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Eigenvalue implicit sensitivity and uncertainty analysis with the subgroup resonance-calculation method

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ABSTRACT

Response sensitivity coefficients with respect to nuclide cross sections consist of two parts, explicit sensitivity coefficients and implicit sensitivity coefficients. The explicit sensitivity coefficients, which account the direct impact of cross sections on the responses through neutron transport equation, can be calculated efficiently with the classical Perturbation Theory. The implicit sensitivity coefficients, which account the indirect impact of cross sections on the responses through resonance self-shielding, are either omitted in most sensitivity analysis codes, or accounted for based on simple resonance-calculation methods which are not applicable for complex fuel designs. In order to expand the implicit sensitivity analysis method to wider application domain, a method based on the Generalized Perturbation Theory (GPT) is proposed in this paper to calculate the implicit sensitivity coefficients by using the subgroup method in the resonance self-shielding calculation. Based on the in-house-developed 2-D general-geometry method-of-characteristic neutron-transport code AutoMOC and subgroup resonance self-shielding code SUGAR, the proposed method has been implemented in the COLEUS code for the sensitivity and uncertainty analysis. Numerical analysis is then performed to investigate the impact of the implicit sensitivity coefficients of eigenvalue on non-resonance nuclide cross sections in two single-cell cases with different enrichments. The eigenvalue sensitivity coefficients predicted by the COLEUS code are consistent with those calculated by the direct-perturbation method, the reference solution. The results show that the implicit sensitivity has an important impact on both sensitivity and uncertainty in some analyzed cases.

1. Introduction

The results of reactor physics calculation are used for reactor design, predicting the properties and behavior under various operating conditions. The accuracy of the results affects the margin of design, limitation of controlling, and even the economy and safety of the reactor. However, because of the hypotheses, approximations in the solution model and the inaccuracy of the input parameters, the results lie in a certain range, which mean that the results are uncertain. Traditionally, conservative assumptions and large safety margins are used in reactor safety analysis because the size of uncertainty is not quantified. In this situation, the safety may be guaranteed with the sacrifice of economy. For example, the uncertainty of neutron fluence in the pressure vessel will affect the choice of safety margins, and consequently affect the operating conditions, the life of nuclear installations, and the cost (Kodeli, 2001). However, if the size of the uncertainty can be determined, the design and operation will be more valid. As a result, the economy can be realized on the premise of the assurance of safety.

Neutron-transport calculation is the first calculation step that will introduce uncertainties. The uncertainties will be propagated through this step to the subsequent calculation steps. Therefore, neutron-transport calculation uncertainty analysis is one of the basic uncertainty analysis in reactor calculation. It is generally believed that the uncertainties of calculated responses in neutron-transport calculation stem from three sources (Weisbin et al., 1976; Laletin and Kovalishin, 2002): (1) modeling error, which is related to inaccuracy of mathematic-physical model, (2) numerical error, which is related to inaccuracy numerical methods, (3) input-parameter error including error in the nuclear data library. Uncertainty introduced by the nuclear data is considered as one of the most significant uncertainty in neutron-transport calculation (Pusa, 2012). As a consequence, the research of response sensitivity and uncertainty with respect to nuclide cross sections obtains more and more attention.

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Sensitivity calculation is a necessary calculation step in deterministic-method-based uncertainty analysis. Response (eigenvalue, reaction rate, etc.) sensitivity with respect to cross sections can be divided into two parts, namely explicit sensitivity and implicit sensitivity. The former is the direct impact of cross sections perturbation on the responses through neutron transport equation, while the latter is the indirect impact of cross sections perturbation on the responses through resonance self-shielding procedure (Williams et al., 2001). As an indirect impact related with resonance calculation, implicit sensitivity is often neglected in many sensitivity and uncertainty analysis, and many sensitivity and uncertainty analysis codes lack the ability to perform implicit sensitivity calculation. However, from the original research of Greenspan et al. (1978) to the subsequent research of Williams et al. (2001), the results indicated that the implicit sensitivity had a non-negligible importance relative to the explicit sensitivity and the implicit effect had a magnitude that was more that 40% of the explicit effect in some cases.

Therefore, it is necessary and important to take implicit sensitivity into account when sensitivity and uncertainty analysis is performed. Up to now, however, most implicit sensitivity studies are mainly established for simple resonance-calculation methods such as Bondarenko method (Williams et al., 2001), generalized Stamm'ler method (Dion and Marleau, 2013), and so on (Kimura and Kitada, 2012), which are not applicable for complex fuel and core designs. Moreover, the impact of the implicit sensitivity on the uncertainty results was not publically reported before. Recently, the subgroup resonance-calculation method (Hébert, 2007) and the method-of-characteristics (MOC) transport-calculation method (Askew, 1972) have been widely used for complex geometry fuel and core designs and show high adaptability. In order to extend the implicit sensitivity analysis method to a wider application extent and investigate the impact of the implicit sensitivity on the uncertainty results, the eigenvalue implicit sensitivity and uncertainty analysis with the subgroup resonance-calculation method are carried out in this paper. The sensitivity-calculation methods are based on the classical Perturbation Theory (PT) for the explicit sensitivity and the Generalized Perturbation Theory (GPT) for the implicit sensitivity. And then the eigenvalue uncertainty is determined based on the Sandwich rule (Alfassi, 2004) and the covariance library is created based on ENDF/B-VII.1 using NJOY (MacFarlane and Muir, 1994).

This paper is organized as follows: Theoretical models of this work are described in Section 2. Section 3 describes the implementation of the calculation procedure based on the method presented in Section 2. Section 4 gives the calculation results of two representative fuel-pin cells with different enrichments. Finally, Section 5 summarizes and concludes the work.

2. Theoretical models

2.1. Sensitivity coefficient

In this paper, the mathematical model is multigroup neutron transport equation that can be written in operator form as:

$$(\boldsymbol{L}-\lambda\boldsymbol{F})\Phi=0 \tag{1}$$

where $\boldsymbol{L}$ is multigroup form of the Boltzmann loss operator for neutrons; $\boldsymbol{F}$ is multigroup form of the Boltzmann production operator for neutrons; $\lambda = 1/k_{\text{eff}}$ is the minimum eigenvalue for this equation; $\Phi = \Phi(\boldsymbol{r}, \boldsymbol{\Omega}, g)$ is multigroup neutron angular flux; and $\boldsymbol{r}$ is position, $\boldsymbol{\Omega}$ is direction of travel, g is energy group; k_{eff} is effective multiplication factor.

When a parameter perturbation is small enough, the change of k_{eff} can be expressed through the linear relationship:

$$\frac{\Delta k_{\text{eff}}}{k}=S^{tot}_{k_{\text{eff}},\alpha}\frac{\Delta\alpha}{\alpha} \tag{2}$$

where α stands for a multigroup microscopic cross section of a particular nuclide; $S^{tot}_{k_{\text{eff}},\alpha}$ stands for the total sensitivity coefficient that indicates the relative percent change of k_{eff} when α is perturbed with a relative value of 1%.

