

Method research and analysis for assembly few-group homogenized cross-section sensitivity and uncertainty

LIU Yong¹, CAO Liang-zhi¹, WU Hong-chun¹, LI Yun-Zhao¹, LIU Zhou-yu¹

1. School of Nuclear Science and Technology, Xi'an Jiaotong University, Xi'an 710049, China.

Abstract: Assembly few-group homogenized cross-sections are the most basic input parameters for core calculation in the traditional two-step method. Therefore, it is necessary to perform few-group homogenized cross-section sensitivity and uncertainty analysis for the subsequent sensitivity and uncertainty analysis of core calculation. Based on generalized perturbation theory, the method to calculate the sensitivity coefficients of few-group homogenized cross-sections with respect to nuclear cross-sections is studied, which can take the implicit sensitivity into account with the subgroup method for resonance calculation. A covariance library is created based on ENDF/B-VII.1 data. The few-group homogenized cross-section uncertainties are obtained based on the sandwich rule. A sensitivity and uncertainty analysis code called NECP-COLEUS is developed based on the platform of lattice-physics code NECP-CACTI. Two typical PWR cell cases are calculated and analyzed. The response sensitivity coefficients show good agreement with those obtained by the reference method, i.e. direct perturbation method. The numerical results indicate that the uncertainties of some PWR few-group homogenized cross-sections exceed 1%, and the capture and non-elastic scattering cross-section of U238 are often the most significant uncertainty contributors. In the case of MOX fuel, the capture cross-sections of plutonium isotopes are also important uncertainty contributors.

Keyword: sensitivity; uncertainty; perturbation theory; covariance; subgroup method

1 Introduction

Generally, there are three uncertainty sources in the reactor physics calculation: 1) module; 2) numerical method; 3) input parameter. Because of the unavoidable deficiency of measuring equipment and measuring method, the nuclear data values are usually given with uncertainties. As significant input parameters for reactor physics calculation, the uncertainties of nuclear data will affect the calculation results of reactor physics. The assessment of sensitivity and uncertainty related to nuclear data has become a hot issue internationally^{[1][2]}. A lot of numerical results show that the nuclear data is a very important uncertainty source in reactor physics calculation^[3].

The framework of sensitivity and uncertainty(S&U) analysis for LWR was proposed by OECD LWR UAM in 2006^[2], which is widely recognized. The reactor physics calculation is based on the traditional two-step scheme in this framework. The few-group homogenized cross-sections connect the assembly calculation and core calculation. To evaluate the core parameter uncertainties, the sensitivity and uncertainty analysis of assembly parameters should be performed firstly. To perform the assembly

few-group homogenized cross-section S&U analysis, a code named NECP-COLEUS is developed based on the lattice-physics code NECP-CACTI^[4]. The main contents include:

- (1) The S&U analysis method for few-group homogenized cross-sections is proposed based on the generalized perturbation theory, and the implicit sensitivity can be taken into account with the subgroup method being used for resonance calculation;
- (2) The uncertainties of few-group homogenized cross-sections, which are induced by the nuclear data, are quantified, and the uncertainty sources are analyzed.

2 Methodology

A few-group homogenized cross-section has the form of

$$\bar{\Sigma}_{x,h} = \frac{\langle \Sigma_x \Phi \rangle}{\langle \Phi \rangle} \quad (1)$$

where x is the cross-section type; h is the group index of few-group cross-sections; $\bar{\Sigma}_{x,h}$ is the few-group cross-sections; Σ_x is the multi-group macro

cross-sections; Φ is neutron flux; $\langle \rangle$ denotes integration over appropriate phase space.

The Generalized Perturbation Theory(GPT) is well suitable for the sensitivity analysis of response which has the form of linear ratio of flux^[5]. The corresponding generalized adjoint equation is given as follow according to GPT^{[5][6]}

$$\mathbf{M}^* \Gamma^* = \frac{\sum_x}{\langle \sum_x \Phi \rangle} - \frac{1}{\langle \Phi \rangle} \quad (2)$$

where \mathbf{M}^* is the adjoint operator of neutron transport operator; Γ^* is the generalized adjoint flux.

Then the relative sensitivity coefficients can be evaluated as follow

$$S_{\bar{\Sigma}_{x,h},\sigma} = \frac{d\bar{\Sigma}_{x,h} / \bar{\Sigma}_{x,h}}{d\sigma / \sigma} = \sigma \frac{\langle (d\bar{\Sigma}_x / d\sigma) \Phi \rangle}{\langle \bar{\Sigma}_x \Phi \rangle} - \sigma \left\langle \Gamma^* \frac{d\mathbf{M}}{d\sigma} \Phi \right\rangle \quad (3)$$

where \mathbf{M} is the neutron transport operator; σ is a specific multi-group cross-section. R will represent arbitrary response which has the Eq. (1) form hereinafter for simplification.

