

RESONANCE SELF-SHIELDING EFFECT IN UNCERTAINTY QUANTIFICATION OF FISSION REACTOR NEUTRONICS PARAMETERS

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In order to properly quantify fission reactor neutronics parameter uncertainties, we have to use covariance data and sensitivity profiles consistently. In the present paper, we establish two consistent methodologies for uncertainty quantification: a self-shielded cross section-based consistent methodology and an infinitely-diluted cross section-based consistent methodology. With these methodologies and the covariance data of uranium-238 nuclear data given in JENDL-3.3, we quantify uncertainties of infinite neutron multiplication factors of light water reactor and fast reactor fuel cells. While an inconsistent methodology gives results which depend on the energy group structure of neutron flux and neutron-nuclide reaction cross section representation, both the consistent methodologies give fair results with no such dependences.

KEYWORDS : Uncertainty Quantification, Covariance Data, JENDL-3.3, ERRORJ

1. INTRODUCTION

In recent years, numerical techniques for reactor physics simulations have been drastically improved and accurate calculations without introducing any significant numerical approximations have been realized with advanced high-performance computers. Even numerical results obtained by such advanced calculations inevitably include an uncertainty which comes from the uncertainty in employed nuclear data with a certain degree. Quantification of this nuclear data-induced uncertainty has become one of the important issues in the reactor physics field, and much effort has been devoted to it so far.

There are several methodologies for quantifying reactor neutronics parameter uncertainties, such as the sensitivity-based method (adjoint method) and the random sampling method. Most of them are based on multi-group representation of neutron-nuclide reaction cross sections and neutron flux. This is because covariance data of multi-group cross sections are generally used in actual uncertainty quantification calculations. In evaluated nuclear data files, covariance data have been evaluated for reaction cross sections and resonance parameters in the resonance range. Since it is very cumbersome to directly treat such covariance data in uncertainty quantification calculations, these covariance data are processed into simple representations,

i.e., covariance data of multi-group cross sections, by so-called nuclear data processing codes such as ERRORJ [1] and PUFF [2].

Reactor neutronics parameter uncertainty induced by nuclear data uncertainty can be quantified using a simple error propagation formula with the covariance data of multi-group cross sections and sensitivity profiles of reactor neutronics parameters to multi-group cross sections. Sensitivity profiles can be easily calculated by the generalized perturbation theory for an arbitrary reactor neutronics parameter of an arbitrary nuclear system. As pointed out by several authors [3, 4], we have to take care to maintain consistency between multi-group cross sections for which covariance data are given and those for which the sensitivity of the reactor neutronics parameter is calculated. Existing covariance data processing codes generate covariance data of infinitely-diluted multi-group cross sections. On the other hand, we usually use sensitivities to self-shielded multi-group cross sections in uncertainty quantification calculations. Thus there is inconsistency between these two sets of multi-group cross sections.

When the random sampling method is employed, we prepare several hundreds/thousands of sets of multi-group cross sections which are randomly distributed around expected values according to their covariance data, calculate reactor neutronics parameters using these cross section

sets, and then obtain the statistical distribution of a reactor neutronics parameter. Finally the neutronics parameter uncertainty can be quantified. If we use the covariance data of infinitely-diluted cross sections, we have to prepare sets of multi-group infinitely-diluted cross sections and perform resonance self-shielding calculations prior to the multi-group neutron transport calculations to obtain reactor neutronics parameters. In the resonance energy range, not only infinitely-diluted cross sections but also self-shielding factors (or resonance integrals) should have their covariance data. Existing covariance data processing codes, however, do not have the capability to generate covariance data for such resonance-related quantities. Furthermore, it is expected that the covariance matrix of these nuclear data should be extremely large because we have to consider correlations among infinitely-diluted cross sections and the resonance-related quantities.

Previously, one of the present authors attempted to generate covariance data of multi-group self-shielded cross sections with a modified version of ERRORJ and to quantify uncertainty of the infinite neutron multiplication factors of light water fuel cells, keeping the consistency between two sets of multi-group cross sections [3]. Just recently Takeda and Foad have shown that there is a large difference between sensitivity profiles to infinitely-diluted cross sections and those to self-shielded cross sections [4].

The present paper addresses the consistency between two sets of multi-group cross sections: those for which covariance data are given and those for which sensitivity is calculated. This paper is organized as follows. Section 2 gives a theoretical background of two different approaches to keeping the consistency; one is based on self-shielded cross sections and the other is based on infinitely-diluted cross sections. In Section 3, numerical results of uncertainty quantification of infinite neutron multiplication factors of light water reactor and fast reactor fuel cells are provided. Section 4 gives a short comment on the group collapsing procedure for a covariance matrix based on a conservation principle, which is a different way to perform uncertainty quantification calculations with a coarse energy group library. Finally, Section 5 summarizes the present study.

2. THEORETICAL BACKGROUND

2.1 Self-Shielded Cross Section-Based Consistent Methodology

The covariance data processing code ERRORJ generates covariance data of infinitely-diluted multi-group cross sections. The numerical algorithm of covariance processing by ERRORJ in the resolved resonance range is briefly described in the following.

