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Application of Perturbation-based Sensitivity Analysis to Nuclear Characteristics*

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섭동론적 감도해석 이론의 원자로 핵특성에의 응용

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Abstract

An equation of material number density sensitivity coefficient is derived using first-order perturbation theory. The beginning of cycle of Super-Phenix I is taken as the reference system for this study. Effective multiplication factor of the reference system is defined as system response function and fuel enrichment and fuel effective density are chosen for the variation of reference input data since they are described by material number density which is a component of Boltzmann operator. The nuclear computational code system (KAERI-26 group cross section library/1DX/2DB/PERT-V) is employed for this calculation. Sensitivity coefficient of fuel enrichment on effective multiplication factor is 4.576 and sensitivity coefficient of effective fuel density on effective multiplication factor is 0.0756. This work shows that sensitivity methodology is lesser timeconsuming and gives more informations on important design parameters in comparison with the direct iterative calulation through large computer codes.

요 약

일차섭동이론을 이용하여 물질밀도 감도 계수의 표현식을 유도하였다. Super-Phenix I 평형노심의 초기상태를 기준계로 택했으며 유효증배계수를 계의 응답함수로 정의했다. 볼츠만 연산자의 구성요소인 물질밀도로 표현되는 핵연료의 농축도와 실효밀도를 입력변화로 선정했다. 위 계산을 수행하는데 전산코드시스템 (KAERI-26군 단면적 library/1DX/2DB/PERT-V)가 사용되었다. 핵연료 농축도의 유효증배계수에 대한 감도계수는 4.576로 계산되었으며, 핵연료 실효밀도의 감도 계수는 0.0756으로 계산되었다. 본 연구는 감도해석법이 대형전산코드를 이용한 직접반복계산법에 비해 계산시간의 단축과 아울러 많은 정보를 준다는 것을 보여준다.

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1. Introduction

Sensitivity analysis in nuclear field deals with the way of obtaining the relative change in system response due to a relative change in nuclear data or design parameters.

Although we have no accumulated case-by-case experience for the reference reactor which is expected to be introduced, we can predict or cope with the modification of the reference system through the utilization of sensitivity. In addition, we can derive the important design parameters which require our attention. Hence, we attempt this work as an example for the application of sensitivity methodology.

For this work, our emphasis has been placed on the space-dependent material density which is a component of the Boltzmann linear operator. Sensitivity study of material number density provides us with the information about the effects of different variations in the compositions of a reference design on its nuclear properties. This information is valuable for assessing the potential design change related to a large number of materials and compositions in the conceptual phase of a design.

When coupled with the geometrical boundary displacement, this material number density sensitivity can be utilized for the transient analysis in case where reactor core deformation due to thermal expansion takes place.

In this study, first-order perturbation theory was adopted within the context of linear perturbation theory. The beginning of cycle (BOC) of equilibrium core of the liquid metal fast breeder reactor, Super-Phenix I was chosen for the reference system. And effective multiplication factor was selected as the system response function. Input parameters for case studies were single isotope, fuel enrichment, and fuel effective density. The latter two input parameters are described by combinations of each relevant material number densities.

The nuclear computational code system for a large LMFBR (KAERI-26 group cross section library[1]/1DX[2]/2DB[3]/PERT-V)[4] was employed for the calculation.

2. Calculational Method

In general, a sensitivity function of a system response or performance parameter, R, with respect to an input variable, q, is defined as the relative change in R due to a relative change in q.[5]

$$S_{R,q}(\rho)=\frac{dR}{R}\Big/\frac{dq(\vec{\rho})}{q(\vec{\rho})} \tag{1}$$

where ρ stands for a subset of the phase space variables $(\vec{r}, E, \vec{\Omega})$. As the functional dependence of R with q is, in general, not linear, the sensitivity function $S_{R,q}$ can express accurately the change in R due only to a relatively small change in q.

