Universal Journal of Physics and Application 11(6): 239-246, 2017 http://www.hrpub.org
DOI: 10.13189/ujpa.2017.110604

Sensitivity and Uncertainty Analysis on the Keff Produced by the ^{1}H, ^{16}O, ^{239}Pu and ^{240}Pu Cross Sections Uncertainties

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Abstract In criticality and stability studies of the nuclear reactor, it is important to evaluate the impact of the uncertainties of the basic nuclear data (cross sections) on the different neutron parameters. So this work is interested in the analysis of the sensitivity and uncertainties due to the nuclear data of ^{1}H, ^{16}O, ^{239}Pu and ^{240}Pu Isotopes in the ENDF/B-VII.1 cross sections processed by the latest version of NJOY code on the effective multiplication factor. Different rapid and thermal cases of the different IHECSBE benchmarks have been studied to calculate the sensitivity vectors for ^{1}H, ^{16}O, ^{239}Pu and ^{240}Pu Isotopes. These sensitivity vectors are calculated by using the adjoint-weighted perturbation method based on the Ksen card of the Monte Carlo code MCNP6.1. Thus, the uncertainties induced by nuclear data have been calculated by combining the sensitivity vectors with the covariance matrices that are generated by the ERRORJ module of NJOY2016. We found several cross sections and covariance matrices lack the adjustment: The capture and fission cross sections of the ^{239}Pu and their covariance matrices lack the adjustment in the thermal energies. And all of the four cross sections (elastic, inelastic, capture and fission) and their covariance matrices for the same isotope lack the adjustment in the rapid energies. For ^{16}O; the elastic cross section and its covariance matrix lack the adjustment in the thermal energies. The elastic and capture cross sections of the ^{1}H and their covariance matrices lack the adjustment especially in the thermal energies.

Keywords Cross Section, Sensitivity, Covariance Matrix, Nuclear Uncertainty, MCNP6.1, NJOY2016

1. Introduction

Recently, there are several continuous-energy Monte Carlo codes developing capabilities of computing eigenvalue sensitivity coefficients with regard to nuclear data, including MONK , Mc CARD, MCNP6 ,the continuous-energy version of TSUNAMI-3D in SCALE 6.2 ,RMC, SERPENT [1] , etc. The key point to compute sensitivity coefficients is to compute the change in keff (the effective multiplication factor) caused by a small perturbation in the nuclear data. The sensitivity with continuous energy spectrum has no problem of the self-shielding effect than the sensitivity with multigroup energy spectrum [2]. For this, we used the adjoint-weighted technique with continuous energy spectrum to calculate the sensitivity profiles. A sensitivity and uncertainty analysis have been performed in this work for certain cases of the different IHECSBE (International Handbook of Evaluated Criticality Safty Benchmark Experiments) [3] benchmarks using the MCNP6.1 and the recently updated of the nuclear data processing system NJOY2016 [4] codes. Two previous studies were performed in our laboratory (Radiations and Nuclear Systems Laboratory, University Abdelmalek Essaadi-Morocco) [2,5] to validate the calculation of the sensitivities coefficients by the adjoint-weighted technique in the code MCNP6. These studies were adopted on the calculation of sensitivity vectors for ^{1}H, ^{16}O, ^{235}U and ^{238}U isotopes using the card **KPERT/MCNP6** "**reactivity perturbations**" which cannot give the overall sensitivity of the cross section of an isotope that exists in several cells of a benchmark with different densities in one cell to another, That's why they calculated, separately. Our study is performed using the new card **KSEN/MCNP6.1** "**keff sensitivity coefficients**" that solves the problem of the isotopes that exist in several cells of a benchmark, Firstly we calculated the sensitivity coefficients of (ENDF/B-VII.1) cross sections processed by the recently updated of the nuclear data processing system NJOY2016 to validate this new version, Then we estimate cross section uncertainties of ^{1}H, ^{16}O, ^{239}Pu and ^{240}Pu isotopes on the effective multiplication factor.

2. Methodology

This study will be restricted to the calculation of sensitivity profiles for some different criticality safety cases of IHECSBE benchmarks that were chosen because their relative differences between the experimental and calculated Keff are higher than their experimental uncertainties and their standard deviations [6]. Once the sensitivity vectors are obtained, they are used with the covariance matrices to study the impact of the cross sections uncertainties [7] on the effective multiplication factor uncertainty in each selected case. The selected isotopes are generally known by their important contribution in the effective multiplication factor calculation. Inputs are the MCNP6.1 input file and ENDF/B-VII.1 file containing the matrices of covariance. ENDF/B-VII.I file is processed by NJOY2016 in order to produce cross sections in the ACE format and covariance matrices used by program for calculating ΔKeff–nucl.