Covariance data between the m th group cross section σ_m and the n th group cross section σ_n , $\text{cov}(\sigma_m, \sigma_n)$, is calculated from covariance data between the i th resonance

parameter Γ_i and the j th resonance parameter Γ_j , $\text{cov}(\Gamma_i, \Gamma_j)$, as

$$\text{cov}(\sigma_m, \sigma_n) = \sum_i \sum_j S_i^m S_j^n \text{cov}(\Gamma_i, \Gamma_j), \quad (1)$$

where S_i^m is a derivative of σ_m to Γ_i , and is defined as:

$$S_i^m = \frac{d\sigma_m}{d\Gamma_i}. \quad (2)$$

The m th group cross section σ_m is calculated as:

$$\sigma_m = \frac{\langle \sigma(E)\phi(E) \rangle}{\langle \phi(E) \rangle}, \quad (3)$$

where $\sigma(E)$ and $\phi(E)$ denote energy-dependent cross section and neutron flux, and brackets denote integration over the energy range included in the m th energy group. In ERRORJ, a smooth function representing an asymptotic neutron flux energy spectrum $W(E)$ is used for $\phi(E)$. Thus the resonance self-shielding effect is neglected in covariance processing and the covariance data of infinitely-diluted multi-group cross sections are calculated.

In order to obtain covariance data of self-shielded multi-group cross sections, we have to consider depression in the neutron flux energy spectrum by resonances when calculating the derivatives shown as Eq. (2). In the present study, we calculate all these derivatives with the following simple numerical procedure: in the case of calculating $\frac{d\sigma_m}{d\Gamma_i}$, a value of Γ_i is increased by 1% and a point-wise cross section at a specific temperature is constructed from this perturbed set of resonance parameters. Then the multi-group cross section is calculated and a change in σ_m , $\Delta\sigma_m$, is derived. Finally the derivative is numerically calculated as:

$$\frac{d\sigma_m}{d\Gamma_i} \approx \frac{\Delta\sigma_m}{0.01 \times \Gamma_i}. \quad (4)$$

With these derivatives we can calculate the covariance data of self-shielded multi-group cross sections by using Eq. (1).

In a previous study done by one of the present authors, ERRORJ was modified to take into account the resonance self-shielding effect in covariance processing.[3] The modified ERRORJ, however, has a restriction that covariance data of self-shielded multi-group cross sections can be calculated only at zero kelvin. On the other hand, this restriction is removed and temperature dependence of the resonance self-shielding effect is rigorously considered in the present study.

2.2 Infinitely-Diluted Cross Section-Based Consistent Methodology

When we use covariance data of infinitely-diluted cross sections in uncertainty quantification calculations, we have to use sensitivities to infinitely-diluted cross sections for consistency. If we can calculate the sensitivity of self-shielded cross section σ to infinitely diluted cross section σ_∞ , the sensitivity of reactor neutronics parameter

R to σ_∞ can be obtained as:

$$\left(\frac{dR}{d\sigma_\infty} \cdot \frac{\sigma_\infty}{R}\right) = \left(\frac{dR}{d\sigma} \cdot \frac{\sigma}{R}\right) \cdot \left(\frac{d\sigma}{d\sigma_\infty} \cdot \frac{\sigma_\infty}{\sigma}\right), \quad (5)$$

where $\left(\frac{dR}{d\sigma} \cdot \frac{\sigma}{R}\right)$ is the sensitivity of R to σ , which has been conventionally used in uncertainty quantification calculations. Note that the index of the energy group is omitted for simplicity. A derivative of σ to σ_∞ , however, cannot be uniquely defined since both the energy-averaged parameters σ and σ_∞ depend on several dozens of parameters, such as resonance parameters, and the dependence of σ and σ_∞ cannot be uniquely expressed. This difficulty can be overcome by introducing several assumptions described in the following.

A self-shielded multi-group cross section weighted by neutron flux based on the narrow resonance (NR) approximation is written as:

$$\sigma = \frac{\left\langle \frac{\sigma(E)W(E)}{\sigma_i(E) + \sigma_0} \right\rangle}{\left\langle \frac{W(E)}{\sigma_i(E) + \sigma_0} \right\rangle}. \quad (6)$$

Similarly, an infinitely-diluted cross section σ_∞ is defined as:

$$\sigma_\infty = \frac{\langle W(E)\sigma(E) \rangle}{\langle W(E) \rangle}. \quad (7)$$

Here, let us introduce the following relationship:

$$\sigma(E) = \sigma_\infty g(E), \quad (8)$$

where:

$$\frac{\langle W(E)g(E) \rangle}{\langle W(E) \rangle} = 1, \quad (9)$$

and assume that the energy distribution function $g(E)$ has no uncertainty. It means that the relative uncertainty of $\sigma(E)$ is constant in an energy group and that the cross sections at two different energies in the same energy group have full correlation.

