Sensitivity and Uncertainty Analysis for UAM TMI-1 Pin-cell with UNIST Monte Carlo Code MCS

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1. Introduction

There have been several studies to perform sensitivity and uncertainty analysis with Monte Carlo codes. Reactor analysis codes such as McCARD [1-3], MCNP6 [4], SERPENT [5], TSUNAMI (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) [6] and RMC [7] have developed capabilities of computing sensitivity of the effective multiplication factor to nuclear data.

Recently, a sensitivity and uncertainty (S/U) analysis function has been implemented in MCS, which is an in-house Monte Carlo code developed by UNIST. The S/U analysis for nuclear data is highly related with generalized perturbation theory (GPT) [8].

In this paper, a brief review of GPT and a sandwich rule will be presented in Section 2.1. Specifications of UAM TMI-1 fuel pin-cell problem will be described in Section 2.2. The comparison of numerical results between MCS and SERPENT will be presented for the UAM TMI-1 fuel pin-cell problem in Section 2.3.

2. Methods and Results

2.1 Methodology

In generalized perturbation theory, the effect of perturbation of the nuclear parameter x to the response Q, which is the normalized tally in Monte Carlo simulation, can be expressed as Eq. (1) [2].

$$Q = \frac{\langle \mathbf{R}_Q S \rangle}{\langle S \rangle}, \tag{1}$$

where $\boldsymbol{R}_Q$ is the response operator of the tally Q. The brackets, ⟨ ⟩, indicate the inner product over the phase space.

The sensitivity coefficients, which is the change in the response Q due to a perturbation of some nuclear parameters can be written as Eq. (2) by neglecting products of perturbations which is the first order approximation of perturbation [2].

$$\frac{\Delta Q}{Q} \simeq \frac{\langle \Delta \mathbf{R}_Q S \rangle}{\langle \mathbf{R}_Q S \rangle} + \frac{\langle \mathbf{R}_Q \Delta S \rangle}{\langle \mathbf{R}_Q S \rangle} - \frac{\langle \Delta S \rangle}{\langle S \rangle}. \tag{2}$$

The first term on the right side of Eq. (2) is called the perturbed operator effect of the perturbation, and the last two terms are called the perturbed source effect of the perturbation. The perturbed operator effect term is caused by the perturbed nuclear data such as the macroscopic cross section. The perturbed source effect term is caused by the perturbed source that is affected by the perturbation of nuclear data.

The generalized adjoint equation is needed to compute the perturbed source effect term. The generalized adjoint equation is defined as

$$\left(\mathbf{I} - \lambda \mathbf{H}^*\right)\Gamma^* = S_{ex}^*, \tag{3}$$

where Γ^* is the solution to Eq. (3), which is called a generalized adjoint function. $\mathbf{I}$, $\mathbf{H}^*$ and λ are the identity operator, the adjoint fission operator and the eigenvalue, respectively. S_{ex}^*, which is the generalized adjoint source, can be written as Eq. (4) [2].

$$S_{ex}^* \equiv \frac{1}{Q}\frac{\partial Q}{\partial S} = \frac{\mathbf{R}_Q^*}{\langle \mathbf{R}_Q S \rangle} - \frac{\mathbf{I}}{\langle S \rangle}. \tag{4}$$

The uncertainty of the response Q can be calculated as Eq. (5).

$$u_Q^2 = S_Q C S_Q{}^T, \tag{5}$$

where S_Q and C are the sensitivity coefficients of response Q and the relative covariance matrix, respectively. The multigroup covariance data have been produced by NJOY with ENDF/B-VII.1 nuclear data library.

2.2 Model description

Two-dimensional infinitely reflected TMI-1 fuel pin from UAM-LWR benchmark [9] has been tested for S/U analysis in MCS. Fig. 1 shows the geometry of TMI-1 fuel pin-cell. The cell pitch is 1.4427 cm. The fuel pellet and cladding outside diameters are 0.9391 cm and 1.0928 cm, respectively. The cladding thickness is 0.0673 cm. The fuel pellet material is 4.85 w/o UO_2 with 10.283 g/cm^3.