It should be noted that the sensitivity coefficients obtained above are direct effects of multi-group cross-sections on the responses during the solution process of neutron transport equation. However, resonance calculation is necessary before multi-group neutron transport calculation is performed. The perturbation of the cross-sections will influence the responses through resonance calculation indirectly, which is called implicit sensitivity^[7]. Therefore, the key point to take the implicit sensitivity into account is to calculate the resonance cross-section sensitivity coefficients. The subgroup method is applied in resonance calculation in this study. In the subgroup method, the effective self-shielding cross-section is defined as

$$\sigma_{x,g} = \frac{\int_{\Delta E_g} \alpha_x(E) \phi(E) dE}{\int_{\Delta E_g} \phi(E) dE} = \frac{\sum_{i=1,N} \sigma_{x,g,i} \phi_{g,i}}{\sum_{i=1,N} \phi_{g,i}} \quad (4)$$

where x is the reaction index; g is the energy-group index; i is the subgroup index; $\sigma_{x,g}$ is the effective self-shielding cross-section; $\alpha_x(E)$ is the continuous-energy cross-section; $\phi(E)$ is the weight flux; ΔE_g is the energy rang of the g -th group; $\sigma_{x,g,i}$ is the subgroup cross-section; $\phi_{g,i}$ is the subgroup flux and N is subgroup total number.

Applying the GPT-based method, the sensitivity coefficient of effective self-shielding cross-section with respect to the continuous-energy cross-sections is given as^[8]

$$S_{\sigma_{x,g},\alpha} = \frac{\sum_{i=1}^N \sigma_{x,g,i} S_{\sigma_{x,g,i},\alpha} \phi_{g,i}}{\sum_{i=1}^N \sigma_{x,g,i} \phi_{g,i}} + \sum_{i=1}^N \int_V \int_{\Omega} \Gamma_{x,g,i}^* \left(Q_{g,i} S_{Q_{g,i},\alpha} - \alpha \frac{\partial \mathbf{L}_s}{\partial \alpha} \phi_{g,i} \right) d\Omega dV \quad (5)$$

where $Q_{g,i}$ is the source term of subgroup transport equation, which is equal to $\sum_p P_i$ in the NR-approximation-based subgroup method. Σ_p is the potential scattering cross-section. \mathbf{L}_s is the subgroup transport operator. Γ_g^* is the generalized adjoint subgroup flux, which is the solution of generalized adjoint subgroup transport equation given as following.

$$-\Omega \cdot \nabla \Gamma_g^*(\mathbf{r}, \Omega) + \Sigma_{t,g}(\mathbf{r}) \Gamma_g^*(\mathbf{r}, \Omega) = Q_g^* \quad (6)$$

where Q_g^* is the generalized adjoint source.

There are two terms on the right hand of Eq. (5). The first term is called direct term. When α and $\sigma_{x,g}$ are the cross-sections of a same resonance nuclide, this term is nonzero. The second term is called indirect term. It is caused by the perturbation of subgroup flux when the cross-sections are perturbed.

When α is the cross-sections of a non-resonance nuclide, the indirect term can be calculated after the generalized adjoint subgroup flux is obtained. However, when α and $\sigma_{x,g}$ are the cross-sections of the same resonance nuclide, the subgroup parameter sensitivity coefficients need to be calculated. According to the narrow resonance(NR) approximation, the subgroup flux can be described as

$$\phi_i \approx \frac{\sigma_0 P_i}{\sigma_{t,i} + \sigma_0} \quad (7)$$

where σ_0 is the background cross-section; p_i is the subgroup weight and $\sigma_{t,i}$ is subgroup total cross-section. The resonance cross-section can be approximately given as

$$RI_x \approx \sum_i \frac{\sigma_{x,i} P_i \sigma_0}{\sigma_{t,i} + \sigma_0} \quad (8)$$

Taking the derivative of both side of Eq. (8), the following relationship can be obtained

$$S_{RI_x,\alpha} \approx \frac{\sigma_0}{RI_x} \sum_i \frac{(S_{\sigma_{x,i},\alpha} + S_{P_i,\alpha}) \sigma_{x,i} P_i (\sigma_{t,i} + \sigma_0) - \sigma_{x,i} P_i \sigma_{t,i} S_{\sigma_{t,i},\alpha}}{(\sigma_{t,i} + \sigma_0)^2} \quad (9)$$

The left-side hand term can be obtained by NR approximation^{[9][10]}. The unknown subgroup parameter sensitivity coefficients are included in the right-side hand term. It can be found that there is a linear relationship in Eq. (9). Therefore, the linear least-squares method can be applied to solve this problem.

On the other hand, when α is the cross-section of a non-resonance nuclide, the $S_{Q_{g,i},\alpha}$ is equal to zero.