If the perturbation of α just affects the corresponding multigroup macro cross section, and then affects the eigenvalue through transport calculation, the sensitivity coefficient can be considered as explicit sensitivity coefficient. If the perturbation of α affects the self-shielding cross sections and then affects the multigroup macro cross section, and then affects the eigenvalue through transport calculation, the sensitivity coefficient can be considered as implicit sensitivity coefficient. So the total sensitivity coefficient of eigenvalue can be expressed as:

$$\begin{aligned}S^{\text{tot}}_{k_{\text{eff}},\alpha}&=\frac{\alpha}{k_{\text{eff}}}\frac{\mathrm{d}k_{\text{eff}}}{\mathrm{d}\alpha}=\frac{\alpha}{k_{\text{eff}}}\frac{\partial k_{\text{eff}}}{\partial\alpha}+\frac{\alpha}{k_{\text{eff}}}\sum_{j,x,g}\frac{\partial k_{\text{eff}}}{\partial\sigma^{(j)}_{x,g}}\frac{\partial\sigma^{(j)}_{x,g}}{\partial\alpha}\\&=S^{\text{exp}}_{k_{\text{eff}},\alpha}+S^{\text{imp}}_{k_{\text{eff}},\alpha}\end{aligned} \tag{3}$$

$S^{\text{exp}}_{k_{\text{eff}},\alpha}$ is explicit sensitivity coefficient and $S^{\text{imp}}_{k_{\text{eff}},\alpha}$ is implicit sensitivity coefficient. $\sigma^{(j)}_{x,g}$ is the gth group effective self-shielding cross section of reaction type x for nuclide j.

2.1.1. Explicit sensitivity

If α is explicitly included in the multigroup Boltzmann transport operator, the explicit sensitivity coefficient of k_{eff} with respect to α is defined as:

$$S^{\text{exp}}_{k_{\text{eff}},\alpha}=\frac{\alpha}{k_{\text{eff}}}\frac{\partial k_{\text{eff}}}{\partial\alpha} \tag{4}$$

The explicit sensitivity coefficient can be efficiently calculated utilizing classical Perturbation Theory and it equals to Weisbin et al. (1976):

$$S^{\text{exp}}_{k_{\text{eff}},\alpha}=\frac{\alpha}{k_{\text{eff}}}\frac{\partial k_{\text{eff}}}{\partial\alpha}=-\frac{\alpha}{k_{\text{eff}}}\frac{\left\langle\Phi^{*},\left(\frac{\partial L}{\partial\alpha}-\frac{1}{k_{\text{eff}}}\frac{\partial F}{\partial\alpha}\right)\Phi\right\rangle}{\left\langle\Phi^{*},\frac{1}{k^{2}_{\text{eff}}}F\Phi\right\rangle} \tag{5}$$

where $\langle,\rangle$ indicates integration over space, direction, energy group. Φ^* is adjoint flux, which is the solution of the corresponding adjoint multigroup transport equation:

$$(\boldsymbol{L}^{*}-\lambda\boldsymbol{F}^{*})\Phi^{*}=0 \tag{6}$$

where $\boldsymbol{L}^*$ and $\boldsymbol{F}^*$ is the adjoint operators of $\boldsymbol{L}$ and $\boldsymbol{F}$, respectively.

From Eq. (5), it can be found that the explicit sensitivity coefficients of k_{eff} with respect to all parameters directly appearing in the transport operator can be efficiently obtained with only once forward calculation and once adjoint calculation. In this paper, a subgroup method based code SUGAR (Cao et al., 2011 and He et al., 2014) is applied to the resonance calculation, and a transport code AutoMOC (Chen et al., 2010) based on two-dimensional arbitrary-geometry method-of-characteristics is applied to solve the forward and adjoint neutron transport equation calculation.

2.1.2. Implicit sensitivity

To simplify notation, let α stand for the multigroup cross section of a non-resonance nuclide, and $\sigma^{j}_{r,x,g}$ stand for the self-shielding multigroup cross section of isotope j in region r for reaction type x and energy group g, and $\phi_r(E)$ stand for neutron scalar flux in region r. The symbols j and r are omitted in the following equations for simplicity. Generally, $\sigma_{x,g}$ is given by:

$$\sigma_{x,g}=\frac{\int_{g}\sigma_{x}(E)\phi(E)dE}{\int_{g}\phi(E)dE} \tag{7}$$

In general, the weight function $\phi(E)$ used to average the energy-dependent cross section $\sigma_x(E)$ is not known, and it depends on different geometrical configurations and material compositions. Generally, the weight function $\phi(E)$ is obtained form of an auxiliary equation (e.g. neutron slowing-down equation) if the nuclide cross section has a resonant behavior in an energy group. If the perturbation of α affects the weight function $\phi(E)$ in the solution procedure of the auxiliary equation, then it will affect the resonance self-shielding multigroup cross section $\sigma_{x,g}$ and consequently affect the eigenvalue. To determine this implicit effect of non-resonance nuclide cross sections on the system eigenvalue, which is the main purpose of this paper, the resonance-cross-section sensitivity coefficient of $\sigma_{x,g}$ with respect to a non-resonance cross section α needs to be calculated firstly. Differentiate Eq. (7) with respect to α and rearrange terms to obtain the resonance cross section sensitivity coefficients $S_{\sigma_{x,g},\alpha}$:

$$\begin{aligned} S_{\sigma_{x,g},\alpha} &= \frac{\alpha}{\sigma_{x,g}}\frac{\partial\sigma_{x,g}}{\partial\alpha} \\ &= \alpha\left\{\frac{\int_g \frac{\partial\sigma_x(E)}{\partial\alpha}\phi(E)dE}{\int_g \sigma_x(E)\phi(E)dE} + \frac{\int_g \sigma_x(E)\frac{\partial\phi(E)}{\partial\alpha}dE}{\int_g \sigma_x(E)\phi(E)dE} - \frac{\int_g \frac{\partial\phi(E)}{\partial\alpha}dE}{\int_g \phi(E)dE}\right\} \\ &= \alpha\frac{\int_g \frac{\partial\sigma_x(E)}{\partial\alpha}\phi(E)dE}{\int_g \sigma_x(E)\phi(E)dE} \\ &\quad + \alpha\int_g\left(\frac{\sigma_x(E)}{\int_g \sigma_x(E)\phi(E)dE} - \frac{1}{\int_g \phi(E)dE}\right)\frac{\partial\phi(E)}{\partial\alpha}dE \end{aligned} \tag{8}$$

The first term on the right hand of Eq. (8) is considered as direct effect and the second term is indirect effect. If α is not a fundamental physics parameter, such as resonances width, the first term is always zero. Since this paper focuses on the non-resonant nuclides, the first term vanishes. So $\partial\phi(E)/\partial\alpha$ in the second term is the unknown quantity that needs to be calculated. If $\partial\phi(E)/\partial\alpha$ is solved directly, it will need a different solution for different type of α. It is not easy to modify a transport solver to calculate the derivatives. Besides, when the number of the response $\sigma_{x,g}$ is big, this method is time consuming. An alternative to the directly calculating $\partial\phi(E)/\partial\alpha$ can be formulated by utilizing GPT. The derivation is described as follows.