Furthermore, we assume that the energy dependence of a total cross section can also be described as $g(E)$. Thus the total cross section can be approximated as follows:

$$\sigma_i(E) \approx \sigma_{i,\infty} g(E). \quad (10)$$

With the above assumptions, the self-shielded cross section can be written as

$$\sigma = \frac{\left\langle \frac{\sigma(E)g(E)}{\sigma_{i,\infty}(E) + \sigma_0} \right\rangle}{\left\langle \frac{W(E)}{\sigma_{i,\infty}(E) + \sigma_0} \right\rangle} \sigma_\infty = f(\sigma_0) \sigma_\infty, \quad (11)$$

where $f(\sigma_0)$ denotes a self-shielding factor dependent on σ_0 . Let us consider that a perturbation $\Delta\sigma_\infty$ is given to σ_∞ (and $\sigma_{i,\infty}$) and σ changes to $\sigma' = \sigma + \Delta\sigma$. We can write σ'

with $\sigma'_\infty = \sigma_\infty + \Delta\sigma_\infty$ as:

$$\begin{aligned} \sigma' &= \sigma'_\infty \frac{\left\langle \frac{W(E)g(E)}{(\sigma_{i,\infty} + \Delta\sigma_\infty)g(E) + \sigma_0} \right\rangle}{\left\langle \frac{W(E)}{(\sigma_{i,\infty} + \Delta\sigma_\infty)g(E) + \sigma_0} \right\rangle} \\ &= \sigma'_\infty \frac{\left\langle \frac{W(E)g(E)}{\sigma_{i,\infty}g(E) + \frac{\sigma_{i,\infty}}{\sigma_{i,\infty} + \Delta\sigma_\infty} \sigma_0} \right\rangle}{\left\langle \frac{W(E)}{\sigma_{i,\infty}g(E) + \frac{\sigma_{i,\infty}}{\sigma_{i,\infty} + \Delta\sigma_\infty} \sigma_0} \right\rangle} \\ &= \sigma'_\infty \frac{\left\langle \frac{W(E)g(E)}{\sigma_{i,\infty}g(E) + \frac{\sigma_0}{1 + \Delta\sigma_\infty/\sigma_{i,\infty}}} \right\rangle}{\left\langle \frac{W(E)}{\sigma_{i,\infty}g(E) + \frac{\sigma_0}{1 + \Delta\sigma_\infty/\sigma_{i,\infty}}} \right\rangle} \\ &\approx \sigma'_\infty \frac{\left\langle \frac{W(E)g(E)}{\sigma_{i,\infty}g(E) + \sigma_0 - \frac{\sigma_0 \Delta\sigma_\infty}{\sigma_{i,\infty}}} \right\rangle}{\left\langle \frac{W(E)}{\sigma_{i,\infty}g(E) + \sigma_0 - \frac{\sigma_0 \Delta\sigma_\infty}{\sigma_{i,\infty}}} \right\rangle} \\ &= \sigma'_\infty \frac{\left\langle \frac{W(E)g(E)}{\sigma_{i,\infty}g(E) + \sigma'_0} \right\rangle}{\left\langle \frac{W(E)}{\sigma_{i,\infty}g(E) + \sigma'_0} \right\rangle} = \sigma'_\infty f(\sigma'_0), \end{aligned} \quad (12)$$

where $\sigma'_0 = \sigma_0 + \Delta\sigma_0 = \sigma_0 - \sigma_0 \Delta\sigma_\infty / \sigma_{i,\infty}$.

The self-shielded cross section change $\Delta\sigma$ can be written as:

$$\begin{aligned} \Delta\sigma &= \sigma'_\infty f(\sigma'_0) - \sigma_\infty f(\sigma_0) = (\sigma_\infty + \Delta\sigma_\infty) f(\sigma'_0) - \sigma_\infty f(\sigma_0) \\ &= \Delta\sigma_\infty f(\sigma'_0) + \sigma_\infty (f(\sigma'_0) - f(\sigma_0)) \\ &= \Delta\sigma_\infty f(\sigma'_0) + \sigma_\infty \frac{f(\sigma'_0) - f(\sigma_0)}{\Delta\sigma_0} \left(-\frac{\sigma_0 \Delta\sigma_\infty}{\sigma_{i,\infty}} \right). \end{aligned} \quad (13)$$

By taking the limit as $\Delta\sigma_\infty \rightarrow 0$ we can obtain:

$$\frac{d\sigma}{d\sigma_\infty} = f(\sigma_0) - \frac{df}{d\sigma_0} \frac{\sigma_0}{\sigma_{i,\infty}}. \quad (14)$$

The relative sensitivity of σ to σ_∞ can be written as:

$$\frac{d\sigma}{d\sigma_\infty} \cdot \frac{\sigma_\infty}{\sigma} = 1 - \frac{df}{d\sigma_0} \frac{\sigma_0}{f} \frac{\sigma_\infty}{\sigma_{i,\infty}}. \quad (15)$$

If the wide resonance (WR) approximation is introduced instead of the NR approximation, the following equation is derived:

$$\frac{d\sigma}{d\sigma_\infty} \cdot \frac{\sigma_\infty}{\sigma} = 1 - \frac{df}{d\sigma_0} \frac{\sigma_0}{f} \frac{\sigma_\infty}{\sigma_{a,\infty}}, \quad (16)$$

where σ_a denotes an absorption cross section.

Using the sensitivities of σ to σ_∞ , we can obtain the sensitivity of reactor neutronics parameter R to σ_∞ from Eq. (5). Using this sensitivity, we can realize a consistent uncertainty quantification calculation in conjunction with the covariance data of σ_∞ , which are generated by existing covariance data processing codes without any modifications. Here we refer to this methodology as the infinitely-diluted cross section-based consistent methodology.

Takeda and Foad have also derived sensitivities of R to σ_∞ . Even though their derivation is different from the present one, the same results were derived. [4] In their derivation, however, an assumption introduced to derive $\frac{d\sigma}{d\sigma_\infty} (\frac{df}{d\sigma_\infty}$ in their study) is not explicitly described, whereas the present study clearly describes the introduced assumptions.

