International Journal of Innovation and Applied Studies
ISSN 2028-9324 Vol. 4 No. 1 Sep. 2013, pp. 171-181

http://www.issr-journals.org/ijias/

Impact of the atomic density on the uncertainty of the effective multiplication factor due to nuclear data uncertainties

M. Kaddour[1], T. El Bardouni[1], Y. Boulaich[2], O. Allaoui[1], B. El Bakkari[2], C. El Younoussi[2], M. Azahra[1], H. Boukhal[1], S. EL Ouahdani[1], and E. Chakir[3]

[1]Radiations and Nuclear Systems Laboratory, University Abdelmalek Essaadi,
Faculty of Sciences, Tetuan, Morocco

[2]CEN-Maamora, CNESTEN, Rabat, Morocco

[3]Nuclear Physic Laboratory, Faculty of Sciences, Kenitra, Morocco

ABSTRACT: The main objective of this study is the knowledge of the impact of the atomic density on the uncertainty of the effective multiplication factor (Keff) due to the uncertainties in elastic and inelastic scattering, capture and fission cross sections. Six thermal cases of the benchmark (HEU-SOL-THERM-001) have been studied by using a recently updated nuclear data evaluation JENDL4 to calculate the sensitivity vectors for ^{1}H, ^{16}O, ^{235}U and ^{238}U isotopes. These sensitivity profiles are calculated by using the adjoint-weighted perturbation method based on the Kpert card; and we validated them with the KENO code results, with the differential operator technique of the MCNP5 code and with two nuclear data evaluations (ENDF/B-VI.8 and ENDF/B-VII.0). Kpert card is used by the Monte Carlo code MCNP6. Thus, the Keff uncertainties induced by nuclear data uncertainties have been calculated by combining the sensitivity vectors with the covariance matrices that are generated by the ERRORJ module of the recently updated of the nuclear data processing system NJOY99. This study shows that: it must the cross sections and covariance matrices adjustment of the isotopes that have the great atomic densities and it must the cross sections and covariance matrices adjustment of the fissile isotopes even if they have small atomic density in nuclear reactors.

KEYWORDS: Atomic density, cross section, Keff, sensitivity, covariance matrix, nuclear uncertainty, MCNP6.

1 INTRODUCTION

The average of neutrons from one fission that cause another fission or the effective multiplication factor (Keff) is related to the nuclear interaction probabilities (cross sections), these cross sections have the experimental uncertainties; then, these uncertainties have the effects on the Keff. Now, these experimental uncertainties are available in the covariance files, as in the JENDL4 [1] nuclear data evaluation.

The Monte Carlo code MCNP6 [2] computes the sensitivity on the Keff using the adjoint-weighted methodology [3], [4] and the ERRORJ module of the recently updated of the nuclear data processing system NJOY99 [5] process the covariance matrices. This sensitivity profiles and covariance matrices are combined in order to obtain the final uncertainties in Keff [6].

In this work, a sensitivity and uncertainty analysis is performed for certain cases of the benchmark 'HEU-SOL-THERM-001'[7], the impact of the atomic density on the total uncertainty produced by elastic, inelastic, capture and fission nuclear data on the Keff uncertainty is studied.

Corresponding Author: M. Kaddour (moh-gad@live.fr)

2 METHODOLOGY AND STUDY APPROACH

2.1 ADJOINT-WEIGHTED TECHNIQUE

Starting from the nuclear transport equation and applying a first-order perturbation, the following expression for the change in reactivity ρ can be derived [3]:

$$\Delta\rho = -\frac{<\psi^{+},P\psi>}{<\psi^{+},F'\psi>} \quad (1)$$

The reactivity is related to Keff in the typical way, $\rho = \frac{(\mathrm{Keff}-1)}{\mathrm{Keff}}$. The angular flux in the unperturbed system is ψ and its adjoint is denoted by ψ^{+} . P is the operator for the perturbation taking the form: $P = \Delta\Sigma_t - \Delta S - \lambda\Delta F$. The eigenvalue $\lambda = \frac{1}{\mathrm{Keff}}$, and the tree terms from left to right, are the change in the total cross section, the change in scattering operator, and the change in the fission multiplication operator. F' is the perturbed fission operator.

Monte Carlo technique can be used to sample the numerator and the denominator in continuous-energy forward calculation [4] and the change in reactivity can be estimated by taking the ratio in Eq.(1).

We express change in cross section as: $\Delta\sigma_x = f\sigma_x$

We apply the relationship: $\Delta K_{eff} = K_{eff}\frac{K_{eff}\Delta\rho}{1-K_{eff}\Delta\rho}$

We compute sensitivity coefficients by: $S_{K_{eff},\sigma_x} \approx \frac{1}{f}\frac{K_{eff}\Delta\rho}{1-K_{eff}\Delta\rho}$

The quantity $K_{eff}\Delta\rho$ scales linearly with f; can make arbitrarily small until sensitivity becomes sufficiently precise.

2.2 STUDY APPROACH

During this study:

- We have selected a six of the criticality safety cases of the thermal benchmark 'HEU-SOL- THERM-001' from IHECSBE [8], they have different atomic densities.
- We have studied the impact of the atomic density on the effective multiplication factor uncertainty due to nuclear data uncertainties for ^{1}H, ^{16}O, ^{235}U, and ^{238}U isotopes in each selected case. The selected isotopes are generally known by their important contribution in the effective multiplication factor calculation.
- The sensitivity vectors for multiplication factor were generated by using Kpert card of MCNP6 code in 15 energy groups, are represented in (table 1).