Suppose $\phi(E)$ is determined by an auxiliary equation:

$$\boldsymbol{L}\phi(E) = Q(E) \tag{9}$$

Differentiate both side of Eq. (9) with respect to α:

$$\boldsymbol{L}\frac{\partial\phi(E)}{\partial\alpha} = \frac{\partial Q(E)}{\partial\alpha} - \frac{\partial\boldsymbol{L}}{\partial\alpha}\phi \tag{10}$$

Introduce a generalized adjoint function $\Gamma^*_{x,g}(E)$ for reaction type x and energy group g, and multiply both sides of Eq. (10) by $\Gamma^*_{x,g}(E)$, and then integrate over energy:

$$\int_g \Gamma^*_{x,g}(E)\left(\boldsymbol{L}\frac{\partial\phi(E)}{\partial\alpha}\right)dE = \int_g \Gamma^*_{x,g}(E)\left(\frac{\partial Q(E)}{\partial\alpha} - \frac{\partial\boldsymbol{L}}{\partial\alpha}\phi(E)\right)dE \tag{11}$$

The property of adjoint can give the following relationship:

$$\int_g \Gamma^*_{x,g}(E)\left(\boldsymbol{L}\frac{\partial\phi(E)}{\partial\alpha}\right)dE = \int_g \boldsymbol{L}^*\Gamma^*_{x,g}(E)\left(\frac{\partial\phi(E)}{\partial\alpha}\right)dE \tag{12}$$

where $\boldsymbol{L}^*$ is the adjoint operator of $\boldsymbol{L}$.

Through the comparison of the right side of Eq. (12) and the second term of the right side of Eq. (8), it can be found that their structure are similar. So it is natural to define the generalized adjoint equation as:

$$\boldsymbol{L}^*\Gamma^*_{x,g}(E) = \frac{\sigma_x(E)}{\int_g \sigma_x(E)\phi(E)dE} - \frac{1}{\int_g \phi(E)dE} \tag{13}$$

After establishing such a generalized adjoint equation for a specific resonance cross section and substituting the generalized adjoint function into the right side of Eq. (11), and utilizing the equivalence relation of Eq. (11) and Eq. (12), it can be obtained ultimately:

$$\begin{aligned} S_{\sigma_{x,g},\alpha} &= \alpha\int_g\left(\frac{\sigma_x(E)}{\int_g \sigma_x(E)\phi(E)dE} - \frac{1}{\int_g \phi(E)dE}\right)\frac{\partial\phi(E)}{\partial\alpha}dE \\ &= \alpha\int_g \Gamma^*_{x,g}(E)\left(\frac{\partial Q(E)}{\partial\alpha} - \frac{\partial\boldsymbol{L}}{\partial\alpha}\phi(E)\right)dE \end{aligned} \tag{14}$$

Now the GPT equation to calculate $S_{\sigma_{x,g},\alpha}$ with regular resonance-calculation method has been derived. Once $\Gamma^*_{x,g}(E)$ is derived via solving Eq. (13), it is straightforward to calculated $S_{\sigma_{x,g},\alpha}$ by using Eq. (14). The aforementioned general derivation can be extended to the subgroup resonance-calculation method as illustrated below.

Resonance cross section is divided into several bands (subgroups) from its minimum value to its maximum value in the subgroup resonance-calculation method. The definition of subgroup cross section is expressed as:

$$\sigma_{x,i,g} = \frac{\int_{\Delta E_i}\sigma_{x,g}(E)\phi(E)dE}{\int_{\Delta E_i}\phi(E)dE} \tag{15}$$

where subscript g and i stands for energy group and subgroup respectively, and the range of ΔE_i is $\Delta E_i \in \{E|\sigma_{x,i} \leqslant \sigma_{x,g}(E) \leqslant \sigma_{x,i+1}\}$.

The definition of the subgroup probability for subgroup i is:

$$p_i = \frac{\Delta E_i}{\Delta E_g} \tag{16}$$

where ΔE_i the energy width of subgroup i and ΔE_g is the energy width of group g.

Because the corresponding each range of every band is contained in the energy range of energy group g, the average micro cross section of energy group g can be expressed as follows:

$$\begin{aligned} \sigma_{x,g} &= \frac{\int_{\Delta E_g}\sigma_x(E)\phi(E)dE}{\int_{\Delta E_g}\phi(E)dE} = \frac{\sum_{i=1}^N\int_{\Delta E_i}\sigma_x(E)\phi(E)dE}{\sum_{i=1}^N\int_{\Delta E_i}\phi(E)dE} \\ &= \frac{\sum_{i=1}^N\sigma_{x,i,g}\int_{\boldsymbol{\Omega}}\phi_{g,i}d\boldsymbol{\Omega}}{\sum_{i=1}^N\int_{\boldsymbol{\Omega}}\phi_{g,i}d\boldsymbol{\Omega}} \end{aligned} \tag{17}$$

where $\phi_{g,i}$ is called subgroup angular flux and is used as weight function. $\phi_{g,i}$ is the solution of subgroup transport equation in this

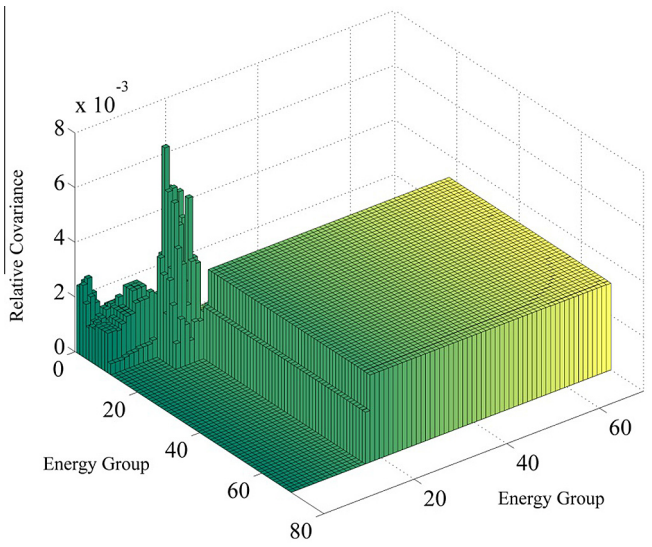

Fig. 1. The relative covariance matrix of Zr-90 total micro cross section.

paper. The subgroup transport equation can be expressed as follows:

$$\Omega \cdot \nabla \phi_{g,i}(r,\Omega) + \Sigma_{t,g,i}(r)\phi_{g,i}(r,\Omega) = Q_{g,i}(r,\Omega) \tag{18}$$

where $\Sigma_{t,g,i}(r)$ is subgroup total macro cross section. $Q_{g,i}(r,\Omega)$ is source term.

Eq. (18) is spatially-dependent because $\phi_{g,i}$ is the solution of a transport equation, which is solved by the method-of-characteristics.