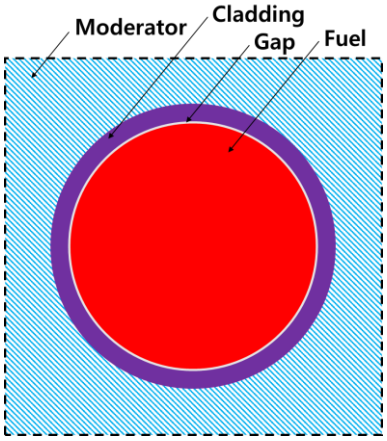

Fig. 1. Geometry for TMI-1 fuel pin

2.3 Numerical Results

S/U analysis has been performed for the TMI-1 pin-cell problem with MCS and SERPENT. The ENDF/B-VII.1 library has been used for the continuous-energy cross section and covariance data in both codes. A 238-group energy structure is used for tallies of sensitivity coefficients in MCS and SERPENT. Table I shows the k-eff, statistical error and its difference for the UAM TMI-1 pin-cell problem.

Table I: Comparison of k-eff in UAM TMI-1 pin-cell.

MCS	SERPENT	Diff.
1.43414 ± 0.00012	1.43414 ± 0.00005	0.00000

Fig. 2~4 show the energy independent k-eff sensitivity coefficients to ^{235}U total nubar cross section, ^{238}U capture cross section and ^{1}H elastic scattering cross section, respectively. The sensitivity coefficients are calculated by MCS and SERPENT. For the verification, SERPENT estimates are set as reference results. The sensitivity profiles show a good agreement between MCS and SERPENT.

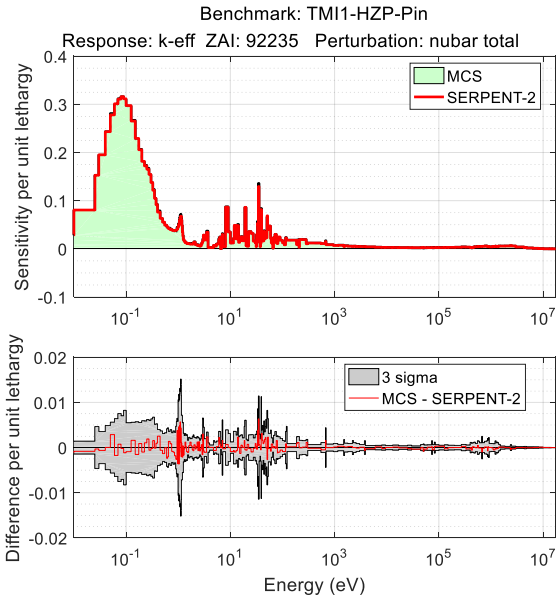

Fig. 2. Energy independent k-eff sensitivity coefficients to ^{235}U total nubar cross section in UAM TMI-1 pin-cell.

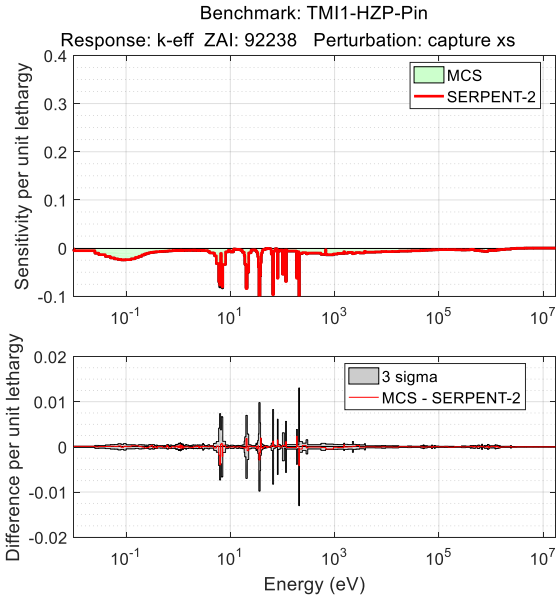

Fig. 3. Energy independent k-eff sensitivity coefficients to ^{238}U capture cross section in UAM TMI-1 pin-cell.