Otherwise,

$$S_{Q_{g,i},\alpha} = \frac{\alpha}{Q_{g,i}} \frac{dQ_{g,i}}{d\alpha} = S_{P_i,\alpha} \quad (10)$$

The resonance cross-section sensitivity coefficients can be obtained according to Eq. (5) up to now. Therefore, the total sensitivity coefficient which takes the implicit effect into account is expressed as

$$\begin{aligned} S_{R,\alpha_{\omega,g}^{(i)}}^{\text{tot}} &= \sum_x S_{R,\sigma_{x,g}^{(i)}}^{\text{exp}} S_{\sigma_{x,g}^{(i)},\alpha_{\omega,g}^{(i)}} + \sum_{\substack{j,y,h \\ j \neq i}} S_{R,\sigma_{y,h}^{(j)}}^{\text{exp}} \sum_x S_{\sigma_{y,h}^{(j)},\sigma_{x,g}^{(i)}} S_{\sigma_{x,g}^{(i)},\alpha_{\omega,g}^{(i)}} \\ &= S_{R,\alpha_{\omega,g}^{(i)}}^{\text{exp}} + S_{R,\alpha_{\omega,g}^{(i)}}^{\text{imp}} \end{aligned} \quad (11)$$

where x , y and ω are reaction indexes; i and j are nuclide indexes; g , g and h are group indexes; α is continuous-energy cross-section; σ is the multi-group cross-section.

2.2 The solution of generalized adjoint equation

For generalized adjoint equation shown as Eq. (2), the adjoint transport operator is singular because the eigenvalue has been known. In order to ensure the existence of solution, the generalized source term needs to be orthogonal to the forward flux. Obviously, the right hand of Eq. (2) meets the criteria. The equation will have infinitely many solutions under this circumstance, which can be described as

$$\Gamma^* = \Gamma_0^* + c\Phi \quad (12)$$

The generalized adjoint equation is a neutron transport equation with fixed source and the eigenvalue has been known. It can be solved referring to the iteration scheme of general eigenvalue problem. The iteration takes the scheme

$$\mathbf{L}^* \Gamma^{*(n+1)} = \lambda \mathbf{F}^* \Gamma^{*(n)} + \mathbf{S}^* \quad (13)$$

where λ is the known eigenvalue; \mathbf{F}^* is the adjoint fission operator; \mathbf{L}^* is the operator in \mathbf{M}^* except for fission term and \mathbf{S}^* is generalized adjoint source.

Because of the existence of $d\mathbf{M}/d\sigma$ in Eq. (3), the generalized adjoint flux is always needed to be orthogonal to the fission source in order to avoid calculating the derivative of eigenvalue. Therefore, the orthogonal condition will be applied during the

iteration to ensure the orthogonal condition is fulfilled and the final iteration scheme is given as

$$\mathbf{L}^* \Gamma^{*(n+1)} = \lambda \mathbf{F}^* \left(\Gamma^{*(n)} - \frac{\langle \mathbf{F}^* \Gamma^{*(n)}, \Phi \rangle}{\langle \mathbf{F}^* \Phi^*, \Phi \rangle} \Phi^* \right) + \mathbf{S}^* \quad (14)$$

The transport solver of NECP-CACTI is based on the Method of Characteristic (MOC). Some modifications are needed to perform adjoint calculation:

- (1) Transpose the matrix of scattering cross-sections;
- (2) Interchange the vector of $\bar{v}\Sigma_f$ and χ .

It should be noted that the up-scattering may be enhanced because of the transposition of scattering matrix, which may reduce the convergence rate. The energy-group index can be inverted before the iteration is performed. The transport solver can perform adjoint calculation after above operations. Additional operations are needed to perform generalized adjoint calculation:

- (1) The generalized adjoint source is treated as an external source;
- (2) The update of fission source complies with the following form:

$$FS_g = \frac{\bar{v}\Sigma_f^g}{4\pi k_{\text{eff}}} \sum_{h=1}^G \chi_h \left(\Gamma_h^* - \frac{\langle \mathbf{F}^* \Gamma^*, \Phi \rangle}{\langle \mathbf{F}^* \Phi^*, \Phi \rangle} \Phi_h^* \right) \quad (15)$$

The iteration scheme is similar with that of the neutron transport equation with some differences:

- (1) The eigenvalue does not need to be updated. The value is fixed to the eigenvalue of the forward solution;
- (2) The fission source is updated according to Eq. (15).

Additionally, because the generalized adjoint source may be negative, the transport solver needs to exclude the limitation of nonnegative flux or source.

2.3 Uncertainty

The covariance describes the information about the uncertainties of nuclear data and the correlations between them. The response uncertainties can be determined by combining the sensitivity coefficients with the covariance using the first-order uncertainty propagation formula, which is defined as:

$$\text{rcov}(\mathbf{R}) \approx \mathbf{S} \mathbf{C} \mathbf{S}^T \quad (16)$$

where $\text{rcov}(\mathbf{R})$ is the relative covariance of the responses; \mathbf{S} is the sensitivity coefficient matrix; and \mathbf{C} is the relative covariance of nuclear data.

3 Numerical verification and analysis

The verification and analysis are performed based on two typical PWR pin-cells which are from NECP resonance benchmark^[11]. RB3.1 is a UOX case with 5% ²³⁵U-enrichment and RB3.3 is a MOX case with 7% Pu-enrichment. The calculation is performed based on ENDF/B-VII data. The covariance library is created using NJOY^[12] based on ENDF/B-VII.1 data. The direct perturbation(DP) method is treated as the reference method in this paper. The DP method can be described as Eq. (17):

$$S_{R,\alpha} = \frac{\alpha}{R} \frac{dR}{d\alpha} = \frac{\alpha}{R^0} \frac{\Delta R}{\Delta\alpha} \quad (17)$$

where R^0 is the unperturbed results; α is a given input parameter; and ΔR and $\Delta\alpha$ are the corresponding changing amount. When the perturbations are appropriate and the non-linear relationship is not strong, this method can obtain accurate results. The sensitivity and uncertainty analysis for eigenvalue and two-group spatially homogenized cross-sections are carried out.