After making a comparison between Eqs. (7) and (17), it can be found several differences. For general resonance-calculation method, the multigroup resonance cross section is obtained through integrating over energy, while for the subgroup resonance-calculation method the multigroup resonance cross section is obtained through adding over bands. Moreover, the weight function of Eq. (7) is the solution of a spatially-independent slowing-down equation while the weight function of Eq. (17) is the solution of a spatially-dependent subgroup transport equation. Hence it is easy to generalize the result of Eq. (14) to subgroup resonance-calculation method:

$$S_{\sigma_{x,g},\alpha} = \alpha \sum_{i=1}^{N} \int_V \int_{\Omega} \Gamma^*_{x,g,i}\left(\frac{\partial Q_{g,i}}{\partial \alpha} - \frac{\partial \boldsymbol{L}}{\partial \alpha}\phi_{g,i}\right) d\boldsymbol{\Omega} dV \tag{19}$$

Eq. (13) can be transferred into the following form, from which $\Gamma^*_{x,g,i}$ is calculated. In the following discussions, this equation is named as subgroup generalized adjoint transport equation:

$$\boldsymbol{L}^*_i \Gamma^*_{x,g,i} = \frac{\sigma_{x,g,i}}{\sum_{i=1}^{N} \int_V \int_{\Omega} \sigma_{x,g,i}\phi_{g,i} d\boldsymbol{\Omega} dV} - \frac{1}{\sum_{i=1}^{N} \int_V \int_{\Omega} \phi_{g,i} d\boldsymbol{\Omega} dV} \tag{20}$$

where $\boldsymbol{L}^*_i$ is the subgroup adjoint transport operator for each band.

The source term $Q_{g,i}$, in SUGAR is composed of scattering sources from fast energy group and scattering sources from upstream resonance energy group. The fission sources and scattering sources among subgroups are neglected in consideration of their slight importance. The source term can be divided into two parts:

$$Q_{fast,g,i} = p_i \sum_{g' \in G_{fast}} \int_{\Omega} \Sigma_{s,g' \to g} \phi_{g'}(r,\Omega) d\Omega \tag{21}$$

$$Q_{res,g,i} = p_i \sum_{g' < g} \Sigma_{s,g' \to g,i} \sum_{i=1}^{N} \int_{\Omega} \phi_{g',i}(r,\Omega) d\Omega \tag{22}$$

The derivative of source term with respect to α can also be solved with GPT because the source term is the linear function of flux. Since the derivation is similar to the derivation of the sensitivity coefficient of resonance cross section with respect to α, the formula is presented as follows without derivation process for simplicity:

$$\frac{\partial Q_{g,i}}{\partial \alpha} = p_i \sum_{g'} \left[\sum_{i=1}^{N} \int_V \int_{\Omega} \frac{\partial \Sigma_{s,g' \to g,i}}{\partial \alpha} \phi_{g',i} d\boldsymbol{\Omega} dV + \sum_{i=1}^{N} \int_V \int_{\Omega} \Psi^*_{g',i}\left(\frac{\partial Q_{g',i}}{\partial \alpha} - \frac{\partial \boldsymbol{L}}{\partial \alpha}\phi_{g',i}\right) d\boldsymbol{\Omega} dV \right] / V \tag{23}$$

where Ψ^* is the corresponding generalized adjoint flux and V is the region volume.

After obtaining the resonance-cross-section sensitivity coefficient $S_{\sigma_{x,g},\alpha}$ and taking into account the isotope j and region r, the implicit sensitivity coefficients of non-resonance nuclide cross sections can be expressed as:

$$S^{\mathrm{imp}}_{k_{\mathrm{eff}},\alpha} = \sum_{j,r,x,g} S_{k_{\mathrm{eff}},\sigma^{(j)}_{r,x,g}} S_{\sigma^{(j)}_{r,x,g},\alpha} \tag{24}$$

where $S_{k_{\mathrm{eff}},\sigma^{(j)}_{r,x,g}}$ is the explicit sensitivity coefficient of eigenvalue with respect to the resonance cross section of a resonance nuclide j in region r for reaction type x and energy group g, which can be calculated by using Eq. (5).

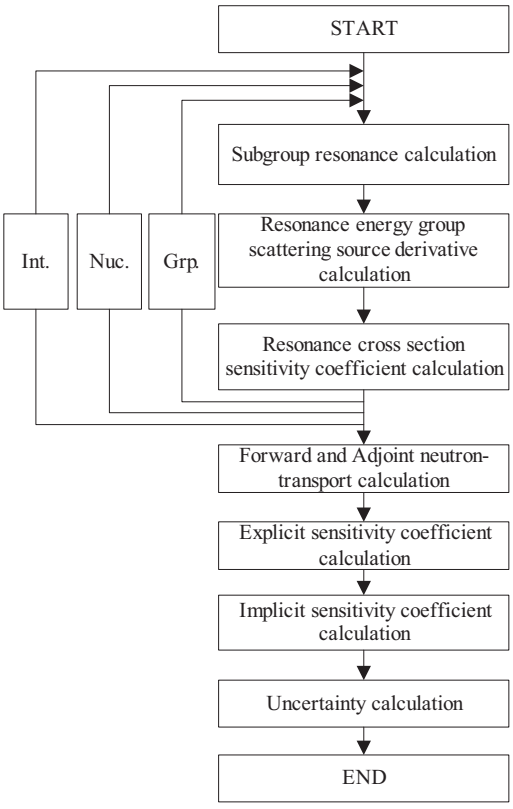

Fig. 2. Calculation flow chart of sensitivity and uncertainty analysis.

2.2. Uncertainty

In deterministic methods for sensitivity and uncertainty analysis, uncertainty can be obtained through the Sandwich rule after sensitivity coefficients are obtained. The uncertainty of k_{eff} can be expressed as:

$$\frac{V(k_{\mathrm{eff}})}{k^2_{\mathrm{eff}}} = S^{\mathrm{tot}}_{k,\alpha_i} C_{\alpha_i \alpha_j} (S^{\mathrm{tot}}_{k,\alpha_j})^T \tag{25}$$

where $V(k_{\mathrm{eff}})$ is the variance of k_{eff}. $S^{\mathrm{tot}}_{k,\alpha_i}$ is the total sensitivity coefficients of k_{eff} with respect to an input parameter α_i. $C_{\alpha_i \alpha_j}$ is the covariance matrices between input parameter α_i and α_j. The covariance matrices describe the uncertainty related to the cross sections.

3. Implementation

In order to utilize Eq. (25) to determine the uncertainty of k_{eff}, the energy-group structure of covariance matrices should be same as the sensitivity profiles. The EPRI-CPM 69-group structure (MacFarlane and Muir, 1994) is used in this paper, so a corresponding covariance library is created using NJOY99 based on ENDF/B-VII.1. Fig. 1 shows the 69-group total micro cross section relative covariance matrix of Zr-90. With the covariance data, the uncertainty of k_{eff} can be determined by Eq. (25).

