Cross sections data adjustment for KRITZ-2:13

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Abstract

Over the past years, the cross-sections reaction data has been re-evaluated several times, in order to approximate the nuclear model measurements with the predictions with great reliability. In our work, uncertainty analysis caused by the data on the neutron factor (K_{eff}) and the reactivity temperature coefficient (RTC), in addition to nuclear data adjustment related to the nuclear reactor physics have been done for KRITZ-2:13 reactor, with ENDF/B - VII.1, ENDF/B - VIII.0 and JENDL - 4.0 evaluations by the nuclear code MCNP6.1. Our analysis detects that the greatest uncertainty on K_{eff} and RTC in the studied libraries comes from the capture and fission reaction contributions respectively, for U-238 and U-235. The previous reactions and their covariances were adjusted using the generalized least squares method (GLLSM), in order to contribute to improve the data needed for neutron simulation of experiments and to ensure the installations safety, where K_{eff} and RTC represent neutron parameters reflecting the modification effects in the data.

Keywords: Covariance matrix; KRITZ; nuclear uncertainty; sensitivity; temperature coefficient.

1. Introduction

Practical necessity is the main motivation for research in the field of nuclear uncertainty and its re-evaluation. These uncertainties can propagate through nuclear system simulations into safety and operation related parameters. Inaccurate treatment of uncertainty in nuclear reactor operating and design can affect the economic efficiency and thus the sustainability of nuclear power. It is therefore important in the study and design of nuclear reactors to carry out an accurate re-evaluation of the cross section uncertainties on the critical neutron coefficients as K_{eff} and RTC.

Cross-section data helps reveal the reaction phenomenon's mechanisms within the process of a nuclear reaction (Hasan Özdoğan *et al*., 2021). This data depended on nuclear experiments, is the fundamental component of Monte Carlo and deterministic methods that are constantly being improved to reduce the uncertainties related to this data. Nuclear uncertainty can be improved by a variety of statistical techniques (C. de Saint-Jean *et al*., 2010) such as Lagrange multipliers, Monte Carlo total, etc. But the generalized least squares technique stays the most suitable. This current work is dedicated to the study and re-evaluation of data uncertainty regarding nuclear reactor physics for the important isotopes in a structure of 15-group energy. The capture cross-section of U-238 and fission of U-235 have significant uncertainty values on both K_{eff} and RTC coefficients in all the libraries studied ENDF/B - VII.1 (Chadwick *et al*., 2011), ENDF/B - VIII.0 (D. A. Brown *et al*., 2018) and JENDL - 4.0 (K. SHIBATA *et al*., 2011) (that will be mentioned later as the two ENDF/Bs and JENDL libraries). These reactions are the main cause of deviations between the calculated and benchmark values of the two coefficients. It is recommended to modify these cross-sections as well as their covariance matrices in all libraries. Adjustment of these reactions data will contribute to reducing the uncertainty values on K_{eff} and RTC and thus correcting the calculated values of these neutron coefficients.

KRITZ benchmarks performed in Sweden, during the 70s and included three experiments that will be critical at cod temperatures (KRITZ-2:1C ,KRITZ-2:13C and KRITZ-2:19C) and at hot temperatures (H configurations), the first two are with uranium rods, and the last one with fuel of mixed-oxide. The rods are on a square pitch, surrounded by a light water reflector. KRITZ-2:13 core (the study axis) was square and consisted of a regular lattice of UO2 fuel rods on a 1.635 cm pitch. Its C configuration was at 22.1C and the H configuration at 243.0 C. Additional details on KRITZ benchmarks are in Refs. (L. SNOJ *et al*., 2009; I. REMEC *et al*., 2002; International Handbook of Evaluated Reactor Physics Benchmark Experiments, 2011; Benchmark on the KRITZ-2 LEU and MOX Critical Experiments, 2006).

Experimental uncertainties of the benchmark values of K_{eff} were 210 and 200 pcm, respectively, for C and H configurations of KRITZ-2:13, where the modeling uncertainties were 8 pcm for both configurations. The small value of the statistical uncertainty was obtained from the following data: 40,000 neutrons per cycle for 1600 effective cycles from total number of 1750.

The old versions (4B and 4C) of the code MCNP with old versions of some libraries: (3.2 and 3.3) of JENDL, (90.2 and 2002) of IRDF and (V and VI) of ENDF/B have been used in one of the studies of the KRITZ reactor (Benchmark on the KRITZ-2 LEU and MOX Critical Experiments, 2006), which is concerned with the analysis of sensitivity and nuclear uncertainty about the K_{eff}. This study showed that the greatest participation in sensitivity and nuclear uncertainty for KRITZ-2:13 comes from the capture reaction of U-238. Sensitivities were nearly identical for all libraries, while uncertainty varied from one library to another.