3.1 UOX case

The integrated sensitivity coefficients are given in Fig. 1. The results of GPT-based method(PT) agree well with those of DP method(DP). It can be found that different response are sensitive to different cross-sections. For example, the $\nu\Sigma_{f1}$ are more sensitivity to the fission cross-sections of U235 and U238 while the Σ_{s1-1} are more sensitivity to the elastic cross-sections.

Fig. 2 shows the covariance matrix of k_{eff} and two-group homogenized cross-sections. It can be found that the uncertainty of k_{eff} is about 0.5% while the uncertainties of two-group homogenized cross-sections can exceed 1%, including the capture cross-sections of both the 1st group and the 2nd group and the scattering cross-sections of the 1st group, etc. It is interesting to find that the uncertainties of fast-group homogenized cross-sections are usually larger than those of thermal-group. In order to investigate this phenomenon, Fig. 3 shows the five most significant uncertainty contributors for different responses.

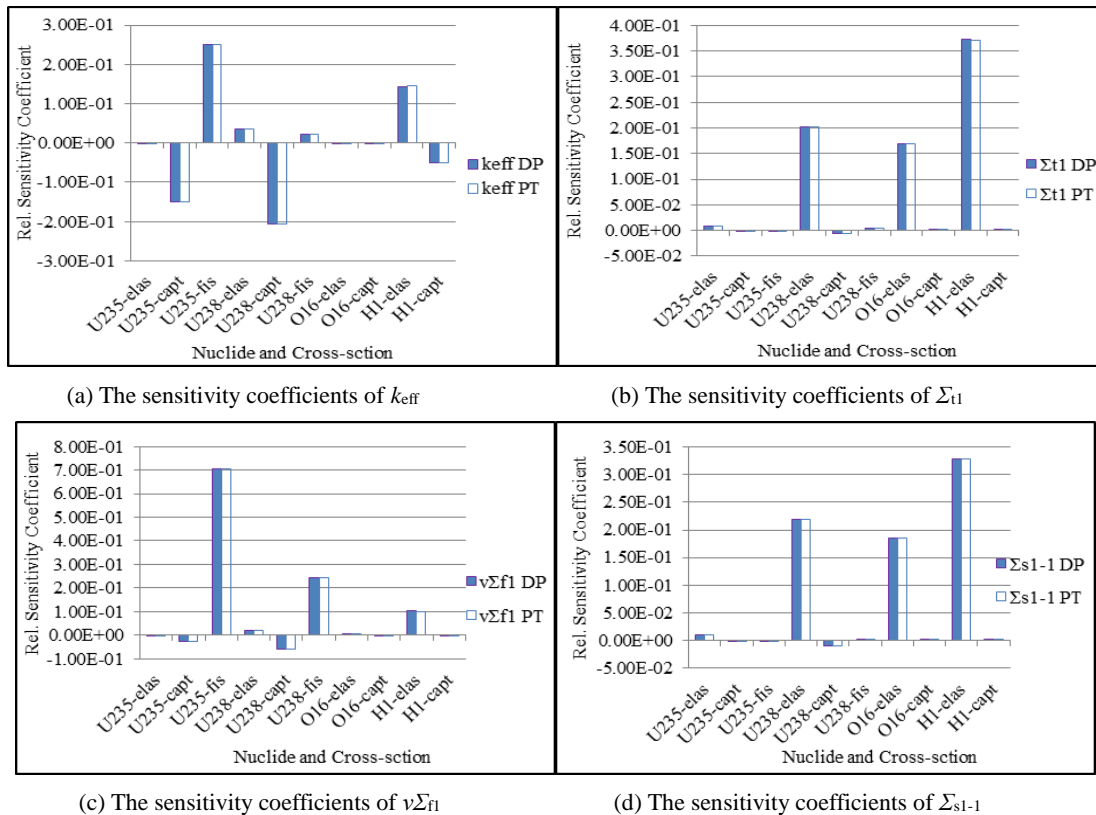


Fig.1 The comparison of integrated sensitivity-coefficient of some important responses between DP and PT methods for the UOX case.