AutoMOC is applied as a subgroup transport-equation solver in the resonance calculation of SUGAR, and the problem geometry will be subdivided into many meshes with the flat-source approximation. Hence for each mesh that contains resonance nuclides or sources, a generalized subgroup adjoint equation is needed for

each resonance nuclide and each source respectively. Besides, in consideration of resonance interference effects, SUGAR will perform resonance interference iterations. These situations will lead to complexities and large computation demands. Therefore, some simplifications and assumptions are made as follows in this paper:

(1) Because the perturbation of fast-energy-group cross section just affects the fast scattering sources and this effect is indirect, neglecting the effects of fast-energy-group cross section may have negligible impact on the results and is helpful to reduce the computing time. The validity of this approximation can be confirmed through numerical results.
(2) In order to take the resonance interference effect into account, resonance interference iteration is performed twice or more. Resonance cross section sensitivity coefficients will be calculated in each iteration if the influences of iteration are taken into account strictly. However, the nuclide cross section influences transferred from the previous iteration to the next iteration are indirect, which are considered negligibly small. So the resonance cross section sensitivity coefficients are calculated in the final iteration. The validity of this simplification can be confirmed through numerical results.
(3) The meshes of the geometry are user-defined in AutoMOC. If two meshes are equivalent to each other (it implies that the meshes are exactly equivalent, including material, geometrical shape, location and boundary condition, etc.), it can be regarded as that the resonance cross sections or the source terms in the two meshes have equal sensitivity coefficients with respect to a nuclide cross section over the whole problem region. Hence the sensitivity coefficients only need to be calculated once for equivalent meshes in order to reduce computation time.

Based on the above derivations and analyses, the calculation of eigenvalue implicit and explicit sensitivity coefficients and uncertainties can be summarized in the following steps, as illustrated in Fig. 2.

As stated above, the solution is performed in the last resonance interference iteration of the subgroup resonance calculation, and the equivalent meshes just need to be solved once.

Firstly, the derivative of the resonance energy group scattering source needs to be solved. The basic numerical method is the same as the method utilized to calculated resonance cross section sensitivity coefficients. A corresponding generalized adjoint equation needs to be established and solved for a specific source. And the derivative can be calculated with Eq. (23).

Secondly, a subgroup generalized adjoint equation should be established according to Eq. (20) for a certain resonance energy group g and a certain resonance reaction type x of a certain resonance nuclide j in region r.

Thirdly, the subgroup generalized adjoint equation is solved by a transport solver which can perform adjoint calculation. The transport solver AutoMOC in this paper is based on method-of-characteristics. When MOC method is applied, it is worth noting that the subgroup generalized adjoint equation is a fixed sources problem, and the source is just located in a small mesh, so it is necessary to choose a relatively high order quadrature set to prevent the ray effect. Besides, because of the particularity of the generalized adjoint source on the right side of Eq. (20), the source term may be negative in some situations. Therefore, the transport solver should exclude the assumption of the nonnegative flux or the sources.

The above three steps are repeated for all scattering sources and resonance cross sections of all resonance nuclides.

Fourthly, after quantifying the resonance self-shielding cross section sensitivity coefficients, a forward and an adjoint neutron-transport calculation are performed. And then explicit sensitivity coefficients are calculated based on classical Perturbation Theory described by Eq. (5).

Fifthly, implicit sensitivity coefficients of non-resonant nuclides can be quantified with Eq. (24). And finally, uncertainty can be computed using the Sandwich rule.

Table 1
Comparison of implicit sensitivity coefficients of k_{eff} with respect to group-wide total micro cross sections of non-resonance nuclides for case NECP-RB3.1.

GRP	H-1		O-16 in the fuel		O-16 in the moderator		Zr-nat	
	PT	DP	PT	DP	PT	DP	PT	DP
1	–	6.24E−10	–	1.16E−10	–	1.65E−10	–	1.53E−10
2	–	1.10E−09	–	5.80E−11	–	1.42E−10	–	3.47E−10
3	–	3.48E−09	–	6.91E−11	–	2.62E−11	–	9.45E−10
4	–	5.92E−09	–	4.47E−10	–	3.52E−10	–	6.90E−10
5	–	4.89E−09	–	7.81E−10	–	6.06E−10	–	5.42E−10
6	–	4.84E−09	–	5.74E−10	–	3.17E−10	–	2.11E−10
7	–	2.94E−09	–	1.08E−09	–	2.20E−10	–	2.01E−10
8	–	5.38E−09	–	1.13E−09	–	2.72E−10	–	4.26E−10
9	–	5.01E−09	–	1.58E−09	–	2.37E−10	–	5.42E−10
10	–	4.58E−09	–	1.09E−09	–	−4.86E−10	–	7.46E−10
11	–	2.80E−08	–	4.48E−09	–	1.01E−09	–	2.67E−09
12	–	5.99E−09	–	2.68E−09	–	−9.23E−10	–	7.57E−10
13	–	5.28E−08	–	−2.91E−08	–	−1.72E−08	–	−1.09E−09
14	–	9.62E−07	–	−9.08E−07	–	1.54E−08	–	3.36E−08
15	−7.26E−05	−7.50E−05	−2.83E−05	−2.82E−05	−7.23E−06	−7.46E−06	−7.40E−06	−7.35E−06
16	−9.46E−05	−9.75E−05	−3.92E−05	−3.91E−05	−9.33E−06	−9.62E−06	−8.63E−06	−8.58E−06
17	−1.90E−04	−1.95E−04	−7.87E−05	−7.84E−05	−1.84E−05	−1.89E−05	−1.84E−05	−1.83E−05
18	−2.65E−04	−2.72E−04	−1.13E−04	−1.13E−04	−2.56E−05	−2.62E−05	−1.83E−05	−1.82E−05
19	−3.90E−04	−3.99E−04	−1.67E−04	−1.67E−04	−3.73E−05	−3.82E−05	−2.23E−05	−2.22E−05
20	−1.04E−03	−1.07E−03	−4.63E−04	−4.63E−04	−9.99E−05	−1.02E−04	−6.65E−05	−6.61E−05
21	−1.86E−03	−1.89E−03	−8.56E−04	−8.55E−04	−1.77E−04	−1.80E−04	−1.34E−04	−1.33E−04
22	−1.85E−03	−1.88E−03	−8.47E−04	−8.47E−04	−1.75E−04	−1.77E−04	−1.15E−04	−1.15E−04
23	−8.03E−04	−8.13E−04	−4.58E−04	−4.59E−04	−7.80E−05	−7.91E−05	−5.25E−05	−5.22E−05
24	−2.02E−03	−2.06E−03	−1.03E−03	−1.03E−03	−1.91E−04	−1.93E−04	−1.30E−04	−1.29E−04
25	−2.90E−03	−2.94E−03	−1.33E−03	−1.34E−03	−2.69E−04	−2.74E−04	−1.83E−04	−1.82E−04
26	−8.05E−05	−8.59E−05	−1.90E−04	−1.90E−04	−1.41E−05	−1.47E−05	−1.08E−05	−1.08E−05
27	−5.51E−03	−5.60E−03	−2.61E−03	−2.63E−03	−5.08E−04	−5.17E−04	−3.51E−04	−3.50E−04

Table 2
Integral sensitivity coefficients of k_{eff} with respect to total micro cross sections for case NECP-RB3.1.

