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Sensitivity to nuclear data of Es-Salam fuel assembly eigenvalue using TSUNAMI-3D/SCALE 6.2.3

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ABSTRACT

Currently, in the design and safety studies of nuclear reactor cores, great interest is given to sensitivity and uncertainty studies because of the deviations observed due to the values of the neutron cross sections, which are important in neutronic calculations. The main objective of this study is to evaluate the influence of neutron cross section uncertainties on the effective multiplication factor k_{eff} and its sensitivity to nuclear data. This paper presents the obtained results of the sensitivity analysis performed for Es-Salam fuel assembly using SCALE 6.2.3 package. Similarity was found with the reference direct perturbation results for some nuclides but not for others. Furthermore, the study shows that differences between the TSUNAMI-3D and the direct perturbation results vary 1.9 % for 235U, 8% for 238U up to 53% for ^{2}H for multigroup calculations and 11% for 235U, 2 % for 238U and 53.7% for ^{2}H in case of continuous energies calculations. These differences for the ^{2}H nuclide, were decreased with the spatial mesh technique implemented in TSUNAMI-3D. The sensitivity analysis applied in this study could be the reference for Es Salam reactor core analyses to estimate the nuclear data uncertainty contributions to key physical parameters such as reactivity coefficients.

1. Introduction

Simulation of reactor core parameters always depends on the quality of the model and the calculation tools. These computational tools are mainly based on neutron transport methods using nuclear data such as cross sections. They can predict neutron parameters with high accuracy, but with some deviations from experimental values. It is believed that computational biases, when using simulation codes, often turn out to be uncertainties in cross-section data, manufacturing inaccuracies, or approximations implemented in computer codes. It is therefore necessary to carry out sensitivity and uncertainty analyses to assess the quality of the simulation results. A sensitivity analysis is defined by how much a physical parameter would change due to a change in a particular cross section.

Over the past 40 years, the usefulness of sensitivity analyses, in the context of reactor safety application, has been demonstrated several times. The theory of sensitivities includes the evaluation of the impact of small variations in reactor parameters, in particular variations in cross sections on the effective multiplication coefficient k_{eff} [1]. Various methods have been developed for sensitivity and uncertainty analyses such as the adjoint-weighted perturbation capability in MCNP6, a discrete ordinates sensitivity formulation of the first-order perturbation theory in the SUSD3D code and a fine group calculation from TSUNAMI-3D [2]. We are particularly interested in the sensitivity and uncertainty analysis implemented in the SCALE 6.2 system code [3]. Cross section uncertainties, referred to as covariance data, have been a consideration in SCALE since the introduction of the TSUNAMI tools and their application to criticality safety in SCALE 5.0. The SCALE 6.2 covariance library is based on ENDF/B-VII.1 data for 187 nuclides, combined with previous SCALE 6.1. Thus, SCALE 6.2 has a complete set of uncertainties for important data of all nuclides in the multigroup cross sections [3,4].

This study is the first step in the sensitivity/uncertainty analysis of Es-Salam reactor core; it focuses on neutronic calculations carried out on the fuel assembly. Because assessment of simulation parameters for design and safety operation of a nuclear reactor is essential, it is advantageous to perform such sensitivity analysis. To carry out this study, SCALE 6.2.3 code package [3] was used by means of KENO-VI and TSUNAMI-3D codes [5,6]. The first one performs eigenvalue calculations of the system while the second provides the sensitivity coefficients. Both

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sequences uses the ENDF/B-VII.0 and ENDF/B-VII.1 continuous energy (CE) and multigroup energy (MG) libraries with the 44 and 56 group covariance data. This study allows the identification of the main contributors to sensitivity of the k_{eff} for the fuel assembly.

2. SCALE 6.2 and TSUNAMI sequence

SCALE 6.2 provides several new features such as the ENDF/B-VII.1 CE and MG nuclear data libraries with improved group structures, Neutron covariance data based on ENDF/B-VII.1, CE sensitivity/uncertainty analysis [3].