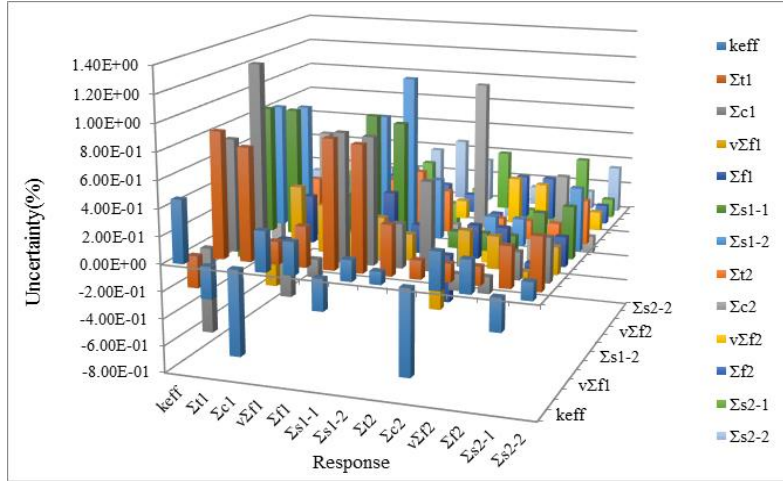
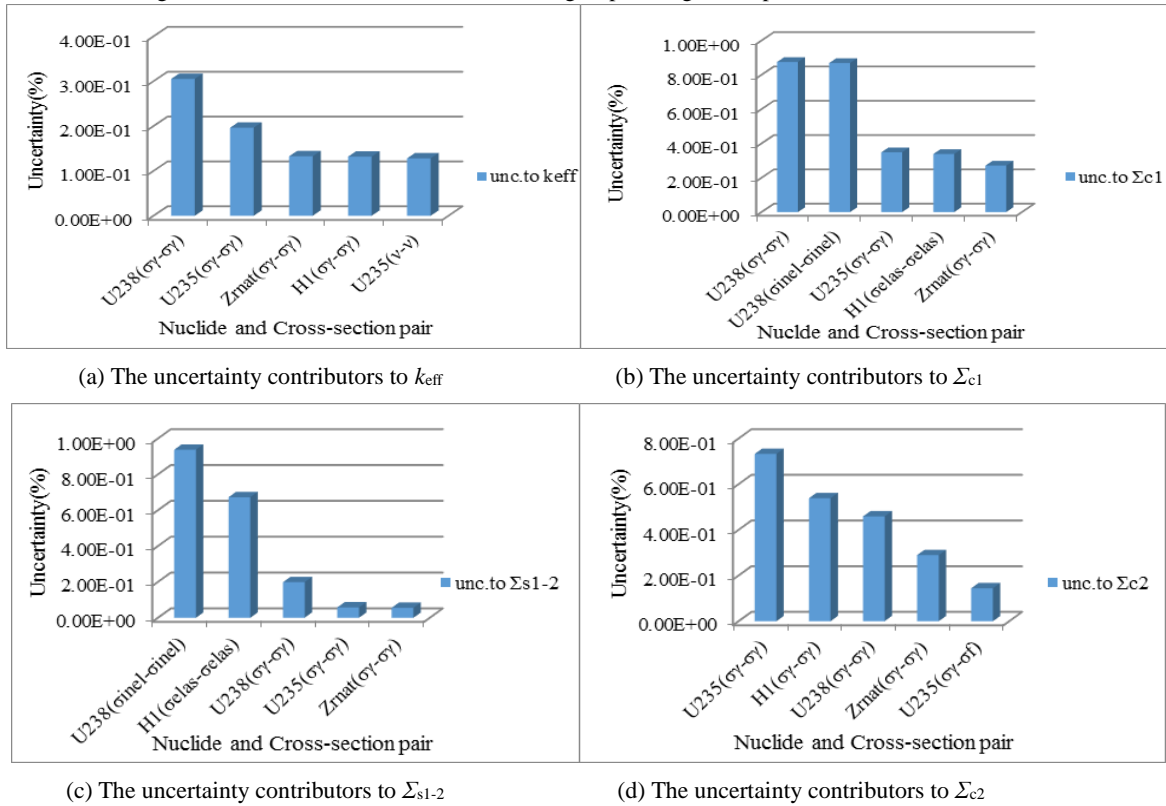


Fig. 2 The covariance matrix of k_{eff} and two-group homogenized parameters of the UOX case.



(a) The uncertainty contributors to k_{eff}

(b) The uncertainty contributors to Σ_{c1}

(c) The uncertainty contributors to Σ_{s1-2}

(d) The uncertainty contributors to Σ_{c2}

Fig. 3 The five most significant uncertainty sources for some important responses in the UOX case.

It can be found in Fig. 3 that the uncertainty contributors for various responses are different. However, the σ_γ of U238 is important uncertainty contributors for most responses. Although the σ_{inel} is a threshold-energy reaction in fast-group, the uncertainty contributions are considerable to most responses. This is one of the reasons why the fast-group homogenized cross-section uncertainties are usually larger. From the numerical results and analysis above, it can be found that the σ_γ and σ_{inel} of U238 are very significant uncertainty sources. As an

example, Fig. 4 gives the sensitivity coefficients of Σ_{c1} to σ_γ and σ_{inel} of U238 and the relative standard deviations(RSD) of these cross-sections. It can be seen that the uncertainties and the sensitivity coefficients of σ_{inel} are considerable, causing a significant uncertainty contribution. The uncertainties of σ_γ are also large in the whole energy range, while the corresponding sensitivity coefficients are considerable. Therefore, it is understandable that the uncertainty contributions are very large.

