

Research Article

Perturbation Theory-Based Whole-Core Eigenvalue Sensitivity and Uncertainty (SU) Analysis via a 2D/1D Transport Code

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For nuclear reactor physics, uncertainties in the multigroup cross sections inevitably exist, and these uncertainties are considered as the most significant uncertainty source. Based on the home-developed 3D high-fidelity neutron transport code HNET, the perturbation theory was used to directly calculate the sensitivity coefficient of k_{eff} to the multigroup cross sections, and a reasonable relative covariance matrix with a specific energy group structure was generated directly from the evaluated covariance data by using the transforming method. Then, the “Sandwich Rule” was applied to quantify the uncertainty of k_{eff} . Based on these methods, a new SU module in HNET was developed to directly quantify the k_{eff} uncertainty with one-step deterministic transport methods. To verify the accuracy of the sensitivity and uncertainty analysis of HNET, an infinite-medium problem and the 2D pin-cell problem were used to perform SU analysis, and the numerical results demonstrate that acceptable accuracy of sensitivity and uncertainty analysis of the HNET are achievable. Finally, k_{eff} SU analysis of a 3D minicore was analyzed by using the HNET, and some important conclusions were also drawn from the numerical results.

1. Introduction

Due to the fact that the nuclear reactor is a complex nonlinear multiphysics, multiscale coupling system, the high-fidelity simulations and modelling with full consideration of the coupling among neutronics, thermal hydraulics, fuel performance, and so on have now become the powerful numerical tool for the detailed analysis of both the current and advanced reactor design. However, the uncertainties in the basic data, such as the multigroup cross sections, manufacturing tolerance of fuel and materials, naturally exist, and these uncertainties inevitably propagate in the progress of nuclear reactor simulations. So, understanding these uncertainties and quantifying the total uncertainty of the nuclear reactor key parameters is important for improving the reliability of the best estimated results, identifying the importance of uncertainty sources and ensuring appropriate design margins, and also to establish best-estimate calculations for nuclear reactor design and safety analysis. As research progressed,

it matures a move toward Best-Estimation plus Uncertainty (BEPU) analysis, and BEPU has now become the standard for the modern evaluation of the nuclear reactor system.

Nuclear reactor physics is the branch of science that deals with the study and application of the chain reaction to induce a controlled rate of fission in the nuclear reactor for the production of energy, so understanding the nuclear reactor physics is very important for each nuclear reactor design, operation, and safety analysis. As a result, uncertainty analysis on nuclear reactor physics simulation results has been a rising topic in recent years. In general, there are three basic uncertainty sources in nuclear physics calculations, including modelling error, numerical solution error, and input parameter uncertainties [1]. The first two errors can be significantly reduced by the arbitrary-geometry modelling method and fast-growing high-fidelity numerical method for transport calculation, respectively. However, the uncertainties of input parameters, especially the multigroup cross sections,

inevitably exist, and these uncertainties are considered as the most significant uncertainty source in the reactor neutronics calculation [2]. For nuclear reactor physics, multiplication factor is one of the most important integral parameters that need to quantify its uncertainty propagated from the multigroup cross sections.

Uncertainty quantification method includes the perturbation theory- (PT-) based method and the statistics sampling-based method. The statistics sampling based method has no approximation with the simulation models and codes and is easy to be implemented. Although the statistical sampling based uncertainty and sensitivity analysis method has less simplifications and approximations and no limit to the system responses compared with the perturbation theory-based method, this method is costly in time and efforts to perform and to interpret the results, and the more challenging problem is that the probability density functions (PDF) are usually unknown being replaced by approximations of good or worse fidelities. For the problems with good adjoint system and easy to solve its associated adjoint system, such as the eigenvalue problem of the nuclear reactor physics, the perturbation theory-based method is efficient, and the superiority is more obvious. As for the implementation progress of the perturbation theory-based uncertainty and sensitivity analysis of the eigenvalue due to the cross section, the sensitivity coefficient of k_{eff} with respect to multigroup macroscopic cross sections should be quantified by using the perturbation theory based on the forward and adjoint solutions, and a reasonable nuclear cross-section covariance matrix in the specific multigroup form, which represents uncertainty and correlation information of different cross sections, should also be built. Then, the ‘‘Sandwich Rule’’ is applied to quantify the uncertainty of k_{eff} propagated from nuclear cross sections.

Indeed, much effort has been put in the development of the perturbation theory-based sensitivity and uncertainty analysis methods by using the forward and adjoint solutions obtained by deterministic transport methods or Monte Carlo methods for the past years. For the deterministic transport methods, perturbation-based sensitivity and uncertainty analysis is always performed by using the 2D forward and adjoint transport solutions, and some well-known lattice codes already have the SU analysis ability, such as the Polaris in SCALE6.2.1 [3], CASMO5 [4], and AutoMOC [5]. For the direct 3D whole-core SU analysis, the Monte Carlo methods are preferred to perform the forward and adjoint calculations, and then the perturbation theory-based SU method is applied, and the SU analysis ability is also developed in some famous Monte Carlo codes in recent years, such as the TSUNAMI-3D module in SCALE [6], RMC [7], and McCARD [8]. Even more important, significant advances in high performance computing clusters have enabled the direct 3D whole-core heterogeneous transport simulation in the subpin level by using the deterministic transport methods, and extending the direct 3D whole-core high-fidelity deterministic transport simulation capabilities to the SU

analysis has attracted more and more research efforts in recent years [9].

A 3D whole-core high-fidelity deterministic neutron transport code based on 2D/1D fusion method has been developed in our research group, which adopts the 2D MOC and 1D NEM with a global multilevel CMFD acceleration to solve the forward and adjoint neutron transport equations directly from the multigroup microscopic cross sections [10, 11]. Based on this new code, the generalized perturbation theory is used to directly calculate the sensitivity coefficient of k_{eff} to the multigroup cross sections, and then a new SU module is developed to directly quantify the k_{eff} uncertainty with one-step deterministic transport methods. It is worthy to note that the multigroup relative covariance matrix is also important for the SU analysis, and the ZZ-SCALE6.0/COVA-44G [12] built in SCALE6.0 is very comprehensive. But some other deterministic transport codes cannot directly use this library due to a different energy group structure. Although a new covariance matrix can be processed from the Evaluated Nuclear Data File ENDF/B-VII.1 by using the NJOY code, an alternative efficient and convenient transforming method is developed in our research to generate a reasonable relative covariance matrix with a specific energy group structure from the evaluated 44g covariance data library.

In the following sections, the theory background of uncertainty analysis with Sandwich Rule, perturbation theory-based sensitivity analysis, and the covariance matrix transforming method is firstly present. Especially the detailed form of sensitivity coefficients for individual nuclide reaction type is given. Then, the sensitivity and uncertainty analysis scheme is described in detail. In order to verify the accuracy of SU results, the analytical solutions of the three-group infinite medium problem and the direct perturbation (DP) sensitivity analysis and uncertainty analysis of the VERA single cell problem are performed. Finally, SU analysis is performed on the VERA 3 × 3 patterned minicore, and the calculated SU results are given.