For this study, the sensitivity function of effective multiplication factor to macroscopic cross section is defined as follows;

$$S_{k,\Sigma}(\vec{\rho})=\frac{\delta k_{\text{eff}}}{k_{\text{eff}}}\Big/\frac{\delta\Sigma(\vec{\rho})}{\Sigma(\vec{\rho})}. \tag{2}$$

Boltzmann operator consists of microscopic cross section and material number density. Then, with fixed microscopic cross section data, Eq. (2) becomes

$$S_{k,N}(\vec{r})=\frac{\delta k_{\text{eff}}}{k_{\text{eff}}}\Big/\frac{\delta N(\vec{r})}{N(\vec{r})} \tag{3}$$

where $N(\vec{r})$ is material number density distribution for arbitrary nuclide. Eq. (3) is the sensitivity traverse of effective multiplication factor to material number density.

The total sensitivity coefficient can be obtained from the sensitivity traverse as follows:

$$S_{k,N}=\int d\vec{r}\, S_{k,N}(\vec{r})$$
$$=\int d\vec{r}\left[\frac{\delta k_{\text{eff}}}{k_{\text{eff}}}\Big/\frac{\delta N(\vec{r})}{N(\vec{r})}\right]. \tag{4}$$

The resulting sensitivity coefficient of material number density, S_{kN}, can be used for estimating the effect on the system response, k_{eff}, due to uniform relative changes in the concentration of any material throughout the reactor.

The system response change, $\delta k_{eff}/k_{eff}$, which is the ratio of a bilinear functional was evaluated using the PERT-V code. The PERT-V code computes the reactivity coefficient, δ_{eff}/k_{eff} per k_g of a specific nuclide, at each mesh point in the specified row or column using the first-order perturbation theory. This value can be converted into $\delta k_{eff}/k_{eff}$ per atom of specific nuclide. The expression for reactivity coefficient used in the PERT-V code is as follows[4]

$$\frac{\delta k_{eff}}{k_{eff}}=\frac{F+A+L+S}{I} \tag{5}$$

where

$$I=\frac{1}{k_{eff}}\int dV\left\{\sum_{j=1}^{IGM}(\chi_j\phi_j^*)\sum_{i=1}^{IGM}(\nu\Sigma_f^i\phi_i)\right\}$$

$$F=\frac{1}{k_{eff}}\int dV\left\{\sum_{j=1}^{IGM}(\chi_j\phi_j^*)\sum_{i=1}^{IGM}(\delta[\nu\Sigma_f^i]\phi_i)\right\}$$

$$A=-\int dV\left\{\sum_{i=1}^{IGM}(\delta[\Sigma_a^i]\phi_i\phi_i^*)\right\}$$

$$L=\int dV\left\{\sum_{i=1}^{IGM}(\nabla\phi_i\cdot\nabla\phi_i^*)\frac{\delta[\Sigma_{tr}{}^i}{3(\Sigma_{tr}{}^i)^2}\right\}$$

$$S=\int dV\left\{\sum_{i=1}^{IGM}\left(\sum_{j=i+1}^{IGM}\delta[\Sigma(i\to j)]\phi_i(\phi_j^*-\phi_i^*)\right)\right\}$$

where

IGM=number of energy groups

ϕ_i=flux in group i (#/cm^2 sec)

χ_i=fission source born in group i $\left(\sum_{i=1}^{IGM}\chi_i=1.0\right)$

Σ_a^i=macroscopic absorption cross section for group i (cm^{-1})

Σ_{tr}^i=macroscopic transport cross section for group i (cm^{-1})

$\Sigma(i\to j)$=macroscopic transfer cross section from group i to group j

k_{eff}=effective multiplication factor

$(\nu\Sigma_f)^i$=macroscopic fission source cross section for group i

$\delta\Sigma$=perturbed operator for macroscopic cross section.

Furthermore, a sensitivity function can be defined in any of the independent variables and can be expressed in terms of different combinations of the independent variables. As an application of this case, the sensitivity traverse of fuel enrichment on k_{eff} can be described as follows;

$$S_{k,EN}(\vec{r})=\frac{\delta k_{eff}}{k_{eff}}\Big/\frac{\delta EN(\vec{r})}{EN(\vec{r})} \tag{6}$$

where $EN(\vec{r})$ is the fuel enrichment distribution. And the mixed oxide fuel enrichment is defined as

$$EN=\frac{\text{Pu-fissile}}{\text{Pu-fissile}+\text{Pu-fertile}+\text{U}} \tag{7}$$

In this case the relative change of fuel enrichment have to be transformed into the terms of the relevant material number denstiy variation. Then, Eq. (6) can be expressed as the following formula.[7]

$$S_{k,EN}(\vec{r})=\sum\left(\frac{\delta k_{eff}}{k_{eff}}\Big/\frac{\delta N^l(\vec{r})}{N^l(\vec{r})}\right) \tag{8}$$

where l means the isotopes related to the definition of MOX (PuO_2+UO_2) fuel enrichment.