2. Methodology

By using the card KSEN from the code MCNP6.1 (Denise *et al*., 2014) we have generated the sensitivity coefficients of isotope reactions at 22.1C and 243C, respectively, for KRITZ-2:13C and KRITZ-2:13H in an energy range partitioned into 15 groups (table 1) for the neutron coefficients K_{eff} and RTC. These sensitivities have been calculated based on the adjoint-weighting technique that does not take into account disturbances that may appear from fission spectra or scattering laws (Romojaro *et al*., 2017), which may lead to spurious and false results in the measurements (Denise *et al*., 2014). NJOY system (Macfarlane *et al*., 2017) has been used to convert the ENDF6 data of the libraries into ACE format necessary for

MCNP code, as well as to generate the covariances, by means of ERRORJ module. Sensitivities G and covariances M will be combined according to the first equation in order to calculate the nuclear uncertainty on K_{eff}:

$$\frac{\Delta \boldsymbol{keff}}{\boldsymbol{keff}} = \boldsymbol{G}^{+}\boldsymbol{MG}\ ,\ \boldsymbol{G}^{+} \text{ is a transpose of } \boldsymbol{G} \tag{1}$$

Table 1. Energy groups (A. Ahmed *et al.*, 2019)

Numbers	Energy groups (ev)
1	1.00E-5 - 0.110
2	0.110 – 0.540
3	0.540- 4.00
4	4.00 - 22.6
5	22.6 - 454
6	454 - 2030
7	2030 - 9120
8	9120 - 24800
9	24800 - 67400
10	67400 - 1.83E+5
11	1.83E+5 - 4.98E+5
12	4.98E+5 - 1.35E+6
13	1.35E+6 - 2.23E+6
14	2.23E+6 - 6.07E+6
15	6.07E+6 - 1.96E+07

For a temperature range [T1, T2], with neutron factors [K_{eff1}, K_{eff2}], the RTC could be obtained by the following formula (El Ouahdani *et al.*, 2015):

$$\alpha = \frac{1}{\Delta T}\frac{K_{eff2}-K_{eff1}}{K_{eff1}K_{eff2}} \tag{2}$$

Considering the quantity $\Delta T = T_2 - T_1$ is constant, we can find:

$$\Delta\alpha = \left[\frac{\Delta K_{eff2}}{(K_{eff2})^2} - \frac{\Delta K_{eff1}}{(K_{eff1})^2}\right]\frac{1}{\Delta T}$$

So, the nuclear uncertainty on the RTC can be expressed as:

$$\frac{\Delta\alpha}{\alpha} = \left[\frac{K_{eff1}\frac{\Delta K_{eff2}}{K_{eff2}} - K_{eff2}\frac{\Delta K_{eff1}}{K_{eff1}}}{K_{eff2}-K_{eff1}}\right] \tag{3}$$

K_{eff1}: Is the neutron multiplication factor at T_1

$\frac{\Delta K_{eff1}}{K_{eff1}}$: Is the relative uncertainty on K_{eff1}due to nuclear data at T_1
K_{eff2}: Is the neutron multiplication factor at T_2
$\frac{\Delta K_{eff2}}{K_{eff2}}$: Is the relative uncertainty on K_{eff2}due to nuclear data at T_2

Statements requiring adjustments in nuclear data (reactions that are important in the sensitivity analysis with uncertainty larger than 100 pcm (C. de Saint-Jean *et al*., 2010)) that would produce the best agreement between the measured and calculated values of integral experiments - as GLLSM supposes-, have been carefully selected. Depending on GLLSM, this reactions data can be adjusted according to these equations (C. de Saint-Jean *et al*., 2010 ; H. Kuroi & H. Mitani, 1975; V. Sobes *et al*., 2016; Makhloul *et al*, 2018):

$$T^{Adj} = T_0 + MG^t[GMG^t + V_e + V_m]^{-1}[R_e - R_c(T_0)] \quad (4)$$

$$M^{Adj} = M - MG^t[GMG^t + V_e + V_m]^{-1}GM \quad (5)$$

Where
$T_0\ and\ T^{Adj}$ are the cross sections before and after adjustment
$M\ and\ M^{Adj}$ are the covariances before and after adjustment
$R_e\ and\ R_c$ are measured and analytical values of integral experiments
$V_e\ and\ V_m$ are experimental and modeling errors of integral experiments

3. Results

3.1. Critical Calculations

One of the advantages of the Monte Carlo method is to focus on the nuclear uncertainties by reducing the errors related to modeling and design. The critical coefficients (K_{eff} and RTC) for KRITZ-2:13 were calculated by the card KCODE from the code MCNP6.1, which offers complex geometry modeling capabilities with high accuracy 3-D calculations of the physical system (Zuhair *et al*., 2021).

The calculated values of K_{eff} for the two configurations of KRITZ-2:13 with the three evaluations, the benchmark values, the experimental uncertainties and the relative differences are listed on table 2.

Table 2. Benchmark (Ivan Kodeli & Luka Snoj, 2012) And Calculated Values Of K_{eff}

KRITZ-Experiment		Benchmark		JENDL - 4.0		ENDF/B - VII.1		ENDF/B - VIII.0	
		K_{eff}	S.d pcm	K_{eff}	|C/E-1| (%)	K_{eff}	|C/E-1| (%)	K_{eff}	|C/E-1| (%)
2:13	C	1.0013	210	0.99887	0.24	0.99892	0.23	0.99896	0.23
	H	1.0019	200	0.99800	0.38	0.99797	0.39	0.99835	0.35

For our two configurations of KRITZ-2:13 in the two ENDF/Bs and JENDL libraries, the simulated values of K_{eff} were underestimated from benchmark values. This underestimation will be explained by the uncertainty analysis. Due to the temperature effect, the underestimation in H configuration is less than of the C. There was a noticeable agreement between these calculated values for the three investigated libraries, with large deviations between them and the benchmark values. For all the studied configurations and libraries, the relative deviations are greater than the analytical and modeling errors, this calls for an uncertainty analysis of the nuclear data.