3. NUMERICAL RESULTS

3.1 Calculation Condition

Through the present study, we quantify the uncertainties of infinite neutron multiplication factors (k_∞ s) of three types of fuel cell: a light water reactor (LWR) cell with uranium-oxide (UO₂) fuel of 4.7 wt% uranium-235 enrichment, a LWR cell with a mixed-oxide (MOX) fuel of 13 wt% fissile plutonium enrichment, and a fast reactor (FR) cell with a MOX fuel. The two LWR cells are rectangular

and the FR cell is hexagonal. Nuclide compositions of fuel, cladding, and coolant regions of these cells are simplified in order to ease numerical calculations. The temperatures of all the included nuclides are set to the room temperature (300K). The nuclide number densities of these cells are summarized in Table 1.

All the numerical calculations are performed by the general-purpose reactor physics code system CBZ, which is being developed at Hokkaido University. Resonance self-shielded cross sections are generated with the equivalence theory using a Bondarenko-type multi-group library. Cell heterogeneity is considered by the one-term rational approximation with energy group-wise optimized Bell factors and the Dancoff factor method. Calculated background cross sections of uranium-238 are shown in Fig. 1. Thermal scattering is considered below 3.93 eV. With the obtained multi-group cross sections, eigenvalue calculations are performed with the collision probability method. Sensitivity profiles of k_∞ are calculated by the perturbation theory. The validity of CBZ has been confirmed through an experimental analysis against post-irradiation examination data.[5]

Three multi-group libraries are prepared for the present study: 107-, 231-, and 386-group libraries. The energy group structure of the 107-group library is the same as that of the SRAC2006 code system [6]. In the 231- and 386-group libraries, every energy group of the SRAC2006 107-group structure from 5.04 eV to 11.709 keV is divided

Table 1. Number Densities of Fuel Cells (unit:10²⁴/cm³)

Region	Nuclide	LWR-UO ₂	LWR-MOX	FR
Fuel	U-235	1.072 × 10 ⁻³	4.104 × 10 ⁻⁵	3.097 × 10 ⁻⁵
	U-238	2.146 × 10 ⁻²	2.022 × 10 ⁻²	1.526 × 10 ⁻²
	Pu-238		4.731 × 10 ⁻⁵	
	Pu-239		1.223 × 10 ⁻³	2.543 × 10 ⁻³
	Pu-240		5.586 × 10 ⁻⁴	1.048 × 10 ⁻³
	Pu-241		2.069 × 10 ⁻⁴	6.088 × 10 ⁻⁴
	Pu-242		1.418 × 10 ⁻⁴	1.732 × 10 ⁻⁴
	Am-241		6.007 × 10 ⁻⁵	
	O-16	4.505 × 10 ⁻²	4.500 × 10 ⁻²	3.843 × 10 ⁻²
Cladding	Zr-90	3.786 × 10 ⁻²	3.786 × 10 ⁻²	
	Fe-56			8.000 × 10 ⁻²
Coolant	H-1	5.572 × 10 ⁻²	5.572 × 10 ⁻²	
	O-16	2.786 × 10 ⁻²	2.786 × 10 ⁻²	
	B-10	4.592 × 10 ⁻⁶	4.592 × 10 ⁻⁶	
	Na-23			2.250 × 10 ⁻²

into five or ten groups with equal lethargy width, respectively.

Since the resonance self-shielding effect of uranium-238 capture cross section is important in the nuclear systems considered in the present study, we quantify the k_{∞} uncertainty induced by the uranium-238 capture cross section uncertainty. We use the covariance data of capture reaction-related nuclear data of uranium-238 given in JENDL-3.3[7], in which the covariance data of resonance parameters are evaluated in the resonance range.

To see the fine structure of uncertainty of uranium-238 capture cross section in the resolved resonance range, the uranium-238 covariance data of JENDL-3.3 is processed by ERRORJ into a multi-group form where fine energy meshes with equal lethargy width (0.003) are assigned

from 5 eV to 30 eV. Figure 2 shows the cross section and its relative standard deviation of uranium-238 capture reaction. Dips of relative standard deviations observed around some small resonance peaks are due to the fact that resonance parameter covariance data for these resonances are not provided. Significant energy dependence is observed in the relative uncertainty of cross sections around peaks of large resonances.

3.2 Numerical Results of Self-Shielded Cross Section-Based Consistent Methodology

When we use the self-shielded cross section-based consistent methodology, we have to prepare covariance data of self-shielded cross sections. These are calculated