The subroutine "CALC" in the PERT-V code, which calculates reactivity coefficient traverses according to Eq. (5), is modified in order to calculate the sensitivity coefficients by using Eq. (8).

3. Applications and Results

3.1. Description of Reference System

The forward and adjoint fluxes for the reference reactor[6] are assumed to be given by the nuclear computational code system (KAERI-26 group cross section library/1DX/2DB).

The R-Z geometry model for the beginning of cycle(BOC) of equilibrium core of Super-Phenix I is shown in Fig. 1.

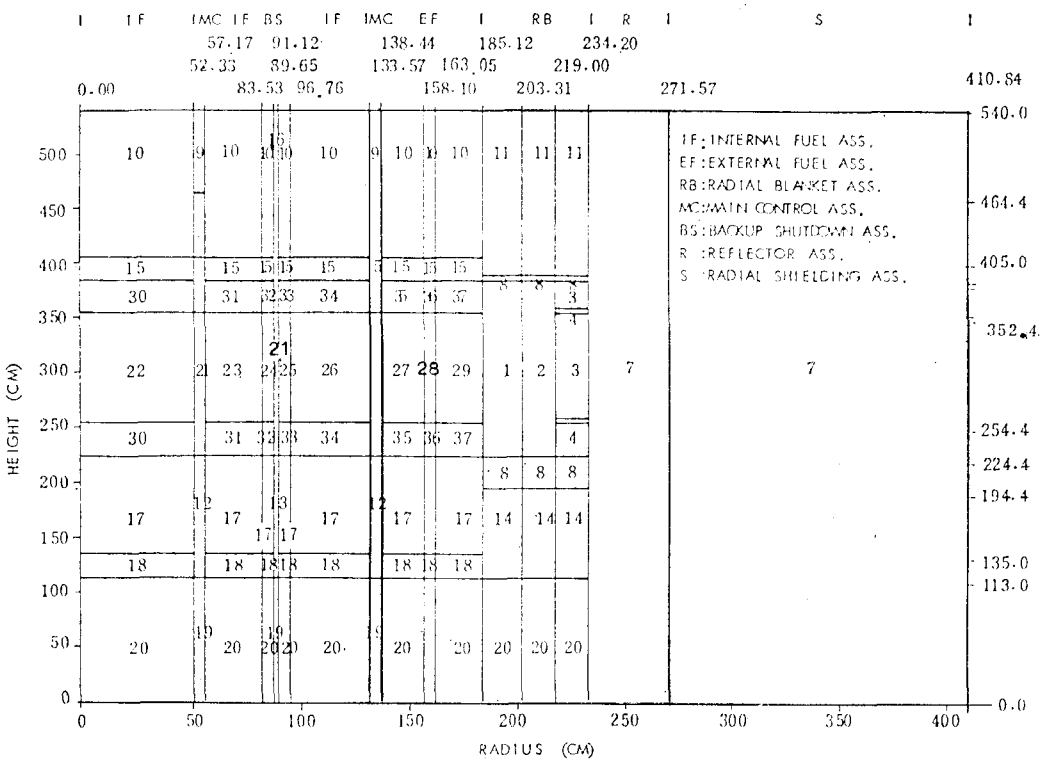

Fig. 1. R-Z Geometry Model with All Control Rods Out for the Core of Super-Phenix I

For this study the effect of system response is confined to the active fuel region such as internal and external fuel assembly region which correspond to the zone number 22, 23, 24, 25, 26, 27, 28, and 29 in Fig. 1 and control assembly regions are excluded.