2.1. Sensitivity and Uncertainty Approach

MCNP/KSEN card can compute the sensitivity coefficients of the keff to nuclear data [8,9]. A method based on linear-perturbation theory using adjoint-weighting -the same method as used by TSUNAMI- is employed for this purpose. The adjoint weighting is performed in a single forward calculation using the Iterated Fission Probability method. An important limitation of the adjoint-based methods as implemented in MCNP is that they do not consider perturbations that may arise from scattering laws or from fission emission spectra. This limitation has been shown to lead to spurious results [7]. The only addition to the input files used for sensitivity calculations is the specific ‘‘KSEN” card. The default options for the ‘‘KSEN” card are used (especially for the ‘‘BLOCKSIZE” option, set to 5) [10]. Sensitivity vectors are calculated for different isotopes using two cases of energy groups:

1) 15 energy groups used in our sensitivity and uncertainty analysis.
2) 30 energy groups used in calculate the sensitivities coefficients for cross sections processed by NJOY2016 and comparison these sensitivities coefficients with the sensitivities coefficients which are in IHECSBE and calculated by the KENO code “validation NJOY2016”.

All of the “15 and 30” energy groups is distributed between “1.00E-11 and 1.96E+01” Mev.

Sensitivity profiles $\boldsymbol{S_{keff,\sigma_x,g}}$ are defined as the relative change in a response **Keff** with respect to cross section $\boldsymbol{\sigma_x}$ in a particular energy group **g** [11,12], it is defined as:

$$\boldsymbol{S_{keff,\sigma_x,g}} = \frac{\boldsymbol{\sigma_{x,g}}}{\boldsymbol{keff}}\frac{\boldsymbol{\Delta keff}}{\boldsymbol{\Delta\sigma_{x,g}}}$$

The covariance matrices generated by ERRORJ module of the NJOY2016 processing system based on the same discretization of the sensitivity energy. The values of the covariance were computed for fifteen energy groups by using a weighting flux that corresponds to the $1/E$ + fission spectrum + thermal maxwellian shape. For all cases, an infinite dilution condition was assumed ($\sigma_0 = 1.10^{10}\ barns$) and the temperature was considered to be 300K.

The uncertainty in the keff that results from the uncertainties in the nuclear data is computed as a combination of the sensitivity to a particular cross section and the uncertainty for that cross section. The total uncertainty is calculated by using the following equation [2]:

$$\frac{\boldsymbol{\Delta keff}}{\boldsymbol{keff}} = \sqrt{\sum_i\sum_{\sigma_x i}\sum_g [\frac{\boldsymbol{\Delta keff}}{\boldsymbol{keff}}]^2_{i,\sigma_x,g}}$$

i: index of material
$\boldsymbol{\sigma_x}$: index of reaction cross section
$\boldsymbol{g}$: index of energy group

The contribution of every nuclide-reaction in $\frac{\boldsymbol{\Delta keff}}{\boldsymbol{keff}}$ is calculated as follows:

$$\begin{cases} \sqrt{\boldsymbol{S_{keff,\sigma_x,g}}\, cov(\boldsymbol{\sigma_{x,g}},\boldsymbol{\sigma_{y,g'}})\boldsymbol{S_{keff,\sigma_y,g'}}}\ , if\ \boldsymbol{S_{keff,\sigma_x,g}}\, cov(\boldsymbol{\sigma_{x,g}},\boldsymbol{\sigma_{y,g'}})\boldsymbol{S_{keff,\sigma_y,g'}} > 0 \\ -\sqrt{\left|\boldsymbol{S_{keff,\sigma_x,g}}\, cov(\boldsymbol{\sigma_{x,g}},\boldsymbol{\sigma_{y,g'}})\boldsymbol{S_{keff,\sigma_y,g'}}\right|}\ , if\ \boldsymbol{S_{keff,\sigma_x,g}}\, cov(\boldsymbol{\sigma_{x,g}},\boldsymbol{\sigma_{y,g'}})\boldsymbol{S_{keff,\sigma_y,g'}} < 0 \end{cases}$$

$cov(\boldsymbol{\sigma}_{x,g}, \boldsymbol{\sigma}_{y,g'})$: Covariance matrix that comprises covariance data for two cross sections $(\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y)$ in the energy groups $\boldsymbol{g}$ and $\boldsymbol{g}'$.