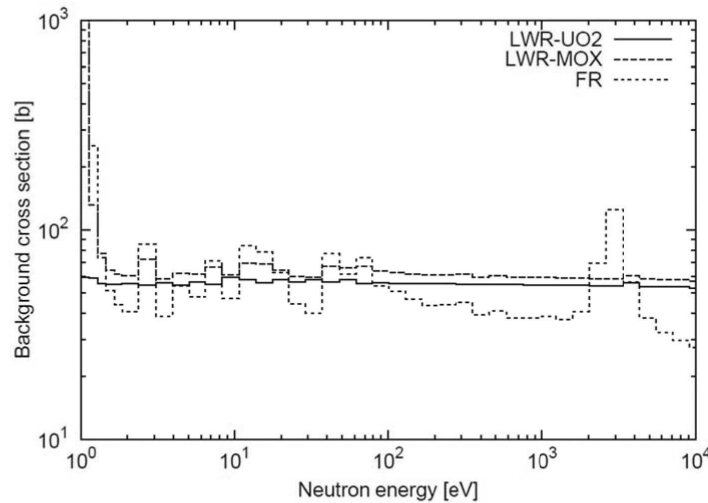


Fig. 1. Background Cross Sections of Uranium-238

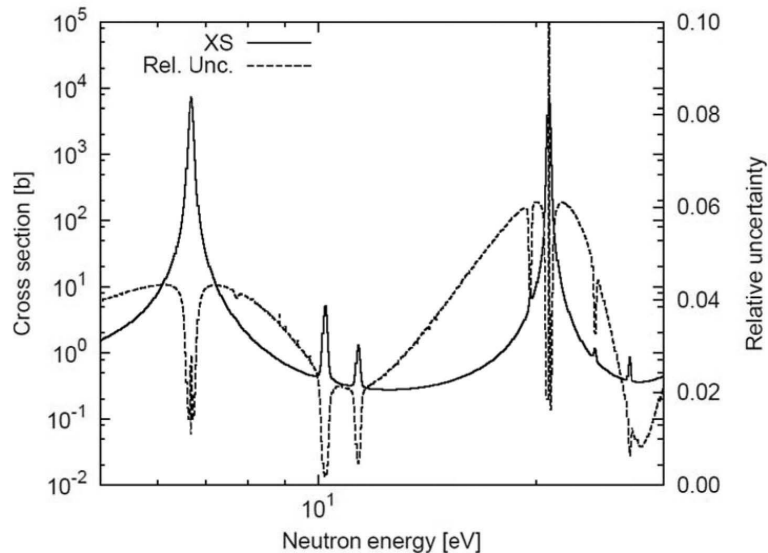


Fig. 2. Relative Standard Deviation of Uranium-238 Capture Cross Section in JENDL-3.3

with an in-house numerical tool consisting of the PREPRO code [8] for point-wise cross section construction and a computer program for multi-group cross section calculation. In the latter computer program, neutron flux $\phi(E)$ is represented by the NR approximation as:

$$\phi(E) = \frac{1}{E(\sigma_c(E) + \sigma_0)}, \tag{17}$$

or by the WR approximation as

$$\frac{1}{E(\sigma_a(E) + \sigma_0)}. \tag{18}$$

With this in-house tool, we can calculate the covariance data of multi-group cross sections for an arbitrary value of σ_0 . In the present calculations we set 60 barn for σ_0 since Fig. 1 suggests that the energy group and fuel composition dependence of σ_0 are not so severe in the resonance energy range. Since this in-house tool can calculate covariance data only in the resolved resonance range, covariance data in the unresolved resonance range and upper energy range are calculated by ERRORJ. It is confirmed that the covariance data of infinitely-diluted cross sections calculated with this in-house tool agree well with those calculated with ERRORJ in the resolved resonance range.

Obviously it is better to use a rigorous neutron flux energy spectrum which can be calculated by the neutron slowing-down equation instead of the NR or WR approximation. The use of the rigorous neutron flux remains a future subject.

Relative standard deviations of uranium-238 capture cross sections are shown in Fig. 3 with the 107-group structure. Large differences are observed between the uncertainties of infinitely-diluted cross sections and those of self-shielded cross sections. It should also be noted that

the model for neutron flux energy spectrum representation significantly affects the uncertainties of self-shielded cross sections. When the WR approximation is adopted, the neutron flux depends on the capture cross section only. Thus the contribution of neutron width uncertainties is not large and that of gamma width uncertainties seems to be dominant. On the other hand, if the NR approximation is assumed, the neutron flux depends on the total cross i.e., sum of capture and elastic scattering cross sections. Thus, both the neutron width uncertainty and the gamma width uncertainty affect the uncertainty of the multi-group cross section. This is the reason why the covariance data of self-shielded cross sections significantly depend on the neutron flux representation model.

Figure 4 shows the correlation matrices of uranium-238 capture cross section in the 107-group structure. Similar to the relative standard deviations of this cross section, the correlation matrices also depend on treatment of the resonance self-shielding effect. In infinitely-diluted cross sections, more positive correlations are observed between two resonances at 6.67 eV and 20.87 eV and between two resonances at 20.87 eV and 36.68 eV than self-shielded cross sections.

Covariance data of self-shielded cross sections are generated for the 107-, 231- and 386-group structures with the NR/WR approximation-based neutron flux representation, and then uncertainty quantification calculations for k_{∞} are carried out using the sensitivity profiles of k_{∞} to self-shielded cross sections. These sensitivities are calculated with the corresponding energy group libraries. For a comparison, we also perform calculations with the conventional inconsistent methodology, which uses covariance data of infinitely-diluted cross sections and sensitivities to self-shielded cross sections. The numerical results are shown