Nuclides	Method	Explicit	Implicit	Total	Explicit + implicit
H-1	DP	1.1115E−01	−1.7378E−02	9.4356E−02	9.3767E−02
	PT	1.1088E−01	−1.7078E−02	–	9.3805E−02
O-16 in the fuel	DP	−1.0084E−03	−8.3058E−03	−9.3235E−03	−9.3142E−03
	PT	−1.0084E−03	−8.2130E−03	–	−9.2213E−03
O-16 in the moderator	DP	−6.1668E−04	−1.6376E−03	−2.1418E−03	−2.2542E−03
	PT	−6.5871E−04	−1.6094E−03	–	−2.2681E−03
Zr-nat	DP	−8.3021E−03	−1.1121E−03	−9.5452E−03	−9.4142E−03
	PT	−8.3676E−03	−1.1182E−03	–	−9.4858E−03

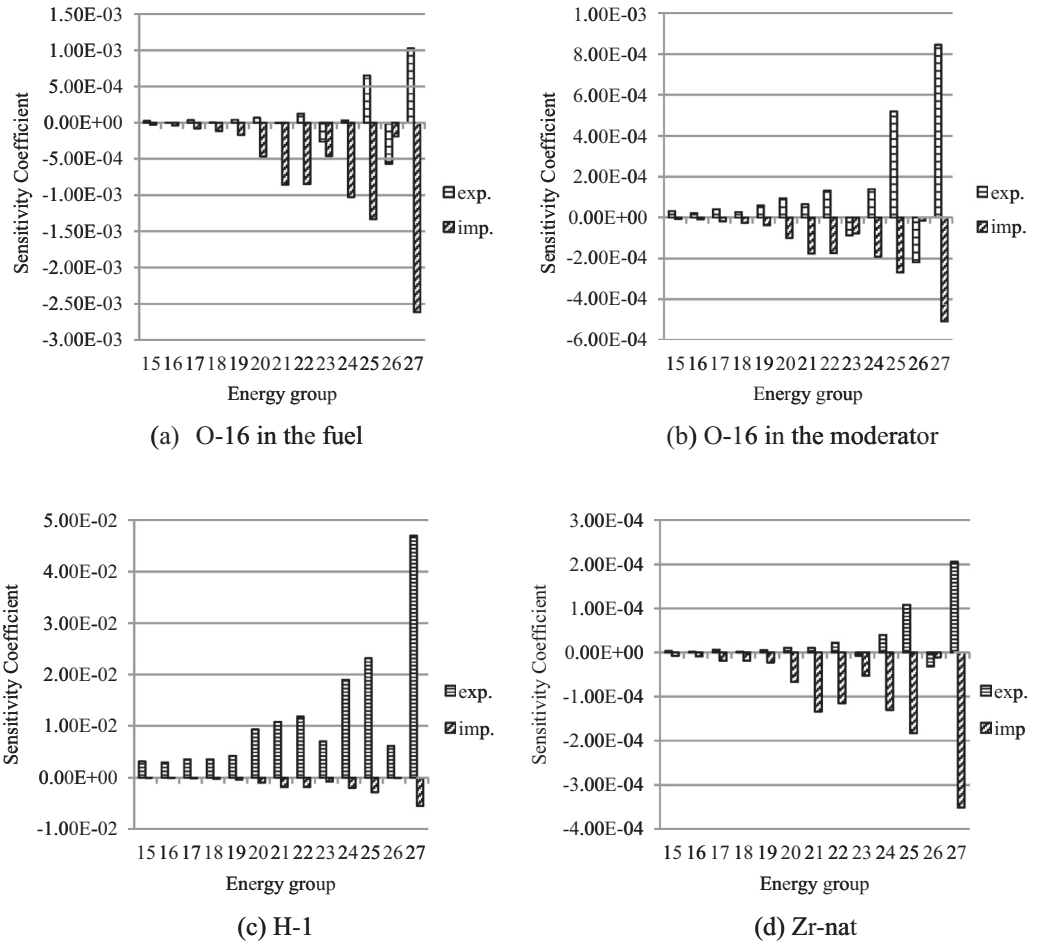

Fig. 3. The comparison between explicit sensitivity and implicit sensitivity for case NECP-RB3.1.

4. Numerical results

The sensitivity coefficients can be calculated with Direct Perturbation (DP) method, which is precise when the perturbation is small and the linear relation is strong. So the results given by the DP method are usually treated as reference results. This method can be described as Eq. (26):

$$S_{k_{\mathrm{eff}},\alpha} = \frac{\alpha}{k_{\mathrm{eff}}}\frac{\mathrm{d}k_{\mathrm{eff}}}{\mathrm{d}\alpha} = \frac{\alpha_0}{k^0_{\mathrm{eff}}}\frac{k^+_{\mathrm{eff}} - k^-_{\mathrm{eff}}}{\alpha^+ - \alpha^-} \tag{26}$$

where α_0, α^+ and α^- are the unperturbed, positive perturbed and negative perturbed value of a cross section respectively, and k^0_{eff},k^+_{eff} and k^-_{eff} is the corresponding k_{eff}. To obtain different types of reference sensitivity coefficients for comparison, the DP method was implemented as follows (Dion and Marleau, 2013):

(1) To obtain the total sensitivity coefficients, a full calculation (e.g., both resonance calculation and transport calculation) with reference cross sections and two full calculations with positive and negative perturbed cross sections (applied before resonance calculations) are performed respectively.
(2) To obtain the explicit sensitivity coefficients, a full calculation with reference cross sections and two full calculations with positive and negative perturbed cross sections (applied after resonance calculations) after resonance calculation are performed respectively.
(3) To obtain the implicit sensitivity coefficients, a full calculation with reference cross sections is performed first, and two resonance calculations with positive and negative per-

Table 3
Comparison of implicit sensitivity coefficients of k_{eff} with respect to group-wide total micro cross sections of non-resonance nuclides for case NECP-RB3.2.