3. Comparison Sensitivity Coefficients between MCNP6.1 and Keno Codes "Validation NJOY2016"

Firstly we calculate the sensitivities coefficients of ^{239}Pu fission, capture, inelastic and elastic scattering cross sections (ENDF/B-VII.1) processed by NJOY2016. And to validate it, we compared our results for sensitivities coefficients obtained by the code MCNP6.1 with the sensitivities coefficients which are in IHECSBE and calculated by the KENO code. This comparison is used in 30 energy groups.

Figures '1, 2 and 3' show the results of the sensitivity coefficients "**in unit %/% versus energies in ev**" for rapid experiments: pmf020.001 (SPHERE OF PLUTONIUM REFLECTED BY DEPLETED URANIUM), pmf024-001(Polyethylene-Reflected Spherical Assembly of PU239), and for thermal experiment pst002-001(WATER-REFLECTED 12-INCH DIAMETER SPHERES OF PLUTONIUM NITRATE SOLUTIONS); for ^{239}Pu fission, capture, inelastic and elastic scattering cross sections.

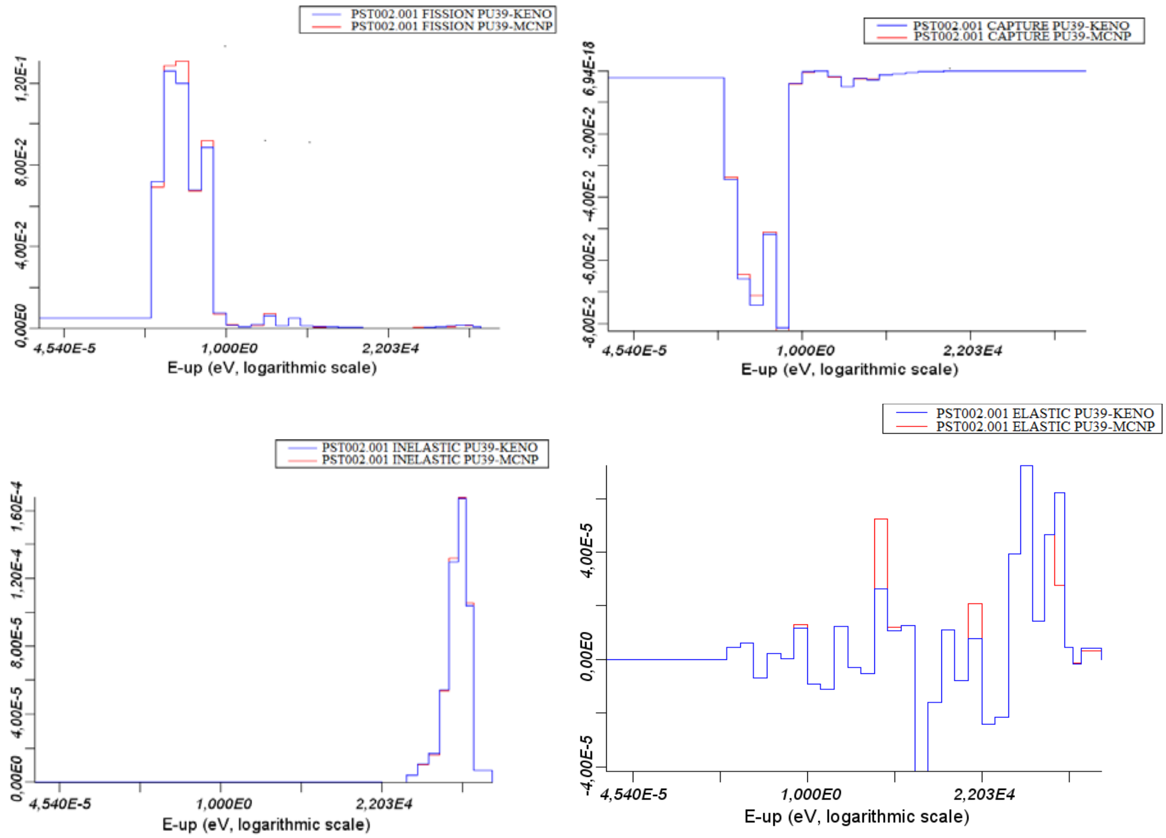
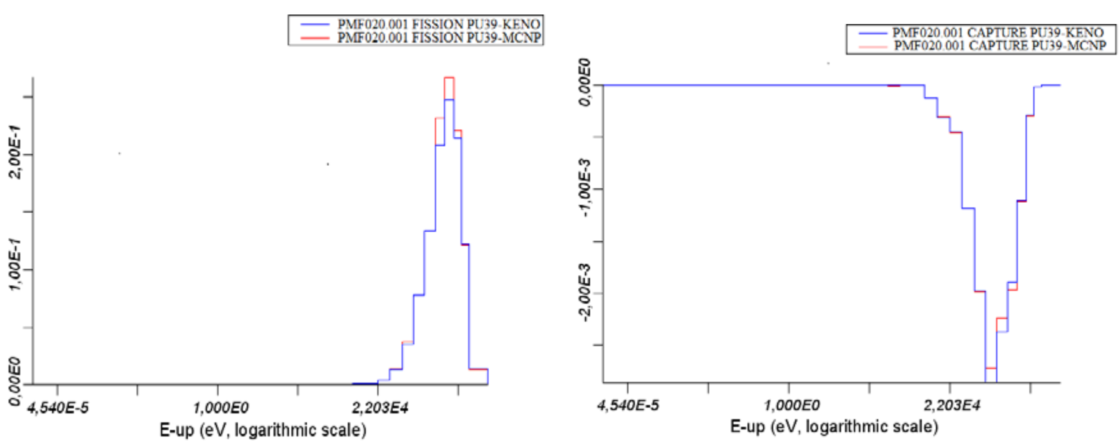