3.1 MOX case

The integrated sensitivity coefficients of the MOX case are given in Fig. 5. Good agreement can be found between the results of GPT-based method and those of DP method. Same phenomena can be found as the UOX case. In addition, it can be seen that the plutonium isotopes show a non-negligible effect in the sensitivity analysis.

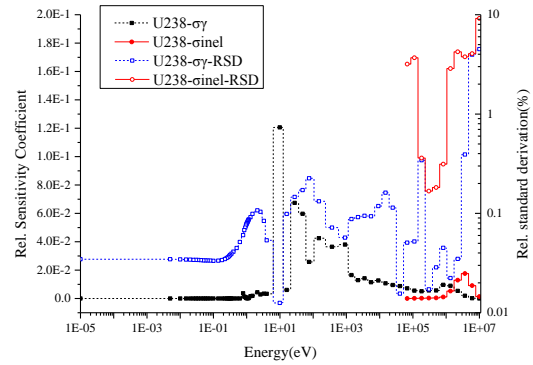
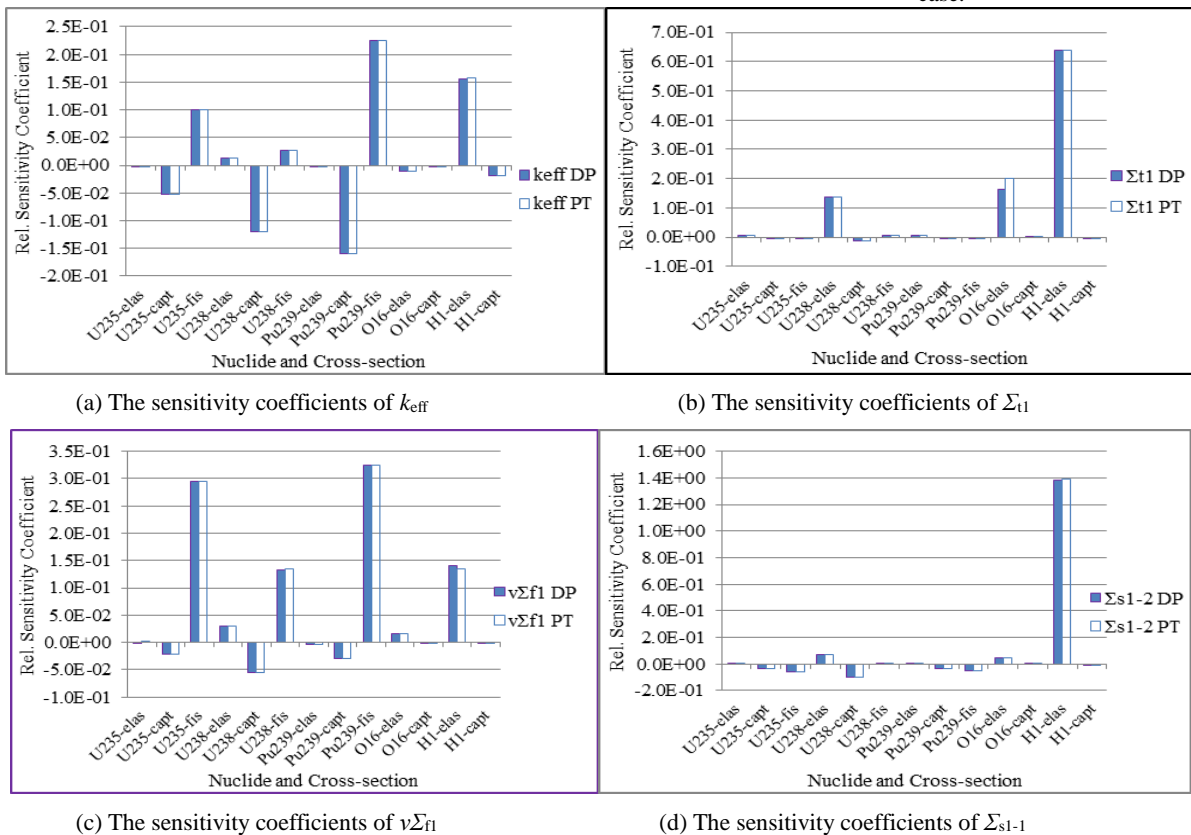


Fig. 4 The relative standard derivation and sensitivity coefficients of σ_γ and σ_{inel} of U238 related to Σ_{c1} in the UOX case.



Fi. 5 The comparison of integral sensitivity-coefficient of some important responses between DP and PT methods for the MOX case.