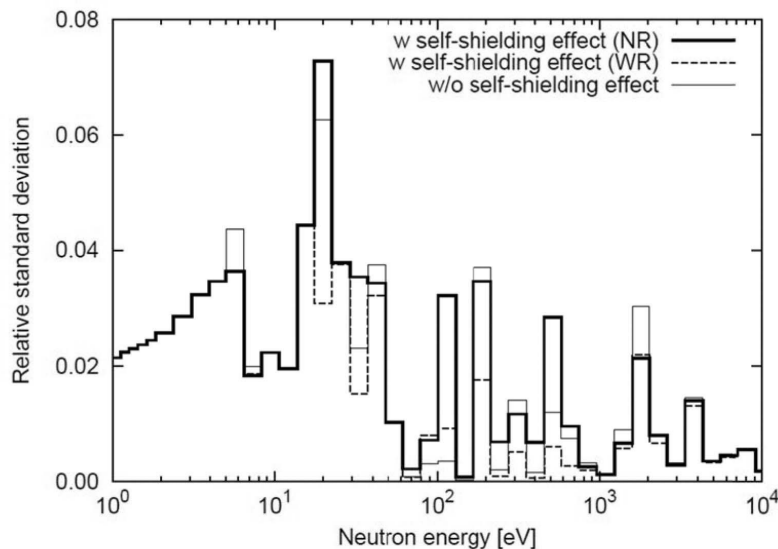


Fig. 3. Relative Standard Deviation of Uranium-238 Capture Cross Section in a 107-Group Structure

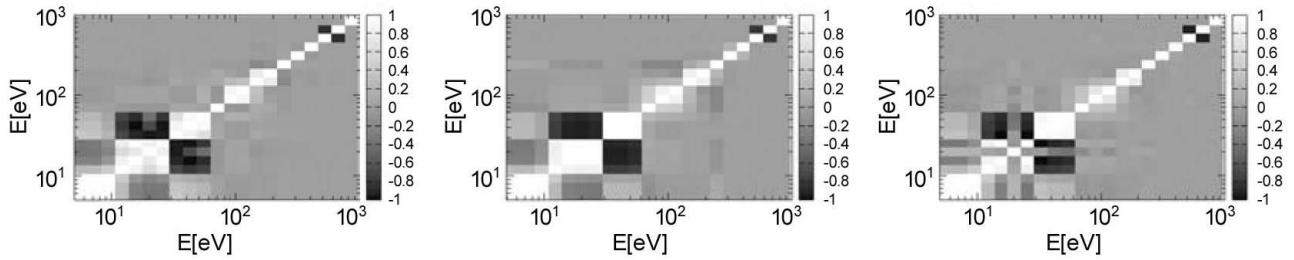


Fig. 4. Correlation Matrices of Uranium-238 Capture Cross Sections (Left: Self-Shielded Cross Section (NR), Center: Self-Shielded Cross Section (WR), Right: Infinitely-Diluted Cross Section)

Table 2. Uncertainty in k_{∞} Based on Self-Shielded Cross Sections (unit: % dk/k)

	LWR-UO ₂		LWR-MOX		FR	
	Consistent	Incon.	Consistent	Incon.	Consistent	Incon.
107-group	0.241*/0.238**	0.300	0.136/0.127	0.189	0.408/0.408	0.412
231-group	0.237/0.236	0.245	0.129/0.126	0.136	0.412/0.412	0.413
386-group	0.235/0.234	0.238	0.128/0.126	0.130	0.411/0.411	0.412

* NR approximation, ** WR approximation.

in Table 2. When the number of energy groups increases, the difference between the results of the consistent and inconsistent methodologies becomes small. This is because the difference between self-shielded cross sections and infinitely-diluted cross sections becomes small when a fine energy group library is used. In the two LWR cells, the inconsistent methodology clearly overestimates the uncertainty when the coarse-group library is used. On the other hand, the consistent methodology based on the NR or WR approximation gives almost constant uncertainties independent of the number of energy groups. It is interesting to point out that the k_{∞} uncertainties calculated with the consistent methodology based on the NR and WR approximations are very close to each other in the 107-group calculations even though the two covariance data derived with these approximations are different. In the LWR-MOX cell result, the consistent methodology with the WR approximation gives a slightly better result than the consistent methodology with the NR approximation. The k_{∞} uncertainties of the LWR cells mainly come from cross section uncertainties below 100 eV. The WR approximation is better than the NR approximation in this energy range, so the consistent methodology with the WR approximation shows better performance. Since the performance of the proposed consistent methodology seems to depend on the covariance data of resonance parameters and sensitivity profiles of target neutronics parameters, further numerical tests are required.

In the FR cell, no significant differences between the two methodologies are observed because the k_{∞} uncertainty mainly comes from cross section uncertainty in the unre-

solved energy range. As shown in Fig. 3, the relative standard deviations of multi-group cross sections are not affected by the resonance self-shielding effect above 2 keV. In this energy range all the resonances are so narrow that the resonance self-shielding effect on multi-group cross sections itself is small. Thus the resonance self-shielding effect on covariance data of multi-group cross sections in the unresolved energy range is expected to be negligible.

3.3 Numerical Results of Infinitely-Diluted Cross Section-Based Consistent Methodology

When we use the infinitely-diluted cross section-based consistent methodology, we have to prepare sensitivities of reactor neutronics parameter R to infinitely-diluted cross section σ_{∞} . Under the assumptions described in the preceding section, these sensitivities can be expressed as a product of the sensitivity of R to self-shielded cross section σ and the sensitivity of σ to σ_{∞} as shown in Eq. (5). Here we calculate the sensitivities of σ to σ_{∞} using Eq. (15) or (16). In this calculation, we set $\sigma_0=60$. Figures 5 and 6 show these sensitivities in the 107-, 231-, and 386-group structures based on the NR or WR approximation. It is clearly shown that fine energy group libraries give sensitivities close to 1.0 below 100 eV since energy groups in this energy range have wide resonances which can be explicitly represented by the fine group libraries. On the other hand, above 1 keV, these three libraries give similar results with each other since resonances in this energy range are narrow relative to the energy group width. In the unresolved resonance range the sensitivities take values close to unity in the case of the NR approximation.

