Nuclear Data and Fuel/Assembly Manufacturing Uncertainties Analysis and Preliminary Validation of SUACL

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1. Introduction

As the sensitivity and uncertainty analysis of nuclear system can provide more confident bounds for the Best-estimate Prediction used to assess the performance and safety of nuclear plant, the uncertainty and sensitivity analysis has been a component of analysis of nuclear system. There are hundreds of uncertainty sources in reactor physics calculation, only epistemic or subjective uncertainties can be analyzed. And the imprecise input parameters are recognized as epistemic uncertainties[1]. The objective of uncertainty analysis is to quantify the uncertainty of output derived from the relative inputs uncertainty[2]. The cross section and parameters of fuel/assembly manufacturing are the fundamental inputs of the neutron transport equation. The imprecise nuclear data has been treated as one of the major uncertainty sources[3]. But the parameters of fuel/assembly manufacturing uncertainties are paid little attention. Both the cross section uncertainty and the uncertainty of parameters of fuel/assembly manufacturing are analyzed in this paper.

Generally, all cross section can be divided into the basic and integralones. The integral cross sections are composed of basic cross sections. The cross section uncertainties are stored in their covariance data. Different evaluate approaches used in nuclear data library may lead to the different of analysis result. For verify the effect, the covariance library uses the covariance data from NJOY99 based on ENDF/B-VII.1 and JENDL4.0. Other important inputs are the parameters of fuel/assembly manufacturing uncertainties which are crucial to the simulation model. The uncertainty of these parameters can propagate to the result through the simulating model and affect the accuracy of the result.

The code SUACL based on Monte Carlo sampling method wereprogrammed to do the uncertainty analysis of cross section. The Monte Carlo sampling method and the SUACL is introduced in section 2. The perturbation model of cross section and parameters of fuel/assembly manufacturing is in section 3. All results and discussions are described in section 4. Summary is in the last section.

2. MC Sampling Method and SUACL

2.1 Monte Carlo Sampling Method

The implementation of MC sampling method can often be performed as follow[4]: define an appropriate probability distribution function of inputs; generate enough analysis samples in the distribution; deliver the samples to neutron physics calculation; determine the uncertainty of desired output; determine the sensitivity of the desired output. The sample size is calculated by Wilks’ formula (1)[5].

\[
(1 - \alpha^2) - N(1 - \alpha)^{\alpha - 1} \geq \gamma
\]

Here, N is the minimum sampling number, \( \gamma \) is confidence coefficient.

2.2 The code of SUACL

The code SUACL has been developed to perform the uncertainty analysis of cross section. The procedure of uncertainty analysis like introduced in figure 1.

3 Perturbation model

3.1 Cross section Perturbation model

In WIMS-69, a few types of basic cross section are stored in their integral cross section like the capture cross section etc. So before build perturbation model of cross section, it is required to obtain the actual value of the cross section. It is related to the relationship between the integral cross section and their components. The relationship is given in eq. (2)-eq. (3).

\[
\sigma_i = \sigma_f + \sigma_p + \sigma_{el} + \sigma_{inel} - 2\sigma_{sc}
\]

\[
\sigma_{sc} = \sigma_{el} + \sigma_{inel} + 2\sigma_a + 3\sigma_{sc}
\]

Secondly is to obtain the perturbation factor based on the covariance matrix. The variance and covariance of cross section are elements kept in corresponding covariance matrix, so its uncertainty stored in covariance matrix. The Jacobi Rotation decomposition method is impl
mented to perform the decomposition of covariance matrix. After decomposition, one diagonalizable matrix $D$ consists of eigenvalues and two matrices $V$ composed by the vector of eigenvalue can be obtained.

