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Generation and analysis of independent fission yield covariances based on GEF model code

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Abstract. The fission yield data provided by the evaluated nuclear data files do not contain covariance information, which is not conducive to uncertainty analysis. To generate covariance information, the model parameters of the code GEF which describes the fission process are sampled and the independent fission yield samples are calculated. The covariances of independent fission yields of ^{235}U, ^{239}Pu, and ^{241}Pu thermal neutron-induced fissioning systems are generated individually based on the above samples. This method is verified by comparing the uncertainties of burnup-related responses based on fission yield samples calculated by GEF and based on fission yield samples generated with the covariances. The influence of correlations among fissioning systems is also quantified and the joint covariances among different fissioning systems calculated with GEF are demonstrated correct. In addition, the Bayesian Monte Carlo method is adopted to adjust the model parameters of GEF, and the numerical results prove the effectiveness of the adjustment.

1 Introduction

Fission yields are the basic nuclear data in nuclear fuel cycle calculation. As input data of reactor burnup calculation, fission yields play an important role in the prediction of inventories of fission product nuclides. The inventories of fission products determine the calculation accuracy of macro parameters of reactor physics, such as eigenvalue. The fission yield data are mainly obtained through theoretical model evaluation [1]. During the evaluation process, imperfect model parameters propagate uncertainties to fission yields. Therefore, it is necessary to further analyze the uncertainties of fission yields propagated to macro parameters. However, the most commonly used fission yield data in ENDF-6 format [2] only contain the mean value and uncertainty of each fission yield itself, lacking the correlations among different fission yields of fission products or fissioning systems. This affects the accuracy of the uncertainties of the macro parameters.

To provide the correlations among fission yield data and quantify the uncertainties more accurately, many studies have been carried out worldwide. Subgroup 37 (SG37) of the Working Party on International Nuclear Data Evaluation Co-operation (WPEC) was established with the goal of developing "Improved Fission Product Yield evaluation methodologies" [3]. Katakura proposed a Bayesian/general least-squares method to construct covariances among fission yields of fission products with the same mass number [4]. Fiorito et al. considered the different physical constraints of fission yields and generated the covariances of independent fission yields through an iterative generalized least-square method [5]. At the Oak Ridge National Laboratory (ORNL), Wahl's systematics and its random parameters were used to generate random fission yields, and a Bayesian approach based on constraints from the mass yields, the conservation of the mass and charge number was proposed to generate the covariances among different fission yields [6]. Recently, the covariance matrices of independent fission yields were determined based on the generalized least-square method by Kohsuke Tsubakihara, et al [7].

GEF (**GE**neral description of **F**ission observables) code [8, 9] is a semi-empirical model designed to give a complete description of the fission process [10]. GEF code determines the corresponding fission products of different fission events through model parameters and determines the yields of different fission products through the Monte-Carlo process. Some important model parameters of GEF exist in the form of normal distribution, so the parameter samples are obtained by perturbation based on the probability distribution, and then fission yield samples are obtained by running GEF with the parameter samples. In this paper, the independent fission yield covariances of ^{235}U, ^{239}Pu, and ^{241}Pu thermal neutron-induced fissioning systems are generated respectively using the fission yield samples. These covariances are verified based on uncertainties of burnup-related responses. At the same time, the influence of the correlations among fissioning systems on the uncertainties of the burnup-related responses is analyzed. In addition, the model parameters of GEF are preliminarily adjusted through the Bayesian Monte Carlo method [10, 11]. All uncertainty calculations in this paper are based on random sampling.

This paper is organized as follows. Section 2 expounds on the detailed process of generating and

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verifying independent fission yield covariances for individual fissioning systems. Section 3 shows the influence of correlations among fissioning systems. Section 4 introduces the preliminary adjustment of GEF model parameters. Conclusions and perspectives are summarized in Section 5.

2 Fission yield covariance generation for individual fissioning systems

2.1 Generation of fission yield covariances

The process of generating independent fission yield covariances mainly includes three steps, which are summarized below.

(1) Sample the GEF model parameters.
(2) Calculate independent fission yield samples with the above parameter samples.
(3) Calculate covariances among different fission products with the above fission yield samples.

The GEF code version used in this paper is 2021.1.1 [12]. The GEF2021.1.1 determines the normal distribution of the 23 most important parameters for calculating fission yields, and these parameters are independent of each other. In the present work, we sample these parameters. The specific information on these model parameters is shown in Table 1.

Table 1. Specific information on sampled model parameters in GEF2021.1.1 [12].