2. Theories

2.1. Uncertainty Quantification with the Sandwich Rule. Consider the k_{eff} of a reactor system which can be expressed as a function of a set of multigroup macroscopic cross sections:

$$k_{\text{eff}} = R(\sigma_1, \sigma_2, \dots, \sigma_n), \quad (1)$$

where σ represents the multigroup macroscopic cross section for a nuclide reaction type, i.e., effective multigroup resonance cross section, and \bar{k} and $\bar{\sigma}$ represent the expected value. This function can be rewritten by using Taylor expansion and the first order linearity approximation as

$$k_{\text{eff}} = \bar{k}_{\text{eff}} + \delta k_{\text{eff}} = R(\bar{\sigma}_1, \bar{\sigma}_2, \dots, \bar{\sigma}_n) + \sum_i^n \frac{\partial k_{\text{eff}}}{\partial \sigma_i} \delta \sigma_i. \quad (2)$$

Assuming that input parameters are random and satisfy a joint probability density function $p(\sigma_1, \sigma_2, \dots, \sigma_n)$, then the variance of k_{eff} can be quantified by

$$\begin{aligned} \text{var}(k_{\text{eff}}) &= \int \left(\sum_{i=1}^n \left(\frac{\partial k_{\text{eff}}}{\partial \sigma_i} \right) \delta \sigma_i \right)^2 p(\sigma_1, \sigma_2, \dots, \sigma_n) d\sigma_1, d\sigma_2, \dots, d\sigma_n \\ &= \sum_{i=1}^n \left(\frac{\partial k_{\text{eff}}}{\partial \sigma_i} \right)^2 \text{var}(\sigma_i) + 2 \sum_{i \neq j=1}^n \frac{\partial k_{\text{eff}}}{\partial \sigma_i} \frac{\partial k_{\text{eff}}}{\partial \sigma_j} \text{cov}(\sigma_i, \sigma_j), \end{aligned} \quad (3)$$

where cov represents the covariance and var represents variance. Thus, the relative variance of k_{eff} , i.e., the square of the relative k_{eff} uncertainty due to cross sections could be written as

$$\begin{aligned} \frac{\text{var}(k_{\text{eff}})}{k_{\text{eff}}^2} &= \sum_{i=1}^n \left(\frac{\sigma_i}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma_i} \right)^2 \frac{\text{var}(\sigma_i)}{\sigma_i^2} + 2 \sum_{i \neq j=1}^n \left(\frac{\sigma_i}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma_i} \right) \\ &\quad \cdot \left(\frac{\sigma_j}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma_j} \right) \frac{\text{cov}(\sigma_i, \sigma_j)}{\sigma_i \sigma_j} \\ &= \sum_{i=1}^n (S_{k_{\text{eff}}, \sigma_i})^2 \text{Rvar}(\sigma_i) + 2 \sum_{i \neq j=1}^n S_{k_{\text{eff}}, \sigma_i} S_{k_{\text{eff}}, \sigma_j} \text{Rcov}(\sigma_i, \sigma_j), \end{aligned} \quad (4)$$

with the new definition of the sensitivity coefficient vector and the relative covariance matrix as

$$\begin{aligned} S_{k_{\text{eff}}, \sigma} &= (S_{k_{\text{eff}}, \sigma_1}, S_{k_{\text{eff}}, \sigma_2}, \dots, S_{k_{\text{eff}}, \sigma_n}) \\ &= \left(\frac{\sigma_1}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma_1}, \frac{\sigma_2}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma_2}, \dots, \frac{\sigma_n}{k_{\text{eff}}} \frac{\partial k_{\text{eff}}}{\partial \sigma_n} \right), \end{aligned} \quad (5a)$$

$$\text{Rcov} = \begin{bmatrix} \frac{\text{var}(\sigma_1)}{\sigma_1^2} & \dots & \frac{\text{cov}(\sigma_1, \sigma_n)}{\sigma_1 \sigma_n} \\ \vdots & \ddots & \vdots \\ \frac{\text{cov}(\sigma_n, \sigma_1)}{\sigma_n \sigma_1} & \dots & \frac{\text{var}(\sigma_n)}{\sigma_n^2} \end{bmatrix}, \quad (5b)$$

and the sensitivity coefficient reflects the relative change of the independent response k_{eff} with respect to the relative perturbation of a dependent parameter σ , which is defined as

$$S_{k_{\text{eff}}, \sigma} = \frac{\delta k_{\text{eff}} / k_{\text{eff}}}{\delta \sigma / \sigma}. \quad (5c)$$

Then, the relative k_{eff} uncertainty can be rewritten by using the matrix form as

$$\frac{\text{var}(k_{\text{eff}})}{k_{\text{eff}}^2} = S_{k_{\text{eff}}, \sigma} \text{Rcov} (S_{k_{\text{eff}}, \sigma})^T. \quad (6)$$

Equation (6) is the well-known ‘‘Sandwich Rule’’. Once the sensitivity coefficient and the relative covariance matrix are known, the relative uncertainty of k_{eff} can be quantified by equation (6).

2.2. Sensitivity Analysis of k_{eff} by Using Perturbation Theory. For uncertainty analysis based on the Sandwich Rule, the sensitivity coefficient of k_{eff} to different cross sections should be quantified firstly by using different methods, such as the

central difference direct perturbation method and perturbation theory-based sensitivity analysis method. For each sensitivity coefficient calculated by the direct perturbation, k_{eff} of the system is computed first with the normal values of the input multigroup cross sections, then with a selected nominal input cross section increased by a certain percentage, and then with the same nominal value decreased by the same percentage. Finally, the direct perturbation sensitivity coefficient of k_{eff} to a certain input cross section σ is calculated as

$$S_{k_{\text{eff}}, \sigma} = \frac{(k_{\text{eff}}^{\sigma^+} - k_{\text{eff}}^{\sigma^-}) / k_{\text{eff}}}{(\sigma^+ - \sigma^-) / \sigma}, \quad (7)$$

where σ^+ and σ^- represent the increased and decreased input cross sections, respectively, and $k_{\text{eff}}^{\sigma^+}$ and $k_{\text{eff}}^{\sigma^-}$ represent the corresponding values of the k_{eff} . The direct sensitivity coefficients are easily determined since they depend only on the response functions and do not require an adjoint calculation compared with the perturbation theory-based sensitivity analysis method. This method is feasible and accurate as long as a linear relationship between k_{eff} and cross sections is maintained. However, the central difference direct perturbation method for sensitivity coefficient calculations is computationally cost and even impracticable if all isotopes, reaction types, and energy groups are taken into consideration. Even more important, the relative perturbation factor needs to be chosen carefully, as too small perturbation could be overwhelmed by the numerical calculation errors, whereas too large perturbation may destroy the linear relationship between k_{eff} and cross sections. In this way, the central difference direct perturbation method is always considered as an adequate test for verification of other sensitivity calculation methods. So, the sensitivity coefficient results obtained by using the direct perturbation method are also used to verify the perturbation theory-based sensitivity results in this paper.

In this paper, the perturbation theory is used to calculate the sensitivity coefficient of k_{eff} to the multigroup macroscopic cross sections of different nuclides. The details of each sensitivity coefficient are summarized in this section. In nuclear reactor physics, the operator form of the forward and adjoint neutron transport equations can be written as

$$(L - \lambda F)\Psi = 0, \quad (8a)$$

$$(L^* - \lambda^* F^*)\Psi^* = 0, \quad (8b)$$

where L is the operator that represents neutron leakage, absorption, and scattering term and F represents the fission source operator; Ψ is the forward neutron angular flux; L^* and F^* are the adjoint operators of L and F , respectively. Ψ^* represents the adjoint neutron angular flux. λ and λ^* are the eigenvalues of forward and adjoint neutron transport equations, respectively (for details, see [10] and [11]). It is important in sensitivity calculations to ensure that the k_{eff} value of the forward and adjoint solutions closely agree. If the k_{eff} values do not agree, then the quality of at least one of the transport calculations may be in question. Typically, the transport calculation of concern is the adjoint calculation.

For nuclear reactor physics, k_{eff} is an integral key parameter and determined by several dependent parameters, such as geometry information, nuclide compositions, and cross sections. As research of high-fidelity simulation and modelling progressed, the uncertainty of nuclear cross sections become more and more important to the total uncertainty of k_{eff} .

