Generalized Perturbation Formulation for Monte Carlo Eigenvalue Calculations with Constraint Condition

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1. Introduction

The existing generalized perturbation formulation [1] applied in the eigenvalue calculations within the McCARD [2] code was derived using the constraint that the sum of the fission source density (FSD) over the entire phase space is equal to one. This constraint is a normalization condition commonly employed in Monte Carlo (MC) codes to express results per unit source in the output file.

In this paper, a first-order generalized perturbation formulation is derived to account for cases where additional constraint conditions exist beyond the FSD sum normalization, such as when a thermal power constraint is imposed in burnup calculations. Furthermore, the differences in calculation results are examined when applying the thermal power constraint compared to the conventional approach.

2. Formulation

2.1 Unperturbed system with constraint condition

The operator form of the steady-state MC eigenvalue equation is given as:

$$S = \frac{1}{k}\mathbf{H}S, \tag{1}$$

$$\mathbf{H}S = \int d\mathbf{P}' H(\mathbf{P}' \to \mathbf{P}) S(\mathbf{P}'). \tag{2}$$

where k and S represent the eigenvalue and fundamental-mode FSD, respectively. $H(\mathbf{P'}\to\mathbf{P})$ represents the number of first-generation fission neutrons born per unit phase space volume about **P**, due to a parent neutron born at **P'**. In this MC calculations, the reactor core performance parameter Q can be evaluated as follows:

$$Q = \langle \mathbf{R}_Q S \rangle. \tag{3}$$

The angle brackets <·> denote integration over the phase space $\mathbf{P}=(\mathbf{r},E,\mathbf{\Omega})$, and S represents the fundamental-mode FSD. The response operator $\mathbf{R}_Q$ of the tally Q can be expressed as follows:

$$\mathbf{R}_Q S = \int d\mathbf{P}' R_Q(\mathbf{P}' \to \mathbf{P}) S(\mathbf{P}'), \tag{4}$$

where $R_Q(\mathbf{P'}\to\mathbf{P})$ represents the extent to which the tally Q at **P** responds to a unit fission source born at *P'*.

The solution S of Eq. (1) is an arbitrary solution. Therefore, to specify a unique solution, the following constraint condition is imposed:

$$c = \langle \mathbf{R}_c S \rangle. \tag{5}$$

Here, c is the constraint constant, and $\mathbf{R}_c$ is the response function operator used to calculate c, which can be expressed in the same manner as Eq. (4).

2.2 Perturbed system

Equation (3) in the perturbed system is given as Eq. (6).

$$Q + \Delta Q = \langle (\mathbf{R}_Q + \Delta\mathbf{R}_Q)(S + \Delta S) \rangle. \tag{6}$$

Applying the first-order approximation here, the relative change in tally Q can be expressed as shown in Eq. (7).

$$\frac{\Delta Q}{Q} \simeq \frac{\langle \Delta\mathbf{R}_Q S \rangle}{\langle \mathbf{R}_Q S \rangle} + \boxed{\frac{\langle \mathbf{R}_Q \Delta S \rangle}{\langle \mathbf{R}_Q S \rangle}}. \tag{7}$$

The first term on the right-hand side of Eq. (7) can be computed during the Monte Carlo forward calculation using either the differential operator sampling (DOS) method or the correlated sampling (CS) method. However, since the perturbed source cannot be directly calculated, the second term is evaluated by introducing the generalized adjoint equation as follows:

$$\Gamma^\dagger = \frac{1}{k^\dagger}\mathbf{H}^\dagger \Gamma^\dagger + S_{ex}^\dagger, \tag{8}$$

$$S_{ex}^\dagger = \frac{\mathbf{R}_Q^\dagger}{\langle \mathbf{R}_Q S \rangle} - \frac{\mathbf{R}_c^\dagger}{\langle \mathbf{R}_c S \rangle}. \tag{9}$$

The superscript dagger (†) denotes the adjoint. $\Gamma^\dagger$ and $S_{ex}^\dagger$ represent the generalized adjoint function and the external source term of the generalized adjoint equation, respectively. Here, $S_{ex}^\dagger$ must satisfy the condition that its inner product with S is zero, as given in Eq. (10), and the $S_{ex}^\dagger$ presented in Eq. (9) satisfies this condition.

$$\begin{aligned} \langle S_{ex}^\dagger, S \rangle &= \langle (\mathbf{I} - \mathbf{H}^\dagger / k^\dagger)\Gamma^\dagger, S \rangle \\ &= \langle \Gamma^\dagger, \cancel{(\mathbf{I} - \mathbf{H}/k)S} \rangle \quad , \\ &= 0 \end{aligned} \tag{10}$$

where <*a*,*b*> denotes the inner product of functions *a* and *b*.