Table 1. Fifteen energy groups used in our sensitivity and uncertainty analysis

Groups numbers	Energy groups (Mev)
1	0.00E 00 - 1.10E-07
2	1.10E-07 - 5.40E-07
3	5.40E-07 - 4.00E-06
4	4.00E-06 - 2.26E-05
5	2.26E-05 - 4.54E-04
6	4.54E-04 - 2.04E-03
7	2.04E-03 - 9.12E-03
8	9.12E-03 - 2.48E-02
9	2.48E-02 - 6.74E-02
10	6.74E-02 - 1.83E-01
11	1.83E-01 - 4.98E-01
12	4.98E-01 - 1.35E00
13	1.35E00 - 2.23E00
14	2.23E00 - 6.07E00
15	6.07E00 - 19.60E00

- The covariance matrices generated by ERRORJ module of the NJOY99 processing system based on the same discretization of the sensitivity energy. Results for ^{1}H are based on JENDL3.3 [1] data since JENDL4 does not contain uncertainty information for this isotope. The values of the covariance were computed for fifteen energy groups mentioned above 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 (σ_0=$1 \cdot 10^{10}$ barns) and the temperature was considered to be 300K.
- The steps adopted in this study are presented in fig.1.

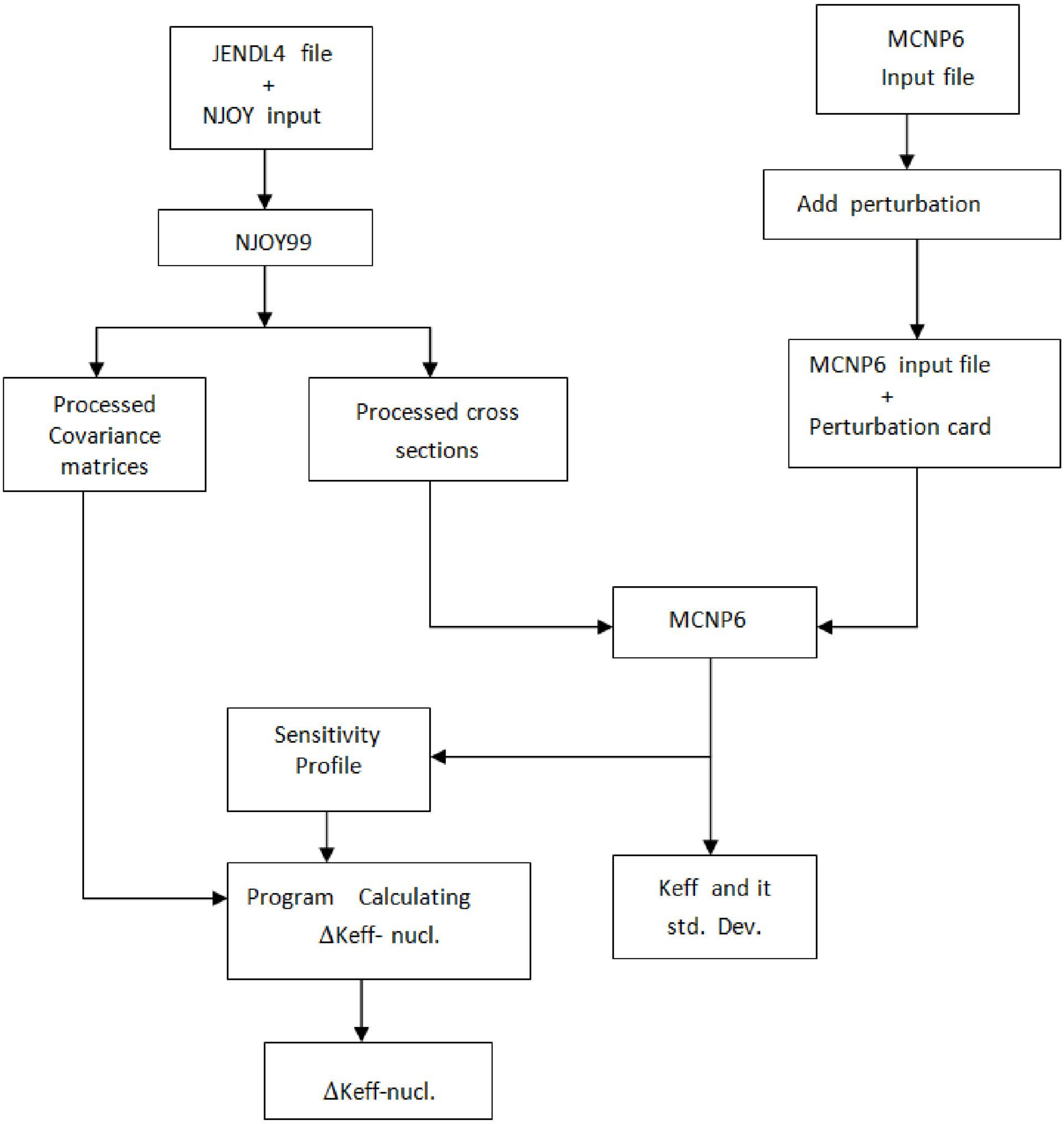

Fig. 1. flowchart of the uncertainty calculation by MCNP6 and NJOY99 codes

- The perturbation approach is generally based on the NJOY99 processing system, the MCNP6 code and the program for calculating the total uncertainty produced by nuclear data (ΔKeff-nucl.).
- Inputs are the MCNP6 input file and JENDL4 file containing the matrices of covariances. As shown in fig.1, JENDL4 file is processed by NJOY99 in order to produce cross sections in the ACE format and covariance matrices used by program for calculating ΔKeff–nucl. .
- The sensitivity vectors were calculated by using the most commonly used radiation transport code MCNP6. The sensitivity profiles $S_{Keff,\sigma_{x,g}}$ are defined as the relative change in a response Keff(the effective multiplication factor) with respect to cross section σ_x in a particular energy group g, is defined as:

$$S_{Keff,\sigma_{x},g} = \frac{\sigma_{x,g}}{Keff}\frac{\Delta Keff}{\Delta\sigma_{x,g}} \approx \frac{1}{f}\frac{K_{eff}\Delta\rho}{1-K_{eff}\Delta\rho} \qquad (2)$$

- The sensitivity profile $S_{Keff,\sigma_{x,g}}$ was obtained by using the perturbation option of MCNP6 that is defined in Kpert card by using the first-order perturbation by the adjoint- weighted technique.
- The cross sections were perturbed as described in the following steps:

1. Four cross sections will be considered: elastic, inelastic, capture and fission cross section, and only one specific cross section in one energy group and one isotope varied each time.
2. Then a material card is created in which the atomic density for the relevant isotope is increased by 1% .
3. The Kpert card is then created specifying that: the relevant material is replaced by the perturbed material in each of the cells in which the material is present. Perturbation cards are given for all energy groups.
4. Finally, MCNP6 is run with this modification in the input; and in the output file a table is given with the results of different perturbations and their related statistical uncertainties.

- These sensitivity vectors must be combined with covariances matrices (see eqs. (4) and (5)), by using a program calculating Keff uncertainties in similar energy groups.
- The total uncertainty is calculated by using the following equation:

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

i: index of material.
σ_x: index of reaction cross section.
g: index of energy groups.

- The contribution of every nuclide-reaction was calculated as follows:

$$\left[\frac{\Delta K_{eff}}{K_{eff}}\right]_{(\sigma_{x,g},\sigma_{y,g'})} = \begin{cases} \sqrt{S_{Keff,\sigma_{x,g}} cov(\sigma_{x,g},\sigma_{y,g'}) S_{Keff,\sigma_{y,g'}}} & (4) \\ -\sqrt{\left|S_{Keff,\sigma_{x,g}} cov(\sigma_{x,g},\sigma_{y,g'}) S_{Keff,\sigma_{y,g'}}\right|} & (5) \end{cases}$$

If $S_{Keff,\sigma_{x,g}} cov(\sigma_{x,g},\sigma_{y,g'}) S_{Keff,\sigma_{y,g'}} \geq 0$, we have to use equation (4).
If $S_{Keff,\sigma_{x,g}} cov(\sigma_{x,g},\sigma_{y,g'}) S_{Keff,\sigma_{y,g'}} < 0$, we have to use equation (5).

$S_{Keff,\sigma_{x,g}}$: Sensitivity coefficient for Keff to neutron cross sectionσ_x, and energy group g.
$cov(\sigma_{x,g},\sigma_{y,g'})$: Covariance matrix that comprises covariance data for two cross sections (σ_x,σ_y) in the energy groups g and g'.

3 OVERVIEW OF EXPERIMENTS (CASES) BENCHMARK

HEU-SOL-THERM-001 is teen critical experiments (cases) were performed in the mid-1970's at the Rocky Flats Plant which was operated at the time by Rockwell international, each involving a tank of highly enriched uranyl nitrate. The critical height for each experiment was determined by linear interpolation between reactor periods of slightly supercritical and slightly subcritical states. The tanks were cylindrical in shape and suspended in approximate center of a large room. Critical configurations had height to diameter ratios less than 1.2. Uranium concentration varied between 50 and 360 grams of uranium per litre. All teen cases are considered acceptable for use as benchmark experiments [7].

In the following parts, we analyse six cases of this benchmark by MCNP6 code for K_{eff} and its related nuclear uncertainty due to the different reactions types for ^{235}U, ^{238}U, ^{1}H, and ^{16}O isotopes and we conclude how varied the effective multiplication factor uncertainty with the atomic density of these isotopes.

4 MULTIPLICATION FACTORS CALCULATED BY MCNP6

The K_{eff} values with its related standard deviation for thermal systems studied throughout this study are listed in table 2. The third column represent values from the International Criticality Safty Benchmark experements (IHECSBE) and our results calculated by MCNP6 code and JENDL4 nuclear data evaluation are represented in the second column.

Table 2. HEU-SOL-THERM-001-cases Keff and its standard deviation

Benchmark	$\mathbf{Keff} \pm \mathbf{std.dev.}^{1}$ (MCNP6)	$\mathbf{Keff} \pm \Delta\mathbf{Keff}^{2}$ (IHECSBE)
HEU-SOL-THERM-001-001	0.98531 ±0.00012	1.0004±0.0060
HEU-SOL-THERM-001-002	0.99453 ±0.00021	1.0021±0.0072
HEU-SOL-THERM-001-003	0.98765±0.00020	1.0003±0.0035
HEU-SOL-THERM-001-004	0.99574 ± 0.00021	1.0008±0.0053
HEU-SOL-THERM-001-005	0.97169 ± 0.00017	1.0001±0.0049
HEU-SOL-THERM-001-006	0.97612 ± 0.00017	1.0002±0.0046

[1]This uncertainty means the statistical uncertainty or standard deviation in MCNP6 calculated with the Monte Carlo technique.