The SCALE sensitivity and uncertainty (S/U) analysis sequences known as the Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) quantify the predicted change in k_{eff}, reaction rates, or reactivity differences due to changes in the cross-section data. Sensitivity coefficients are given by [2,7]:

$$S_{x,g}^{i} = \frac{\Delta keff}{keff} / \frac{\Delta \Sigma_{x,g}^{i}}{\Sigma_{x,g}^{i}} \quad (1)$$

TSUNAMI provides automated problem-dependent cross sections using the same methods and input as the Criticality Safety Analysis Sequences (CSASs). Calculations can be performed either with the MG TSUNAMI-3D-K6 sequence or CE TSUNAMI-3D simulation, following the flow diagram in Fig.1a and Fig.1b respectively. The sensitivity and uncertainty analysis is performed with the SAMS 6 sequence [8]. To catch the uncertainties in k_{eff} due to tabulated cross section covariance data, the calculated sensitivity coefficients and the cross-section uncertainties are combined.

In order to check the validity of the calculated sensitivity coefficients it was necessary to compare them to reference values given by the direct perturbation method. This technique is applied to generate reference sensitivity coefficients ($S_{k,\alpha}$) that express the sensitivity of k_{eff} to the changes in the number density of a nuclide. Those sensitivity coefficients are defined as:

$$S_{k,\alpha} = \frac{\alpha}{k} \times \frac{dk}{d\alpha} = \frac{\alpha}{k} \times \frac{k_{\alpha^+} - k_{\alpha^-}}{\alpha^+ - \alpha^-} \quad (2)$$

$\alpha+$ and $\alpha-$ represent the increased and decreased densities values of the input quantity α, respectively, and $k_{\alpha+}$ and $k_{\alpha-}$ represent the corresponding values of k_{eff} [3].

Statistical uncertainties in the computed values of k_{eff} are propagated to uncertainties in direct perturbation sensitivity coefficients by standard error propagation techniques as [8]:

$$\sigma_s = \left(\left(\frac{\sigma_{k^+}^2 + \sigma_{k^-}^2}{\left(k_{\alpha^+} - k_{\alpha^-}\right)^2} + \frac{\sigma_k^2}{k_{eff}^2} \right) \times \left(\frac{k_{\alpha^+} - k_{\alpha^-}}{k_{eff}} \right)^2 \right)^{1/2} \times \frac{\alpha}{\alpha^+ - \alpha^-} \quad (3)$$

σ_{k+} and σ_{k-} represent the corresponding values of statistical uncertainties for $k_{\alpha+}$ and $k_{\alpha-}$ respectively.

The deviation between TSUNAMI-3D and direct perturbation sensitivity coefficients is computed through the standard deviation Nδ (equ.4). This difference must be less than two standard deviations Nδ to be acceptable.

$$N\delta = \frac{|S_x - S_d|}{\sigma_s} \quad (4)$$

S_x and S_d are the TSUNAMI and direct perturbation sensitivity coefficients respectively and σ_s is the standard error of direct perturbation sensitivity coefficients.

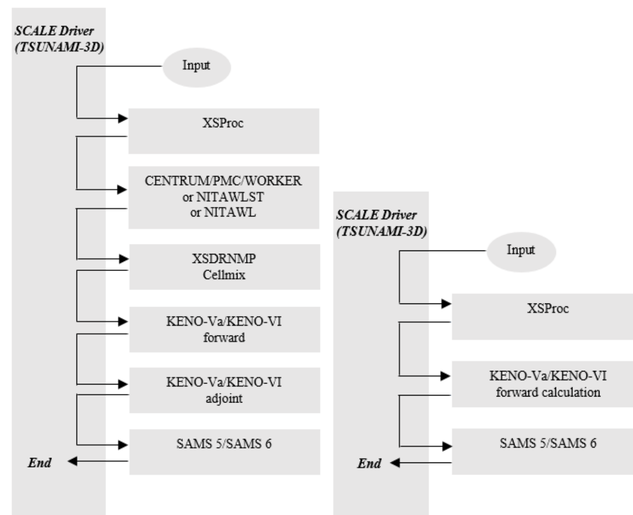

Fig. 1. **(a)** General flow diagram of MG TSUNAMI-3D **(b)** General flow diagram of CE TSUNAMI-3D

3. Methodology adopted for sensitivity analysis of Es salam fuel assembly

Es-Salam is a multipurpose research reactor, cooled and moderated by heavy water using graphite as reflector. It is a tank type reactor with nominal power of 15 MW [9].