Model parameter	GEF name	Mean	Standard deviation
Position of the shell for the S_1 channel	P_DZ_Mean_S1	-0.3	0.06
Position of the shell for the S_2 channel	P_DZ_Mean_S2	-0.4	0.06
Position of the shell for the S_3 channel	P_DZ_Mean_S3	0.2	0.06
Position of the shell at Z≈42	P_DZ_Mean_S4	0.0	0.06
Shell effect for the S_1 channel	P_Shell_S1	-3.0	0.06
Shell effect for the S_2 channel	P_Shell_S2	-4.4	0.06
Shell effect for the S_3 channel	P_Shell_S3	-7.2	0.12
Shell effect at Z≈42	P_Shell_S4	-1.1	0.03
Rectangular contribution to the width of S_2 channel	P_A_Width_S2	11.5	3%
Shell effect at mass symmetry	Delta_S0	0.0	0.06
Curvature of shell for the S_1 channel	P_Z_Curv_S1	0.38	3%
Curvature of shell for the S_2 channel	P_Z_Curv_S2	0.098	3%
Curvature of shell for the S_3 channel	P_Z_Curv_S3	0.09	3%
Curvature of shell at Z≈42	P_Z_Curv_S4	0.05	3%
Weakening of the S_1 shell	T_low_SL	0.31	0.006
$(\hbar\omega)_{\mathrm{eff}}$ for tunneling of the S_1 channel	T_low_S1	0.31	0.006
$(\hbar\omega)_{\mathrm{eff}}$ for tunneling of the S_1 channel	T_low_S2	0.31	0.006
$(\hbar\omega)_{\mathrm{eff}}$ for tunneling of the S_1 channel	T_low_S3	0.31	0.006
$(\hbar\omega)_{\mathrm{eff}}$ for tunneling at Z≈42	T_low_S4	0.31	0.006
Width of the fragment distribution in N/Z	HOMPOL	1.3	6%
Charge polarization	POLARadd	0.35	0.06
Asymmetry in diffuseness of S_2 mass peak	S2leftmod	0.75	3%
General scaling of fragment angular moment	Jscaling	1.0	6%

1000 sets of model parameter samples are generated and based on these samples, independent fission yield samples of ^{235}U, ^{239}Pu, and ^{241}Pu thermal neutron-induced fissioning systems are calculated individually. The number of fission events of GEF is 2×10^5. Based on these samples, the respective fission yield covariances of the three fissioning systems are calculated.

2.2 Verification of fission yield covariances

To verify the fission yield covariances, 1000 samples of fission yield are generated respectively for the three fissioning systems by resampling the above-obtained covariances. Besides, as mentioned above, there are

1000 samples of fission yield by sampling the GEF model parameters. Based on the two types of samples, neutronics-burnup coupling calculation is conducted for the TMI-1 pin cell problem in UAM project [13]. The fuel material of this problem is UO_2, and the ^{235}U enrichment is 4.85%. The calculation is based on the hot full power condition and the power density is 33.58 MW/tU. The burnup of the problem reaches 60 GW·d/tU. Figure 1 shows the geometry of the TMI-1 pin cell. The relative uncertainties of the responses, the infinite multiplication factor (k_{inf}), and the number densities of important fission product nuclides, are calculated based on the fission yield samples resampled based on the above-obtained covariances. The same uncertainties are also calculated based on the fission yield samples by sampling the GEF model parameters, which are taken as the reference results. The neutronics-burnup coupling calculation tool is the high-fidelity reactor physics code NECP-X [14]. Other burnup data and cross section data are extracted from ENDF/B-VII.1 evaluated nuclear data library [15].

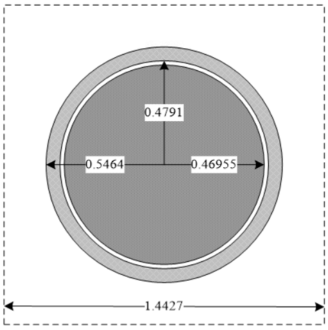

Fig.1. Geometry of the TMI-1 pin cell (unit: cm).

Figure 2 to Figure 4 show the results of the uncertainty comparison. The results show that for the three fissioning systems, the uncertainties of resampling based on the fission yield covariances are all consistent with the reference results. This demonstrates that the method of generating independent fission yield covariances for individual fissioning systems is correct.

