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Numerical sensitivity analysis of rector neutron spectrum

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Highlights

- **Cross section values are the main source of error.**
- **Scattering cross section is the biggest contributor to spectrum uncertainty.**
- **Neutron energy groups are sensitive to each other.**
- **The use of diagonal covariance Matrix is not justified.**

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ABSTRACT

The uncertainty data of a neutron spectrum can be completely described by the corresponding covariance matrix. The main diagonal of such covariance matrix consist of the variances of the energy group flux values, and the off-diagonal elements give the cross-covariance between these values. The major step in evaluating the covariance matrix of a calculated neutron spectrum is the derivation of the sensitivity matrix. The covariance matrix can be evaluated by performing a simple multiplication of the sensitivity matrix and a covariance matrix consisting of basic cross-section covariance data taken from literature. Numerical sensitivity analysis usually made whenever there is a lack of analytical tools. In the frame of this work, a numerical procedure based on the sensitivity analysis theory have been developed to estimate this information. In this procedure, results of several neutron transport calculations are used to derive numerically the sensitivity matrix of the calculated neutron spectrum.

1. Introduction

The covariance matrix cov (∅) of a calculated neutron spectrum can be written according to the sensitivity analysis theory (Cacuci, *et al*., 1980) as follows:

$$cov\ (\emptyset) = S\ cov\ (P) S' \tag{1}$$

where

P: Vector of parameters used in neutron spectrum calculation.
cov(P): Covariance matrix of parameters included in the vector P.
S: Sensitivity matrix of the neutron spectrum with respect to parameters included in P.
S': The transpose of S.

Each column of the sensitivity matrix S consists of partial derivatives of group flux values with respect to one parameter used in their calculations. The element Sij of the ith row and jth column in this matrix is given as follows:

$$Sij = \frac{d\ \emptyset j}{d\ Pi} \tag{2}$$

where

∅j: Total neutron flux of the jth energy group.
Pi: The ith quantity used in calculating ∅ j

The covariance matrix cov(P) can be constructed from the individual covariance matrices of all components of the vector P and from their cross-covariance matrices. The most important parameters used in the neutron spectrum calculations are the cross section values describing various reactions. Due to the increase in the experimental database, evaluated nuclear data files are continuously updated (Zwermann *et al*., 2014). Other parameters (such as fission spectrum, atomic density... etc.) have small uncertainty values, therefore, their effect on the spectrum uncertainty is being ignored (see Table (1) below).

The American library ENDF/B VII.1 (Herman, 2011) has been used in this work. Computed uncertainties based on this library may show differences with others (Augusto, 2012).

Table (I)

Typical uncertainty values of quantities used in neutron spectrum calculations

Types of data used	Typical uncertainty
Cross section	up to 30 %
Fission spectrum	less than 3 %
Atomic density	less than 1 %
Geometrical	less than 1 %

Accordingly, we can represent the vector *p* as follows:

$$P = (\textstyle\sum f_1, \sum a_1, \sum s_1, \sum a_2, \sum s_2) \tag{3}$$

where

∑: macroscopic group cross section values,
f: fission, *a*: absorption, *s*: scattering

The subscript numbers 1 and 2 in Eq. (3) refer to the homogenized core and water reflector regions respectively.

2. Numerical sensitivity analysis

According to Eq (1) the sensitivity matrix is needed for the evaluation of the covariance matrix of the calculated neutron spectrum (Tashani, 2010). The elements of this matrix should be calculated using analytical expressions derived according to Eq. (2). However, the derivation of these expressions is very difficult due to complex functional relationships; therefore, these partial derivatives were evaluated numerically for numerical calculation of the sensitivity matrix S, each parameter included in the vector P has been perturbed separately. The input data (including the perturbed values) were then used to perform neutron transport calculation. The well-known deterministic transport code (ANISN) integrated with the XSUN computer code system was used (Kodeli & Slaviˇc, 2013) and (Slaviˇc & Kodeli, 2013). Furthermore, a 27-neutron energy group structure was adopted.

The propagation of uncertainty was analyzed using statistical approach (Slavickas *et al*., 2017). The results of such calculation are used to approximate linearly the corresponding element (relative) of the sensitivity matrix as follows:

$$s(n,m) = \frac{\{\emptyset_p(n,m) - \emptyset_r(n)\}}{\{d(m)\emptyset_r(n)\}} \qquad (4)$$

where

$s(n,m)$: Relative sensitivity coefficient of the nth group flux with respect to the mth element of P.