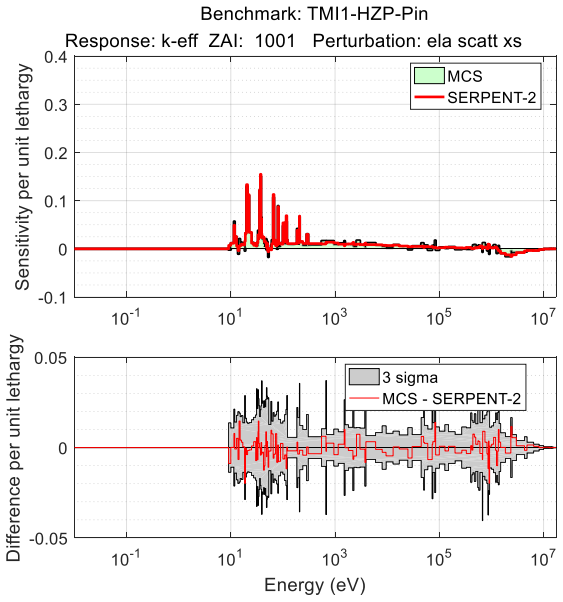

Fig. 4. Energy independent k-eff sensitivity coefficients to ^{1}H elastic scattering cross section in UAM TMI-1 pin-cell.

Table II shows the ten major contributors of energy integrated k-eff sensitivity coefficients. The sensitivity coefficients, statistical errors and relative differences are in %. The relative differences of energy integrated sensitivity between MCS and SERPENT are within 8%. The large discrepancies in the sensitivity to ^{1}H σ_{sab} are due to the high statistical error in MCS.

Table II: Energy integrated k-eff sensitivity coefficients for UAM TMI-1 pin-cell. The sensitivity coefficients, statistical errors and relative differences are in %.

Perturbation		Sensitivity (statistical error)		Rel. diff.
Nuclide	XS	MCS	SERPENT	
^{235}U	$\bar{\nu}_{total}$	0.94000 (0.04)	0.94041 (0.01)	-0.04
^{235}U	σ_{fis}	0.25429 (0.47)	0.25221 (0.15)	0.82
^{238}U	σ_{cap}	-0.19931 (0.19)	-0.19930 (0.08)	0.01
^{235}U	σ_{cap}	-0.15329 (0.16)	-0.15400 (0.08)	-0.46
^{1}H	σ_{ela}	0.11586 (4.24)	0.12057 (0.93)	-3.90
^{238}U	$\bar{\nu}_{total}$	0.05999 (0.60)	0.05958 (0.11)	0.69
^{1}H	σ_{sab}	0.05977 (7.85)	0.05536 (2.90)	7.95
^{1}H	σ_{cap}	-0.03859 (0.19)	-0.03881 (0.20)	-0.56
^{238}U	σ_{fis}	0.02841 (1.28)	0.02809 (0.26)	1.11
^{18}O	σ_{ela}	-0.01148 (31.00)	-0.01144 (7.60)	0.30

Table III shows the uncertainties of k-eff due to the covariance in ^{235}U and ^{238}U ENDF/B-VII.1 library for UAM TMI-1 pin-cell problem. The k-eff uncertainties are in %. The k-eff uncertainty estimates have been calculated with postprocessing due to the lack of uncertainty calculation function in SERPENT. In the postprocessing, the sensitivity coefficients by SERPENT are directly multiplied by the relative covariance matrix as shown in Eq. (5). The same relative covariance data are used in MCS and SERPENT. The total uncertainty shown in Table III is the summation of k-eff uncertainties due to the covariance in ^{235}U and ^{238}U. The total uncertainties agree well between MCS and SERPENT.

Table III: Uncertainty of k-eff due to the covariance in ^{235}U and ^{238}U ENDF/B-VII.1 for UAM TMI-1 pin-cell. The uncertainties are in %.