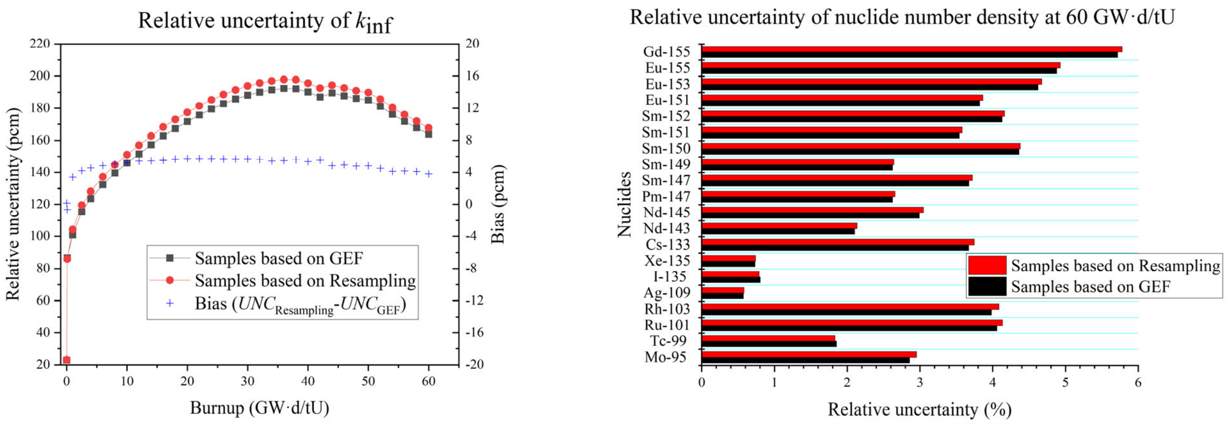

Fig.2. Comparison of uncertainties of the TMI-1 problem based on fission yield samples of $^{235}U+n_{th}$.

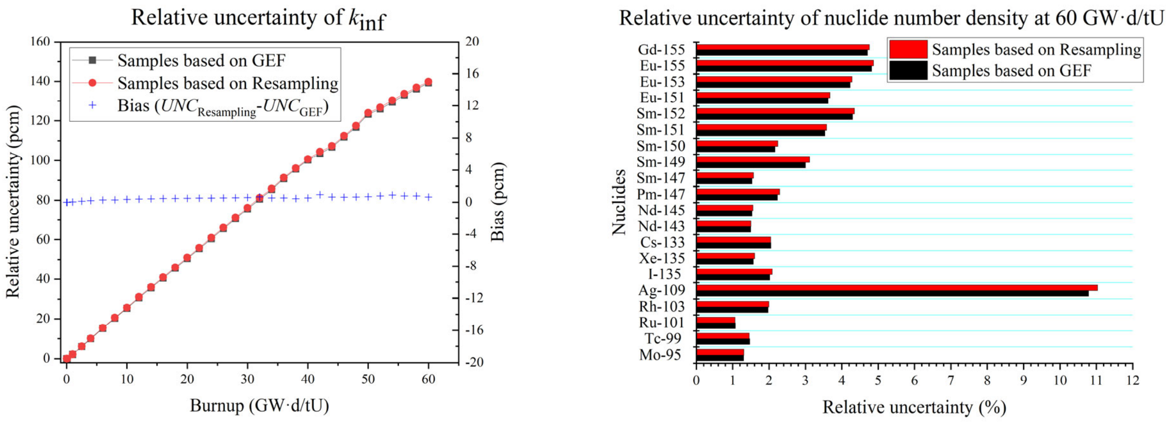

Fig.3. Comparison of uncertainties of the TMI-1 problem based on fission yield samples of $^{239}Pu+n_{th}$.