To construct a TSUNAMI-3D model for Es salam fuel assembly, the TSUNAMI-3D-K6 control module was chosen with the CSASs6 (Criticality Safety Analysis Sequences). Calculations were done using first the multigroup energy cross-section libraries, the v7-238 with 44 covariance data and the v7.1-252 with 56 covariance data, then the continuous energy cross section libraries, the ce_v7_endf and the ce_v7.1_endf. To achieve convergence, a number of 3000 generations with 200 skipped generations and 105 neutrons per generations were specified for the forward calculations.These specified parameters were tripled by TSUNAMI-3D to perform the adjoint solutions in case of multigroup calculations. This choice of parameters is to achieve a good agreement between the forward and adjoint calculations of k_{eff} to obtain accurate sensitivity coefficients, as recommended [8].

To improve the sensitivity coefficients for some system's nuclides the spacial mesh technique in TSUNAMI-3D was used. Computations are run both with and without the mesh option using the four libraries. After some runs, meshes equal to 1, 2 and 6 for MG TSUNAMI-3D, with the MSH option that defines the size of mesh, were fixed. CE TSUNAMI-3D was performed for the same mesh intervals using the CLUTCH sensitivity method (cet=1) [3].

To confirm the accuracy of the calculated sensitivity coefficients, direct perturbation calculations were performed with a perturbation of ±0.36% in the main isotopes densities of the fuel assembly.

The total nuclide sensitivity coefficients, calculated with TSUNAMI-3D, were compared to the direct perturbation calculations. The obtained results reveal similarities for some nuclides, but not for others. In table 1 we notice that the differences between the TSUNAMI-3D results without mesh and the direct perturbation results vary from 1.9% for ^{235}U, 8% for ^{238}U up to 53% for ^{2}H for MG calculations and 11% for ^{235}U, 2% for ^{238}U and 53.7% for ^{2}H in case of CE calculations.

To improve these results, the spacial mesh technique was applied. Therefore, the sensitivity coefficients for ^{2}H were enhanced and the deviation with direct perturbation coefficients were decreased, as shown in tables 2, 3 and 4.

4. Results and discussion

Table 1: Comparison of Sensitivity coefficients for mesh=0

Libraries / Isotopes	MG_V7_238_44			MG_V7.1_252_56			CE_V7			CE_V7.1		
	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ
^{235}U	0.373652	0.38101	0.16234	0.35672	0.37918	0.51498	0.33012	0.38847	0.88506	0.43169	0.38965	0.65563
^{238}U	0.536293	0.49291	0.97572	0.44983	0.49424	0.97989	0.50304	0.51453	0.18028	0.51574	0.50588	0.14767
^{2}H	0.321655	0.19088	2.94067	0.41235	0.18986	5.10102	0.39723	0.42502	0.44816	0.41235	0.42408	0.17592

Table 2: Sensitivity coefficients comparison for mesh=1

Libraries / Isotopes	MG_V7_238_44			MG_V7.1_252_56			CE_V7			CE_V7.1		
	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ
^{235}U	0.37365	0.38408	0.23007	0.35672	0.38225	0.58538	0.37365	0.38847	0.22476	0.43169	0.38781	0.68432
^{238}U	0.53629	0.51533	0.47148	0.44983	0.51653	1.47175	0.53629	0.51453	0.34145	0.51574	0.51359	0.03216
^{2}H	0.32166	0.41531	2.10597	0.41235	0.41248	0.00304	0.32166	0.42502	1.66705	0.41235	0.42312	0.16152

Table 3: Sensitivity coefficients comparison for mesh=2

Libraries / Isotopes	MG_V7_238_44			MG_V7.1_252_56			CE_V7			CE_V7.1		
	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ
^{235}U	0.37365	0.38383	0.22455	0.35672	0.38199	0.57942	0.37365	0.38931	0.23750	0.43169	0.38785	0.68370
^{238}U	0.53629	0.51286	0.52703	0.44983	0.51404	1.41680	0.53629	0.51346	0.35824	0.51574	0.51345	0.03426
^{2}H	0.32166	0.40935	1.97195	0.41235	0.40661	0.13154	0.32166	0.41868	1.56480	0.41235	0.42306	0.16062