[2] This uncertainty means the experimental uncertainty due to uncertainties in critical heights, uncertainties in Solution constituents, and in isotropic constituents [7].

5 VALIDATION OF SENSITIVITY RESULTS

The calculation of the sensitivities coefficients with the adjoint-weighted technique is new in the code MCNP6; for this, we compared the results of this technique with the results of the MCNP6 differential operator technique [2] (old technique) and with the sensitivities coefficients calculated by the KENO code [8]. Also, we compared the results of the adjoint-weighted technique by two nuclear data evaluations ENDF/B-VI.8 [1] and ENDF/B-VII.0 [1]. This comparison is used in 30 energy groups, are represented in table 3.

Table 3. Thirty energy groups used in our sensitivity validation

Groups numbers	Energy groups (Mev)
1	0.00E+0 - 1.00E-02
2	1.00E-02 -2.15E-02
3	2.15E-02 - 4.64E-02
4	4.64E-02 - 1.00E-01
5	1.00E-01 - 2.15E-01
6	2.15E-01 - 4.64E-01
7	4.64E-01 - 1.00E+00
8	1.00E+00 - 2.15E+00
9	2.15E+00 - 4.64E+00
10	4.64E+00 - 1.00E+01
11	1.00E+01 - 2.15E+01
12	2.15E+01 - 4.64E+01
13	4.64E+01 - 1.00E+02
14	1.00E+02 - 2.15E+02
15	2.15E+02 - 4.64E+02
16	4.64E+02 - 1.00E+03
17	1.00E+03 - 2.15E+03
18	2.15E+03 - 4.64E+03
19	4.64E+03 - 1.00E+04
20	1.00E+04 - 2.15E+04
21	2.15E+04 - 4.64E+04
22	4.64E+04 - 1.00E+05
23	1.00E+05 - 2.00E+05
24	2.00E+05 - 4.00E+05
25	4.00E+05 - 8.00E+05
26	8.00E+05 - 1.40E+06
27	1.40E+06 - 2.50E+06
28	2.50E+06 - 4.00E+06
29	4.00E+06 - 6.50E+06
30	6.50E+06 - 6.50E+06

The figures below show the results of the sensitivity validation in rapid benchmark Godiva (highly enriched uranium sphere) for four reactions: elastic and inelastic scattering, capture and fission.