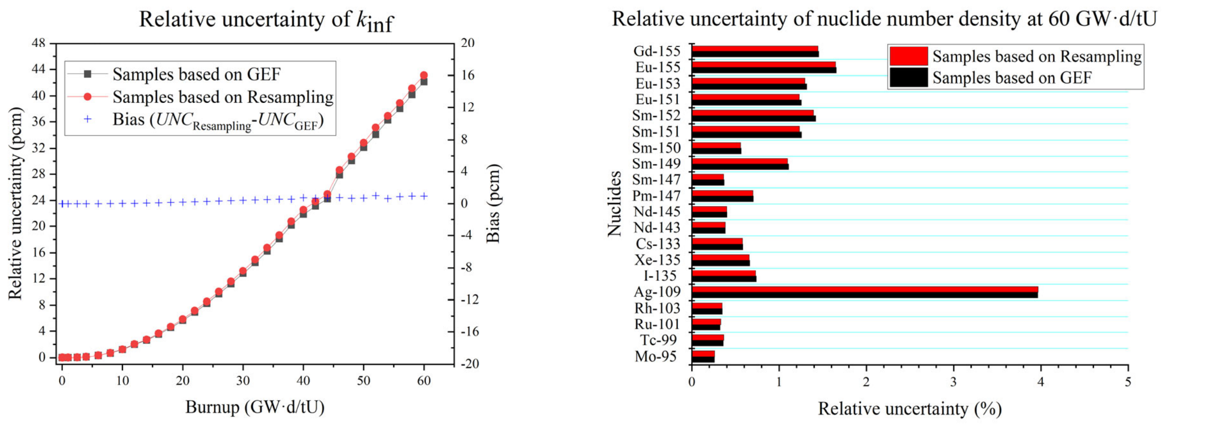

Fig.4. Comparison of uncertainties of the TMI-1 problem based on fission yield samples of ^{241}Pu+n$_{\mathrm{th}}$.

3 Influence of correlations among fissioning systems

Generally, there are correlations among multiple fissioning systems. According to the analysis in Section 2, since the same set of model parameter sample of GEF can calculate one set of fission yield sample for each of the three fissioning systems (^{235}U+n$_{\mathrm{th}}$, ^{239}Pu+n$_{\mathrm{th}}$, and ^{241}Pu+n$_{\mathrm{th}}$) simultaneously, the fission yield samples calculated by GEF actually include the correlations among fissioning systems. To analyze the influence of these correlations, two cases are calculated. Case 1 uses fission yield samples of three fissioning systems calculated by GEF in one random run of the TMI-1 problem. Case 2 uses fission yield samples of one fissioning system calculated by GEF in one random run of the TMI-1 problem and calculates the sum of the uncertainties of three fissioning systems with equation (1) :

$$\Delta_{\mathrm{sum}} = \sqrt{\left(\Delta_{\mathrm{U235}}\right)^2 + \left(\Delta_{\mathrm{Pu239}}\right)^2 + \left(\Delta_{\mathrm{Pu241}}\right)^2} \tag{1}$$

where Δ is relative uncertainties of burnup-related responses (k_{inf} or nuclide number densities).

In other words, Case 1 considers correlations among three fissioning systems and Case 2 assumes that the three fissioning systems are independent. Figure 5 shows the uncertainty results for the two cases. It can be seen that the uncertainties of Case 1 considering correlations are significantly higher than that of Case 2 assuming independence. The bias of relative uncertainty of k_{inf} reaches about 100 pcm at the end of irradiation. For uncertainties of nuclide number densities, the two cases also differ greatly. Therefore, the influence of the correlations among fissioning systems on the quantification of uncertainty cannot be ignored.

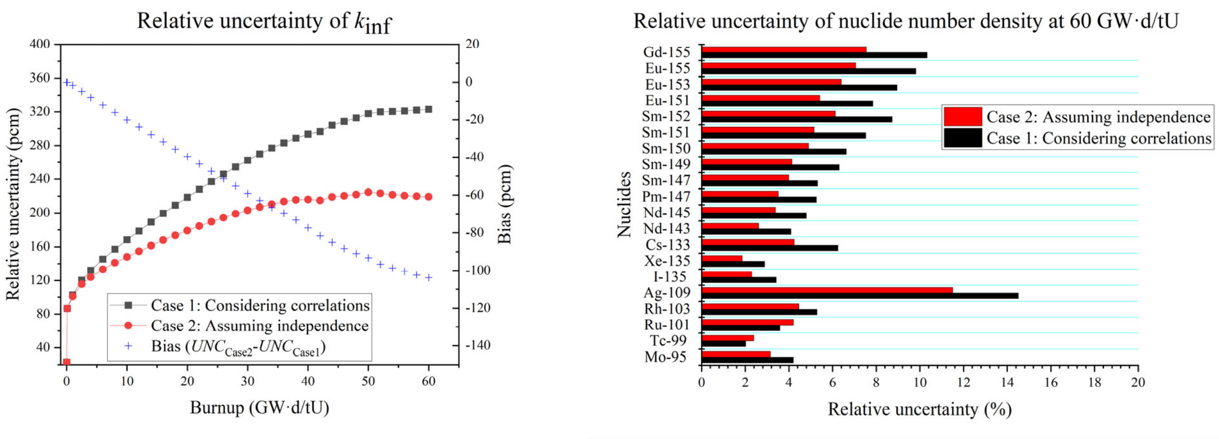

Fig.5. Uncertainty results of the TMI-1 problem for influence of correlations among fissioning systems.