$$\left\langle S_{ex}^{\dagger}, \Delta S \right\rangle = \boxed{\frac{\langle \mathbf{R}_Q \Delta S \rangle}{\langle \mathbf{R}_Q S \rangle}} - \frac{\langle \mathbf{R}_c \Delta S \rangle}{\langle \mathbf{R}_c S \rangle}. \quad (11)$$

The left-hand side of Eq. (11) can be derived using the generalized adjoint function, $\Gamma^{\dagger}$, which satisfies the condition that the inner product of $\Gamma^{\dagger}$ and S is zero ($\langle \Gamma^{\dagger}, S \rangle = 0$), as follows.

$$\begin{aligned} \left\langle S_{ex}^{\dagger}, \Delta S \right\rangle &= \left\langle \left(\mathbf{I} - \frac{\mathbf{H}^{\dagger}}{k^{\dagger}} \right) \Gamma^{\dagger}, \Delta S \right\rangle \\ &= \left\langle \Gamma^{\dagger}, \left(\mathbf{I} - \frac{\mathbf{H}}{k} \right) \Delta S \right\rangle \\ &= \left\langle \Gamma^{\dagger}, \frac{1}{k} (\Delta \mathbf{H} - \Delta k \mathbf{I}) S \right\rangle \\ &= \left\langle \Gamma^{\dagger}, \frac{1}{k} \Delta \mathbf{H} S \right\rangle - \frac{\Delta k}{k} \cancel{\left\langle \Gamma^{\dagger}, S \right\rangle}. \end{aligned} \quad (12)$$

To calculate the second term on the RHS of Eq. (11), the first-order approximation can be applied to Eq. (5) in the perturbed system, thereby transforming the perturbed source effect into the perturbed operator effect as follows:

$$\begin{aligned} c &= \left\langle \left(\mathbf{R}_c + \Delta \mathbf{R}_c \right) \left(S + \Delta S \right) \right\rangle \\ &= \left\langle \mathbf{R}_c S \right\rangle + \left\langle \Delta \mathbf{R}_c S \right\rangle + \left\langle \mathbf{R}_c \Delta S \right\rangle + \cancel{\left\langle \Delta \mathbf{R}_c \Delta S \right\rangle} \end{aligned}, \quad (13)$$

$$\langle \mathbf{R}_c \Delta S \rangle \simeq -\langle \Delta \mathbf{R}_c S \rangle. \quad (14)$$

2.3 The formulation for the relative change in tally Q

By substituting Eqs. (12) and (14) into Eq. (11) and then applying it to Equation (7), the relative change in tally Q can be expressed as follows:

$$\frac{\Delta Q}{Q} \simeq \frac{\langle \Delta \mathbf{R}_Q S \rangle}{\langle \mathbf{R}_Q S \rangle} + \left\langle \Gamma^{\dagger}, \frac{1}{k} \Delta \mathbf{H} S \right\rangle - \boxed{\frac{\langle \Delta \mathbf{R}_c S \rangle}{\langle \mathbf{R}_c S \rangle}}. \quad (15)$$

The second term on the right-hand side of Eq. (15), the generalized adjoint-weighted term, can be calculated as follows according to the method described in previous studies [1].

$$\left\langle \Gamma^{\dagger}, \frac{1}{k} \Delta \mathbf{H} S \right\rangle = \lim_{N \to \infty} \sum_{n=0}^{N} \left[A_{Q,n} - A_{c,n} \right], \quad (16)$$

$$A_{x,n} = \frac{\left\langle \mathbf{R}_x \left(\frac{\mathbf{H}}{k} \right)^n \left(\frac{\Delta \mathbf{H} S}{k} \right) \right\rangle}{\langle \mathbf{R}_x S \rangle}. \quad (17)$$

$A_{x,n}$ represents the effect of the perturbed source generated in the current cycle ($(1/k)\Delta\mathbf{H}S$) on response x after n cycles.

Compared to previous research [1], Equation (15) includes an additional third term on the right-hand side. In previous studies, the condition that the sum of the FSD is 1 ($\langle S \rangle = 1$) was used, leading to $\mathbf{R}_c = 1$, $c = 1$, and $\Delta \mathbf{R}_c = 0$, which eliminated the third term. However, when performing MC depletion analysis, the FSD normalization condition shown in Eq. (18) is applied.

$$\left\langle \mathbf{R}_p S \right\rangle = p_{real}, \quad (18)$$

where, $\mathbf{R}_p$ is the response function operator for calculating thermal power p_{real} generated by fission.