The library that gives calculated values for the K_{eff} closer to the benchmarks - Least deviations according to Figure 1 - in the two configurations, is the new library ENDF/B-VIII.0, ENDF-6 formats for some components and sections of fissile isotopes have been improved for this library.

Simulated values of the RTC for KRITZ-2:13 in the two ENDF/Bs and JENDL libraries are listed on table 3.

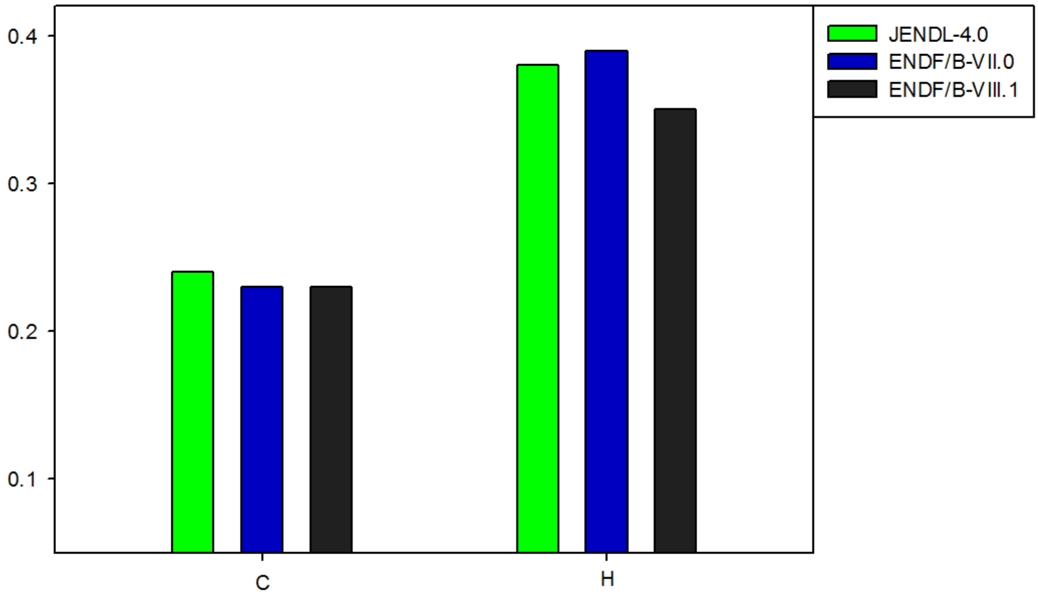

Fig. 1. Deviations Between Benchmark And Simulated Values Of K_{eff} For C and H Configurations Of KRITZ-2:13.

Table 3. Calculated Values Of RTC

α in pcm/°C			
Benchmark*	JENDL-4.0	ENDF/B-VII.1	ENDF/B-VIII.0
-0.03	-0.39	-0.43	-0.27

* *According to the benchmark values of K_{eff}.*

All the simulated values of RTC were systematically negative, as for safety standards, it is required that the RTC be negative (Kaddour *et al.*, 2013). The results showed a very good agreement between the considered libraries in the two configurations of KRITZ-2:13, with big deviations between them and the benchmark values. The absolute values of the RTC obtained in our study for both evaluations JENDL-4.0 and ENDF/B-VII.I are lower than of other study (El Ouahdani *et al.*, 2015) whose results were (-1.49 and -0.88) pcm/°C respectively for JENDL-4.0 and ENDF/B-VII.I. In that study the data was treated using the assistant code Makxsf (interpolation between two temperatures) along with the NJOY code. While in our study, we treated the data only with NJOY code for each temperature without the need for an assistant code.

3.2. K_{eff} Sensitivity

Figures 2 and 3 show the integrated sensitivities over the 15 energies for C and H configurations of KRITZ-2:13. The reactions sensitivity to the K_{eff} is almost identical in the two ENDF/Bs and JENDL evaluations. The KRITZ-2:13 reactor with its critical configurations was very sensitive to the fission reaction of U-235 and the capture of U-238. The negative sensitivity of the latter reaction means that the large uncertainty value of this reaction will cause a decrease in the calculated values of K_{eff} in the three libraries. The reactions of capture for U-235 and the elasticity for H-1 also have important sensitivities in the investigated libraries.