The square root of covariance matrix $\sqrt{\Sigma}$ equals to the square root of diagonalizable matrix $\sqrt{\Sigma} = V \sqrt{\lambda} V^T$. All computations are shown in eq. (5) - eq. (6). The perturbation factor $P$ is the square root of covariance matrix multiply with a vector of random number which was sampled in the standard normal distribution, and plus a unit matrix $I$ of the same dimension with input parameter like eq. (7).

$$\Sigma = V \times D \times V^T$$

$$\Sigma^{\frac{1}{2}} = V \times D^{\frac{1}{2}} \times V^T$$

$$P = \Sigma^{\frac{1}{2}} G_0(0,1) + I$$

The consistency rules of cross section perturbation are detailed displayed in table I to III.

Table I. The consistency rule of perturbed fission and capture cross section

| Basic cross section | Perturbation factor | Perturbed cross section |
|---------------------|---------------------|------------------------|
| $\sigma_i$          | $P = 1 + \delta j$  | $\sigma_i' = \delta j \sigma_i$ |
| $\sigma_{f/\gamma}$ |                     |                         |

Table II. The consistency rule of perturbed elastic scatter and inelastic scatter cross section

| Basic cross section | Perturbation factor | Perturbed cross section |
|---------------------|---------------------|------------------------|
| $\sigma_i$          | $P = 1 + \delta j$  | $\sigma_i' = \delta j \sigma_i$ |
| $\sigma_{f/\gamma}$ |                     |                         |

Table III. The consistency rule of perturbed average total fission neutron

| Basic cross section | Perturbation factor | Perturbed cross section |
|---------------------|---------------------|------------------------|
| $\nu_{fs}$          | $P = 1 + \delta j$  | $\nu_{fs}' = \delta j \nu_{fs}$ |
| $\nu_{f/\gamma}$    |                     |                         |

3.2 Parameters of Fuel/Assembly Manufacturing Perturbation model

Two typical PWR cells have been recommended to quantify the uncertainty of parameters of fuel/assembly manufacturing. One is a traditional UO$_2$ cell called TMI-1, which is described in UAM benchmark. The other is created by cosRMC and filled with MOX fuel. The introduction of models is shown in table 4. According to the reference [6], the 3σof these parameters are defined: (Fuel density: $\pm 0.17$ g/cm$^3$; Fuel pellet diameter: $\pm 0.013$ mm; Gas thickness: $\pm 0.024$ mm; Clad thickness: $\pm 0.025$; 235U concentration: $\pm 0.0024$ w/o). In order to compare the results easily, the same distribution is used to analyze the uncertainty of parameters of MOX cell.

Table IV. The information of TMI-1 cell and MOX cell

| Parameters                  | MOX-cell | TMI-cell |
|-----------------------------|----------|----------|
| Fuel material               | PuO$_2$-UO$_2$(MOX) | UO$_2$ |
| Gap material                | Zircaloy | H$_2$O   |
| Clad material               | 316SS    | Zircaloy-4 |
| moderator                   | H$_2$O   | H$_2$O   |
| Fuel pellet [mm]            | 9.020    | 9.391    |
| Gap thickness [mm]          | 0.000    | 0.955    |
| Clad thickness [mm]         | 0.380    | 0.673    |
| Unit cell pitch [mm]        | 12.600   | 14.427   |

4 Results and Analysis

The paper has researched on the uncertainty of eigenvalue caused by the uncertainty of cross section and the parameters of fuel/assembly manufacturing respectively in framework of TMI-1-cell and MOX-cell. The reference codes are TSUNAMI-1D; UNICORN and SAINT. The covariance data ZZSCALE6.0/COVA-44G, which originates from the SCALE (based on ENDF/B-VII, ENDF/B-VI, and JENDL-3.1) is adopted by TSUNAMI-1D. The covariance matrix produced by JENDL4.0. The uncertainty of 235U capture cross section and the 235U fission yield have occupied the majority of uncertainty source regardless of the covariance origin. The contributions to the uncertainty mainly depend on cross section of 238U and 235U. Considering the enrichment of uranium in UO$_2$-fuel, more attention needs pay to the optimization of 238U and 235U cross section.