Covariance Type			MCS	SERPENT
^{235}U	σ_{ela}	σ_{ela}	0.00127	0.00051
	σ_{ela}	σ_{inl}	-0.00023	-0.00030
	σ_{ela}	σ_{fis}	0.00109	0.00213
	σ_{ela}	σ_{cap}	-0.00857	0.00266
	σ_{inl}	σ_{inl}	0.00046	0.00150
	σ_{fis}	σ_{fis}	0.07673	0.07666
	σ_{fis}	σ_{cap}	0.07639	0.07635
	σ_{cap}	σ_{cap}	0.19629	0.19660
	$\bar{\nu}_{total}$	$\bar{\nu}_{total}$	0.60663	0.60650
^{238}U	σ_{ela}	σ_{ela}	0.00856	0.01023
	σ_{ela}	σ_{inl}	0.01951	-0.01587
	σ_{ela}	σ_{fis}	-0.00052	0.00029
	σ_{ela}	σ_{cap}	0.01451	0.01528
	σ_{inl}	σ_{inl}	0.11184	0.10983
	σ_{fis}	σ_{fis}	0.01463	0.01461
	σ_{fis}	σ_{cap}	0.00104	0.00105
	σ_{cap}	σ_{cap}	0.23854	0.23933
	$\bar{\nu}_{total}$	$\bar{\nu}_{total}$	0.06994	0.06991
Total			0.70240	0.70196

3. Conclusions

S/U analysis has been performed for the TMI-1 pin cell problem in UAM-LWR benchmark with MCS and SERPENT. For the analysis, ENDF/B-VII.1 nuclear data has been used for continuous energy neutron cross section and multi-group covariance matrices. Sensitivity coefficients are calculated based on the GPT and uncertainties are calculated with the sandwich rule.

The energy integrated and independent k-eff sensitivity coefficients are compared between MCS and SERPENT. They show a good agreement within three standard deviastions. For the comparison of k-eff uncertainties due to the covariance in ^{235}U and ^{238}U ENDF/B-VII.1 library, the additional postprocessing has been performed. The k-eff sensitivities from SERPENT are multiplied by the relative covariance matrix as shown in the sandwich rule, and the uncertainties are compared

between MCS and SERPENT. The relative difference of the total uncertainties between MCS and SERPENT are within 1%.

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REFERENCES

[1] H. J. Shim and C. H. Kim, Adjoint Sensitivity and Uncertainty Analysis in Monte Carlo Forward Calculations, *J. Nucl. Sci. Technol.*, Vol. 05, p. 1453-1461, 2013.
[2] S. H. Choi and H. J. Shim, Memory-efficient calculations of adjoint-weighted tallies by the Monte Carlo Wielandt method, *Ann. Nucl. Energy*, Vol. 96, p. 287-294, 2016.
[3] 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, p. 171-187, 2018.
[4] B. C. Kiedrowski, F. B. Brown and P. P. H. Wilson, Adjoint-weighted Tallies for k-eigenvalue Calculations with Continuous-energy Monte Carlo, *Nucl. Sci. Eng.*, Vol. 174, p. 227-244, 2013.
[5] M. Aufiero, A. Bidaud, M. Hursin, J. Leppänen, G. Palmiotti, S. Pelloni and P Rubiolo, A Collision History-based Approach to Sensitivity/Perturbation Calculations in the Continuous Energy Monte Carlo Code SERPENT, *Ann. Nucl. Energy*, Vol. 85, p. 245-258, 2015.
[6] C. M. Perfetti and B. T. Rearden, Continuous-energy Eigenvalue Sensitivity Coefficient Calculations in TSUNAMI-3D, Mathematics and Computational Methods Applied to Nuclear Science & Engineering, *M&C 2013*, Sun Valley, Idaho, USA, May 5-9, 2013.
[7] Y. Qiu, M. Aufiero, K. Wang and M. Fratoni, Development of Sensitivity Analysis Capabilities of Generalized Responses to Nuclear Data in Monte Carlo code RMC, *Ann. Nucl. Energy*, Vol. 97, p. 142-152, 2016.
[8] M. L. Williams, "Perturbation theory for nuclear reactor analysis," CRC Handbook of Nuclear Reactors Calculations, Vol. III, CRC Press, Inc., Boca Raton, 1986.
[9] K. Ivanov, M. Avromova, S. Kamerow, I. Kodel, E. Sartori, E. Ivanov and O. Cabellos, Benchmarks for Uncertainty Analysis in Modelling (UAM) for the Design, Operation and Safety Analysis of LWRs, NEA/NSC/DOC, 2012.