Figure 1. Sensitivities of ^{239}Pu fission, capture, inelastic and elastic scattering cross sections in PMF020.001



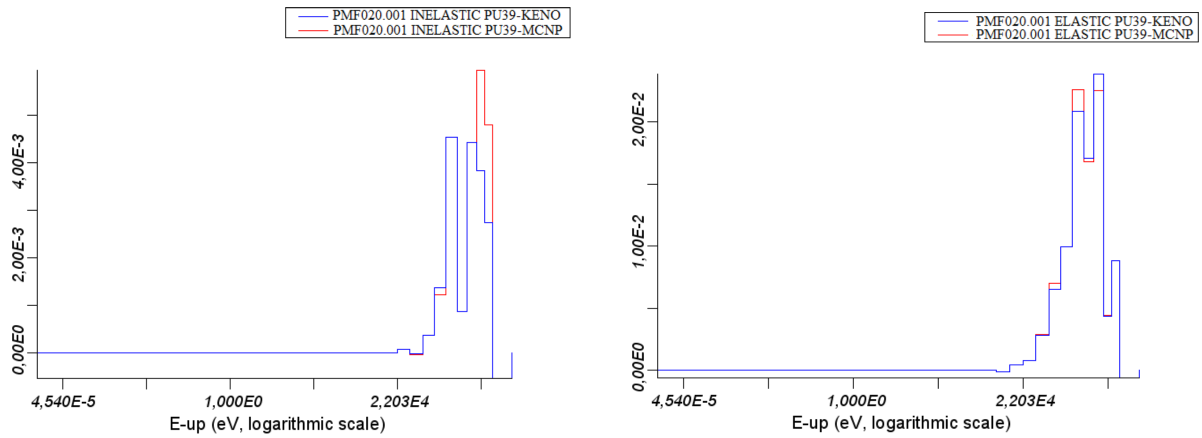


Figure 2. Sensitivities of ^{239}Pu fission, capture, inelastic and elastic scattering cross sections in PMF024.001