Then, the perturbed transport operators and perturbed eigenvalue can be expressed as,

$$\begin{aligned} L' &= L + \delta L, \\ F' &= F + \delta F, \\ \lambda' &= \lambda + \delta \lambda, \end{aligned} \quad (9)$$

where δL and δF represent small perturbations of these transport operators, respectively. $\delta \lambda$ is the corresponding perturbation of the eigenvalue. The perturbed forward neutron transport equation is thus written as

$$(L' - \lambda' F')\Psi' = 0. \quad (10)$$

Multiplying both sides of equation (10) by the adjoint neutron angular flux Ψ^* and integrating over all phase space yields

$$\langle \Psi^* (L' - \lambda' F')\Psi' \rangle = 0, \quad (11)$$

where the bracket $\langle \rangle$ represents the inner product, and integrating over all phase space involves region, energy, and direction. Then, substitute the perturbed term in equation (11) with equation (9):

$$\langle \Psi^* ((L + \delta L) - (\lambda + \delta \lambda)(F + \delta F))\Psi' \rangle = 0. \quad (12)$$

In order to obtain the relative perturbation of the eigenvalue, two approximations are introduced into equation (12): the high order perturbation $\delta F \delta L$ is ignored, and Ψ' is approximated by the unperturbed Ψ as the perturbation of transport operator would not introduce obvious changes in the neutron angular flux. The relative perturbation of eigenvalue is thus obtained as

$$\frac{\delta \lambda}{\lambda} = \frac{\langle \Psi^* (\delta L - \delta F)\Psi \rangle}{\langle \Psi^* (\lambda F)\Psi \rangle}. \quad (13)$$

Here, the perturbation of the operators L and F could be introduced explicitly by the first-order Taylor's expansion with respect to multigroup macroscopic cross sections in their corresponding operator. And, the sensitivity coefficient of k_{eff} due to the perturbation of a certain macroscopic cross section σ can be eventually expressed as

$$S_{k_{\text{eff}},\sigma} = -\sigma \frac{\langle \Psi^* ((\partial L/\sigma) - (1/k_{\text{eff}})(\partial F/\sigma))\Psi \rangle}{\langle \Psi^* (1/k_{\text{eff}})F\Psi \rangle}. \quad (14)$$

Based on the above equation, the sensitivity coefficient can be obtained by using the perturbation theory, and it only requires forward transport calculation and adjoint calculation once.

It can be found from the above equation that the denominator is reaction type-independent, whereas

numerator would vary with different analyzed reaction types. Then, the discretization of denominator can be expressed as follows:

$$\begin{aligned} D = \left\langle \Psi^* \frac{1}{k_{\text{eff}}} F\Psi \right\rangle &= \frac{1}{k_{\text{eff}}} \sum_i^I \sum_z^Z V_z \sum_g^G \chi_{g,z}^i \left(\sum_{m=1}^M w_m \Psi_{m,g,z}^* \right) \\ &\sum_{g'}^G \nu_{g',z}^i \sigma_{f,g',z}^i \left(\sum_{m=1}^M w_m \Psi_{m,g',z} \right), \end{aligned} \quad (15)$$

where i , m , g , and z are the nuclide isotope, direction, energy, and mesh index, respectively. And, w_m is the quadrature weight.

The derivation of numerator term could be easily obtained according to the discrete form of neutron transport equation. The sensitivity coefficients of k_{eff} to different cross sections of the isotope i , energy group g , and reaction type x are summarized as follows:

(1) Capture cross section

$$S_{k_{\text{eff}},\sigma_{\text{cap},g}}^i = -\frac{1}{D} \sum_z^Z V_z \sigma_{\text{cap},g,z}^i \sum_m^M w_m \Psi_{m,g,z}^* \sum_m^M w_m \Psi_{m,g,z}. \quad (16)$$

(2) Fission cross section

$$\begin{aligned} S_{k_{\text{eff}},\sigma_{f,g}}^i &= \frac{1}{D} \left(\lambda \sum_z^Z V_z \nu_g^i \sigma_{f,g,z}^i \sum_m^M w_m \Psi_{m,g,z} \sum_{g'=1}^G \chi_{g'}^i \sum_m^M w_m \Psi_{m,g',z}^* \right. \\ &\left. - \sum_z^Z V_z \sigma_{f,g,z}^i \sum_m^M w_m \Psi_{m,g,z} \sum_m^M w_m \Psi_{m,g,z}^* \right). \end{aligned} \quad (17)$$

(3) Average number of neutrons emitted per fission reaction

$$S_{k_{\text{eff}},\nu_g}^i = \frac{1}{D} \lambda \sum_z^Z \nu_{g,z}^i \sigma_{f,g,z}^i \sum_m^M w_m \Psi_{m,g,z} V_z \sum_{g'=1}^G \chi_{g'}^i \sum_m^M w_m \Psi_{m,g',z}^*. \quad (18)$$

(4) Fission spectrum

$$S_{k_{\text{eff}},\chi_g^i} = \frac{1}{D} \lambda \sum_z^Z V_z \chi_g^i \sum_m^M w_m \Psi_{m,g,z}^* \sum_{g'=1}^G \nu_{g',z}^i \sigma_{f,g',z}^i \sum_m^M w_m \Psi_{m,g',z}. \quad (19)$$

(5) Scattering cross section

$$S_{k_{\text{eff}}, \sigma_{s,g \rightarrow g'}}^i = \frac{1}{D} \sum_z V_z \sigma_{s,g \rightarrow g',z}^i \sum_m^M w_m \psi_{m,g,z} \left(\sum_m^M w_m \psi_{m,g',z}^* - \sum_m^M w_m \psi_{m,g,z}^* \right), \quad (20)$$

where, $\psi_{m,g,z}$ and $\psi_{m,g,z}^*$ are the neutron angular flux and adjoint angular flux of direction m , energy group g , and mesh z , and they are obtained by solving the forward and adjoint neutron transport equations, respectively. V_z is the volume of mesh z , i.e., the flat source region due to the MOC method used in this work.

It is worth to note that the sum of all the k_{eff} sensitivity coefficients to the fission spectrum for all energy groups and nuclides should be equal 1.0 based on equations (14), (15), and (19). Actually, the sum of the fission spectrum must be equal to 1.0 over all energy groups for any nuclide. Thus, the sensitivity of k_{eff} to the fission spectrum should sum to 0.0, as any change in fission spectrum in any energy group must be compensated by changes in other groups to maintain the constraint that all the fission spectra sum to 1.0. In this way, the sensitivity coefficient of k_{eff} to the fission spectrum is corrected by the following equation in our work:

$$S_{k_{\text{eff}}, \chi_g}^{i,C} = S_{k_{\text{eff}}, \chi_g}^i - \chi_g^i \sum_{g'}^G S_{k_{\text{eff}}, \chi_{g'}}^i. \quad (21)$$

2.3. Transforming Method to Generate Multigroup Relative Covariance Matrix. It is worthy to note that the multigroup relative covariance matrix is very important for the sensitivity and uncertainty analysis, and the relative covariance matrix, which contains uncertainties and correlations information between cross sections of different reaction types, is used to propagate uncertainties of nuclear cross sections. At the same time, the relative covariance matrix should be formed in the same energy group structure with the multigroup nuclear cross section library utilized in the neutron transport calculations. Normally, there are two approaches to generate a reasonable relative covariance matrix for uncertainty analysis. One is that the new relative covariance

matrix with a problem-specific energy group structure can be processed from the Evaluated Nuclear Data File ENDF/B-VII.1 by using the NJOY code, and this method is mathematically rigorous, in which it needs more evaluations and some judgements from experts. Another approach is transforming a well-evaluated relative covariance matrix, such as ZZ-SCALE6.0/COV-44G, into an appropriate energy group structure based on the method of flat-flux approximation. Compared with the new generated relative covariance matrix obtained by using the first method, numerical errors are inevitably introduced in the transformed relative covariance matrix due to mathematical approximation. However, these errors are sometimes less than the expert evaluation information contained in the comprehensive-evaluated covariance matrix. Hence, the efficient and convenient transforming method is developed in our research to generate a reasonable relative covariance matrix with a specific energy group structure from the evaluated 44g covariance data library.