The change in tally Q under the <S>=1 condition used in previous studies is given as follows:

$$\left(\frac{\Delta Q}{Q} \right)_{\langle S \rangle = 1} \simeq \frac{\langle \Delta \mathbf{R}_Q S \rangle}{\langle \mathbf{R}_Q S \rangle} + \lim_{N \to \infty} \sum_{n=0}^{N} \left[A_{Q,n} - A_{1,n} \right]$$

$$A_{1,n} = \frac{\left\langle \left(\frac{\mathbf{H}}{k} \right)^n \left(\frac{\Delta \mathbf{H} S}{k} \right) \right\rangle}{\langle S \rangle}. \quad (19)$$

The difference between the new Eq. (16) and the previous Eq. (19) is given by Eq. (20). This corresponds to the relative change Δp_{est} of the estimated value for the constraint condition (p_{est}) under the <S>=1 condition in Monte Carlo calculations. In other words, when performing burnup analysis, the relative change of the real value should be obtained by subtracting the relative change of the total fission power from the conventional value.

$$\begin{aligned} &\left(\frac{\Delta Q}{Q} \right)_{\langle \mathbf{R}_p S \rangle = p_{real}} - \left(\frac{\Delta Q}{Q} \right)_{\langle S \rangle = 1} \\ &= \frac{\langle \Delta \mathbf{R}_p S \rangle}{\langle \mathbf{R}_p S \rangle} + \lim_{N \to \infty} \sum_{n=0}^{N} \left[A_{p,n} - A_{1,n} \right] \\ &= \left(\frac{\Delta p_{est.}}{p_{est.}} \right)_{\langle S \rangle = 1} \end{aligned} \quad (20)$$

Equations (15)–(17) were applied to McCARD, and the perturbed operator effects such as $\Delta\mathbf{R}S$ and $\Delta\mathbf{H}S$ were calculated using first-order DOS method, as described in Reference [1], as follows:

$$\Delta \mathbf{R} S \simeq \Delta x \left(\frac{\partial \mathbf{R}}{\partial x} \right) S. \quad (21)$$

3. Numerical Results

To measure how the relative change in tally Q differs from the conventional case when applying the constraint condition where thermal power is given, sensitivity calculation tests were performed on the two-group infinite homogeneous problem [1] and the GODIVA benchmark problem [3].

3.1 Two-group infinite homogeneous problem

The neutron reaction cross sections for the two-group infinite homogeneous problem are shown in Table I. Σ_{tg} and Σ_{fg} represent the total and fission cross section for neutron energy group g, respectively. $\Sigma_{sg'g}$ and $\chi_{g'g}$ are the transfer scattering cross sections and energy spectrums from energy group g to g'.

Table I: Cross sections for the two-group infinite homogeneous problem

Cross Section	First Group (g=1)	Second Group (g=2)
Σ_{tg}	0.5	0.5
Σ_{fg}	0.025	0.175
ν_g	2.0	2.0
Σ_{s1g}	0.1	0.0
Σ_{s2g}	0.181905	0.2
χ_{1g}	0.8	0.5
χ_{1g}	0.2	0.5
κ_g [MeV/fis.]	200	204

The analytic solution for this problem is shown in Table II. The target Tally Q is the total fission reaction rate, and the change in Tally Q due to cross section perturbations was calculated under the conditions of the sum of FSD being 1 and thermal power being 1 MW_{th}.

Under the condition where the sum of FSD is 1, the change in Q due to xs perturbations is on the order of several hundred pcm, while under the condition where thermal power is given, the change is almost negligible. This is because the target tally Q and the normalized condition of thermal power exhibit similar behaviors, thus canceling each other out.

3.2 GODIVA Benchmark

In the GODIVA benchmark problem, the sensitivities of fission power and various reaction rates were calculated by changing the U-235 (n,fission) and (n,gamma) reaction cross-section by 1% each. The GODIVA benchmark was divided into two equal-volume regions in the radial direction, and calculations were performed for each region. The radius of the GODIVA sphere is 8.7407 cm, and the radius of the inner region, which has an equal volume division, is 6.9375 cm.

For McCARD calculations using direct subtraction, 1,000,000 histories per cycle were used, with a total of 120 cycles including 20 inactive cycles. For McCARD calculations applying GPT, the Wielandt method was used with 100,000 histories per cycle, and a total of 120 cycles including 20 inactive cycles were performed. The number of latent cycles for the generalized adjoint calculation was set to 10, and the Wielandt method used a k_e value of 1.1. The cross-section library used in the McCARD calculations is ENDF/B-VIII.0 [4].

Table III presents the sensitivity calculation results using the McCARD code, comparing the Direct Subtraction method and the perturbation method. Additionally, the calculation results were compared between the case where the constraint condition enforcing the sum of the FSD to be 1 (previous study) and the case where the constraint condition enforcing the thermal power to be 1 MW (this study) was applied.