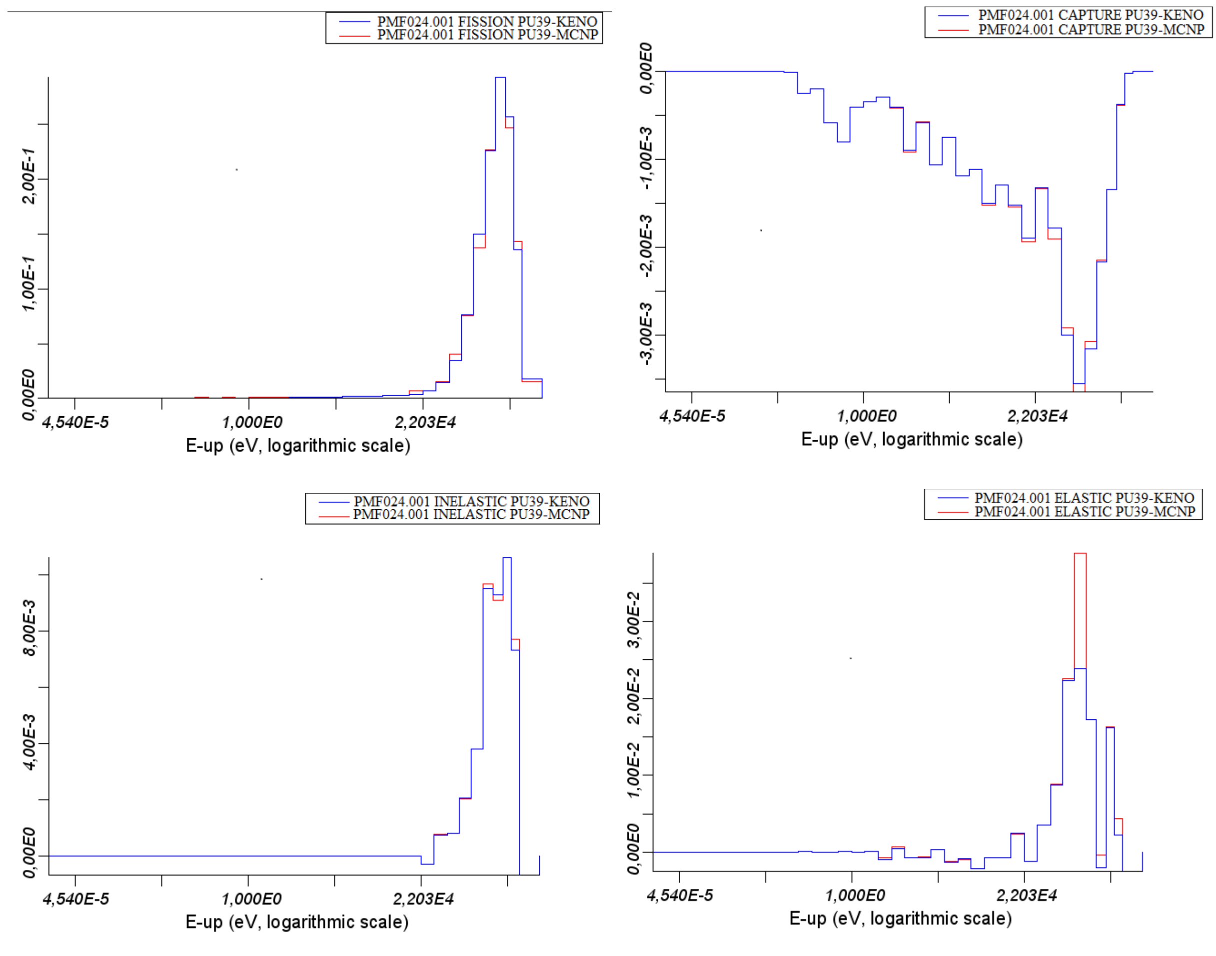


Figure 3. Sensitivities of ^{239}Pu fission, capture, inelastic and elastic scattering cross sections in PST002.001

The slight difference between the results of the two codes attributed to the following:

- The nuclear data evaluations used are different for the two codes.
- The absence of thermal neutron scattering: $S(\alpha, \beta)$ in the KENO code.
- MCNP6.1 is a continuous energy code and KENO is a multigroup energy code.

So, calculating sensitivity vectors for cross sections processed by NJOY2016 code is validated.