The key thought behind this transforming method is liner transformation of the correlation coefficient and relative standard deviation, respectively, between different energy ranges in lethargy, i.e., the integration of relative standard deviation and correlation efficient over the specific energy region is flat. To realize the universality of the transforming method, the idea of constructing a transitional energy group structure is used, as shown in Figure 1 (for more details of this method and the code developed based on this method, see [13, 14]).

Based on this method, a relative covariance matrix in 47g energy group structure, the same as the energy group structure of nuclear data library used in Helios, is generated directly from the ZZ-SCALE6.0/COV-44G library. Due to the fact that the 47 energy group nuclear data library is used as the basic data library for neutron transport calculations and this library contains the total capture and scattering cross sections, while only the relative covariance information for individual cross section are provided in the relative covariance library, the following property of the covariance is applied to estimate the relative covariance information of the total capture and scattering cross section based on the associated individual cross sections [15] as

$$\text{Rcov}(aX + bY, a'X' + b'Y') = aa' \text{Rcov}(X, X') + ab' \text{Rcov}(X, Y') + ba' \text{Rcov}(Y, X') + bb' \text{Rcov}(Y, Y'). \quad (22)$$

In addition, only the relative covariance information is given for the group total scattering cross section $\sigma_{s,g}$, while the covariance information of the self-scattering, downscattering, and upscattering cross section $\sigma_{s,g \rightarrow g'}$, i.e., transfer cross section, is not provided in the relative covariance library. However, equation (20) only calculates the sensitivity coefficient of k_{eff} to the transfer cross section, and it is difficult to directly obtain the corresponding sensitivity coefficient to the group total scattering cross section based on the perturbation theory. However, an approximated sensitivity coefficient can be obtained if some assumptions are made as Pusa suggested [2]:

$$S_{k_{\text{eff}}, \sigma_{s,g}}^i = \sum_{g'}^G S_{k_{\text{eff}}, \sigma_{s,g \rightarrow g'}}^i. \quad (23)$$

3. Overall Calculation Flow

Based on the methods introduced above, the overall calculation flow of the sensitivity and uncertainty analysis is illustrated in Figure 2. The Helios 47g nuclear data library is used as the basic evaluated multigroup cross section library for the forward and adjoint transport calculations, and the

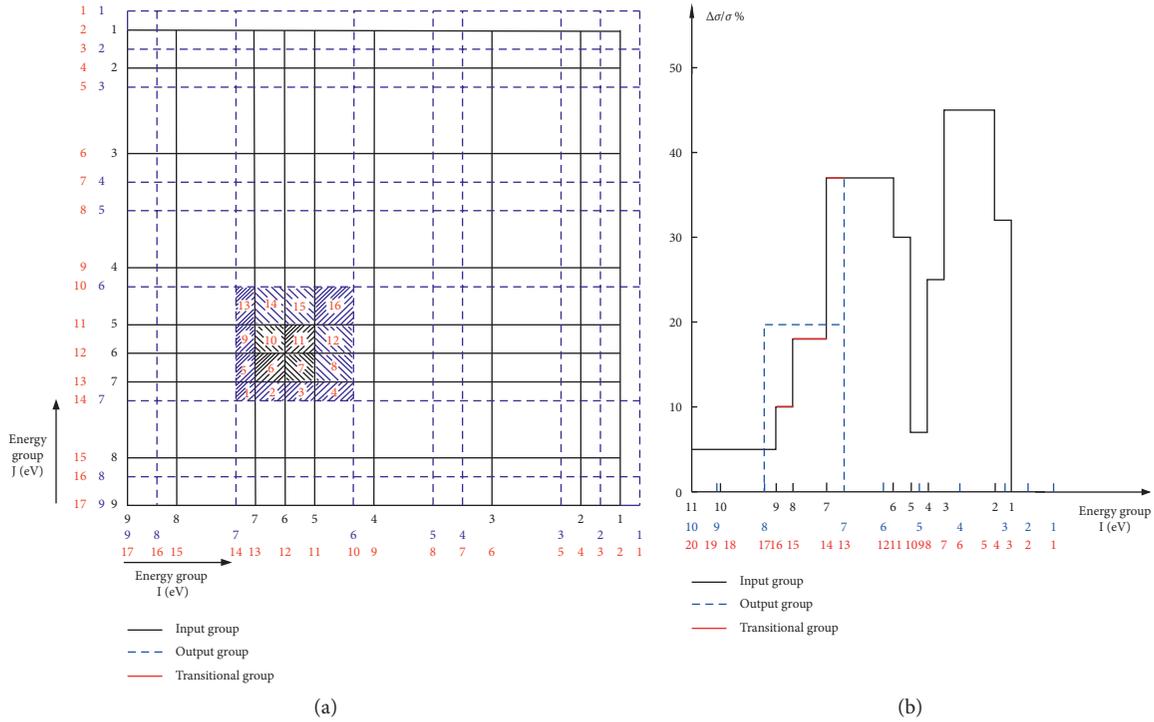


FIGURE 1: Transitional energy group structure for transformation correlation and standard deviation.

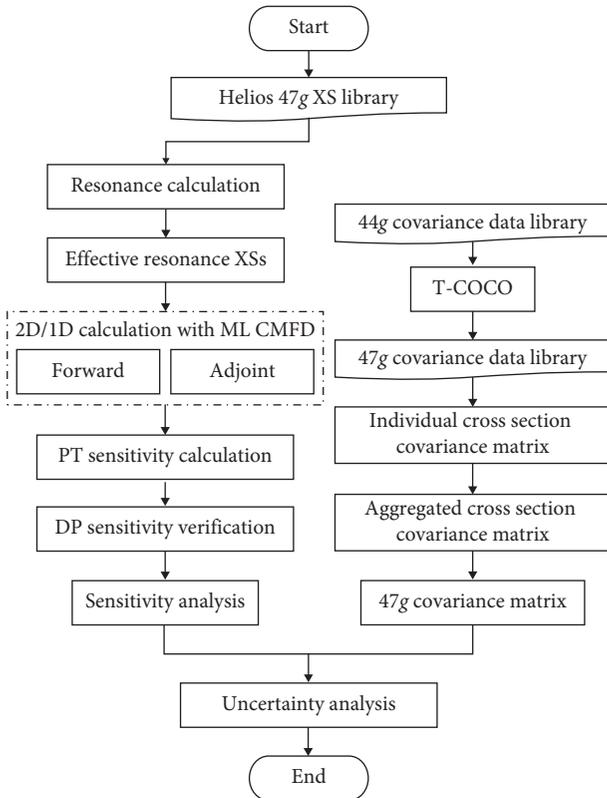


FIGURE 2: Flowchart of perturbation theory based sensitivity and uncertainty analysis.

ZZ-SCALE6.0/COV-44G library is used as the basic relative covariance library. A home-developed 3D whole-core high-fidelity deterministic neutron transport code based on 2D/1D fusion method, which adopts the 2D MOC and 1D NEM with a global multilevel CMFD acceleration, is applied to solve the forward and adjoint neutron transport equations directly from the multigroup microscopic cross sections. Then, an SU analysis module is developed, which is coupled with the home-developed 3D transport code, for sensitivity and uncertainty analysis of k_{eff} due to the uncertainties in the nuclear cross sections. The procedures of perturbation theory-based sensitivity and uncertainty analysis can be summarized as follows:

- (1) The 47g problem-related relative covariance library is generated directly from the evaluated 44g relative covariance library ZZ-SCALE6.0/COV-44G based on a flat-flux approximation.
- (2) The subgroup resonance calculation module in the home-developed 3D high-fidelity neutron transport code HNET firstly uses the 47g Helios library to generate the multigroup macrocross sections of all nuclides. Then, the forward and adjoint 3D transport calculations are performed to generate the forward and adjoint eigenvalue and flux, respectively.
- (3) Based on the forward and adjoint results obtained in step 2, the k_{eff} sensitivity coefficients to different multigroup macrocross sections of each nuclide is calculated by using the perturbation theory, and at

the same time, the direct perturbation method is used to verify the sensitivity results.