The axial region boundary is from 254.4cm to 354.4cm and the radial boundary is from 0cm to 185.12cm. Each zone is divided into one or more columns and each column is divided into 20 axial meshes compatible with the matrices of the forward and adjoint fluxes. The material number density for each homogenized zone are given in the KAERI report.[6]

3.2. Numerical Case Study

3.2.1. Case of Number Density Variation of Single Isotope

For the first case study, fissile isotope Pu-239 number density in the MOX fuel is increased by 1% uniformly over the active fuel assembly region. The amount of Pu-239 number density increase, $\delta N^{239}(\vec{r})$, in each homogenized zone is computed from the given value of the reference reactor.

The column-wise reactivity coefficient is obtained by summing mesh volume-wise reactivity coefficients for the given column through the modified PERT-V code, Then the total sensitivity coefficient is calculated by summing the column-wise reactivity coefficients and dividing the total $\delta k_{eff}/k_{eff}$ by 0.01. Fig. 2 and Table 1 show the sensitivity traverse of Pu-239 number density on k_{eff}. The total sensitivity coefficient is 0.457.

As another case, fertile isotope U-238 is increased by 1%. The results are shown in Table2 and Fig. 3. The total sensitivity coefficient of U-238 number density on k_{eff} is -0.186.

Table 1. Column-wise Sensitivity Traverse of Pu-239 Atom Number Density on k_{eff}

($\times 10^{-2}$)

Zone No.	Column No.	Sensitivity Coefficient
22	1	0.016
	2	0.049
	3	0.082
	4	0.205
	5	0.291
	6	0.375
	7	0.474
	8	0.559
	9	0.638
	10	0.759
	11	0.847
23	17	1.349
	18	1.981
	19	0.821
	20	1.360
	21	1.083
24	22	1.145
25	26	1.302
26	27	1.368
	28	1.437
	29	0.924
	30	1.854
	31	2.260
	32	2.346
	33	2.423
	34	2.476
27	40	1.937
	41	1.976
	42	1.984
	43	1.581
	44	1.939
28	45	1.627
29	46	2.982
	47	0.973
	48	1.329
	49	0.948

Table 2. Column-wise Sensitivity Traverse of U-238 Atom Number Density on k_{eff}

($\times 10^{-2}$)

Zone No.	Column No.	Sensitivity Coefficient
22	1	−0.006
	2	−0.019
	3	−0.032
	4	−0.082
	5	−0.116
	6	−0.151
	7	−0.191
	8	−0.225
	9	−0.260
	10	−0.315
	11	−0.362
23	17	−0.576
	18	−0.822
	19	−0.337
	20	−0.557
	21	−0.445
24	22	−0.480
25	26	−0.534
26	27	−0.549
	28	−0.575
	29	−0.369
	30	−0.742
	31	−0.908
	32	−0.948
	33	−0.909
	34	−1.038
27	40	−1.034
	41	−0.802
	42	−0.786
	43	−0.769
	44	−0.602
28	45	−0.721
29	46	−0.608
	47	−1.078
	48	−0.295
	49	−0.330

From the above results, we can say that the increase of k_{eff} due to 1% increase in Pu-239 number density compensates for the decrease of k_{eff} due to approximately 2.4% increase in U-238 number density.

3.2.2. Case of MOX Fuel Enrichment and Fuel Effective Density Variation

In the case of fuel enrichment variation, the

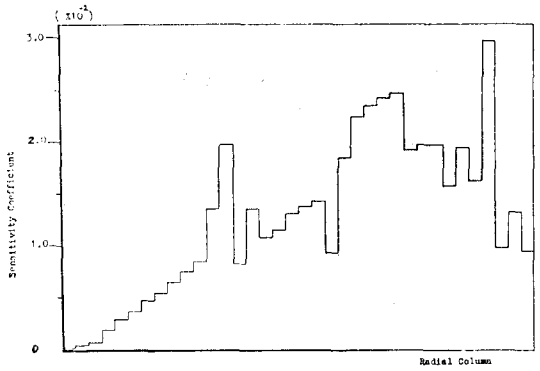

Fig. 2. Column-wise Sensitivity Traverse of Pu-239 Atom Number Density on k_{eff}