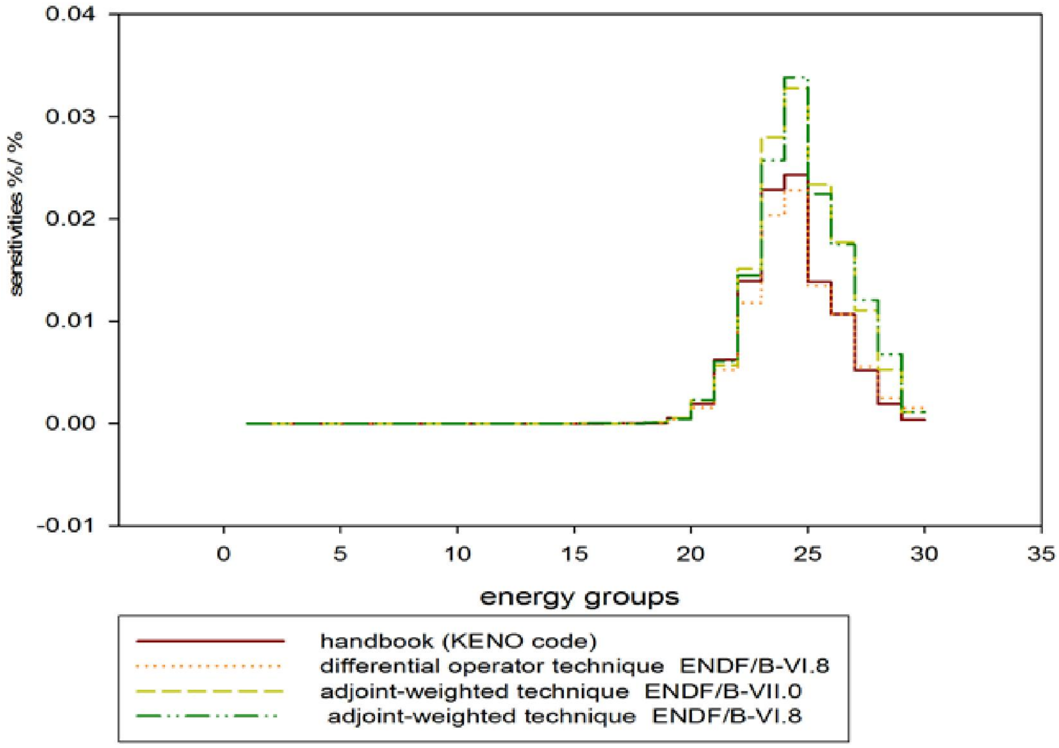

Fig. 2. Sensitivities of ^{235}U elastic scattering cross section in Godiva

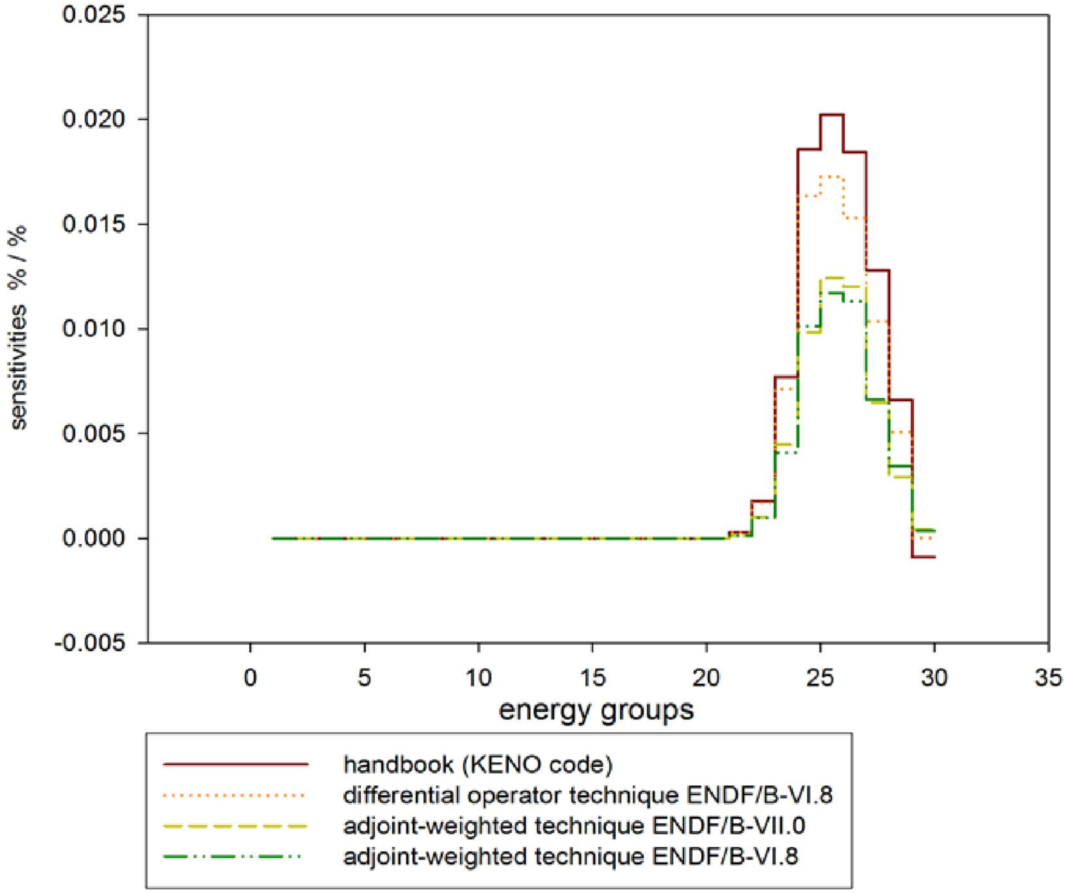

Fig. 3. Sensitivities of ^{235}U inelastic scattering cross section in Godiva

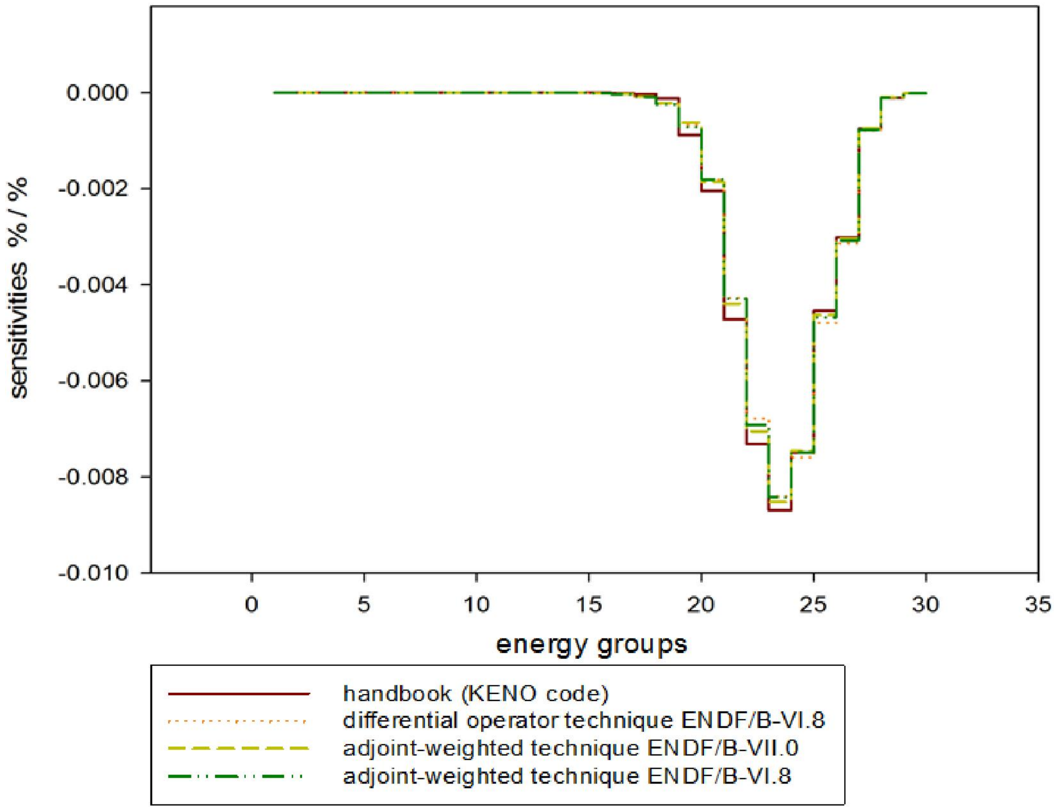

Fig. 4. Sensitivities of ^{235}U capture cross section in Godiva

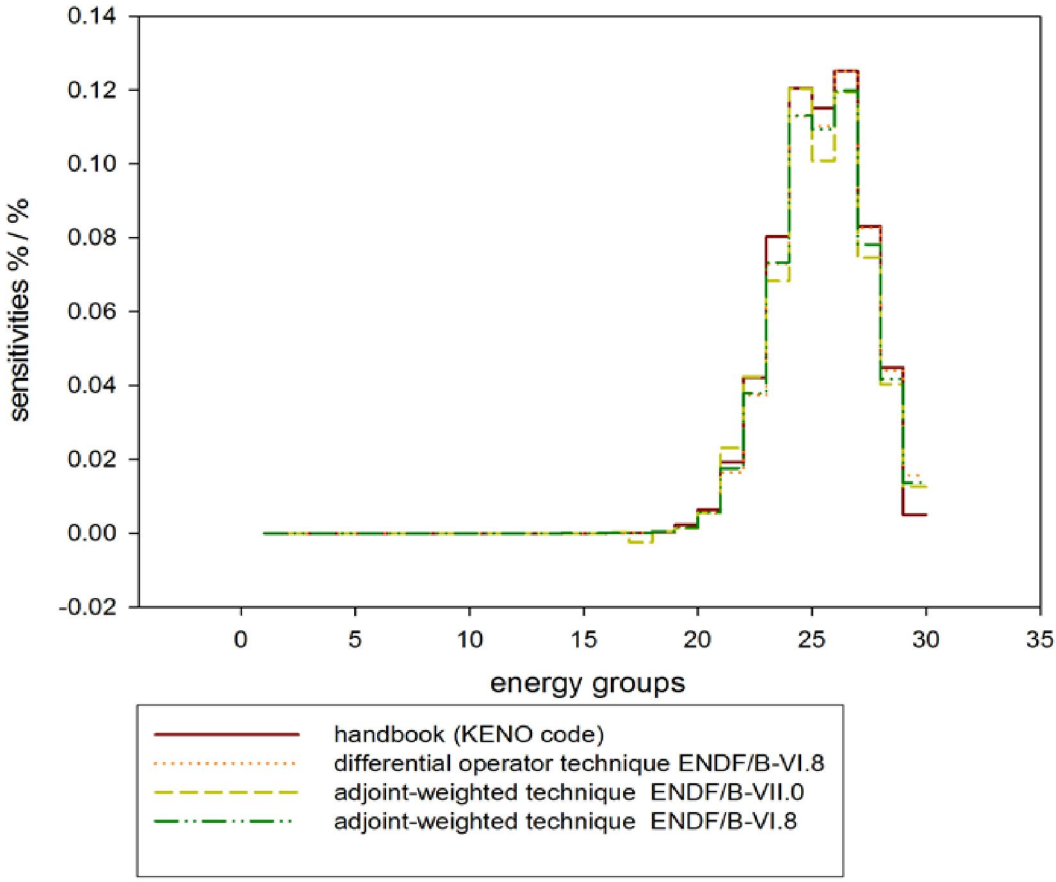

Fig. 5. Sensitivities of ^{235}U fission cross section in Godiva

The differences between the results of sensitivities in the above figures (figs.:2,3,4,5) are due to:

- The difference between the nuclear data evaluation used.
- The difference between the techniques used.