GRP	H-1		O-16 in the fuel		O-16 in the moderator		Zr-nat	
	PT	DP	PT	DP	PT	DP	PT	DP
1	–	1.21E−11	–	4.90E−12	–	−3.91E−13	–	1.21E−11
2	–	7.21E−11	–	3.45E−12	–	5.96E−12	–	5.08E−11
3	–	3.84E−10	–	−1.39E−11	–	−7.74E−12	–	1.13E−10
4	–	9.43E−10	–	2.45E−12	–	1.33E−11	–	9.42E−11
5	–	1.51E−09	–	1.54E−10	–	1.27E−10	–	8.26E−11
6	–	1.75E−09	–	1.76E−10	–	1.00E−10	–	3.14E−11
7	–	5.09E−10	–	2.38E−10	–	4.92E−11	–	3.91E−11
8	–	7.58E−10	–	2.74E−10	–	2.39E−11	–	7.08E−11
9	–	8.02E−10	–	3.71E−10	–	2.04E−11	–	7.24E−11
10	–	5.86E−10	–	5.32E−10	–	−3.90E−13	–	1.03E−10
11	–	3.15E−10	–	7.70E−10	–	−1.62E−11	–	3.33E−10
12	–	2.05E−10	–	1.07E−09	–	−3.40E−11	–	1.19E−10
13	–	−7.01E−10	–	1.06E−09	–	−3.23E−10	–	1.39E−10
14	–	7.92E−09	–	−8.72E−09	–	−7.01E−11	–	7.26E−10
15	−9.43E−07	−1.07E−06	−3.84E−07	−3.82E−07	−1.01E−07	−1.05E−07	−1.05E−07	−1.04E−07
16	−1.65E−06	−1.81E−06	−5.94E−07	−5.88E−07	−1.71E−07	−1.77E−07	−1.57E−07	−1.55E−07
17	2.06E−06	1.99E−06	4.18E−07	4.21E−07	1.69E−07	1.75E−07	1.78E−07	1.80E−07
18	−1.30E−05	−1.35E−05	−5.17E−06	−5.15E−06	−1.27E−06	−1.31E−06	−9.08E−07	−9.06E−07
19	−2.74E−05	−2.84E−05	−1.05E−05	−1.05E−05	−2.66E−06	−2.74E−06	−1.58E−06	−1.58E−06
20	−5.46E−05	−5.68E−05	−2.63E−05	−2.65E−05	−5.54E−06	−5.74E−06	−3.67E−06	−3.69E−06
21	−2.99E−04	−3.08E−04	−1.35E−04	−1.37E−04	−2.85E−05	−2.93E−05	−2.18E−05	−2.19E−05
22	−3.60E−04	−3.70E−04	−1.62E−04	−1.64E−04	−3.40E−05	−3.50E−05	−2.27E−05	−2.29E−05
23	−9.34E−05	−1.00E−04	−6.61E−05	−6.91E−05	−9.54E−06	−1.02E−05	−6.55E−06	−6.88E−06
24	−3.74E−04	−3.92E−04	−2.15E−04	−2.23E−04	−3.58E−05	−3.75E−05	−2.52E−05	−2.58E−05
25	−4.49E−04	−4.73E−04	−2.65E−04	−2.74E−04	−4.23E−05	−4.45E−05	−3.05E−05	−3.13E−05
26	−4.64E−04	−4.69E−04	−2.59E−04	−2.60E−04	−4.36E−05	−4.41E−05	−3.12E−05	−3.09E−05
27	−9.35E−04	−9.82E−04	−4.77E−04	−4.96E−04	−8.66E−05	−9.09E−05	−6.12E−05	−6.29E−05

Table 4
Integral sensitivity coefficients of k_{eff} with respect to total micro cross sections for case NECP-RB3.2.

Nuclides	Method	Explicit	Implicit	Total	Explicit + implicit
H-1	DP	1.1817E−02	−3.1957E−03	8.6263E−03	8.6210E−03
	PT	1.2388E−02	−3.1627E−03	–	9.2256E−03
O-16 in the fuel	DP	−2.9605E−03	−1.6651E−03	−4.6255E−03	−4.6255E−03
	PT	−2.8649E−03	−1.6222E−03	–	−4.4871E−03
O-16 in the moderator	DP	−2.9299E−03	−3.0160E−04	−3.2315E−03	−3.2315E−03
	PT	−3.0236E−03	−2.8991E−04	–	−3.3136E−03
Zr-nat	DP	−4.2860E−03	−2.0894E−04	−4.4949E−03	−4.4949E−03
	PT	−4.2919E−03	−2.0720E−04	–	−4.4991E−03

turbed cross sections are performed next, and then the transport calculations are performed by replacing the perturbed cross sections with the reference values after resonance calculation.

Two resonance benchmark NECP-RB3.1 and NECP-RB3.2 (Wu et al., 2012) were analyzed in this paper. The two benchmark cases are pin cell problems with different U-235 enrichment: 5% for NECP-RB3.1 and 90% for NECP-RB3.2. The clad and moderator for both cases are Zr-nat and light water respectively. It is noteworthy that Zr-nat is not treated as a resonance nuclide in this paper. Because there is no Zr-nat in ENDF/B-VII.1, the covariance of Zr-90 is used instead. Such a treatment is not expected to affect the discussion and conclusion on the results.

Sensitivity coefficients and uncertainty with respect to the total micro cross sections are calculated and analyzed to validate the proposed method in this paper, and to investigate the total effect of the non-resonance nuclides. It is necessary to note that to ensure the perturbation reasonable and physical, the perturbation of the total micro cross sections is implemented by perturbing absorption cross sections and scattering cross section simultaneously with the same relative perturbation amount as that of the total micro cross sections in this paper.

4.1. Sensitivity results

4.1.1. NECP-RB3.1

The implicit sensitivity coefficients of k_{eff} with respect to total micro cross sections calculated with both the PT-based method and the DP method are presented in Table 1. DP method was performed based on ±5% changes in the multigroup total micro cross sections of non-resonance nuclides. It can be found the results of the PT-based method agree well with the DP method in resonance energy groups. The implicit sensitivity coefficients at fast energy group are calculated with the DP method and the results show that the absolute value is very small, which proves that the neglecting of the fast energy group implicit sensitivity coefficients is a reasonable approximation. Because the DP method takes into account the iteration-influence effect, the good agreement between the PT-based method and the DP method in resonance energy groups proves that the neglecting of the iteration influences is a reasonable approximation as well.

Table 2 gives the integral total, explicit and implicit sensitivity coefficients of k_{eff} with respect to total micro cross sections of non-resonance nuclides. The results of the PT based method are also consistent with the DP method.

In order to analyze the relative importance of implicit sensitivity, which is one of the main purpose of this paper, Fig. 3 gives a