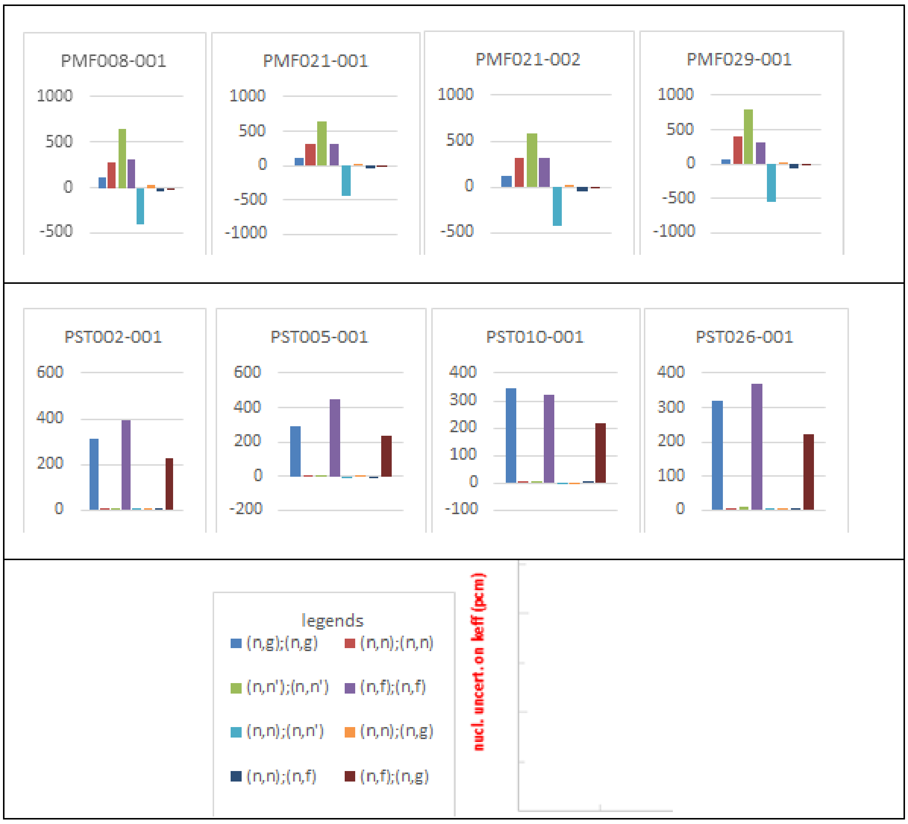


Figure 4. Uncertainties (pcm) produced by different cross sections of ^{239}Pu for rapid (PMF) and thermal (PST) experiences

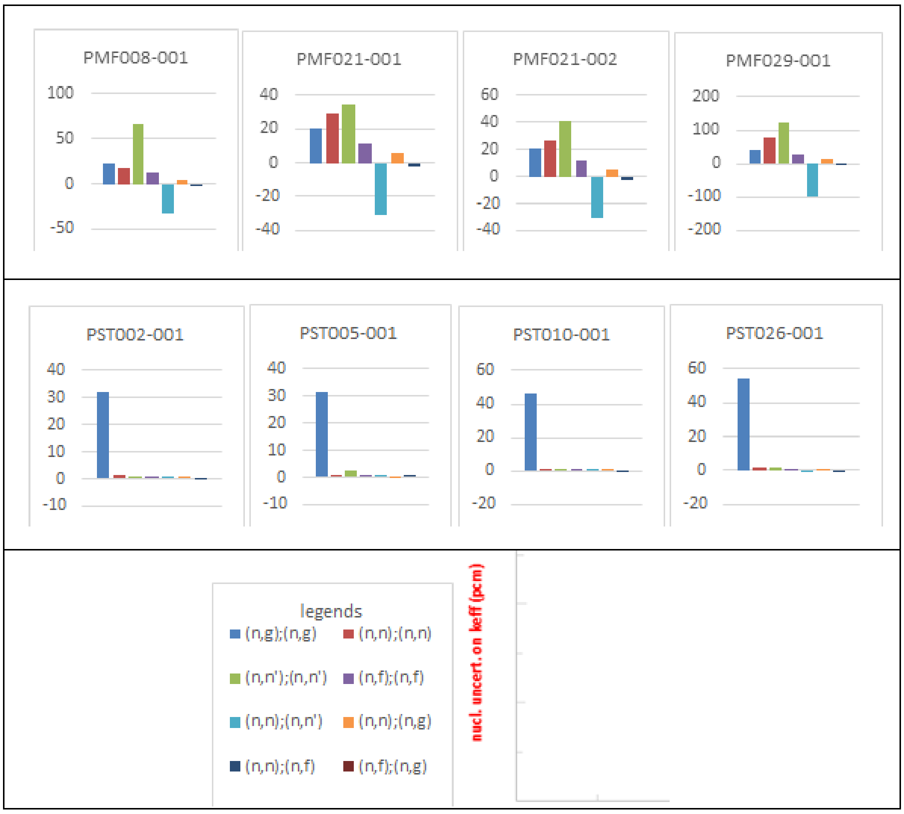


Figure 5. Uncertainties (pcm) produced by different cross sections of ^{240}Pu for rapid (PMF) and thermal (PST) experiences