In general, the adjoint-weighted technique is validated.

6 IMPACT OF ATOMIC DENSITY ON THE NUCLEAR UNCERTAINTY IN EFFICTIVE MULTIPLICATION FACTOR (KEFF)

In this part, we analyse the nuclear uncertainty in Keff due to the elastic, inelastic, capture and fission uncertainties for ^{235}U, ^{238}U, ^{1}H, and ^{16}O isotopes in six cases of the HEU-SOL-THERM-001 by MCNP6 code and we conclude how varied the effective multiplication factor uncertainty with the atomic density of these isotopes (see the figures below).

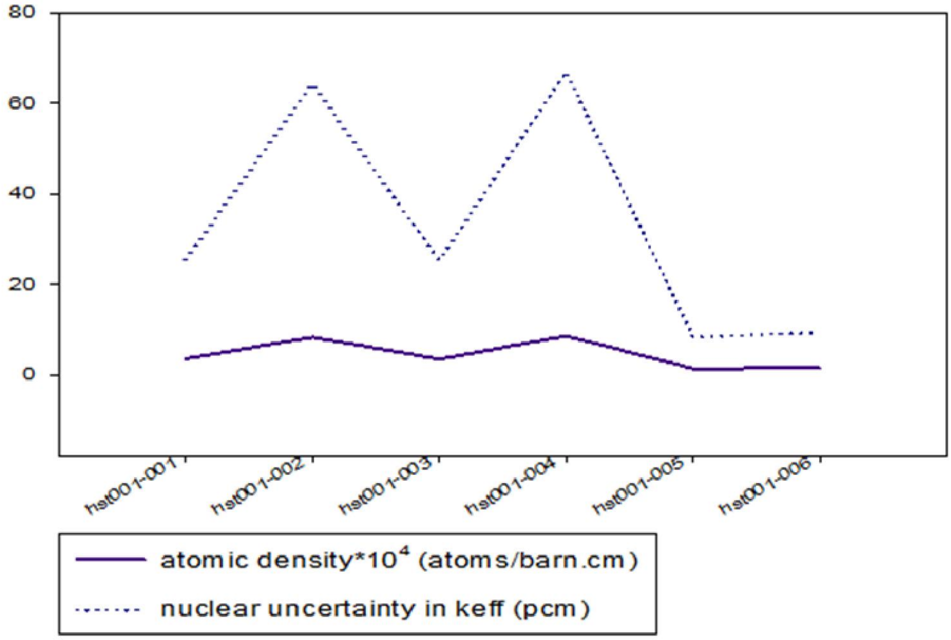

Fig. 6. Variation of the atomic density and ΔKeff-nucl. for ^{235}U in six cases of the benchmark hst001