- (4) The Sandwich Rule is finally used to quantify the k_{eff} uncertainty propagated from the nuclear cross sections based on the relative covariance library and the sensitivity coefficients.

4. Numerical Results

4.1. Verification of the Sensitivity Analysis

4.1.1. Infinite-Medium Problem. In order to verify the sensitivity calculation abilities, a three-group infinite-medium problem was chosen [16] as the k_{eff} of this infinite-medium problem could be obtained analytically, and its associated sensitivity coefficient can be calculated directly from the definition of sensitivity coefficient. The nuclear data used in this problem, including absorption cross sections, fission cross sections, average number of fission neutron, fission spectrum, and scattering matrix are listed in Table 1.

This problem is designed as the critical state, and the analytic solution of k_{eff} can be quantified as

$$k_{\text{eff}} = \frac{\nu_3 \sigma_{f3} \sigma_{s,2 \rightarrow 3}}{\sigma_{r2} \sigma_{r3}} \left(\frac{\sigma_{s,1 \rightarrow 2}}{\sigma_{r1}} \chi_1 + \chi_2 + \frac{\sigma_{r2}}{\sigma_{s,2 \rightarrow 3}} \chi_3 \right) \approx 0.99999656. \quad (24)$$

As mentioned above, the k_{eff} value of the forward and adjoint solutions should closely agree with the sensitivity calculations. For this problem, the calculated k_{eff} of the forward and adjoint solutions quantified by HNET is 0.999997 and 0.999995, respectively. Then, sensitivity coefficients of k_{eff} to different cross sections calculated by using the SU module in HNET and equation (5c) are summarized in Table 2. It is obviously found that the calculated sensitivity coefficients quantified by HNET agree very well with the analytic solutions, which indicates a superior accuracy of the perturbation theory-based sensitivity coefficient calculation of HNET.

4.1.2. VERA 2D Pin-Cell Problem. In order to further verify the sensitivity coefficient calculation abilities of the SU module in HNET, the 2D pin-cell problem proposed in the VERA core physics benchmark [17] was chosen to perform sensitivity analysis, and the direct perturbation method was used for the verification of the sensitivity coefficients results. The problem specifications are summarized in Table 3, and the radial geometry information and subpin meshes are illustrated in Figure 3. For the transport calculations, a Tabuchi-Yamamoto polar quadrature with 3 polar angles per half-space was used, and 40 flat source regions consisting of 3 fuel rings and 2 moderator rings with 8 azimuthal divisions were used and 0.01 cm was chosen for the ray spacing of the MOC calculations. At the same time, the forward and adjoint transport calculations were performed with using the Helios 47 energy group nuclear data library.

The calculated k_{eff} of the forward and adjoint neutron transport solutions and difference from the reference solutions are summarized in Table 4. As expected, the k_{eff}

values for forward and adjoint calculations are same, and it is important in the sensitivity calculations. The difference of the forward eigenvalue is about 20 pcm, which is also in the acceptable range, and the difference derives mainly from the difference in the nuclear data library. The reference value is calculated by using the KENO-VI in SCALE with continuous energy library based on the ENDF/B-VII.0 [17], while the Helios 47g library based on the ENDF/B-VI data is used for the transport calculation in this work.

With the eigenvalues and flux information of the forward and adjoint calculations, sensitivity coefficients of k_{eff} to the different cross sections of each isotope and reaction type can be quantified by using the SU module built in HNET. At the same time, the direct perturbation method was applied for further verification, and a 2% relative perturbation of each cross section was used in the DP method. A linear relation test was performed firstly; the results indicate that the 2% relative perturbation maintains the linear relation between k_{eff} and cross sections and can be selected to perform the DP method. However, the DP method is time consuming, e.g., a total number of 94 forward calculations are required to obtain the sensitivity coefficient for all energy groups for a specific reaction type of an isotope, while only one forward and one adjoint neutron transport calculation is needed for obtaining all the sensitivity coefficients of all energy group, all isotopes and reaction types. The comparisons of sensitivity coefficients calculated by using the DP and PT methods for the total capture cross section, average number of neutrons emitted per fission event, the fission spectrum of ^{235}U , and the scattering cross section of ^1H are illustrated in Figure 4, where the sensitivity coefficients are all integrated over all regions. And, the integrated sensitivity coefficients of some representative cross sections of some isotopes and reaction types are summarized in Table 5 for comparison. As the sum of the k_{eff} sensitivity coefficients to χ for all energies is equal to 0, the sensitivity in group 1 is selected for comparison in this work.

It can be found both in Figure 4 and Table 5 that the sensitivity coefficients calculated by these two methods agree well for all these selected reaction types in almost all the energy groups. But in very few energy groups, such as the total capture cross section of ^{235}U in group 19 and group 20, the relative errors are 7.9% and 1%, respectively, but still are acceptable. So, these comparisons can demonstrate that acceptable accuracy of sensitivity analysis of the HNET is achievable.

4.2. Verification of the Uncertainty Analysis. To verify the uncertainty analysis ability of the SU module in HNET, the Tsunami-2D [18] calculations were performed using the ENDF/B-VI-based cross section library v6-238 for forward and adjoint transport calculations, and the 44g relative covariance library was used for uncertainty quantifications. It is worth to note that the implicit sensitivity analysis is omitted in the Tsunami calculations, in order to facilitate the comparison of the uncertainty results obtained by HNET and Tsunami. At the same time, the reflective boundary conditions were used for the 2D calculations. For uncertainty quantification by using the SU module in HNET, the

TABLE 1: The nuclear cross sections used in infinite-medium problem.

Group	σ_a (cm ⁻¹)	σ_f (cm ⁻¹)	ν	χ	$\sigma_{s,g \rightarrow 1}$ (cm ⁻¹)	$\sigma_{s,g \rightarrow 2}$ (cm ⁻¹)	$\sigma_{s,g \rightarrow 3}$ (cm ⁻¹)
1	1.7273	0.0	0	0.6250	1.1	1.0	0.0
2	1.0	0.0	0	0.2500	0.0	1.1	2.0
3	0.5	1.5	3	0.1250	0.0	0.0	2.1

TABLE 2: The calculated sensitivity coefficients by different methods.

Cross section	$\sigma_{a,1}$	$\sigma_{a,2}$	$\sigma_{a,3}$	$\sigma_{s,1 \rightarrow 2}$	$\sigma_{s,2 \rightarrow 3}$	ν_3	$\sigma_{f,3}$
Analytic solution	-0.2177	-0.2396	-0.2500	0.2177	0.2396	1.0000	0.2500
HNET solution	-0.2177	-0.2396	-0.2500	0.2177	0.2396	1.0000	0.2500

TABLE 3: Main parameters for the 2D pin-cell problem.

Parameter	Value
Rod pitch	1.26 cm
Temperature	565K
Fuel enrichment	3.1%
Fissionable isotopes	²³⁴ U ²³⁵ U ²³⁶ U ²³⁸ U
Boron concentration	1300 ppm

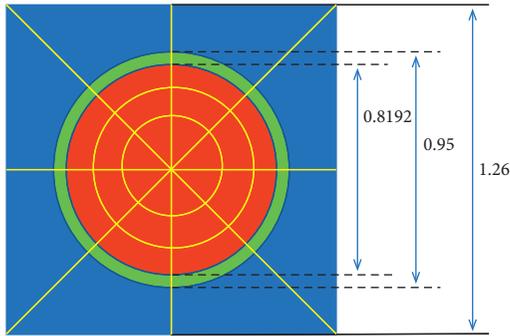


FIGURE 3: Radial geometry information of the 2D pin-cell problem.