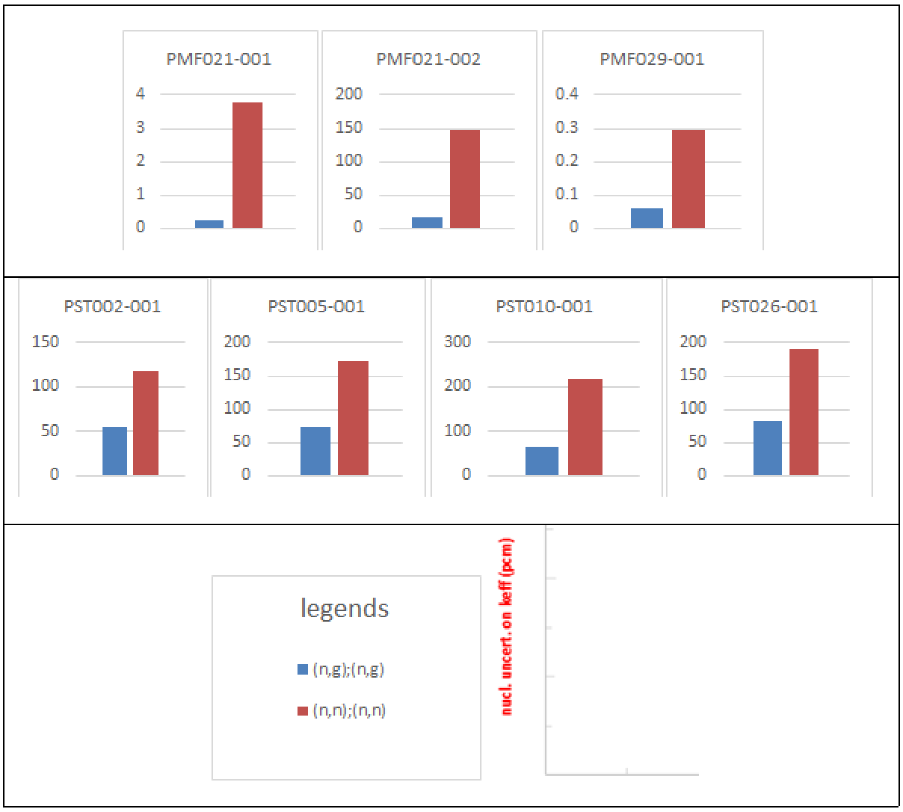


Figure 6. Uncertainties (pcm) produced by different cross sections of ^{16}O for rapid (PMF) and thermal (PST) experiences