This section also adopts the method like Section 2 to calculate the joint covariances among independent fission yields of the three fissioning systems based on the fission yield samples calculated with GEF model parameter samples. The method to verify the joint covariances is also like Section 2. The fission yield samples of three fissioning systems are obtained based on the resampling with joint covariances, and the samples of three fissioning systems are used simultaneously in one random run of the TMI-1 problem to calculate the uncertainties. The reference uncertainty results are also based on fission yield samples calculated with GEF. The comparison of uncertainty results is shown in Figure 6. The uncertainty results of resampling show good consistency with the reference results, which proves that the GEF calculation process for the correlations among fissioning systems is also correct. Thus, when nuclear data users need the covariances of fission yield data, the GEF code can provide covariance data for individual fissioning systems and multiple fissioning systems at the same time.

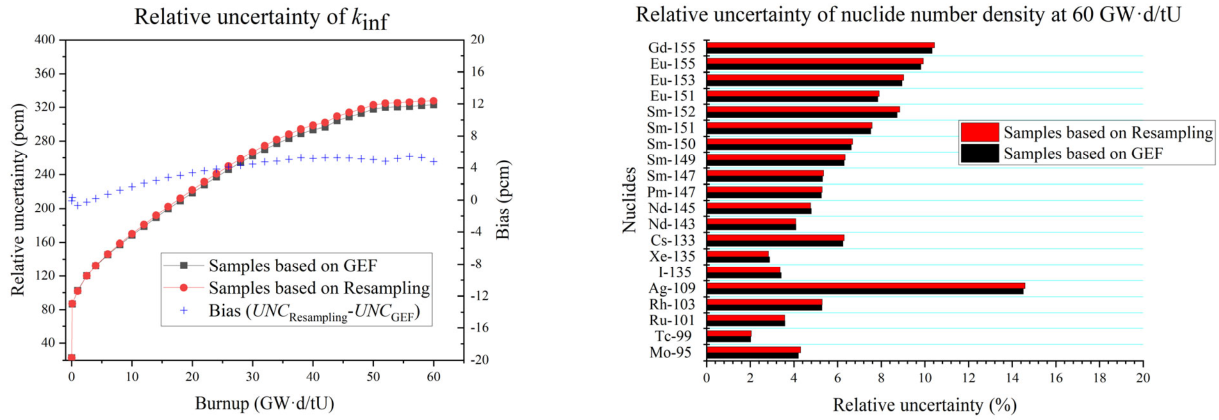

Fig.6. Comparison of uncertainties of the TMI-1 problem based on fission yield samples from joint covariances.

4 Preliminary adjustment of GEF model parameters

This section adopts the Bayesian Monte Carlo method to adjust 23 parameters with normal distribution in GEF2021.1.1 which are shown in Table 1 and presents some preliminary numerical results.

4.1 Bayesian Monte Carlo method

The Bayesian Monte Carlo method combines Bayesian inference theory with Monte Carlo sampling and adjusts the prior nuclear data by calculating the weight of each sample.

Based on the work in this section, Bayesian inference theory is shown in equation (2):

$$p(\boldsymbol{\sigma}'|\ \mathbf{E}) \propto \mathrm{L}(\mathbf{E}|\ \boldsymbol{\sigma})p(\boldsymbol{\sigma}) \tag{2}$$

where $\boldsymbol{\sigma}$ is the prior GEF model parameter vector and $\boldsymbol{\sigma}'$ is the posterior parameter vector; $\mathbf{E}$ is the experimental data vector; $p(\boldsymbol{\sigma})$ is the prior probability density function of parameters; $\mathrm{L}(\mathbf{E}|\ \boldsymbol{\sigma})$ is the likelihood function to use experimental information to adjust prior parameters; $p(\boldsymbol{\sigma}'|\ \mathbf{E})$ is the posterior probability density function of parameters. According to equation (2), Bayesian inference theory adjusts the probability distribution of prior parameters by introducing experimental data. In our work, the experimental data are the inventories of fission product nuclides.