$\emptyset_P(n,m)$: The nth group flux value resulted from calculations using input including the perturbed value of the mth element of P.

$\emptyset r(n)$: The nth group flux value resulted from calculations using unperturbed input data.

$d(m)$: Relative perturbation value of the mth element of P.

As can be seen, numerical evaluation of the partial derivatives of Eq. (2) using Eq. (4) does not require any analytical treatment. However, new problems are introduced which are related to the accuracy and rounding errors of the results in a typical numerical differentiation procedure.

The finite difference quotient of Eq. (4) should accurately describe the actual derivative (*i.e.* Eq. (2)). The accuracy can be improved by making $d(m)$ of Eq. (4) as small as possible. On the other hand, a small value of d(m) may result in a very small change in the neutron flux values. This small change may not appear due to rounding off the results**.**

3. Results and discussion

During calculation of the sensitivity matrix of the neutron spectrum, it was found that 30% perturbation of absorption cross section values produced almost undetectable changes in the neutron flux values. Low absorption cross-section values is one reason for this small effect on the neutron spectrum calculation. Even the large resonance absorption cross section values were lowered due to flux- weighting during cross-section data preparations. A second reason is due to the fact that perturbation of absorption cross section value of one energy group does not affect neutrons of other groups. This is because the absorption reaction plays only a single role with respect to the neutrons in the reactor (*i.e.* neutron consumption).

Unlike absorption, the fission process consumes thermal neutrons and produces fast neutrons. Although cross section values of fission and absorption are comparable, 30% perturbations of the fission cross section values induced changes in the neutron flux values at all energies. On the other hand, the large scattering cross-section values (*i.e.* 100 times that of absorption and fission) make the neutron spectrum very sensitive to their perturbations. Furthermore, perturbation of a scattering cross section value of one energy group affects neutrons in other groups as well. Perturbation of the scattering-out cross section value of a group was accompanied with similar perturbations of the corresponding scatter—in cross-sections of the lower energy groups. In fact, only 10% perturbations were needed to calculate the sensitivity coefficients of the neutron spectrum with respect to the scattering cross-section values.

Fig. 1 gives some of the sensitivity analysis results presented in a curve form. Each curve shows sensitivity coefficients of the neutron spectrum under investigation due to the perturbation of a single group cross section value (*i.e.* elements of a single line of the sensitivity matrix). The shapes of these curves are determined by many factors. Some of these factors are physical and others are related to the different assumptions made during the calculations. The most important of the latter ones are related to the assumption of fixed reactor power. This assumption is satisfied in the calculation by requiring the fission source to be normalized. Since the fission cross section values are constants in each calculation, the normalization is satisfied by re-adjustment of neutron flux values.

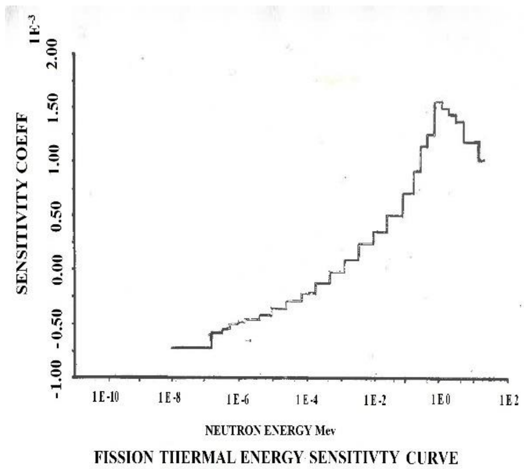

Fig. 1a. Sensitivity coefficients due to perturbation of the fission cross-section of thermal energy group.

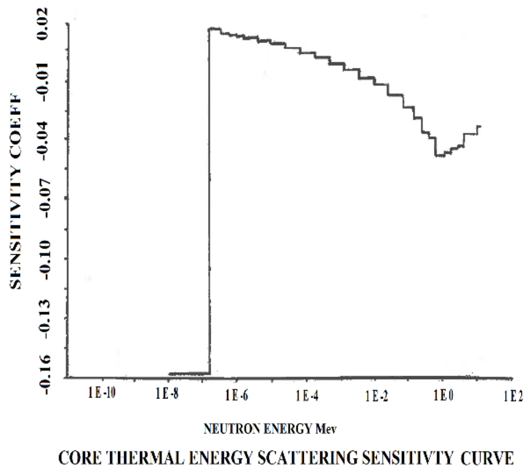

Fig. 1b. Sensitivity coefficients due to perturbation of core thermal scattering cross section.