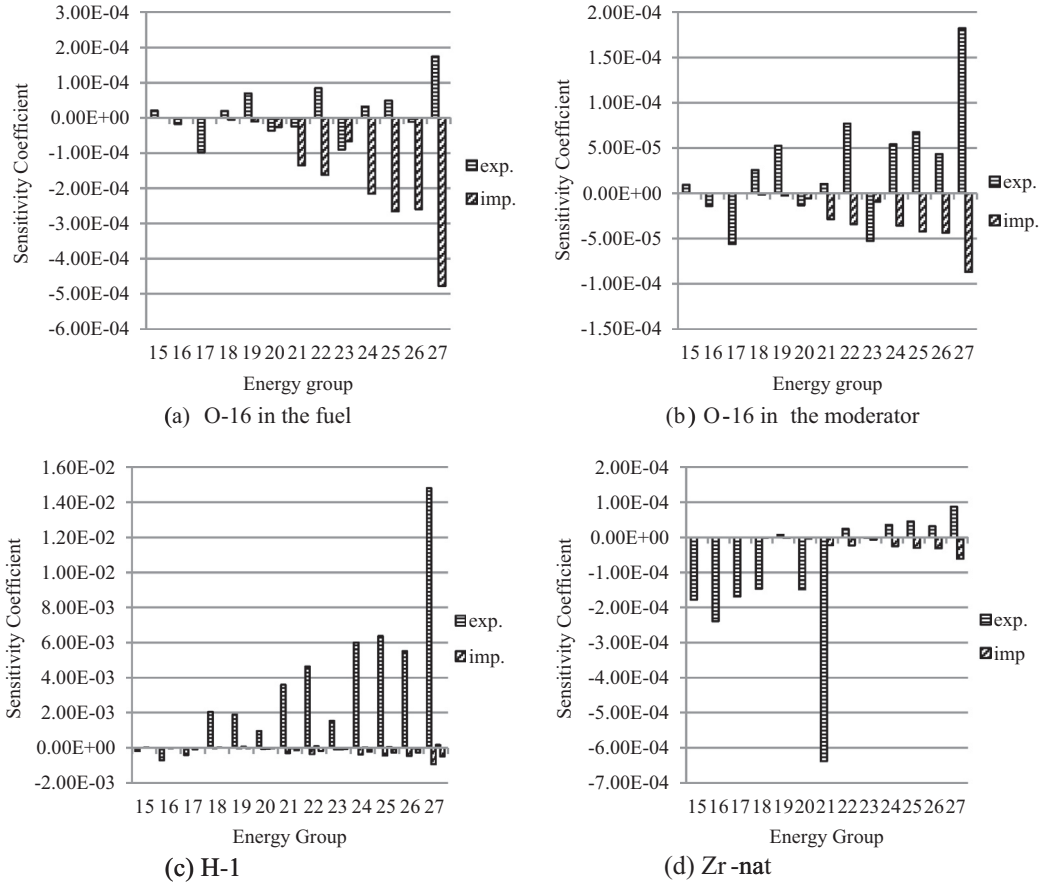

Fig. 4. The comparison between explicit sensitivity and implicit sensitivity for case NECP-RB3.2.

series of histograms comparing the implicit sensitivity coefficients with the explicit sensitivity coefficients with respect to total micro cross sections of non-resonance nuclides.

It can be found from Fig. 3 that the explicit sensitivity coefficients of most energy group are positive, while the implicit sensitivity coefficients are negative. If the absolute value of the explicit sensitivity coefficients is larger than the implicit sensitivity coefficients (e.g. H-1 in this problem), the sensitivity coefficients will be overestimated if the implicit sensitivity coefficients are neglected. On the contrary (e.g. O-16 in the fuel, Zr-nat in this problem), the sensitivity coefficient signs will be contrary to the actual value if the implicit sensitivity coefficients are neglected. It is noteworthy that although the relative importance of H-1 implicit sensitivity is smaller than other nuclides, the absolute values of H-1 implicit sensitivity coefficients are the biggest one, because H-1 is the dominating moderated nuclide in such case.

4.1.2. NECP-RB3.2

The implicit and integral sensitivity coefficients of k_{eff} with respect to total micro cross sections calculated with the two methods are presented in Tables 3 and 4, respectively. The DP method was performed based on ±5% changes in the multigroup total micro cross sections of non-resonance nuclides. It can also be concluded that the results of the PT-based method agree well with the DP method. Neglecting of the fast energy group implicit sensitivity coefficients and the iteration influences are reasonable as well.

Fig. 4 gives a series of histograms to compare the implicit sensitivity with the explicit sensitivity of total micro cross sections of non-resonant nuclides for case NECP-RB3.2. The conclusions are almost the same as the conclusions of case NECP-RB3.1 except Zr-nat. In fact, it can be found that the implicit sensitivity coefficients of all the nuclides decrease when compared with that of NECP-RB3.1. Because in the low enrichment case NECP-RB3.1, the

Table 5
The uncertainty contributions of total micro cross sections.

Case	Nuclide	Uncertainty contribution		Ratio
		With implicit sensitivity	Without implicit sensitivity	
NECP-RB3.1	H-1	2.0635E−02	2.1986E−02	0.9386
	O-16 in the fuel	1.4757E−02	2.7083E−03	5.4488
	O-16 in the moderator	2.2780E−03	3.7203E−03	0.6123
	Zr-nat	3.7064E−02	3.1179E−02	1.1887
NECP-RB3.2	H-1	2.2835E−02	2.2908E−02	0.9968
	O-16 in the fuel	5.4193E−03	2.8623E−03	1.8933
	O-16 in the moderator	3.3408E−03	2.9579E−03	1.1294
	Zr-nat	1.4827E−02	1.4768E−02	1.0040

perturbation of the total micro cross sections affects the absorb cross sections of U-238 mainly. While in the high enrichment case NECP-RB3.2, the perturbation of the total micro cross section mainly affects absorb and fission cross sections of U-235 in the same direction, so the effects on eigenvalue cancel each other out. Therefore, the implicit sensitivity in high enrichment case is smaller than that in the low enrichment case. However, the implicit sensitivity of O-16 is also very import when compared with its explicit sensitivity.

4.2. Uncertainty results

The influences on uncertainty when the implicit sensitivity is neglected are presented in Table 5. It can be found that the uncertainty contributions of H-1 in both cases are not severely influenced by implicit sensitivity because the implicit sensitivity coefficients are relatively small relative to the explicit sensitivity coefficients. When implicit sensitivity is neglected, the uncertainty contribution of O-16 in the fuel is seriously underestimated in both cases, while the uncertainty contribution of O-16 in the moderator is slightly overvalued in NECP-RB3.1 and slightly underestimated in NECP-RB3.2. It is interesting to find that although the implicit sensitivity coefficients of Zr-nat are very important among the resonance energy groups in NECP-RB3.1, the uncertainty contribution is not seriously changed by the neglecting of implicit sensitivity. The main reasons include the multiplicative relationships in the "Sandwich rule" and the covariance magnitude in resonance energy groups.

5. Summary and conclusions

Eigenvalue sensitivity is composed of explicit sensitivity and implicit sensitivity. The former can be calculated efficiently based on classical Perturbation Theory. The latter is an indirect and is not calculated and analyzed widely in sensitivity and uncertainty analysis.

Implicit sensitivity is investigated based on the perturbation-theory-based method presented in this paper with subgroup resonance-calculation method being used in resonance calculation. The numerical results of this method are consistent with the results given by the DP method, which is treated as a reference method. The results of the typical pin cell examples indicate that: (1) the fast energy group cross sections implicit sensitivity coefficients are small, and it is reasonable to neglect these calculations; (2) the sensitivity coefficients may be overestimated or obtained with inverse sign if implicit sensitivity is neglected in some cases; (3) when the sensitivity coefficients are used in uncertainty calculation, because of the complex multiplicative relationships between each sensitivity coefficient in Sandwich rule, it will give unpredictable uncertainty results when implicit sensitivity is neglected. Therefore, it is necessary to perform implicit sensitivity analysis in sensitivity and uncertainty analysis to obtain more rigorous results.

However, because of the properties of subgroup resonance-calculation method, a generalized subgroup adjoint transport equation is necessary for every resonance nuclide mesh and every scatter source mesh. This situation will lead to large computational quantity although some simplifications and assumptions are made in this paper. For the situation where there are many responses, some advanced methods (Abdel-Khalik et al., 2008; Kennedy et al., 2012) are recommended.

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