Table 4. Sensitivity coefficients comparison for mesh=6

Libraries / Isotopes	MG_V7_238_44			MG_V7.1_252_56			CE_V7			CE_V7.1		
	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ	Sd	Stsun.	Nδ
^{235}U	0.37365	0.38362	0.21992	0.35672	0.38178	0.57461	0.37365	0.38961	0.24205	0.43169	0.38786	0.68354
^{238}U	0.53629	0.51000	0.59135	0.44983	0.51114	1.35281	0.53629	0.51370	0.35447	0.51574	0.51337	0.03545
^{2}H	0.32166	0.36845	1.05226	0.41235	0.36602	1.06216	0.32166	0.41963	1.58012	0.41235	0.42293	0.15868

Results indicate the improvement of the number of standard deviation Nδ when the mesh value is increased, for all libraries. The most accurate results are for meshes 2 and 6 in case of multigroup and continuous energies calculations, were the main isotopes of the system agree within less than two standard deviation, particularly calculations with CE-V7.1 in mesh 6 configuration. Thus the standard deviation, Nδ, for ^{235}U is almost constant for all meshes in each case of library. Similarly, for ^{238}U, TSUNAMI-3D agrees within less than two standard deviations for all cases. Sensitivity coefficients for those isotopes are not much impacted by geometry meshing while ^{2}H isotope's sensitivity coefficients, agree well with the direct perturbation results with less than two standard deviation in all meshed cases. Such results could be expected because scattering terms of the sensitivity coefficients are computed using flux moments, which are impacted by the mesh flux, while ^{235}U and ^{238}U have limited scattering cross-sections contrary to ^{2}H. TSUNAMI-3D gives the sensitivity profiles related to nuclide-reaction. The k_{eff} sensitivity curve was generated, by the Integrated user interface FULCRUM, for the largest total sensitivity coefficients. Fig.2. depicts the sensitivity profiles for fission reaction in ^{235}U and ^{238}U. As expected, ^{235}U reveals a high sensitivity at thermal energies, and ^{238}U reveals a high sensitivity at high energies. Fig.3. presents the sensitivity coefficients for ^{235}U fission generated with the MG ENDF/B-VII.0 44 Cov data and the MG ENDF/B-VII.1 56 Cov data. We notice the high sensitivity of k_{eff} in case of library with 56 group covariance data. This result is justified by the fact that the cross sections uncertainties from the new 56-group library are highe