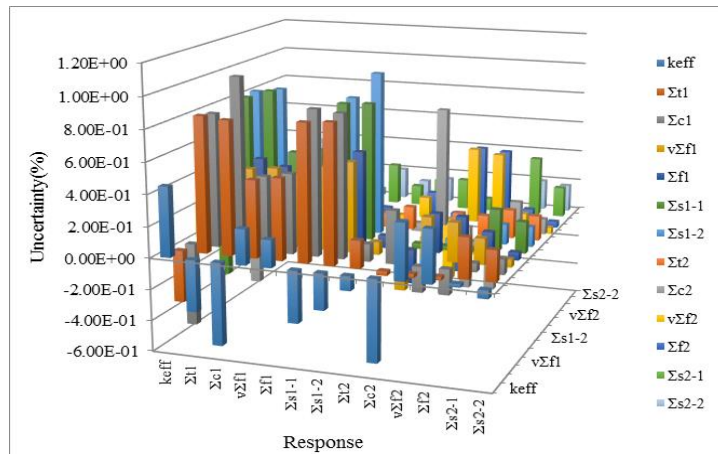


Fig. 6 The covariance matrix of k_{eff} and two-group homogenized parameters of the MOX case.

Fig. 6 shows the covariance matrix of k_{eff} and two-group homogenized cross-sections. The results are similar with that of UOX problem. The uncertainty of k_{eff} is about 0.5%, and the uncertainties of the fast-group homogenized cross-sections are usually larger than those of thermal-group. In order to confirm the uncertainty sources of MOX case, Fig. 7 shows the five most significant uncertainty contributors for

different responses. It can be found that the σ_γ of U238 is still one of the most significant uncertainty contributors, and the σ_γ of plutonium isotopes become important uncertainty sources. For the uncertainties of fast-group homogenized cross-sections, the σ_{inel} of U238 is still the most important contributor.

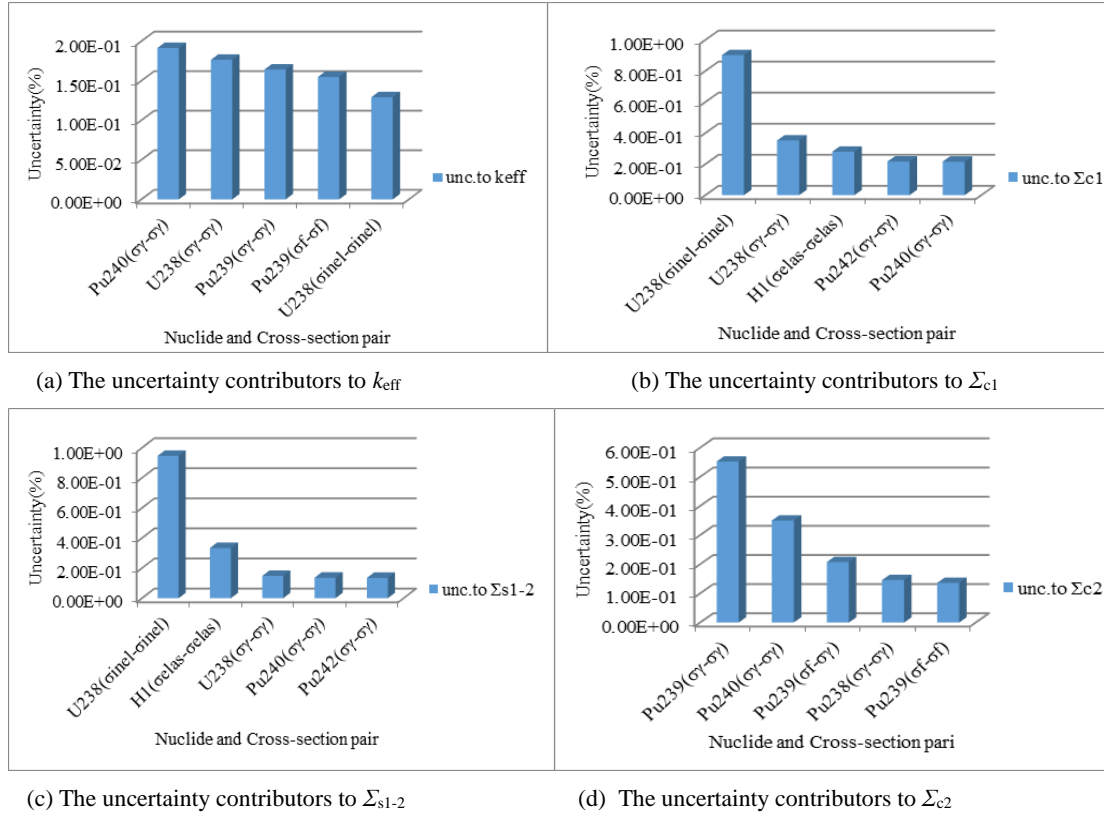


Fig. 7 The five most significant uncertainty sources for some important responses in the MOX case.

Pu239 is a very important plutonium isotope. As an example, Fig. 8 shows the sensitivity coefficients of Σ_{c1} and Σ_{c2} to σ_γ and σ_{inel} of Pu239 and the RSD of these cross-sections. It can be found the inelastic cross-sections have a considerable uncertainty. However, the sensitivity coefficients are negligibly small. Therefore, the uncertainty contribution is not as big as U238. The uncertainties of σ_γ are large, especially in the fast-energy range. However, because of the small sensitivity coefficients of Σ_{c1} , the uncertainty contribution of σ_γ to Σ_{c1} is negligible. On the other hand, the Σ_{c2} are very sensitive to the thermal-group cross-sections, therefore σ_γ has an important uncertainty contribution to the uncertainty of Σ_{c2} .