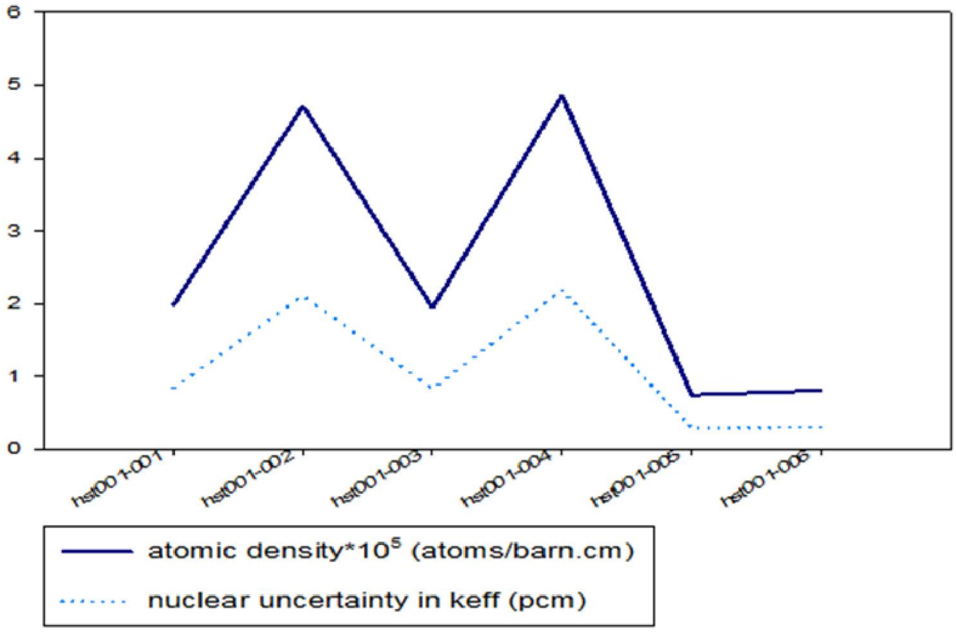

Fig. 7. Variation of the atomic density and ΔKeff-nucl. for ^{238}U in six cases of the benchmark hst001

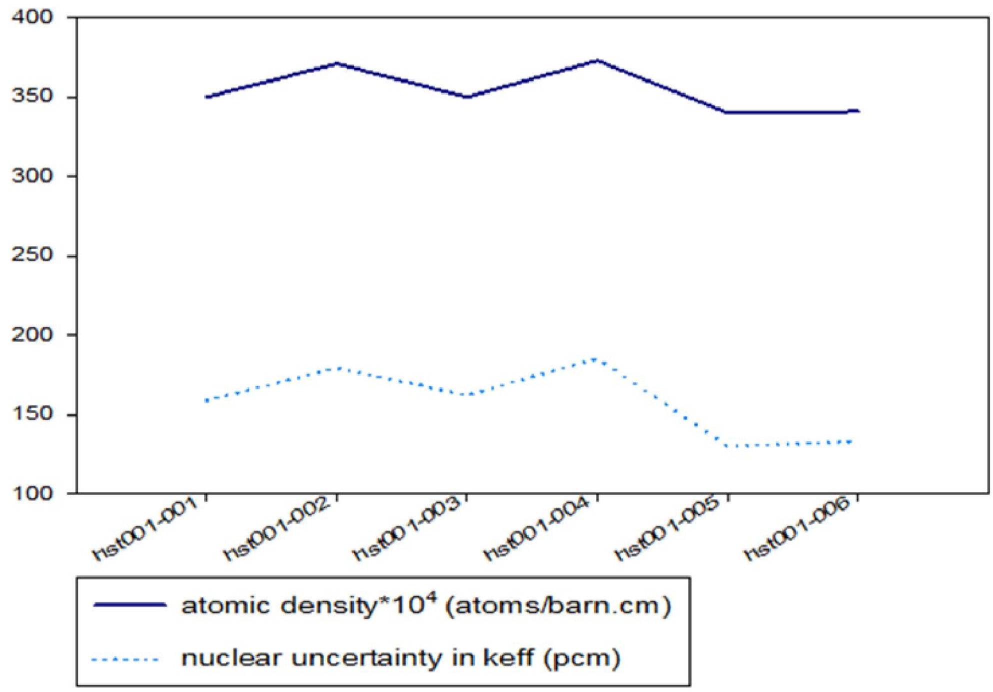

Fig. 8. Variation of the atomic density and ΔKeff-nucl. for ^{16}O in six cases of the benchmark hst001