The relative standard deviation (RSD) of fission power densities and reaction rates in the McCARD results for direct subtraction was in the range of approximately 9–12 pcm, while in the McCARD results for perturbation calculations, it was around 120–200 pcm. In Table III, cases with high differences are due to the large deviations in the Direct Subtraction method when the relative change value is on the order of tens of pcm. This results in inaccurate outcomes, leading to significant discrepancies compared to the perturbation method results.

The sensitivity calculation results of reaction rates during depletion using the new formula show significant differences compared to the previous sensitivity results. Specifically, for fission power density and fission reactions, the sensitivity values are significantly reduced due to cancellation with the estimated values of the constraint condition. In contrast, for reactions like (n, gamma), which exhibit behavior opposite to that of fission power, the sensitivity is amplified, leading to larger values.

4. Conclusions

In this study, the Monte Carlo generalized perturbation formulation was derived under the given constraint condition. After applying the equation to the two-group infinite homogeneous problem and obtaining the analytic solution, the effect of the new equation was investigated. The results revealed that when thermal power input is used as a constraint during depletion calculations, there was a significant difference compared to using the normalized condition where the FSD was 1. Similarly, after applying the equations to McCARD and analyzing the GODIVA benchmark problem, a significant difference was also observed.

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REFERENCES

[1] S. H. Choi, H. J. Shim, and C. H. Kim, Development of Generalized Perturbation Theory Algorithms for Monte Carlo Eigenvalue Calculations, Nucl. Sci. Eng., Vol.189, pp.171-187, 2018.

[2] H. J. Shim, et. al., McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis, Nucl. Eng. Technol., Vol.44, 2, p.161, 2012.

[3] R. J. LaBauve, Bare, highly enriched uranium sphere (Godiva), International Handbook of Evaluated Criticality Safety Benchmark Experiments, HEU-MET-FAST-001, 2003.

[4] D. A. Brown, et. Al., ENDF/B-VIII. 0: the 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data. Nuclear Data Sheets, Vol.148, pp.1-142, 2018.

Table II. Analytic solution for the change [pcm] in reaction rate due to a 1% perturbation in cross section in the two-group infinite homogeneous problem

Target Tally Q	Perturbed Cross Section	Method	<S>=1	Thermal Power = $1MW_{th}$
(n,fis.) reaction rate	(n,fis.) 1% pert.	1st-order perturbation Direct Subtraction	426 426	3 1
		Difference	0%	246%
	(n, γ) 1% pert.	1st-order perturbation Direct Subtraction	-568 -568	3 0
		Difference	0%	2478%

Table III. The sensitivity calculation results using McCARD for a 1% change in the U-235 (n,f) and (n,γ) reaction cross-sections

Constraint Condition	Region	Tally Type	Direct Subtraction (D) [pcm]		MC Perturbation (P) [pcm]		Difference (P-D)/D	
			(n,f)	(n,γ)	(n,f)	(n,γ)	(n,f)	(n,γ)
<S>=1	Inner	FPD*	644	-76	661	-41	2.6%	-45.9%
		Total**	-211	-65	-198	-30	-6.1%	-54.5%
		(n,abs.)	-453	834	-449	878	-0.8%	5.2%
		(n, γ)	-453	834	-439	880	-3.1%	5.5%
		(n,f)	644	-76	661	-41	2.6%	-45.9%
	Outer	FPD*	614	-22	621	-41	1.2%	84.3%
		Total	-238	-13	-235	-30	-1.4%	126.9%
		(n,abs.)	-469	883	-479	878	2.1%	-0.6%
		(n, γ)	-469	883	-468	880	-0.1%	-0.4%
		(n,f)	615	-23	622	-41	1.2%	84.2%
Thermal Power = $1MW_{th}$	Inner	FPD*	9	-17	13	0	33.4%	-100.9%
		Total	-840	-6	-846	12	0.7%	-285.0%
		(n,abs.)	-1080	894	-1097	919	1.6%	2.9%
		(n, γ)	-1080	894	-1087	921	0.6%	3.1%
		(n,f)	10	-17	13	0	32.0%	-100.8%
	Outer	FPD*	-20	36	-27	0	33.4%	-100.9%
		Total	-867	45	-883	11	1.8%	-76.3%
		(n,abs.)	-1096	942	-1126	919	2.8%	-2.5%
		(n, γ)	-1096	942	-1116	921	1.8%	-2.3%
		(n,f)	-20	36	-26	0	34.2%	-101.0%

*FPD: Fission Power Density
**Macroscopic reaction rate