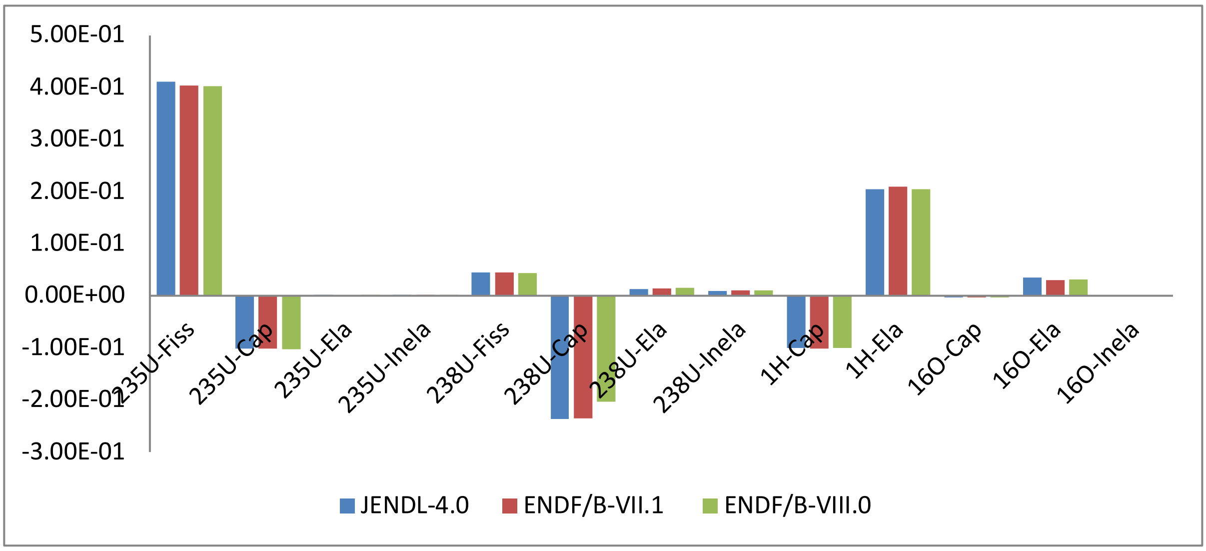

Fig. 2. Integrated sensitivities of K_{eff} for KRITZ-2:13C

Fig. 3. Integrated sensitivities of K_{eff} for KRITZ-2:13H

3.3. RTC Sensitivity

According to equation 3, the uncertainty value of the reactivity coefficient depends to a large degree on the uncertainty values of the K_{eff} and, accordingly, on the values of its sensitivity coefficients. In other words, the values of the RTC uncertainty are not dependent on its own sensitivity values. However, we did analyze the RTC sensitivity to the reaction cross sections of the two ENDF/Bs and JENDL evaluations for KRITZ-2:13 experiment. The purpose of this analysis is to identify reactions for which the sensitivity to the cross-sections is large, whereas those reactions themselves have a significant contribution to the uncertainty on RTC. These will be the reactions that really need to be adjusted.

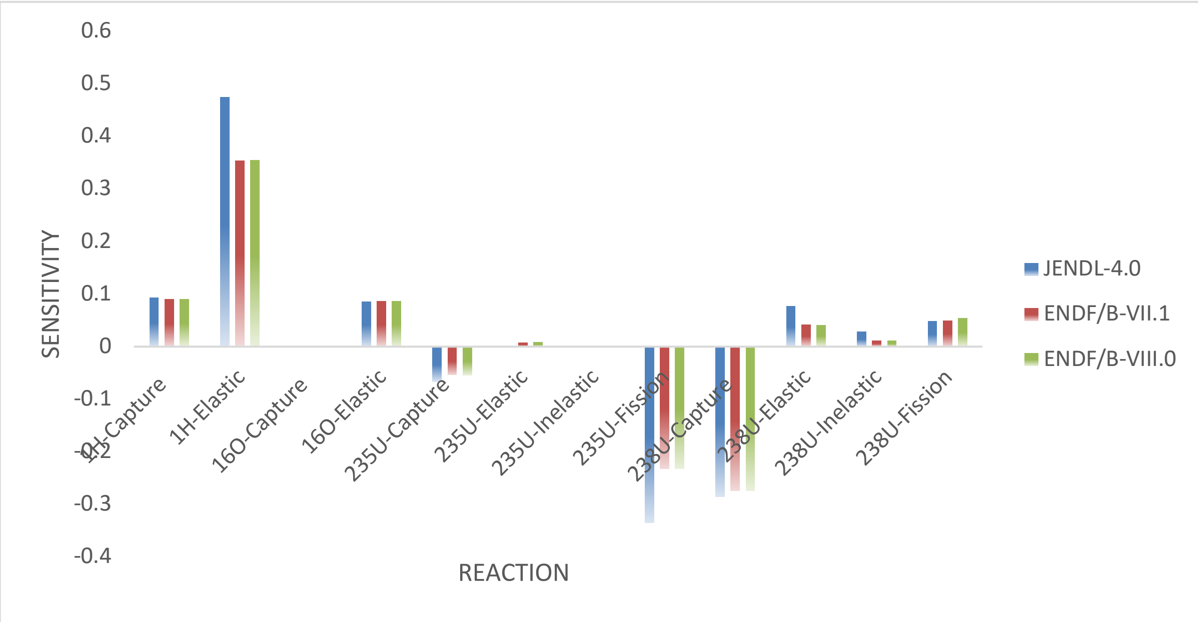

Fig. 4. Sensitivities of *RTC* for KRITZ-2:13

As shown on the previous figure, sensitivity analysis results showed a good consistency between the three different libraries reactions. The RTC in KRITZ-2:13 was large sensitive to fission and capture reactions, respectively of U- 235 and U-238 that are the most sensitive reactions in the three evaluations. Elastic cross section of H-1 is a considered reaction in the sensitivity analysis of RTC in all libraries, but its contribution to uncertainty is small as we will see in the uncertainty analysis.

3.4. Nuclear uncertainty

Data uncertainties on the K_{eff}, due to reactions of the four isotopes: H-1, O-16, U-235 and U-238 are shown on tables 4 and 5, respectively, for C and H configurations of KRITZ-2:13 with the two ENDF/Bs and JENDL evaluations. The reaction that contributes the most to the uncertainty on the K_{eff} and that which gives the greatest contribution to the total uncertainty for this coefficient is the capture reaction of U-238. The underestimation found in the calculated values of K_{eff} is mainly due to the great uncertainty of this reaction, as well as its large negative sensitivity in the three evaluated libraries for the two configurations of KRITZ-2:13. Fission reaction of U-235 in the three libraries, capture of the same isotope in ENDF/B-VII.1 and JENDL-4.0, and elastic of H-1 only in ENDF/B-VII.1 are also important in this analysis for both configurations of KRITZ-2:13. In order to reduce the data uncertainties on the K_{eff}, all cross-sections of the previous reactions must be adjusted as well as their covariance matrices according to their mentioned libraries.