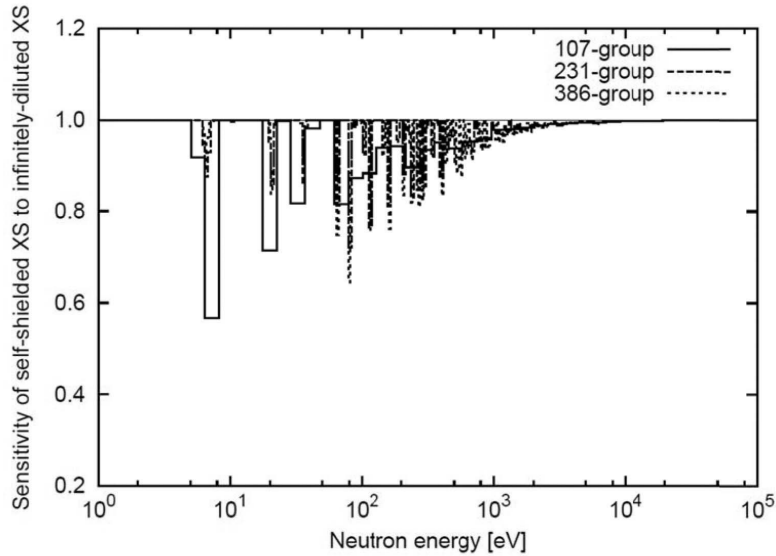


Fig. 5. Sensitivity of Self-Shielded Cross sections to Infinitely-Diluted Cross Sections (NR approximation)

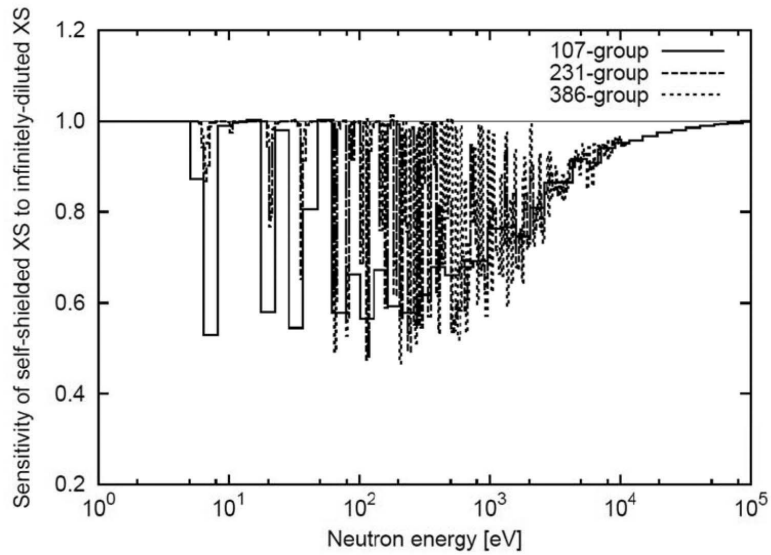


Fig. 6. Sensitivity of Self-Shielded Cross sections to Infinitely-Diluted Cross Sections (WR approximation)

By multiplying the conventional sensitivities of R to σ by these sensitivities of σ to σ_∞ , we can obtain the sensitivities of R to σ_∞ required for uncertainty quantification calculations based on the consistent methodology. Table 3 shows k_∞ uncertainties calculated with the infinitely-diluted cross section-based consistent methodology. Large uncertainties observed in the 107-group calculation based on the inconsistent methodology are reduced when the consistent methodology is adopted, and the consistent methodology gives almost constant uncertainties independent of the number of energy groups. In the 107-group calculations, uncertainties calculated with the consistent methodology are smaller than those with the inconsistent methodology

since the sensitivity of σ to σ_∞ is smaller than unity as shown in Figs. 5 and 6. Let us compare this result with the relative standard deviations shown in Fig. 3. The relative standard deviation of the multi-group cross section of the 58-th group, where the large resonance of uranium-238 at 6.674 eV exists, does not depend on the resonance self-shielding effect. It suggests that the sensitivity of σ to σ_∞ is about unity. On the other hand, this sensitivity is calculated as about 0.6 in the infinitely-diluted cross section-based methodology. This contradiction may come from the assumption introduced in this methodology. Although the infinitely-diluted cross section-based consistent methodology works well in the present numerical testing, it is not

Table 3. Uncertainty in k_∞ Based on Infinitely-Diluted Cross Sections (unit:% dk/kk')

	LWR-UO ₂		LWR-MOX		FR	
	Consistent	Incon.	Consistent	Incon.	Consistent	Incon.
107-group	0.257*/0.244**	0.298	0.151/0.138	0.188	0.409/0.401	0.409
231-group	0.239/0.237	0.244	0.129/0.135	0.131	0.413/0.404	0.413
386-group	0.235/0.234	0.238	0.126/0.130	0.125	0.412/0.403	0.412

* NR approximation, ** WR approximation.

confirmed that the same results can be obtained when different covariance data and sensitivity profiles are used. Further study is required in order to validate this consistent methodology.

4. NOTE ON GROUP COLLAPSING OF COVARIANCE MATRIX ON A CONSERVATION PRINCIPLE

Hiruta et al. have proposed a group collapsing methodology of covariance matrix on a conservation principle [9]. In this section, we briefly review the theory and discuss its relation with the present study.