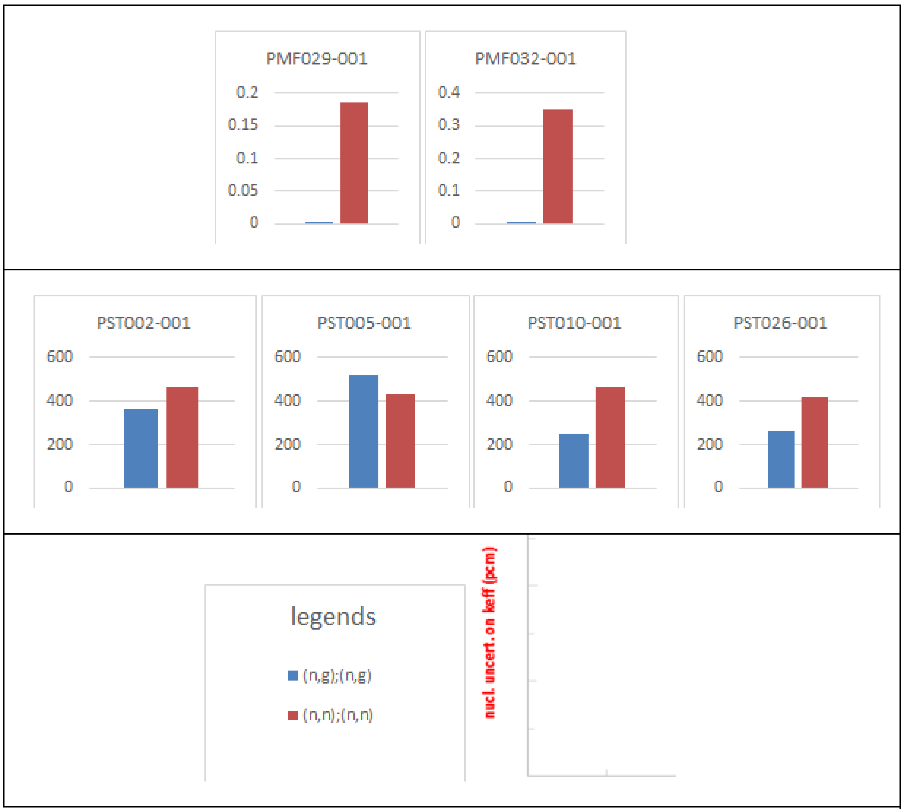


Figure 7. Uncertainties (pcm) produced by different cross sections of ^{1}H for rapid (PMF) and thermal (PST) experiences

4. Uncertainty Analysis

4.1. Uncertainty on the Keff Produced by the Nuclear Data Uncertainties

Figures 4,5,6 and 7 show the effect of cross sections uncertainties related to ^{239}Pu, ^{240}Pu, , ^{16}O and ^{1}H isotopes respectively on the effective multiplication factor (nucl. uncert. On Keff or ΔKeff-nucl.) in different nuclear experiences.

The uncertainties on the Keff produced by capture, fission, elastic and inelastic scattering, cross sections and the effect of the correlation between them are represented by adjoint-weighted technique and by pcm (1pcm = 10-5).

4.2. Interpretation and Conclusion on the Results

- The elastic, inelastic, capture and fission cross sections and the correlations between them for ^{239}Pu in the rapid experiences, they have large contribution of uncertainties in the effective multiplication factor uncertainties (ΔKeff-nucl.). Then, these four cross sections and their covariance matrices require the adjustment in the rapid energies. The capture and fission cross sections and the correlation between them for the same isotope in the thermal experiences have large contribution of uncertainties in the effective multiplication factor uncertainties (ΔKeff-nucl.), these two cross sections and their covariance matrices require the adjustment in the thermal experiences.
- Regarding the ^{240}Pu, the effect of elastic, inelastic, capture and fission cross sections uncertainties on the effective multiplication factor uncertainties is small in the both thermal and rapid experiences, except the inelastic scattering cross section uncertainty has great contribution on the Keff uncertainties in one rapid experience. Then, in this study, we can conclude that: these cross sections and their covariance matrices do not lack the adjustment in the thermal and rapid energies.
- The cross sections uncertainties related to ^{16}O have no effect on the effective multiplication factor (Keff) in all experiences, except the elastic scattering cross section uncertainty has the great contribution on the Keff uncertainties in the thermal experiences and in one rapid experience. Then, the elastic scattering cross section and its covariance matrix for ^{16}O lack the adjustment especially in the thermal experiences.
- For ^{1}H; the cross sections uncertainties have no effect on the effective multiplication factor (Keff) in all experiences, except the elastic scattering and the capture cross sections uncertainties have the great contribution on the Keff uncertainties in the thermal experiences and the elastic scattering cross sections in one rapid experience. Then, the elastic scattering and the capture cross sections and their covariance matrices for ^{1}H lack the adjustment especially in the thermal experiences.

5. Conclusions

In this work we have analyzed the sensitivities and uncertainties on the effective multiplication factor (Keff) produced by ENDF/B-VII.1 nuclear data; especially the four cross sections: capture, fission, elastic and inelastic scattering, and their correlations in the ^{239}Pu, ^{240}Pu, , ^{16}O and ^{1}H isotopes by the adjoint-weighted technique of the MCNP6.1 code. Firstly, we compared and validated our sensitivities coefficients of ^{239}Pu- (ENDF/B-VII.1) cross sections processed by NJOY2016 in three experiences. After that, a series of critical experiences have been studied by using the Monte Carlo code MCNP6.1 and the ERRORJ module of NJOY2016 to calculate the sensitivity vectors and to process the covariance matrices. In the end, the sensitivity vectors and covariance matrices are combined in order to obtain final uncertainties. As a conclusion:

- The four cross sections (elastic, inelastic, capture and fission) of the ^{239}Pu and their covariance matrices lack the adjustment in the rapid energies.

The capture and fission cross sections and their covariance matrices for the same isotope lack the adjustment in the thermal energies.

- The elastic cross section of the ^{16}O and its covariance matrix lack the adjustment especially in the thermal energies.
- The elastic and capture cross sections of the ^{1}H and their covariance matrices lack adjustment especially in the thermal energies.

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