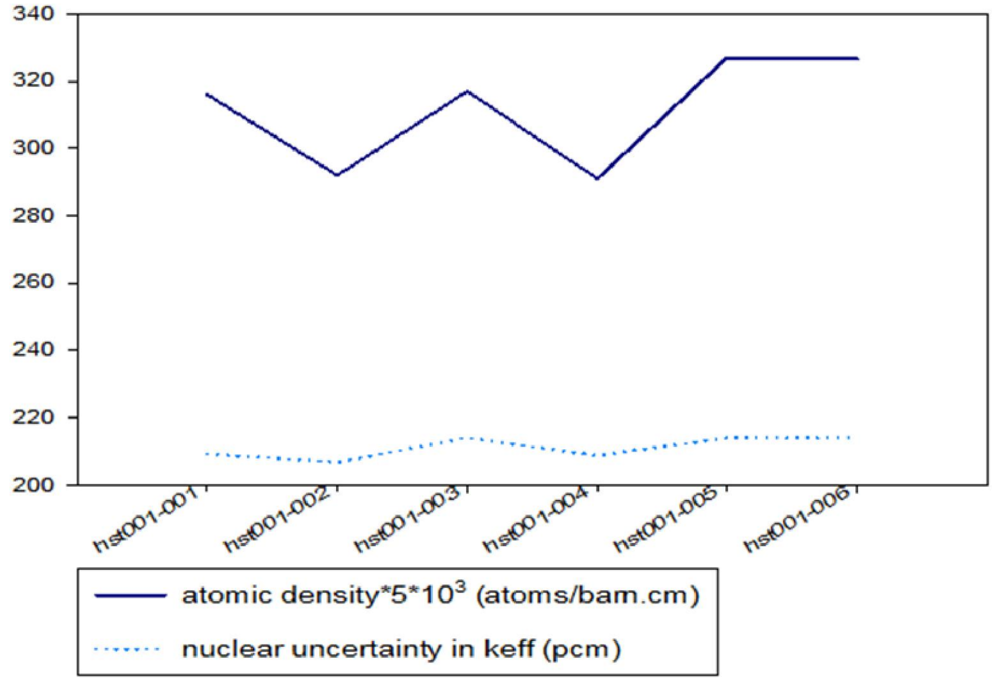

Fig. 9. Variation of the atomic density and ΔKeff-nucl. for ^{1}H in six cases of the benchmark hst001

7 DISCUSSION

- We observed the nuclear uncertainties on Keff due to the elastic, inelastic, capture and fission uncertainty for ^{235}U, ^{238}U, ^{1}H, and ^{16}O isotopes increase when its atomic densities increase. Therefore; it must the adjustment of cross sections and its covariace matrices of the isotopes that have the great atomic densities in nuclear reactors.
- We observed the nuclear uncertainties on Keff due to the elastic, inelastic, capture and fission uncertainty for ^{235}U increase greatly with small increase of the atomic densities than the ^{238}U,^{1}H and ^{16}O uncertainties. This is due to the large contribution of ^{235}U cross sections uncertainties on the Keff uncertainty. Therefore; for small

atomic density it must the cross sections and covariance matrices adjustement of the fissile isotopes such as ^{235}U in nuclear reactors.

8 CONCLUSION

In this work we have analysed the sensitivities and uncertainties on the effictive multiplication factor Keff produced by nuclear data; espicially the elastic and inelastic scattering, capture and fission cross sections and their correlations in the ^{1}H,^{16}O,^{235}U and ^{238}U by the adjoint- weigted technique ; six critical and thermal cases of the 'HEU-SOL-THERM-001' benchmark have been selected in this study by using the Monte Carlo code MCNP6 and the ERRORJ module of the last update NJOY99 to calculate the sensitivities vectors and to process the covarionce matrices. And we studied the impact of the atomic density on the total uncertainty produced by elastic, inelastic, capture and fission nuclear data on the Keff uncertainty. As a conclusion, it must the cross sections and covariance matrices adjustment of the isotopes that have the great atomic densities in nuclear reactors. And for small atomic densities it must the cross sections and covariance matrices adjustement of the fissile isotopes such as ^{235}U in nuclear reactors.

REFERENCES

[1] B. Pritychenko, A. A. sonzogni, *Evaluated Nuclear Data File (ENDF) Retrieval & Plotting*, NNDC, Brookhaven National laboratory, 2012.
[Online] Available: http://www.nndc.bnl.gov/sigma/ (July, 2013)

[2] D. B. Pelowitz, *MCNP User's Manuel*, December 2011, LA-CP-11-01708.

[3] E. E. Lewis, W. F. Miller, "Computational Methods of Neutron Transport," *American Nuclear Society, Inc., Lagrange Park, Illinois*, USA, pp. 52-55, 1993.

[4] B. C. Kiedrowski, F. B. Brown, and P. P. H. Wilson, "Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nuclear Science and Engineering*, vol. 168, no. 3, pp. 226-241, 2011.

[5] R. E. MacFarlane, *NJOY99 Nuclear Data Processing system*, 2002.
[Online] Available: http://t2.lanl.gov/nis/codes/njoy99/index.html (July, 2013)

[6] C. de Saint, E. Dupont, M. Ishikawa, G. Palmiotti, M. Salvatores, *Assessement of existing Nuclear Data Adjustement Methodologies,* NEA/NSC/DOC(2010) 429.

[7] Brian Palmer, Kenneth Woods, Harry F. Lutz, *Minimally reflected cylinders of highly enriched solutions of uranyl nitrate*, NEA/NSC/DOC(95)03/II, Volume II, HEU-SOL-THERM-001.

[8] Nuclear Energy Agency, *International Handbook of Evaluated Criticality Safty Benchmark Experiments*, NEA/NSC/DOC (95)03/III, September 2007 Edition.