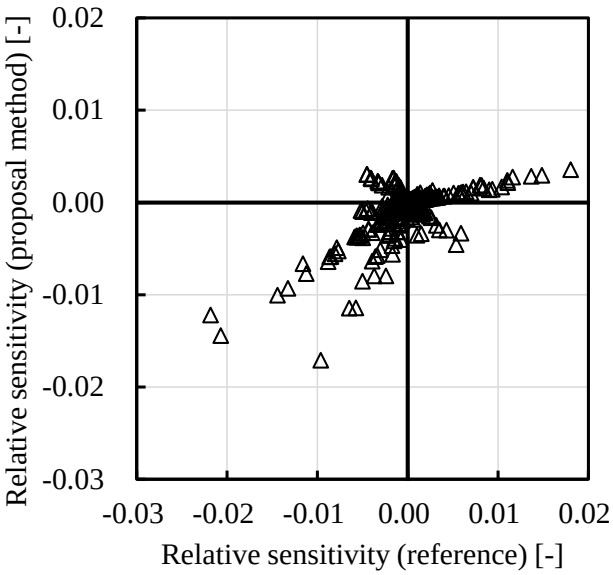


(b) Proposed method: r = 200

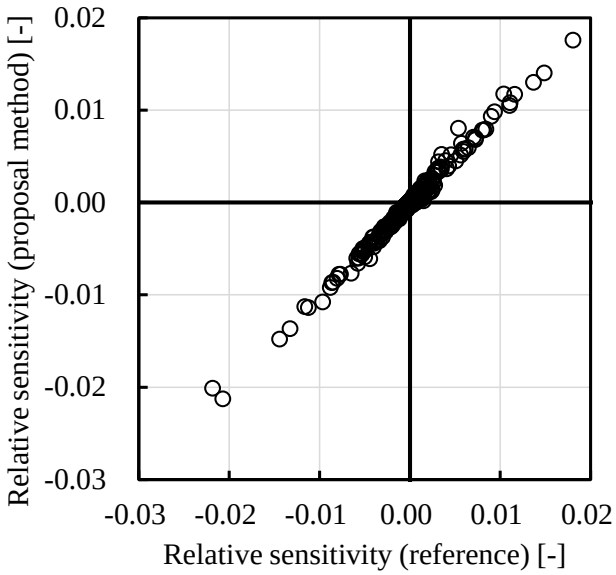
Figure 8. Relative sensitivity coefficients of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3).



(a) r = 1



(b) r = 5



(c) r = 20

Figure 9. Comparison of relative sensitivity coefficients of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3).

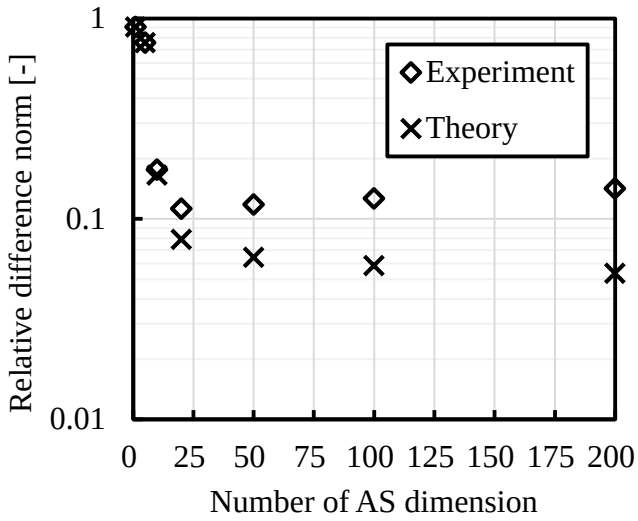


Figure 10. AS dimension versus relative difference norm of relative sensitivity of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3).