Obviously, the uncertainty of $K_{eff}$ obtained from SUACL differs from the results of TSUNAMI with the respect of capture and elastic scattering cross section of $^1$H. But the result is similar to the UNICORN ones. Comparing the energy spectrum of $^1$H which obtained from the covariance library used by TSUNAMI and SUACL, except the $10^{-1}$~$10^{-7}$ of the $^1$H elastic scattering energy spectrum, the others cross sections are just showed the same development trend and significant difference of numerical value. However, the covariance library used by SUACL is processed the ENDF/B-VII.1, which
is also adopted by UNICORN analysis. It is corresponded to the theory—the uncertainty of cross section is determined by its covariance.

For MOX pin cell, filled with PuO₂ and UO₂. The section of ²³⁹Pu and ²³⁸U, especially the ²³⁸U capture section is determined by its covariance. It is corresponded to the theory—the uncertainty of cross section is determined by its covariance.

![Fig.2a. The uncertainty result of Keff in SUACL and SAINT.](image)

![Fig.2b. The different value of ENDF/B-VII.1 and JENDL4.0](image)

**Table V. The uncertainty of Keff in TMI-1 cell (Contributions to \( \frac{\Delta \kappa}{\kappa} (\%) \))**

| nuclide   | Parameter pair | SUACL (ENDF/B_VII.1) | SUACL (JENDL4.0) | TSUNAMI | SAINT (ENDF/B_VII.1) | SAINT (JENDL4.0) | UNICORN |
|-----------|----------------|----------------------|------------------|----------|----------------------|------------------|----------|
| ²³⁵U      | \( \sigma_u, \sigma_f \) | 3.94E-1              | 4.09E-1          | 2.79E-1  | 3.05E-1              | 3.16E-1          | 3.77E-1  |
| ²³⁹Pu     | \( \sigma_u, \sigma_f \) | 2.09E-1              | 1.57E-1          | 2.11E-1  | 1.94E-1              | 1.57E-1          | 1.95E-1  |
| ²³⁸U      | \( \nu \)    | 6.13E-1              | 2.76E-1          | 2.64E-1  | 5.87E-1              | 2.57E-1          | 1.97E-2  |
| ²³⁵U      | \( \sigma_u, \sigma_f \) | 8.40E-2              | 8.93E-2          | 7.67E-2  | 9.53E-2              | 1.01E-1          | 7.89E-2  |
| ²³³H      | \( \sigma_u, \sigma_f \) | 9.42E-2              | N/A              | 1.84E-2  | N/A                  | N/A              | 9.56E-2  |
| ²³³H      | \( \sigma_u, \sigma_f \) | 6.61E-2              | 3.47E-2          | 7.15E-2  | N/A                  | N/A              | 7.00E-2  |

4.2 Result of Cross Section Uncertainty in MOX pin cell

For MOX pin cell, filled with PuO₂ and UO₂. The contributions to the uncertainty mainly depend on cross section of ²³⁹Pu and ²³⁸U, especially the ²³⁸U capture cross section, which means the ²³⁹Pu play important role to determine the uncertainty of Keff in PWR cell.

Comparing the result with TSUNAMI, it is obvious that the total fission yield of ²³⁹Pu is less than the TSUNAMI. The reason is suspected to be similar to the capture cross section of ²³³H in TMI cell, which owns to TSUNAMI. The reason is suspected to be similar to the neutron energy spectrum of the covariance.