As we can see from figure 5, the greatest nuclear uncertainty on the RTC for KRITZ-2:13 is due to the capture reaction of U-238 in the three libraries. The fission reaction of U-235 also has a significant contribution to uncertainty on the RTC in all libraries, but by a smaller range from the capture of U-238.

Table 4. Uncertainties (in pcm) due to cross-sections for the configuration KRITZ-2:13C

cross-sections		JENDL-4.0	ENDF/B-VII.1	ENDF/B-VIII.0
		Uncertainty (pcm)	Uncertainty (pcm)	Uncertainty (pcm)
1H	(n,γ)	50.05	230.01	87.2
	(n,n)	51.95	**118.52**	95.0
16O	(n,γ)	61.50	132.35	16.03
	(n,n)	47.16	72.488	68.5
235U	(n,γ)	**157.2**	**144.1**	41.32
	(n,n)	1.043	0.555	0.269
	(n,n')	1.579	1.323	0.370
	(n,f)	**172.8**	**138.1**	**165.3**
238U	(n,γ)	**322.3**	**356.76**	**202.3**
	(n,n)	30.73	22.349	30.73
	(n,n')	59.32	174.15	30.86
	(n,f)	26.38	23.104	53.95
Total		418	536	310

Table 5. Uncertainties (in pcm) due to cross-sections for the configuration KRITZ-2:13H

cross-sections		JENDL-4.0	ENDF/B-VII.1	ENDF/B-VIII.0
		Uncertainty (pcm)	Uncertainty (pcm)	Uncertainty (pcm)
1H	(n,γ)	49.12	234.8	85.12
	(n,n)	53.51	**123.9**	90.70
16O	(n,γ)	65.50	130.23	18.65
	(n,n)	55.16	74.16	64.3
235U	(n,γ)	**160.73**	**148.1**	44.32
	(n,n)	1.103	1.444	0.634
	(n,n')	1.621	0.755	0.828
	(n,f)	**164.82**	**129.5**	**157.8**
238U	(n,γ)	**342.7**	**395.7**	**224.23**
	(n,n)	32.36	30.03	32.36
	(n,n')	63.16	189.9	29.84
	(n,f)	29.43	25.56	58.63
Total		434	570	320

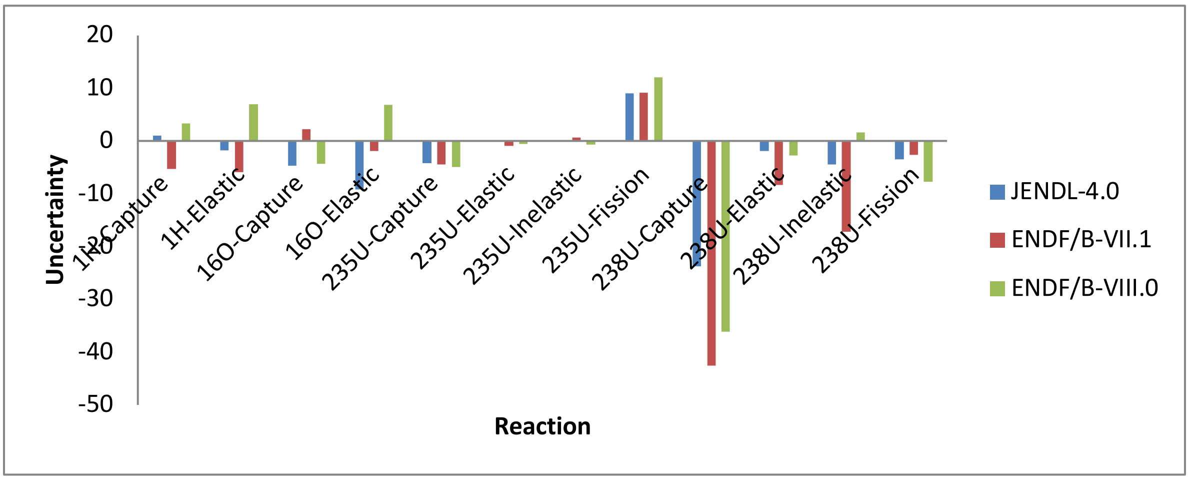

Fig. 5. Cross section uncertainties (in %) on RTC for KRITZ-2:13

4. Nuclear data adjustment

Ad-hoc adjustment were performed in this work on KRITZ:2-13 experiment in the three investigated nuclear data evaluations: the two ENDF/Bs and JENDL. The improvement of the multigroup cross sections for U-235, U-238, and H-1, and of the corresponding covariance matrices are executed using the generalized linear-least-squares methodology (GLLSM). Previous isotopes reactions that required modifications in the nuclear data for the K_{eff} and RTC coefficients were carefully selected. The results obtained for our benchmark will be given in term of adjusted covariance matrices, reduced uncertainty for K_{eff} and corrected values of RTC for the library ENDF/B-VII.1 that has the greatest uncertainty values, corrections for other libraries are not very different from this library.

Figures 6 to 9 illustrate the correlation matrices before and after adjustment for the cross sections of the U-235, U-238 and H-1. In each figure, we had to put the two matrices before and after adjustment in different colors. Drawing the two matrices with the same color - in principle - will give two completely identical shapes, because the differences between prior and posterior matrix are so small. The differences between the two matrices can be discerned by looking at the boundaries of them.