TABLE 4: Calculated eigenvalue of the 2D pin-cell problem.

Parameter	Forward/difference	Adjoint	Reference value
k_{eff}	1.18724/20 pcm	1.18724	1.18703 ± 0.00005

sensitivity profiles were computed using the 47-group structure as mentioned above, which is different with the relative covariance library. So, a 47g relative covariance problem-related library was generated directly from the ZZ-SCALE6.0/COVA-44G library by using the transforming method. Some examples, such as the new generated relative covariance matrix of ²³⁵U (n, f), ²³⁵U (ν), and ²³⁸U (n, γ) in 47 energy group structures, are shown in Figures 5–7.

With the verified sensitivity results and the new generated relative covariance matrix in the 47 energy group, the uncertainty of k_{eff} propagated from nuclear cross sections can be quantified. A summary of the calculated eigenvalue and its associated uncertainties due to cross sections is listed in Table 6. For the total uncertainty, the value calculated by HNET is 3.7% smaller. Table 7 shows uncertainty contributions together with the corresponding energy and region-integrated sensitivity coefficients of some important nuclide reactions.

It can be seen from Table 7 that, in both calculations, the main contribution to the total uncertainty comes from the capture cross section of ²³⁸U. In general, most of sensitivity coefficients and uncertainties quantified by the HNET agree well with those calculated by Tsunami-2D and the conclusion of the UAM benchmark Exercise [1]. This observation can further demonstrate that acceptable accuracy of uncertainty analysis of the HNET is achievable.

4.3. Sensitivity and Uncertainty Analysis of k_{eff} for the Minicore Model. Problem #4 in VERA Core Physics Benchmark, which is a 3D mini reactor core in 3 × 3 pattern, was chosen to perform the whole-core eigenvalue sensitivity and uncertainty analysis via the perturbation theory-based SU module in the home-developed 2D/1D transport code HNET. The configuration of this code model is shown in Figure 8 and detailed geometry and material information can be found in the cited paper [17].

For HNET calculations, the Helios 47g nuclear data library was used as the basic input, and a new generated relative covariance library in 47 energy group was used for uncertainty quantification. As the MOC method was applied for radial transport calculation in HNET, a Tabuchi-Yamamoto polar quadrature with 3 polar angles per half-space was used, and 40 flat source regions consisting of 3 fuel rings and 2 moderator rings with 8 azimuthal divisions were used and 0.01 cm was chosen for the ray spacing. And, the reference eigenvalue is calculated by KENO-VI, a continuous energy (CE) Monte Carlo-based transport solver by using the ENDF/B-VII.0 CE cross section library. A summary of the numerical results for this 3D minicore model is presented in Table 8. The forward and adjoint eigenvalue is nearly the same, and the difference of the forward eigenvalue with the reference value is relatively large, about 202 pcm, but still in acceptable range. This difference mainly derives from the isotropic axial transverse leakage approximation, diffusion approximation for axial calculation, and especially the difference in the basic nuclear cross section library.

Then, the sensitivity analysis of k_{eff} to each cross section of all nuclides was performed, and the energy and region-integrated sensitivity coefficients of some important nuclide reactions are summarized in Table 9. It can be seen from Table 9 that k_{eff} is most sensitive to the ²³⁵U (ν) reaction, which is followed by ²³⁵U (n, f) and ²³⁸U (n, γ), while ²³⁸U

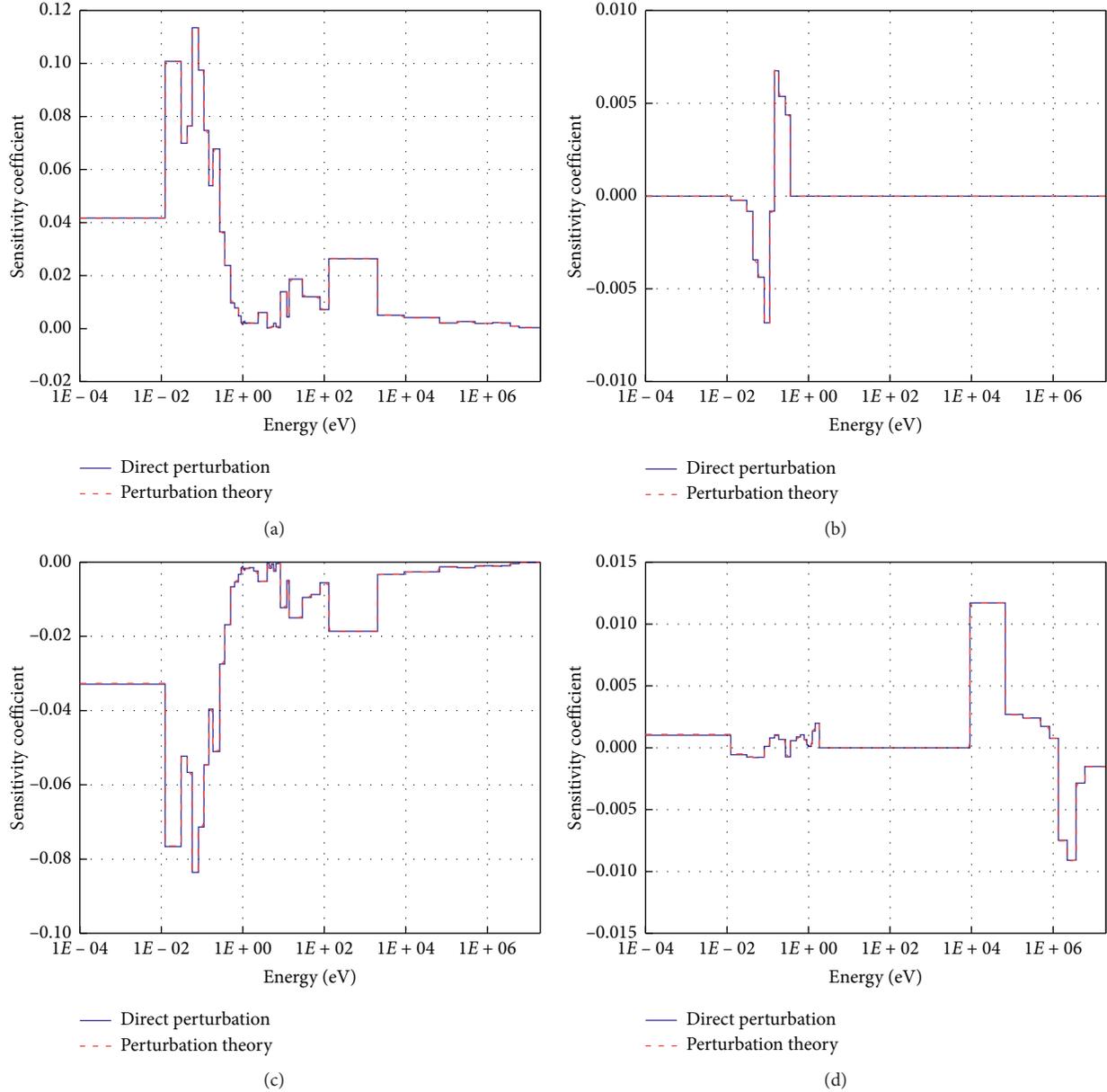


FIGURE 4: Comparisons of sensitivity coefficients calculated by DP and PT methods. Sensitivity verification (a) ^{235}U - ν , (b) ^{235}U - χ , (c) ^{235}U -absorption, and (d) ^1H -total scattering.

TABLE 5: Integral sensitivity coefficients of some representative reaction types.