**Table VI. The uncertainty of Keff in MOX cell (Contributions to \( \frac{\Delta \kappa}{\kappa} (\%) \))**

| nuclide   | Parameter pair | SUACL (ENDF/B_VII.1) | SUACL (JENDL4.0) | TSUNAMI | SAINT (ENDF/B_VII.1) | SAINT (JENDL4.0) | UNICORN |
|-----------|----------------|----------------------|------------------|----------|----------------------|------------------|----------|
| ²³⁵Pu     | \( \sigma_u, \sigma_f \) | 2.11E-1              | 1.88E-1          | 2.04E-1  | 1.94E-1              | 1.93E-01         | 2.40E-01 |
| ²³⁹Pu     | \( \sigma_u, \sigma_f \) | 1.82E-1              | 2.17E-1          | 1.92E-1  | 2.38E-1              | 2.40E-01         | 2.40E-01 |
| ²³³Pu     | \( \nu \)    | 1.08E-1              | 5.20E-2          | 6.51E-1  | 1.12E-1              | 5.74E-02         | 5.74E-02 |
| ²³⁹Pu     | \( \sigma_u, \sigma_f \) | 6.29E-2              | N/A              | 8.84E-2  | 1.59E-1              | 5.6239E-1        | 5.6239E-1 |
| ²³³Pu     | \( \sigma_u, \sigma_f \) | 1.10E-2              | N/A              | 1.19E-2  | 1.78E-1              | 5.9117E-2        | 5.9117E-2 |
| ²³³U      | \( \sigma_u, \sigma_f \) | 2.84E-1              | 2.99E-1          | 2.15E-1  | 2.16E-1              | 2.2838E-1        | 2.2838E-1 |
| ²³³U      | \( \sigma_u, \sigma_f \) | 1.74E-2              | 1.98E-2          | 1.80E-2  | N/A                  | N/A              | 1.46E-2  |

![Fig.3a. The Helastic scattering energy spectrum of the covariance.](image)

![Fig.3b. The ²³³H capture energy spectrum of the covariance.](image)
4.3 Result of uncertainty of parameters of fuel/assembly manufacturing

The parameters of fuel/assembly manufacturing uncertainty for TMI-1 and MOX cell are comparable, and their numerical value is in the same magnitudes the uncertainty caused by some critical cross section like fission. The $^{235}$U concentration uncertainty is the most important uncertainty source to TMI-1 cell. Furthermore, the cell is filled with UO$_2$ and the majority of fission reaction occurs in $^{235}$U. So the $^{235}$U concentration uncertainty plays a decisive role in TMI-1 cell. However, compared with TMI-1 cell, no gas in MOX cell and its whole area is less than the TMI-1, so the impact of clad is greater in it. The fuel density uncertainty has great effect on the eigenvalue uncertainty in typical PWR cell.

| Parameter of geometry and fuel | Contribution to $\Delta_k$ (%) | Contribution to $\Delta_k$ (%) |
|-------------------------------|-------------------------------|-------------------------------|
| $^{235}$U Concentration       | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $3.04E-2$ | N/A          |
| $^{234}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $2.03E-2$ | $2.34E-2$ |
| $^{235}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $5.90E-2$ | $3.99E-2$ |
| $^{239}$Pu                   | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $6.09E-2$ | N/A          |
| $^{238}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $3.47E-2$ | N/A          |
| $^{238}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $3.79E-2$ | $3.57E-2$ |
| $^{238}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $6.79E-2$ | $3.57E-2$ |
| $^{235}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $7.68E-2$ | $9.62E-2$ |
| $^{238}$U                    | $\sigma_{\text{in}}$, $\sigma_{\text{out}}$ | $4.8748E-2$ | $4.8748E-2$ |

5 Conclusions

The uncertainty of various cross sections and manufacturing parameters of fuel/assembly have been analyzed by implementing the Monte Carlo method. Two typical PWR models were constructed to verify the SUACL based on different covariance library.

According to the result of cross section, all results of SUACL were found in accordance with the results of reference codes. $^{235}$U and $^{238}$U play an important role in determining the uncertainty of $K_{eff}$ in TMI-1 cell. The uncertainty of $K_{eff}$ in MOX is mainly affected by $^{239}$Pu and $^{238}$U. It is obvious that the uncertainty mostly depends on the covariance library and insensitivities to cross section library. The uncertainties based on the covariance library obtained from ENDF/B-VII.1 differ from the result of JENDL4.0, which verified the relationship of covariance matrix and the uncertainty of cross section. And the parameters of fuel/assembly manufacturing uncertainty are comparable to uncertainty of some cross section, especially the $^{235}$U concentration, clad thickness. The uncertainty analysis of these parameters is of great significance to evaluate the parameter of actual cell and help to improve the models simulated. More attentions need to paid to improve the accuracy of the parameters analysis talked in the paper.

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