The Bayesian Monte Carlo method first calculates the fission yield samples based on the model parameter samples of GEF and calculates the fission product nuclide inventory samples based on the fission yield samples. Next, the likelihood function in the form of weight for each model parameter sample based on comparing the calculated and experimental values of fission product nuclide inventories is calculated. Finally, the model parameters are adjusted based on Bayesian inference theory. To calculate the weight of each sample, first calculate the square of Mahalanobis distance χ_i^2 for each sample, as shown in equation (3):

$$\chi_i^2 = (\mathbf{E}-\mathbf{C}_i)^{\mathrm{T}}\mathbf{V}_{\mathrm{E}}^{-1}(\mathbf{E}-\mathbf{C}_i) \tag{3}$$

where $\mathbf{C}_i$ is the calculated fission product inventory sample vector based on prior parameter sample i; $\mathbf{V}_{\mathrm{E}}$ is the covariance matrix of experimental data. Then, ω_i, the weight of sample i is calculated with equation (4):

$$\omega_i = \exp(-\frac{\chi_i^2}{\chi_{\min}^2}) \tag{4}$$

where $\chi_{\min}^2$ is the minimum value of all the χ_i^2 values.

We can obtain the posterior model parameters and the posterior parameter covariances through equation (5) and equation (6):

$$\boldsymbol{\sigma}' = \frac{\sum_{i=1}^{N}\omega_i\boldsymbol{\sigma}^i}{\sum_{i=1}^{N}\omega_i} \tag{5}$$

$$\mathrm{cov}(\sigma_l', \sigma_m') = \frac{\sum_{i=1}^{N}\omega_i(\sigma_l^i-\sigma_l')(\sigma_m^i-\sigma_m')}{\sum_{i=1}^{N}\omega_i}, l,m=1,\ldots\ldots,N_\sigma \tag{6}$$

where N is the number of samples; N_σ is the number of model parameters; σ_l^i is the i-th prior sample of model parameter l.

The general steps for adjusting GEF model parameters are:

(1) Sample GEF model parameters.
(2) Calculate fission yield samples with the above parameter samples.
(3) Calculate fission product inventory samples $\mathbf{C}$ corresponding to experimental data $\mathbf{E}$.
(4) Calculate the weight of each sample with equation (3) and equation (4).
(5) Adjust the model parameters with equation (5) and equation (6).

4.2 Generation of pseudo-experimental data

The Bayesian Monte Carlo method has high requirements for experimental data, which requires that experimental data and corresponding calculated data have high consistency [10]. In addition, equation (3) shows that the covariances of experimental data are needed. Nevertheless, common integral experimental data, such as nuclide inventory data in SFCOMPO-2.0 spent fuel experimental database [16], usually have some outliers, and these experimental data do not contain covariances, which will seriously affect the effect of nuclear data adjustment.

Therefore, this section generates pseudo-experimental data based on the fission yield data in the evaluated nuclear data files (ENDF). The accuracy of pseudo-experimental data is high, and covariance data are obtained. The specific steps of generation are:

(1) Generate fission yield samples based on mean values and uncertainties of fission yields in ENDF.

(2) Calculate nuclide number density samples of a burnup problem based on the above samples.

(3) Calculate the sample mean values and covariances based on the above nuclide number density samples.

After this process, the sample mean values are the values of the pseudo-experimental data, and the sample covariances are the covariances of the pseudo-experimental data.

In the process of generating pseudo-experimental data for this work, fission yield data of ^{235}U thermal neutron-induced fission in JEFF-3.3 evaluated nuclear data library [17] are selected for sampling, and the sample size is 10000. The burnup problem is the TMI-1 pin cell and the calculation tool is NECP-X code. The nuclide number densities of 13 fission product nuclides at 60 GW·d/tU are taken as the final pseudo-experimental data. These nuclides are: ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{133}Cs, ^{143,145}Nd, ^{151,152}Sm, ^{151,153,155}Eu, and ^{155}Gd. These nuclides are important in the uncertainty analysis of the burnup credit system [18], so they are selected. The correlation matrix of the pseudo-experimental data of this work is shown in Figure 7. Correlations are shown for the number densities of different nuclides.

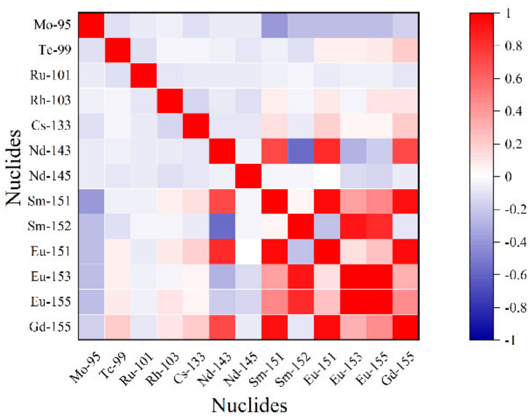

Fig.7. Correlation matrix of pseudo-experimental data.