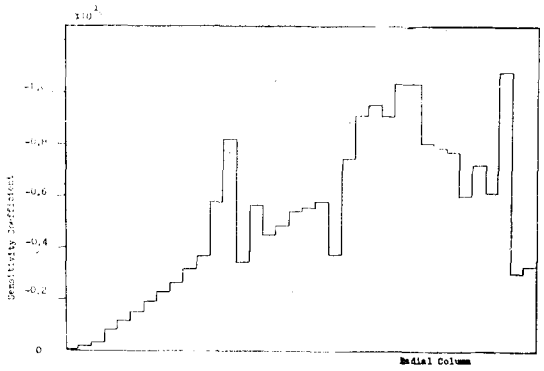

Fig. 3. Column-wise Sensitivity Traverse of U-238 Atom Number Density on k_{eff}

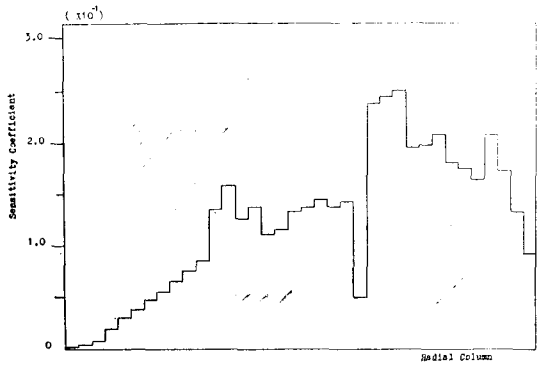

Fig. 4. Column-wise Sensitivity Traverse of Fuel Enrichment on k_{eff}

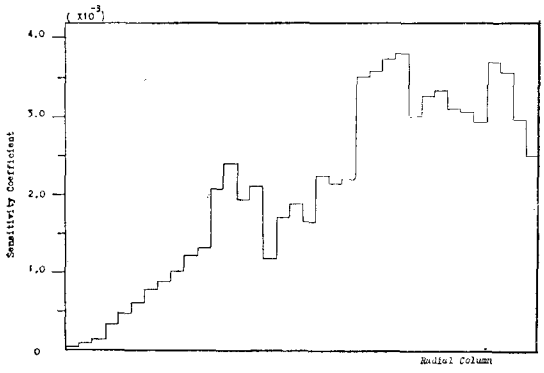

Fig. 5. Column-wise Sensitivity Traverse of Fuel Effective Density on k_{eff}

related isotopes are U-235, U-238, Pu-239, Pu-240, Pu-241, and Pu-242. Among them Pu-fissile isotopes are Pu-239 and Pu-241. And the fuel enrichment of the internal fuel assembly region is 13.79% and that of the external fuel assembly region is 17.60%.[6] For the calculation, it is assumed that the total atom numbers of fuel isotopes remain constant and isotopic abundances in Pu and U are constant, respectively. The remaining calculation procedure is the same as the case of single isotope variation. The total sensitivity coefficient of fuel enrichment on k_{eff} is 4.576. The column-wise sensitivity traverse of fuel enrichment is shown in Fig. 4.

The case study of fuel effective density variation is also investigated. The theoretical density of PuO_2 is 11.465g/cm^3 and that of UO_2 is 10.960g/cm^3. For the reference reactor, MOX fuel effective density is 95.46% TD. With fixed zone volume, 1% increase of fuel effective density is converted into zone-wise fuel mass increase. Then, calculated are the corresponding number density increase in each fuel isotopes, which include 0~16 under the assumption that the isotopic abundances are constant. The total sensitivity coefficient of fuel effective density on k_{eff} is 0.0756. The column-wise sensitivity traverse of fuel effective density is shown in Fig.5.

4. Conclusions and Recommendation

The results of the perturbation-based sensitivity methodology show that the most important input parameter among selected input data sets can be determined quantitatively. Once the

forward and adjoint fluxes have been calculated for the reference system, the system response change due to uncertainties of input data or design modification can be predicted in the context of sensitivity coefficient. The exploitation of sensitivity methodology will contribute to domestic participation in the localization of nuclear power plant.

For further research, this methodology might be extended to design optimization and uncertainty analysis. And more quantitative approaches using generalized perturbation theory and variational method can be applied to the nonlinear problems such as burnup and thermal-hydraulics.

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