Although an explanation of the detailed form of each curve given in Fig. 1 is not possible, the general features can be discussed. In Fig. 1a, results due to perturbation of the core fission cross section value of the thermal energy group are plotted. Fig. 1a shows negative and positive sensitivity coefficients for the thermal and high-energy fluxes respectively. Increasing the fission cross section will lead to drop in the thermal flux due to more neutron consumption, and rise in the high energy flux due to more neutron production. Fig. 1b shows the results of perturbation of the core thermal scattering cross-section; this curve shows negative sensitivity coefficients at thermal and high energies. In a thermal energy group, all scattered neutrons remain in the same group (*i.e.* self-scattering). Decreasing the core scattering cross-section of this group will lead to an increase in the thermal diffusion length (*i.e.* thermal neutrons can travel further) this will lead to an increase in their leakage to the reflector region. At the same time, thermal neutron flux will decrease in the core due to the increase in the thermal leakage; this decrease will be matched by a corresponding increase in the high energy flux in the core (due to normalization) which lead to a similar increase in the reflector region. Table (2) gives the contribution of the uncertainty of fission cross-section values to the uncertainty of the calculated neutron spectrum. These data show that this contribution is indeed very small, due to the low sensitivity of the neutron spectrum to these values (Fig. l). Table (2) gives also an estimate of the contribution of the uncertainty of the scattering cross-section values to the uncertainty of calculated neutron spectrum. This estimation shows a large contribution of scattering cross-section.

Table 2

Contributions of the uncertainty of differential cross-section values to the uncertainty of the neutron spectrum.

Lower limit of energy interval (eV)	% Relative Uncertainty of the calculated Neutron spectrum due to uncertainty of Individual X-SECS		
	Fission	Core. Scatt.	Refl. Scatt.
1.733E+07	0.02	7.78	0.31
1.492E+07	0.01	8.64	0.32
6.065E+06	0.02	8.17	0.25
3.680E+06	0.02	9.79	0.40
2.230E+06	0.03	9.85	0.60
1.350E+06	0.02	9.84	0.98
8.210E+05	0.02	9.46	2.09
4.980E+05	0.02	9.65	2.23
3.020E+05	0.02	9.17	2.32
1.830E+05	0.01	9.07	2.48
8.650E+04	0.01	8.93	2.76
3.180E+04	0.01	8.65	3.13
1.170E+04	0.01	8.25	3.36
4.310E+03	0.01	7.70	3.60
1.580E+03	0.01	7.07	2.61
5.830E+02	0.01	6.13	5.48
2.140E+02	0.01	5.80	4.78
7.890E+01	0.01	5.60	4.44
2.900E+01	0.01	5.47	4.27
1.070E+01	0.01	5.37	4.23
5.040E+00	0.01	5.29	4.25
3.060E+00	0.01	5.28	5.13
1.850E+00	0.02	5.40	4.79
1.120E+00	0.02	5.55	4.54
4.140E-01	0.01	6.85	4.33
2.000E-01	0.01	6.31	3.94
1.000E-04	0.01	8.64	3.33

Fig. 2 (a, b & c) show a visual display of correlation matrices. In the figures, the correlation coefficients are presented by shaded areas, dark areas mean strong positive correlations and white ones mean strong negative correlations. Fig. 2a presents the correlation matrix of the calculated neutron spectrum obtained by considering the effect of the fission cross section only. Figs 2b & 2c presents similar matrices obtained by considering the effect of scattering in core and reflector respectively.