Let us consider energy group collapsing of the covariance matrix of self-shielded cross sections. We represent the multi-group cross sections before and after group collapsing as σ_g and σ_G , respectively. The coarse-group cross section σ_G can be written with fine-group cross section σ_g and fine-group neutron flux ϕ_g as:

$$\sigma_G = \frac{\sum_{g \in G} \sigma_g \phi_g}{\sum_{g \in G} \phi_g} = \frac{\sum_{g \in G} \sigma_g \phi_g}{\phi_G} \quad (19)$$

Using a simple uncertainty propagation formula, the covariance data between σ_G and $\sigma_{G'}$ can be written as:

$$\text{cov}(\sigma_G, \sigma_{G'}) = \sum_g \sum_{g'} \left(\frac{\partial \sigma_G}{\partial \sigma_g} \right) \left(\frac{\partial \sigma_{G'}}{\partial \sigma_{g'}} \right) \text{cov}(\sigma_g, \sigma_{g'}) \quad (20)$$

When the infinitely-diluted situation is assumed, the fine-group neutron flux does not depend on the fine-group cross section. Thus, $\text{cov}(\sigma_G, \sigma_{G'})$ can simply be written as:

$$\text{cov}(\sigma_G, \sigma_{G'}) \approx \sum_{g \in G} \sum_{g' \in G'} \left(\frac{\phi_g}{\phi_G} \right) \left(\frac{\phi_{g'}}{\phi_{G'}} \right) \text{cov}(\sigma_g, \sigma_{g'}). \quad (21)$$

Equation (21) is generally used in existing covariance data processing codes and can be rewritten in a relative form as:

$$r \text{cov}(\sigma_G, \sigma_{G'}) \approx \sum_{g \in G} \sum_{g' \in G'} \left(\frac{\sigma_g \phi_g}{\sigma_G \phi_G} \right) \left(\frac{\sigma_{g'} \phi_{g'}}{\sigma_{G'} \phi_{G'}} \right) r \text{cov}(\sigma_g, \sigma_{g'}), \quad (22)$$

where $r \text{cov}(\sigma_G, \sigma_{G'})$ denotes the relative covariance data between σ_G and $\sigma_{G'}$. This equation suggests that the relative contribution of fine-group reaction rates is used as a weight function in group collapsing of covariance matrix based on the infinitely-diluted assumption. On the other hand, in order to preserve the uncertainty of reactor neutronics parameters the following equation should be preserved:

$$S_g S_{g'} r \text{cov}(\sigma_g, \sigma_{g'}) \approx \sum_{g \in G} \sum_{g' \in G'} S_g S_{g'} r \text{cov}(\sigma_g, \sigma_{g'}), \quad (23)$$

where S denotes the relative sensitivity of a reactor neutronics parameters to a multi-group self-shielded cross section. Thus the covariance matrix of coarse-group self-shielded cross sections should be defined as:

$$r \text{cov}(\sigma_G, \sigma_{G'}) = \sum_{g \in G} \sum_{g' \in G'} \left(\frac{S_g}{S_G} \right) \left(\frac{S_{g'}}{S_{G'}} \right) r \text{cov}(\sigma_g, \sigma_{g'}), \quad (24)$$

The fine-group sensitivity S_g can be written as $S_g = \sum_G S_G \left(\frac{\partial \sigma_G}{\partial \sigma_g} \right) \left(\frac{\sigma_g}{\sigma_G} \right)$. If we assume the infinitely-diluted situation, this expression can be simplified to $S_g = S_G \left(\frac{\phi_g \sigma_g}{\phi_G \sigma_G} \right)$ where the fine-group g is included in the coarse-group G , and we can obtain the intuitive relation $\sum_{g \in G} S_g = S_G$. In this case, Equation (24) agrees with Equation (22); the conventional group collapsing methodology of covariance matrix preserves reactor neutronics uncertainties.

5. CONCLUSION

In order to properly quantify fission reactor neutronics parameter uncertainties, we have to use covariance data and sensitivity profiles consistently. In the present paper, we have established two consistent methodologies for uncertainty quantification: the self-shielded cross section-based consistent methodology and the infinitely-diluted cross section-based consistent methodology. Through numerical assessments for k_∞ uncertainty calculations of LWR and FR fuel cells with the JENDL-3.3 covariance data, both consistent methodologies are found to give fair results; deduced k_∞ uncertainties do not depend on the

energy group structure of neutron flux and neutron-nuclide reaction cross sections.

In the self-shielded cross section-based consistent methodology, we have calculated the covariance data of a self-shielded cross section with an in-house numerical tool in which the narrow resonance or wide resonance approximation is adopted for the neutron flux representation. The Doppler-broadening of resonance cross sections is also properly considered. It has been shown that the covariance data of self-shielded cross sections are different from those of infinitely-diluted cross sections in the coarse group (107-group) structure, and that the covariance data of self-shielded cross sections depend on the neutron flux representation model.

In the infinitely-diluted cross section-based consistent methodology, we calculated the sensitivities of self-shielded cross sections to infinitely-diluted cross sections in the same manner as that previously proposed by Takeda and Foad. Although this methodology has worked well in the present calculations, further study is required to verify the introduced assumption that the shape of the cross section in an energy group has no uncertainty.

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