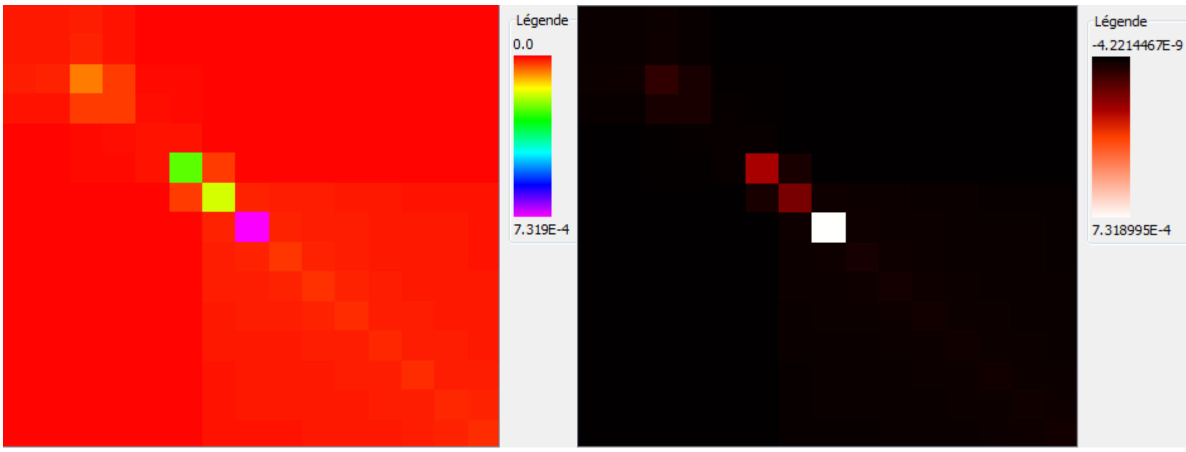

Fig. 6. Prior and posterior correlation matrices of the 235U-fission cross section, respectively

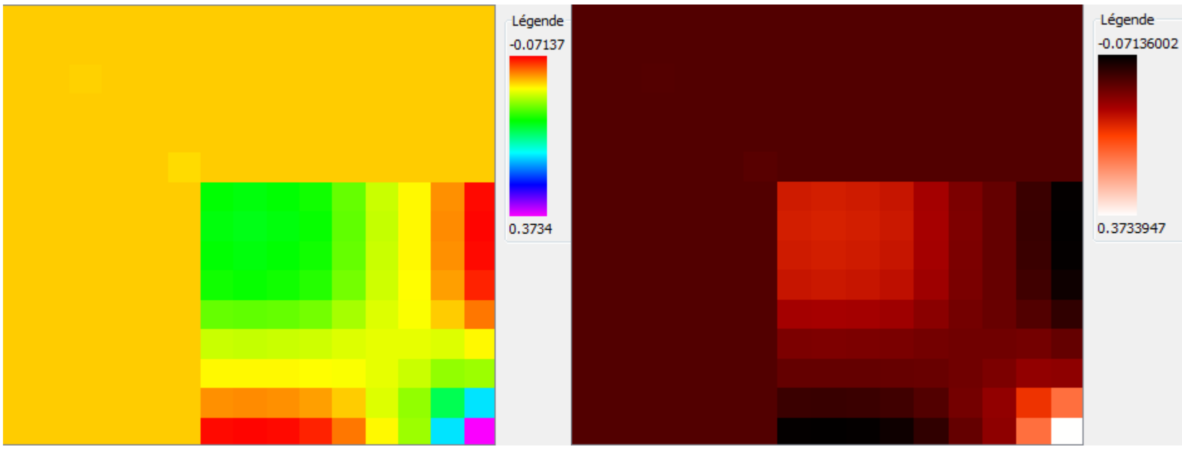

Fig. 7. Prior and posterior correlation matrices of the 235U-capture cross section, respectively

From the latter figures, we notice that the correlations between the multigroup fission and capture cross sections of U-235 are decreased after adjustment, they changed from the range (0 : 7.319E-04) to (-4.22E-09 : 7.318E-04) for fission reaction, and from the range (-0.07137 : 0.3734) to (-0.07136 : 0.3733) for the capture. A reduction in nuclear uncertainty is expected as a result of adjusting the covariance matrices for these reactions.