Reaction type	DP	PT	Relative error (%)
^{235}U σ_γ	-6.91997E-01	-6.91369E-01	0.091
^{235}U ν	9.26186E-01	9.26202E-01	0.001
^{238}U σ_γ	-2.73789E-01	-2.75323E-01	0.560
^{238}U ν	7.36809E-02	7.36677E-02	0.018
^{235}U χ ($g = 1$)	4.37645E-03	4.41066E-03	0.782
^{238}U χ ($g = 1$)	3.38537E-04	3.41451E-04	0.860
^1H σ_s	1.84890E-01	1.85010E-01	0.065

(n, γ) contributes the most to the total uncertainty of k_{eff} due to the uncertainty in ^{238}U (n, γ) itself is much larger.

The sensitivity profiles for some important reactions of ^{235}U and ^{238}U are illustrated in Figures 9 and 10, respectively. It is obviously found that the k_{eff} sensitivity coefficients to the average number of neutrons emitted per fission event, fission and capture cross section of ^{235}U are larger in the thermal energy range, while those values are larger in fast energy range for ^{238}U .

The uncertainty contributions to the total uncertainty of k_{eff} of some important reactions are shown in Table 10. Similar to the 2D pin-cell calculations, the main contribution to the total uncertainty of k_{eff} comes from the capture

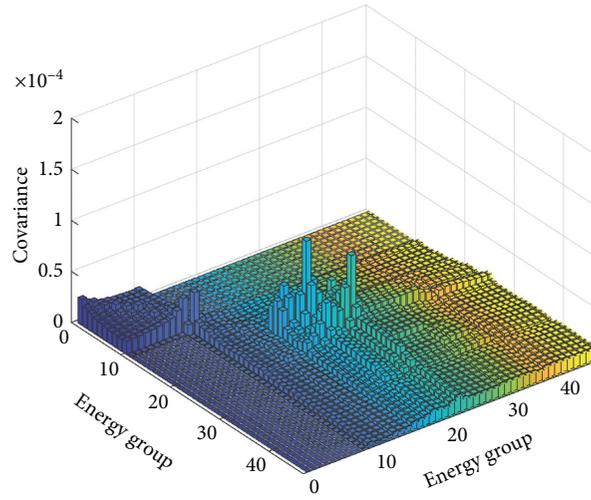


FIGURE 5: Relative covariance matrix in 47 groups for ^{235}U (n, f).

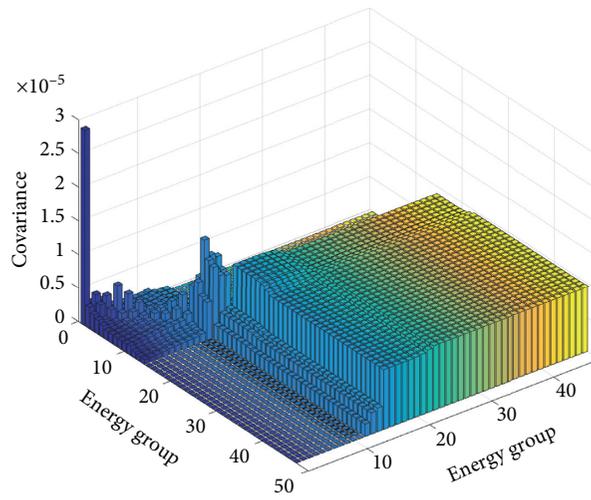


FIGURE 6: Relative covariance matrix in 47 groups for ^{235}U (ν).

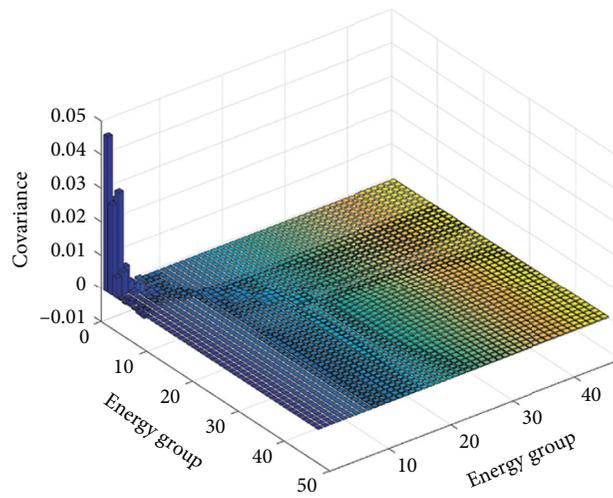


FIGURE 7: Relative covariance matrix in 47 groups for ^{238}U (n, γ).

TABLE 6: Calculated eigenvalue and uncertainties for the 2D pin-cell problem.

Code	Forward/difference	Adjoint	Rel. uncertainty, $\Delta k/k$ (%)
HNET	1.18724/20 pcm	1.18724	0.51
Tsunami-2D	1.17720/984 pcm	1.17710	0.53

^aForward eigenvalue reference is 1.18704 ± 0.000054 .

TABLE 7: Total sensitivity coefficients and uncertainty contributions to $\Delta k/k$ (%) of some important nuclide reactions.

Nuclide	Reaction pair	Sensitivity			Contribution to $\Delta k/k$ (%)		
		HNET	Tsunami-2D	Re (%)	HNET	Tsunami-2D	Re (%)
²³⁸ U	$\sigma_\gamma, \sigma_\gamma$	$-2.753E-01$	$-2.517E-01$	9.40	$3.536E-01$	$3.246E-01$	8.93
²³⁵ U	ν, ν	$9.262E-01$	$9.241E-01$	0.23	$2.654E-01$	$2.648E-01$	0.23
²³⁵ U	$\sigma_\gamma, \sigma_\gamma$	$-1.228E-01$	$-1.226E-01$	0.15	$1.630E-01$	$1.637E-01$	0.43
²³⁵ U	χ, χ	$6.691E-08$	$-2.168E-08$	408.5	$1.225E-01$	$1.249E-01$	1.94
²³⁸ U	σ_s, σ_s	$-8.930E-03$	$-1.061E-02$	15.83	$1.166E-01$	$1.643E-01$	29.02
²³⁵ U	σ_f, σ_f	$3.577E-01$	$3.581E-01$	0.12	$1.140E-01$	$1.133E-01$	0.64
²³⁸ U	ν, ν	$7.367E-02$	$7.580E-02$	2.81	$8.490E-02$	$8.885E-02$	4.44
¹ H	σ_s, σ_s	$1.850E-01$	$1.797E-01$	2.95	$3.418E-02$	$3.453E-02$	1.02
¹ H	$\sigma_\gamma, \sigma_\gamma$	$-4.413E-02$	$-4.448E-02$	0.80	$2.205E-02$	$2.221E-02$	0.74

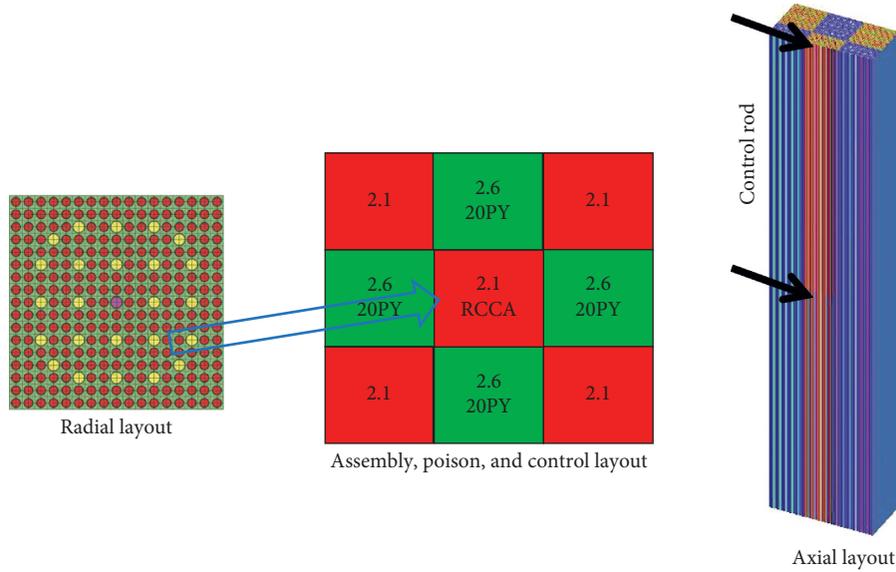


FIGURE 8: The configuration of the VERA 3x3 minicore.