4.3 Numerical results

^{235}U thermal neutron-induced fission is selected as the fissioning system for adjustment of GEF model parameters. The number of model parameter samples is 10000 and each run of GEF uses 2×10^5 fission events. To maintain consistency with the pseudo-experimental data, the calculation of GEF-based prior fission yield samples also uses the burnup data of JEFF-3.3.

The relative adjustment of model parameters is shown in Figure 8. The results show that the adjustment range of all parameters is reasonable and within the prior uncertainties. The uncertainty results of prior and posterior parameters are shown in Figure 9. For most parameters, the posterior uncertainties are reduced, and the effect is more obvious for parameters with larger prior uncertainties.

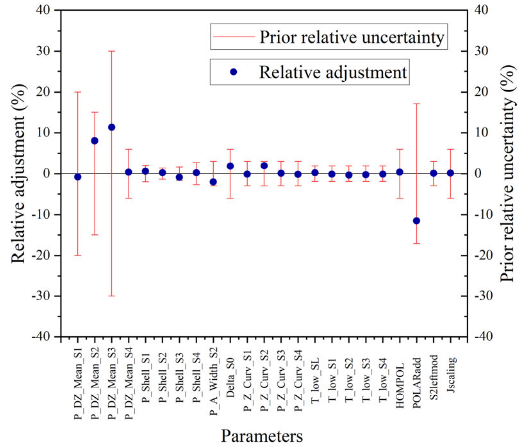

Fig.8. Relative adjustment of model parameters.

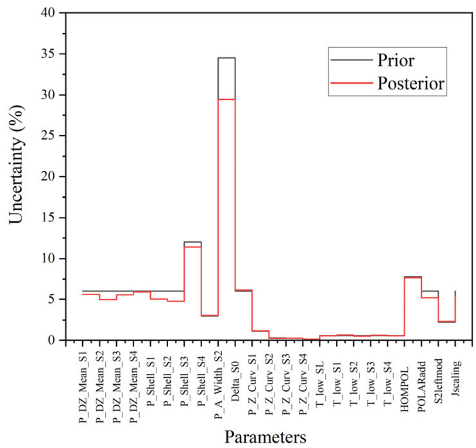

Fig.9. Comparison of uncertainties of prior and posterior parameters.

The fission yield covariances of ^{235}U thermal neutron-induced fission calculated by GEF and the uncertainties of burnup-related responses calculated based on prior and posterior parameters are compared. The prior and posterior lower triangular correlation matrices of fission yields are shown in Figure 10. There are 67 fission product nuclides compared: ^{87,88}Br, $^{88\text{-}92}$Kr, $^{91\text{-}94}$Rb, $^{92\text{-}97}$Sr, ^{95,96m,97,97m,98,98m,99}Y, $^{97\text{-}102}$Zr, ^{101,103}Nb, ^{103,104}Mo, $^{131\text{-}133}$Sb, $^{132,133,133m,134\text{-}136}$Te, ^{135,136,136m,137,138}I, $^{136\text{-}141}$Xe, $^{139\text{-}143}$Cs, $^{141\text{-}145}$Ba, ^{144,145}La, and ^{148}Ce. The fission yields of these nuclides are generally greater than 1%, so the calculation accuracy of GEF is higher. Figure 10 shows that the posterior correlations have decreased for most nuclides. Figure 11 shows the prior and posterior uncertainty results of the TMI-1 problem based on fission yield samples of ^{235}U thermal neutron-induced fission calculated by GEF. The basic setup for the calculation is the same as in Figure 2. The results show that the posterior uncertainties of k_{inf} and nuclide number densities are significantly reduced. The reduction of uncertainty of k_{inf} up to about 80 pcm throughout the process of irradiation. The above numerical results prove that the preliminary adjustment of GEF model parameters is effective.