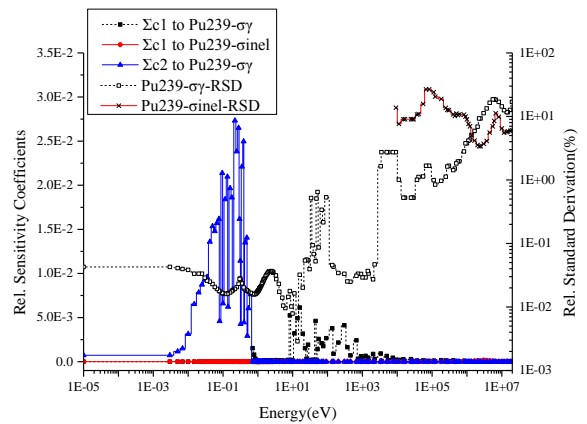


Fig. 8 The relative standard derivation and sensitivity coefficients of σ_γ and σ_{inel} of Pu239 relative to Σ_{c1} and Σ_{c2} in the MOX case.

4 Summary and Conclusions

The method to perform the sensitivity and uncertainty analysis for few-group homogenized cross-section is studied in this paper based on generalized perturbation theory. A new method to take the implicit sensitivity into account is proposed with subgroup method being used for resonance calculation. A code name NECP-COLEUS was developed based on the platform of lattice-physics code NECP-CACTI. A UOX case and a MOX case are calculated and analyzed. The sensitivity coefficients results agree well with the results given by the direct perturbation method. The k_{eff} and few-group homogenized cross-section uncertainties are calculated based on the ENDF/B-VII.1 covariance.

The numerical results show that the σ_{γ} and σ_{inel} of U238 are usually significant uncertainty contributors for both UOX and MOX problems. In the MOX case, the cross-sections of plutonium isotopes are also important uncertainty contributors, especially the capture cross-sections. The precision of current ENDF/B-VII.1 data will lead to considerable uncertainties for lattice calculation. The largest uncertainties of few-group homogenized cross-sections exceed 1%.

Future work should perform core-calculation sensitivity and uncertainty analysis based on the sensitivity and uncertainty results of few-group spatially homogenized cross-sections.

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References

- [1] SALVATORES, M., JACQMIN, R., et al.: OECD/NEA WPEC Subgroup 26 Final Report: Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations, NEA/WPEC-26, 2008.
- [2] IVANOV, K., AVRAMOVA, M., KAMEROW, S., et al.: Benchmarks for Uncertainty Analysis in Modelling (UAM) for the Design, Operation and Safety Analysis of LWRs. Volume I: Specification and Support Data for Neutronics Cases (Phase I), NEA/NSC/DOC, 2013.
- [3] ALIBERTI, G., PALMIOTTI, G., SALVATORES, M., et al.: Nuclear data sensitivity, uncertainty and target accuracy assessment for future nuclear systems, *Annals of Nuclear Energy*, 2006, 33: 700-733.
- [4] LI, Y., TIAN, C., ZHENG, Y., et al.: NECP-CACTI: Pressurized water reactor lattice code development. *Transactions of the American Nuclear Society*, 2015, 112: 814-816.
- [5] TAKEDA, T., ASANO, K., KITADA, T.: Sensitivity Analysis based on Transport Theory. *Journal of NUCLEAR SCIENCE and TECHNOLOGY*, 2006, 43(7): 743-749.
- [6] PUSA, M.: Perturbation-Theory-Based Sensitivity and Uncertainty Analysis with CASMO-4, *Science and Technology of Nuclear Installations*, 2012.
- [7] WILLIAMS, M. L., BROADHEAD, B. L., PARKS, C. V.: Eigenvalue sensitivity theory for resonance-shielded cross sections. *Nucl. Sci. Eng.*, 2001, 138: 177-191.
- [8] LIU, Y., CAO, L., WU, H., et al.: Eigenvalue implicit sensitivity and uncertainty analysis with the subgroup resonance-calculation method, *Annals of Nuclear Energy*, 2015, 79: 18-26.
- [9] BALL, M.R., NOVOG, D.R., LUXAT, J.C.: Analysis of implicit and explicit lattice sensitivities using DRAGON. *Nuclear Engineering and Design*, 2013, 265: 1-12.
- [10] WAN, C., CAO, L., WU, H., et al.: Code development for eigenvalue total sensitivity analysis and total uncertainty analysis. *Annals of Nuclear Energy*, 2015, 85: 788-797.
- [11] WU, H., YANG, W., QIN, Y., et al.: Benchmark Problems and Results for Verifying Resonance Calculation Methodologies, 2012, PHYSOR 2012, Tennessee, USA.
- [12] MACFARLANE, R.E., MUIR, D.W., BOICOURT, R.M., et al: The NJOY Nuclear Data Processing System Version 2012, in: LA-UR-12-27079 (Ed.), Los Alamos National Laboratory, 2012.