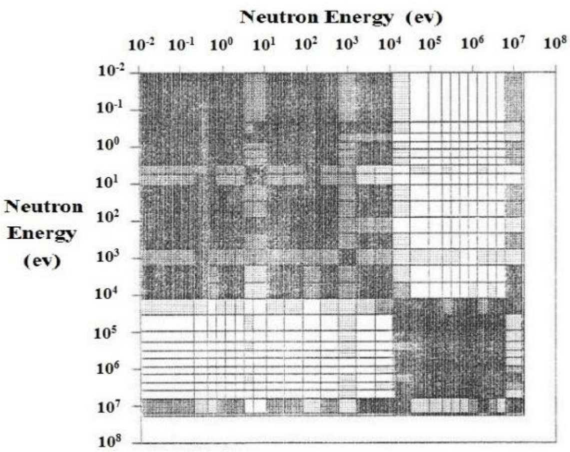

Fig. 2a. Display of contribution of fission reaction to the correlation of the neutron spectrum

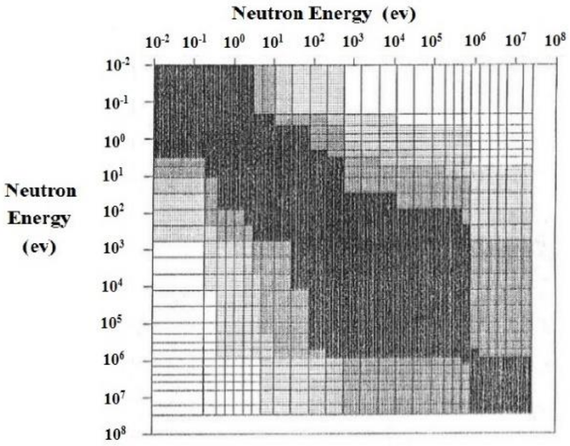

Fig. 2b. Display of contribution of the core scattering to the correlation of the neutron spectrum

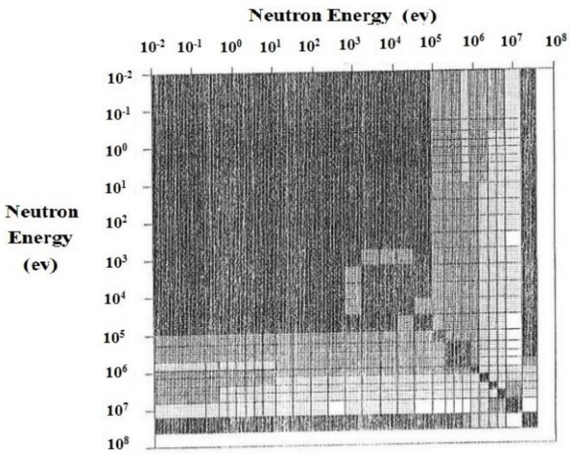

Fig. 2c. Display of contribution of the reflector scattering to the correlation of the neutron spectrum.

The main characteristic of Fig. 2 is that strong and moderate, positive as well as negative correlations between neutron flux values of different energy groups do exist. This observation is a consequence of the fact that changes in neutron flux values of certain energy groups do effect those of other groups. This effect is made through different neutron reactions. For example, increasing in the thermal neutron flux will lead to increase in the fast one (in the core) due to fission. The correlation matrix of the neutron spectrum includes the correlation characteristics due to fission and scattering reactions. Accordingly, it is very clear that a diagonal matrix (*i.e.* no correlation between neutron flux values of different energy groups) does not in any way correspond to the real case. On the other hand, we notice also the difference between the characteristics of the correlations resulting from scattering reactions in the core and the reflector (*i.e.* Figs. 2b & 2c). This is due to different scatter of nuclides in these regions, and also the fact that the effect of a scattering reaction in the core on the neutron spectrum at a position in the reflector is indirect. This effect is a consequence of the contribution of the event investigated to the neutron source outside the reflector consequently, the use of correlation information on the neutron spectrum in different neutron environments is not completely justified and should be made (if necessary) with care.

4. Conclusions

Uncertainty analysis of a calculated neutron spectrum were successfully carried out, unfortunately, a complete evaluation was not possible due to the lack of covariance information on the scattering cross section for some materials. Nevertheless, an estimation of the uncertainty of the neutron spectrum was made using available data. The need of the lacking data is emphasized, in order to avoid non-justified approximations. The results of the covariance matrix estimation of the calculated neutron spectrum showed that an input diagonal covariance matrix for the neutron spectrum adjustment process does not correspond to the real case.

Although the actual values of these results are not exact, they do however, present general real aspects. The most important of these aspects is the large contribution of scattering cross section; this contribution alone can be used to characterize the neutron spectrum uncertainty without any loss of information. The neutron spectrum is highly sensitive to scattering cross section values. The results showed that the common practice of using reported covariance information is not justified.

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