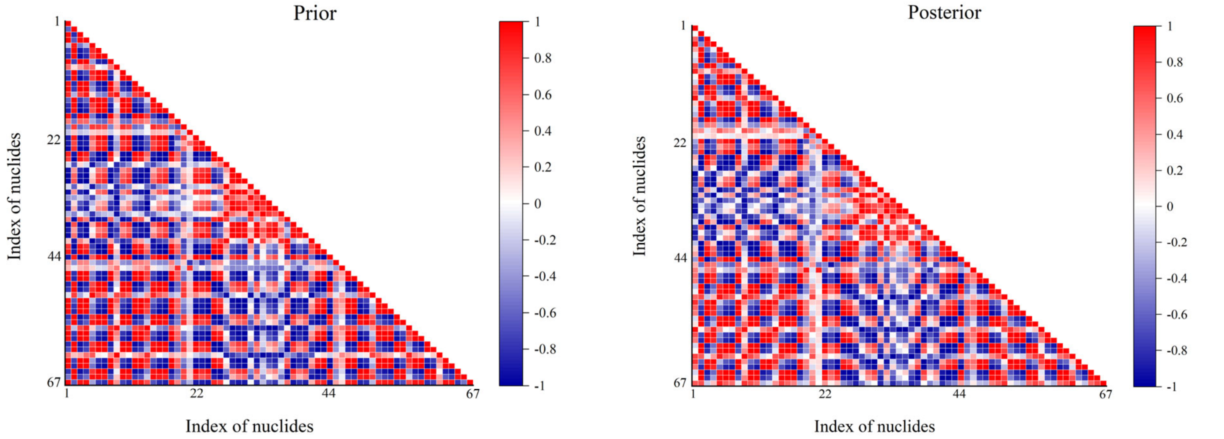

Fig.10. Comparison of prior and posterior fission yields correlation matrices.

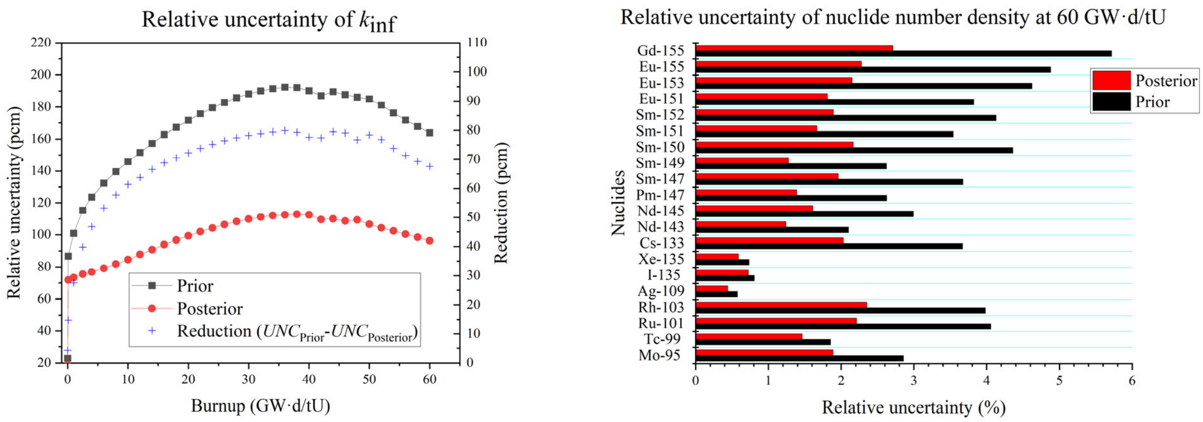

Fig.11. Comparison of prior and posterior uncertainties of the TMI-1 problem.

5 Conclusions and perspectives

The independent fission yield covariances are generated based on the GEF model code in this paper. The samples of fission yield are calculated by sampling model parameters, and the covariances are calculated based on the samples of fission yield. The above process is carried out for ^{235}U, ^{239}Pu, and ^{241}Pu thermal neutron-induced fissioning systems, individually. To verify the correctness of the process, the fission yield samples calculated by GEF and the fission yield samples generated based on the covariances of this work are respectively applied to the random run of the TMI-1 pin cell burnup problem. The uncertainties of the infinite multiplication factor (k_{inf}) and nuclide number densities propagated by two types of fission yield samples are in good consistency for three fissioning systems separately. The correctness of the method of generating fission yield covariance is verified.

The influence of correlations among fissioning systems is also analyzed and quantified. The numerical results show that the influence cannot be ignored. The joint independent fission yield covariances of multiple fissioning systems are calculated with GEF and verified. Finally, the parameters of the GEF model code are preliminarily adjusted with the Bayesian Monte Carlo method based on the pseudo-experimental data. The results show that the adjustment was effective.

The following conclusions are summarized:

(1) Independent fission yield covariances are obtained based on the sampling of GEF model parameters. The influence of correlation among fissioning systems cannot be ignored.

(2) When nuclear data users need the covariances of fission yield data, the GEF code can provide correct covariance data for individual fissioning systems and multiple fissioning systems simultaneously.

(3) Preliminary adjustment of GEF model parameters is performed with the Bayesian Monte Carlo method and the effect is good.

In future work, we will do more numerical tests on the current nuclear data adjustment method and strive to improve the applicability of the method. We will try to apply the adjustment method to other nuclear data, not limited to fission yield-related data.

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