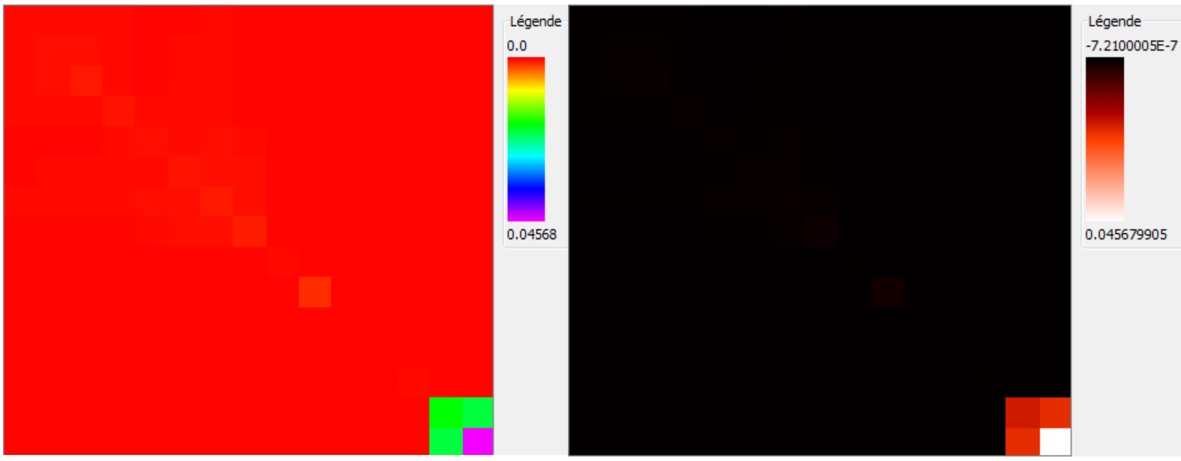

Fig. 8. Prior and posterior correlation matrices of the 238U-capture cross section, respectively

It can be seen from figure 8 that some correlation coefficients are indeed reduced after adjustment and even negative correlations for some energy groups have appeared, where these negative correlation coefficients indicate anti-correlations. Consequently, the nuclear data uncertainties on K_{eff} due to the uncertainties of the capture cross section of U-238 will be reduced after adjustment. Even though some deviations from zero appear in this figure, those remain tiny, since the absolute values of these negative numbers are very small.

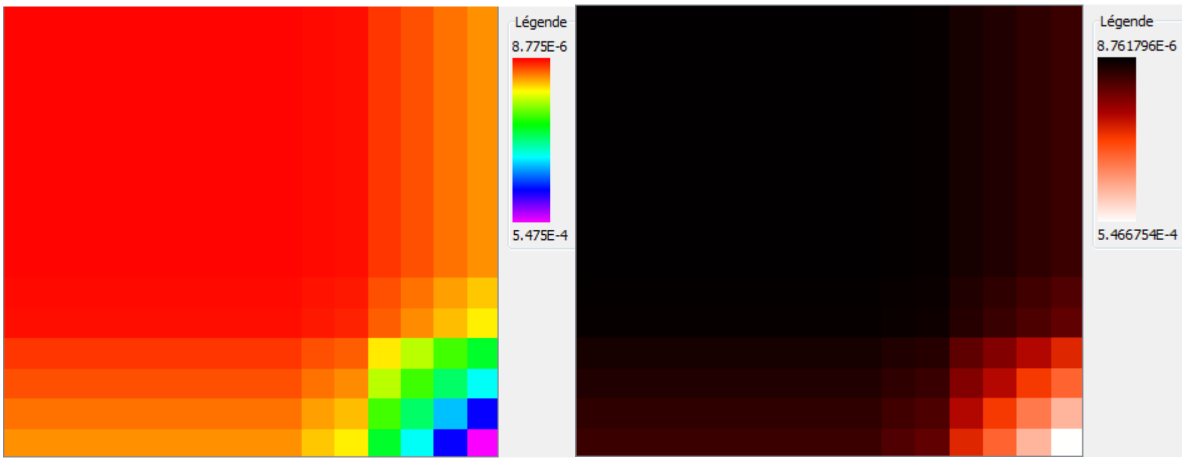

Fig. 9. Prior and posterior correlation matrices of the 1H-elastic cross section, respectively

From the figure 9, we can see that the correlation coefficients of the elastic cross section of H-1 are already reduced after adjustment, they changed from the range (8.77E-06 : 5.47E-04) to (8.76E-06 : 5.46E-04). The K_{eff} uncertainties due to this cross section will be reduced after adjustment, because of the attenuation in correlations.

Figure 10 represents a comparison of the uncertainty values on the K_{eff} for KRITZ-2:13C before and after adjustment.