TABLE 8: The calculated eigenvalues and uncertainties for the minicore model.

Code	k_{eff}				Rel. uncertainty, $\Delta k/k$ (%)
	Forward	Adjoint	Reference	Error	
HNET	1.001009	1.000992	0.998981 ± 0.000005	202 pcm	0.523

TABLE 9: The energy and region integrated sensitivity coefficients of some important reactions.

Reaction type	Sensitivity coefficient	Reaction type	Sensitivity coefficient
²³⁵ U σ_γ	$-9.961E-02$	²³⁸ U σ_γ	$-2.747E-01$
²³⁵ U ν	$9.183E-01$	²³⁸ U ν	$8.163E-02$
²³⁵ U σ_f	$3.708E-01$	²³⁸ U σ_f	$5.114E-02$
²³⁵ U σ_s	$-2.403E-04$	²³⁸ U σ_s	$-7.151E-03$
²³⁵ U χ ($g = 1$)	$4.971E-03$	²³⁸ U χ ($g = 1$)	$4.320E-04$
¹ H σ_γ	$-4.176E-02$	¹⁶ O σ_γ	$-4.323E-03$
¹ H σ_s	$1.425E-01$	¹⁶ O σ_s	$-6.842E-04$

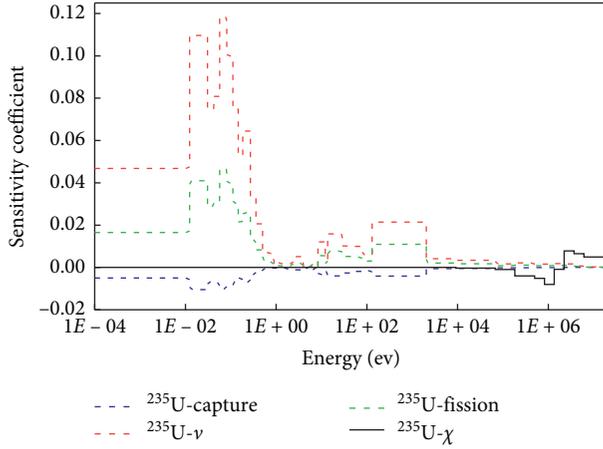


FIGURE 9: k_{eff} sensitivity profiles to different reaction types of ^{235}U .

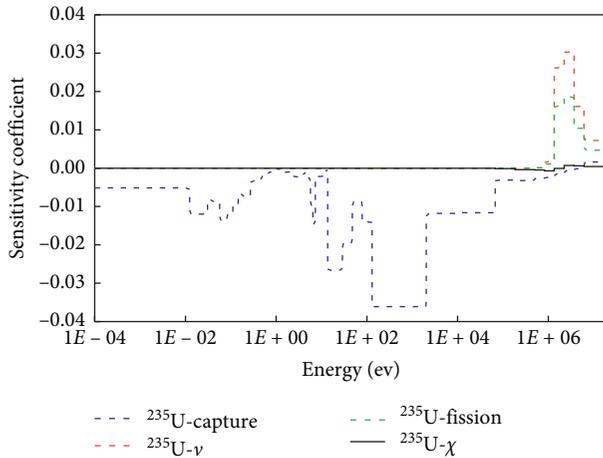


FIGURE 10: k_{eff} sensitivity coefficients to different reaction types of ^{238}U .

TABLE 10: Uncertainty contributions of some important nuclide reactions.

Nuclide	Reaction pair	Contribution to $\Delta k/k(\%)$
^{238}U	$\sigma_{\gamma}, \sigma_{\gamma}$	$3.578E-01$
^{235}U	ν, ν	$2.669E-01$
^{235}U	$\sigma_{\gamma}, \sigma_{\gamma}$	$1.414E-01$
^{235}U	χ, χ	$1.334E-01$
^{235}U	σ_f, σ_f	$1.212E-01$
^{238}U	σ_s, σ_s	$1.005E-01$
^{238}U	N, ν	$9.407E-02$
^1H	σ_s, σ_s	$3.124E-02$
^{238}U	σ_f, σ_f	$2.697E-02$
^1H	$\sigma_{\gamma}, \sigma_{\gamma}$	$2.087E-02$
^{238}U	χ, χ	$1.530E-02$
^{16}O	σ_s, σ_s	$4.889E-03$
^{235}U	σ_s, σ_s	$1.454E-03$
Total	—	0.522

reaction of ^{238}U , and the average number of neutrons emitted per fission event of ^{235}U is another significant contributor to the total uncertainty, which is then followed by the capture reaction of ^{235}U . It can be also seen from

Table 10 that the total contribution of these important reactions is 0.522%, which accounts for the most of k_{eff} uncertainty propagated from the nuclear cross sections and total uncertainty of k_{eff} is 0.523% as shown in Table 8.

5. Conclusions

The Best-Estimation plus Uncertainty (BEPU) analysis has now become the standard for the modern evaluation of the nuclear reactor system. And, uncertainty analysis on nuclear reactor physics simulation results has been a rising topic in recent years. For nuclear reactor physics, uncertainties in the multigroup cross sections inevitably exist, and these uncertainties are considered as the most significant uncertainty source. At the same time, multiplication factor is one of the most important integral parameters that need to quantify its uncertainty propagated from the multigroup cross sections.

Based on the home-developed 3D high-fidelity neutron transport code HNET, the perturbation theory was used to directly calculate the sensitivity coefficient of k_{eff} to the multigroup cross sections by using the forward and adjoint solutions. The multigroup relative covariance matrix is also important for the SU analysis, and then an efficient and convenient transforming method was developed to generate a reasonable relative covariance matrix with a specific energy group structure directly from the evaluated covariance data library ZZ-SCALE6.0/COVA-44G. Then, the ‘‘Sandwich Rule’’ was applied to quantify the uncertainty of k_{eff} propagated from nuclear cross sections based on the sensitivity and relative covariance information. Finally, a new SU module in HNET was developed to directly quantify the k_{eff} uncertainty with one-step deterministic transport methods. At the same time, the direct perturbation method was applied to verify the calculated sensitivity results by using the perturbation theory.

To verify the sensitivity analysis abilities of SU module in HNET, an infinite-medium problem and the 2D pin-cell problem defined in the VERA benchmark were selected to perform sensitivity analysis by HNET, and the analytical method and the direct perturbation method were also used to calculate the sensitivity information for these two problems. For the verification of the uncertainty analysis abilities, the k_{eff} uncertainty for the 2D pin-cell problem was quantified by using HNET and Tsunami-2D, respectively. Overall, the comparisons of numerical results demonstrate that acceptable accuracy of sensitivity and uncertainty analysis of the HNET are achievable, and the SU module in the HNET can be used to perform whole-core eigenvalue sensitivity and uncertainty analysis.

Finally, the k_{eff} sensitivity and uncertainty of the 3D minicore defined in the VERA core physics benchmark to different nuclide cross sections were analyzed by using the HNET. The numerical results indicate that the total uncertainty of k_{eff} due to nuclear cross sections is about 0.52%, and the main contribution to the total uncertainty of k_{eff} comes from the capture reaction of ^{238}U , and the average number of neutrons emitted per fission event of ^{235}U is another significant contributor to the total uncertainty.

However, k_{eff} is most sensitive to ^{235}U (ν), which is followed by ^{235}U (n, f).

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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