R. Katano: Estimation of core sensitivity coefficients based on Reduced-Order Modeling using sensitivity matrix of assembly characteristics

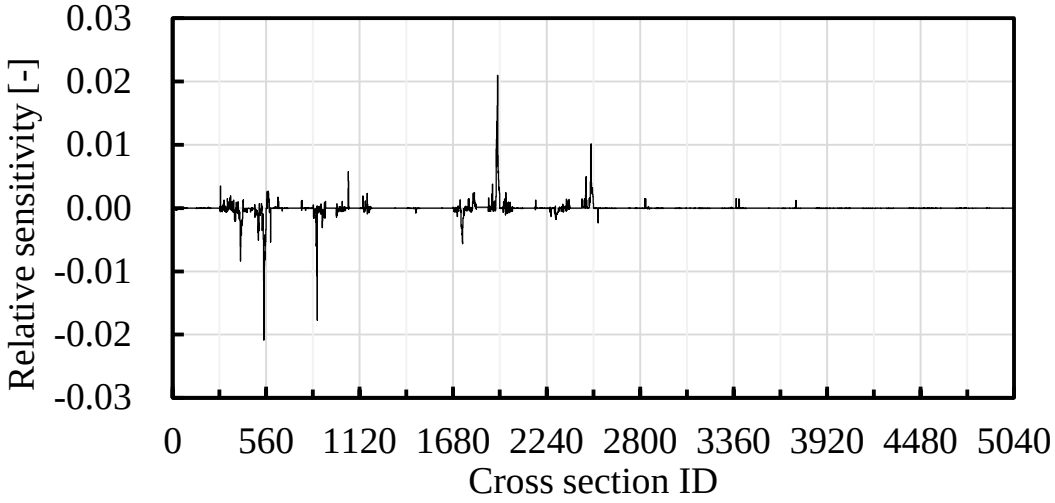


Figure 11. Relative sensitivity coefficients of relative assembly power at EOC (fuel assembly filled by hatched lines in Fig.3) obtained by the direct method with 10% perturbation for input data.

Table 1. ID of input parameters (microscopic cross sections in 70 group)

Nuclide	Capture	Fission	Scattering	ν
U-234	1-70	71-140	141-210	211-280
U-235	281-350	351-420	421-490	491-560
U-236	561-630	631-700	701-770	771-840
U-238	841-910	911-980	981-1050	1051-1120
Np-237	1121-1190	1191-1260	1261-1330	1331-1400
Pu-238	1401-1470	1471-1540	1541-1610	1611-1680
Pu-239	1681-1750	1751-1820	1821-1890	1891-1960
Pu-240	1961-2030	2031-2100	2101-2170	2171-2240
Pu-241	2241-2310	2311-2380	2381-2450	2451-2520
Pu-242	2521-2590	2591-2660	2661-2730	2731-2800
Am-241	2801-2870	2871-2940	2941-3010	3011-3080
Am-242	3081-3150	3151-3220	3221-3290	3291-3360
Am-243	3361-3430	3431-3500	3501-3570	3571-3640
Cm-242	3641-3710	3711-3780	3781-3850	3851-3920
Cm-243	3921-3990	3991-4060	4061-4130	4131-4200
Cm-244	4201-4270	4271-4340	4341-4410	4411-4480
Cm-245	4481-4550	4551-4620	4621-4690	4691-4760
Cm-246	4761-4830	4831-4900	4901-4970	4971-5040

Table 2. Specifications of fuel assemblies.

	UO_2	UO_2-Gd_2O_3
Fuel rod arrangement	17 x 17	
Number of UO2 rods	264	240
Number of Gd bearing rods	0	24
Number of instrumental thimble	1	
Number of control rod guide tubes	24	
Outer diameter of thimble [mm]	12.2	
Inner diameter of thimble [mm]	11.4	
Outer diameter of guide tube [mm]	12.2	
Inner diameter of guide tube [mm]	11.4	
Pitch of fuel rod [mm]	12.6	
Pitch of fuel assembly [mm]	215.0	

Table 3. Specifications of fuel rod.

	UO_2	UO_2-Gd_2O_3
Fuel density [g/cm^3]	10.5	10.1
Uranium enrichment [wt%]	4.8	3.2
Gadolinia concentration [wt%]	0.0	10.0
Pellet diameter [mm]	8.2	
Inner diameter of cladding [mm]	8.4	
Outer diameter of cladding [mm]	9.5	