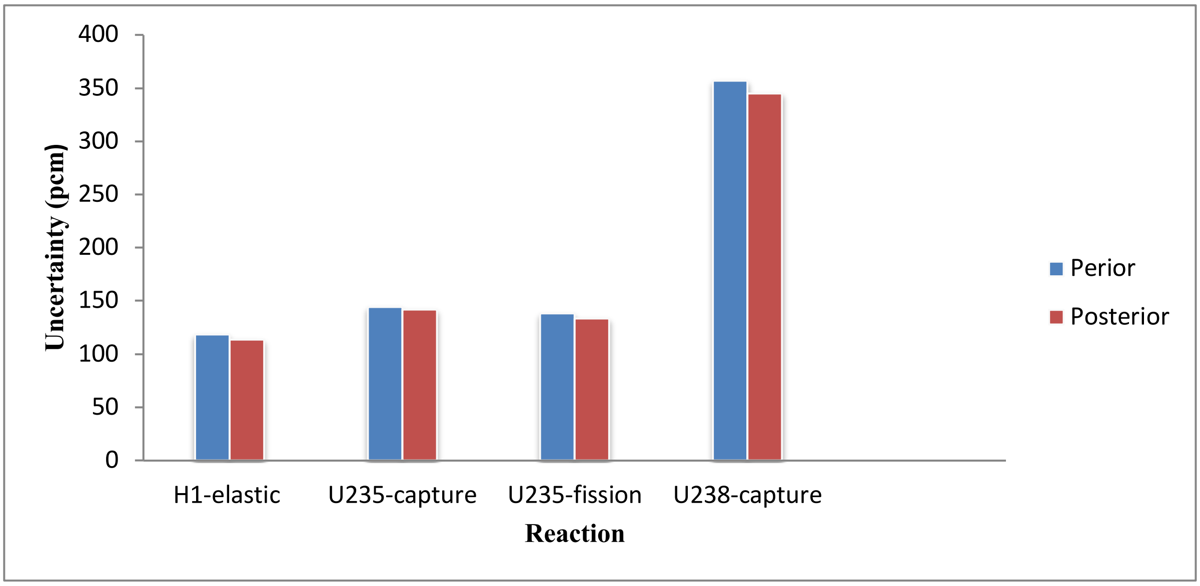

Fig. 10. Prior and posterior K_{eff} uncertainties

Carefully identified cross sections needing adjustments would make significant improvements in the C / E ratios of the benchmark used. Indeed, the use of the adjusted covariance data in the estimation of the posterior nuclear uncertainties has generated - according to figure 10 - noticeable reductions of these uncertainties. The greatest decrease in the uncertainty of the adjusted cross-sections was for the capture reaction of U-238, which we confirmed as the most important cross-section that needs to be modified in this study.

The corrected values of the reactivity temperature coefficient (Absolut values) caused by the improvement of the cross sections are shown on Figure 11.

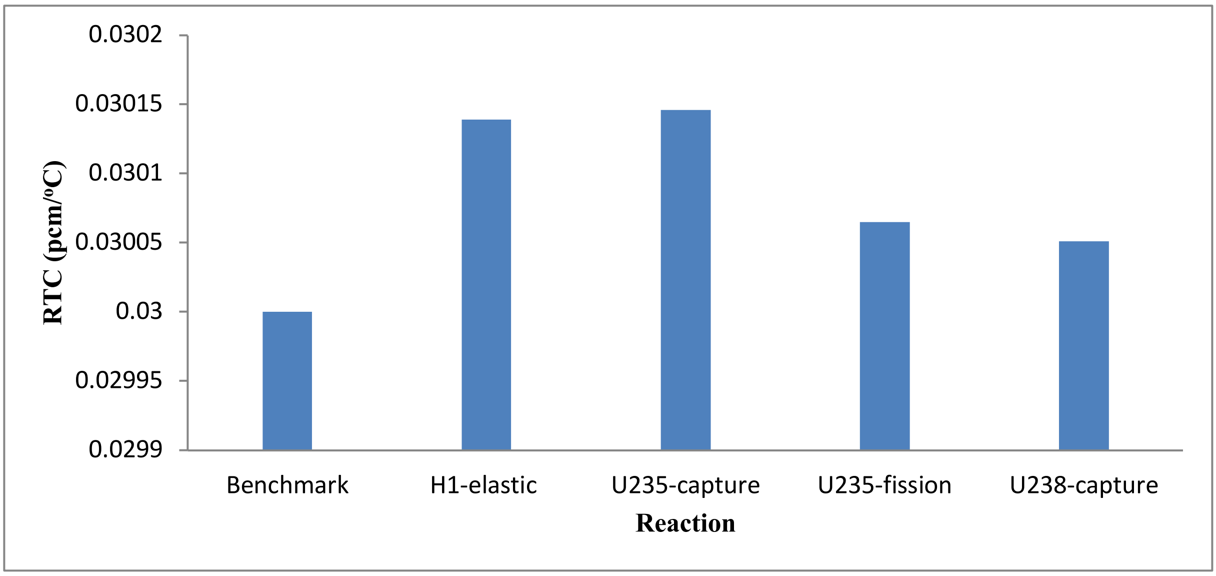

Fig. 11. Corrected valued of RTC

In the framework of our study, we did not take into account the phenomenon of correlation between reactions, we are only interested in the contribution of the individual uncertainty of each cross-section as well as the amount of correction that this cross section will have. According to the previous figure, we note that the improvement performed on the nuclear data individually, made noticeable corrections for the calculated value of RTC, the absolute values of this coefficient were close to the benchmark values, where the calculated values before adjustment reached 0.76 pcm/ºC. The largest correction for the RTC was, respectively, for the capture reaction of U-238 and fission of U-235, that have a significant uncertainty on this coefficient as well as on K_{eff}.

Capture reaction of U-235 and elastic of H-1 do not have a significant effect on the uncertainty of the RTC, yet their correction corrected the calculated value of this parameter. Cross-sections adjustment of these reactions contributed to decreasing the uncertainty value on the K_{eff}, and since the nuclear uncertainty of the RTC depends on the K_{eff} uncertainty, accordingly the RTC uncertainty will be reduced and the calculated value of this coefficient will be corrected.

5. Conclusion

K_{eff} and RTC nuclear uncertainty dependent on the sensitivity of nuclear data of the three libraries was calculated in this work for KRITZ-2:13 reactor at 22.1°C and 243°C using MCNP6.1 code (calculation of sensitivities) and the NJOY system (prepare data in ACE format and calculate covariance matrices).

Capture and fission, respectively, for U-238 and U-235 are the most important reactions in sensitivity as well as uncertainty analysis for both coefficients K_{eff} and RTC in the three libraries. In addition to capture and elastic reactions of U-235 and H-1 respectively, that are important just for the K_{eff}. Previous cross section reactions have been improved depending on GLLSM in an ad-hoc adjustment for KRITZ-2:13.

The results of this improvement, according to our presented study, contributed to decreasing the values of the reactions correlations, thus reducing the data uncertainty on the K_{eff} and correcting the calculated values of the RTC.

Reactions data adjustment for KRITZ-2:13 in parallel with many benchmarks such as those include in the ICSBEP Handbook will be the focus of our future work in order to increase the prediction accuracy of the calculations.

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