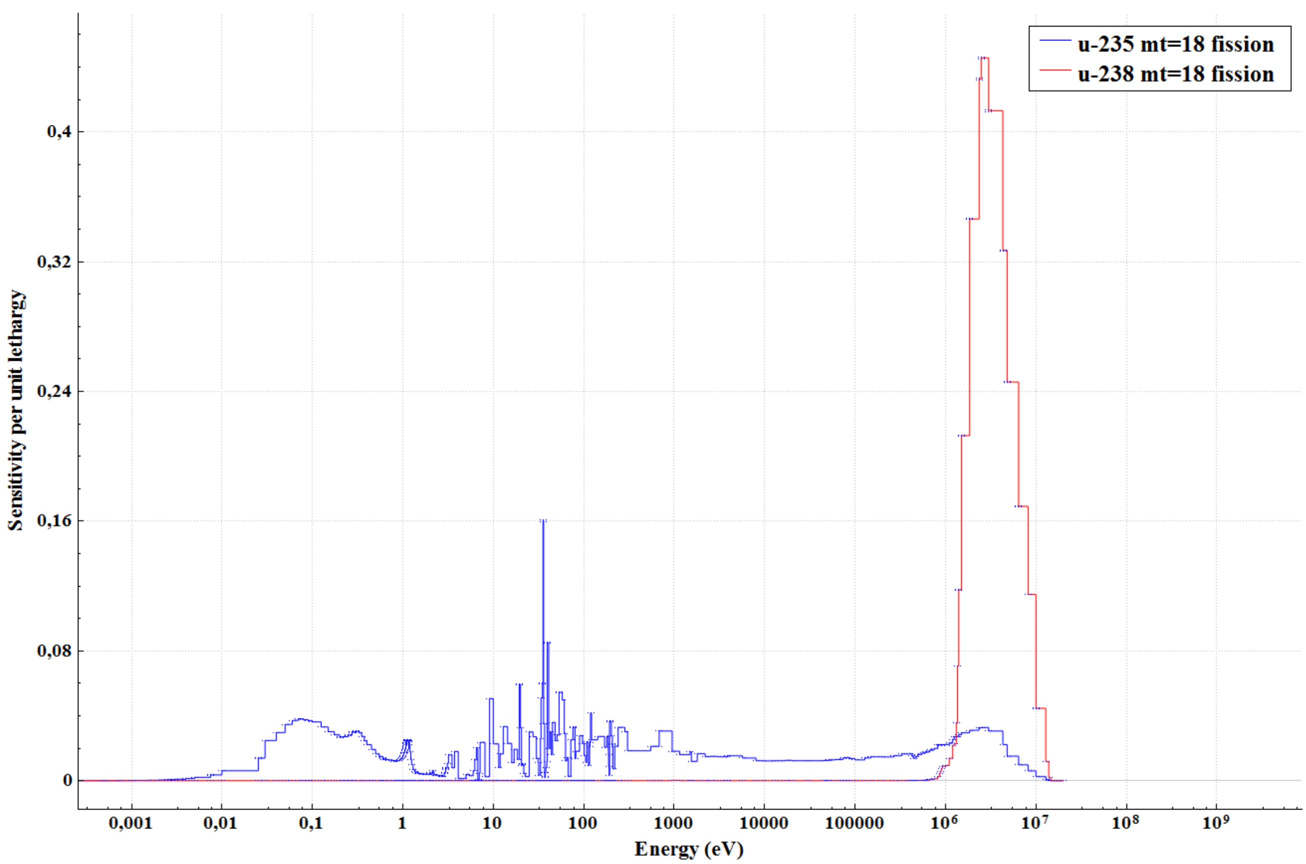

Fig 2. Sensitivity profiles for ^{235}U and ^{238}U fission.

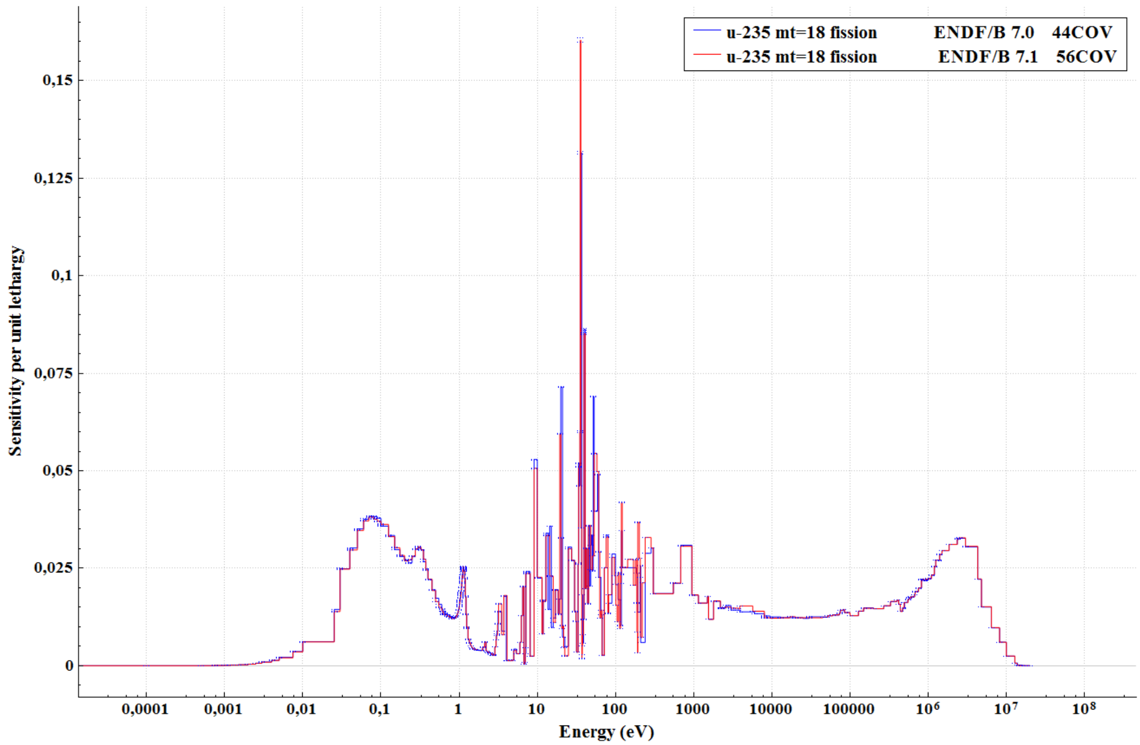

Fig 3. Sensitivity profiles for ^{235}U in case of MG libraries with 44 and 56 group covariance data

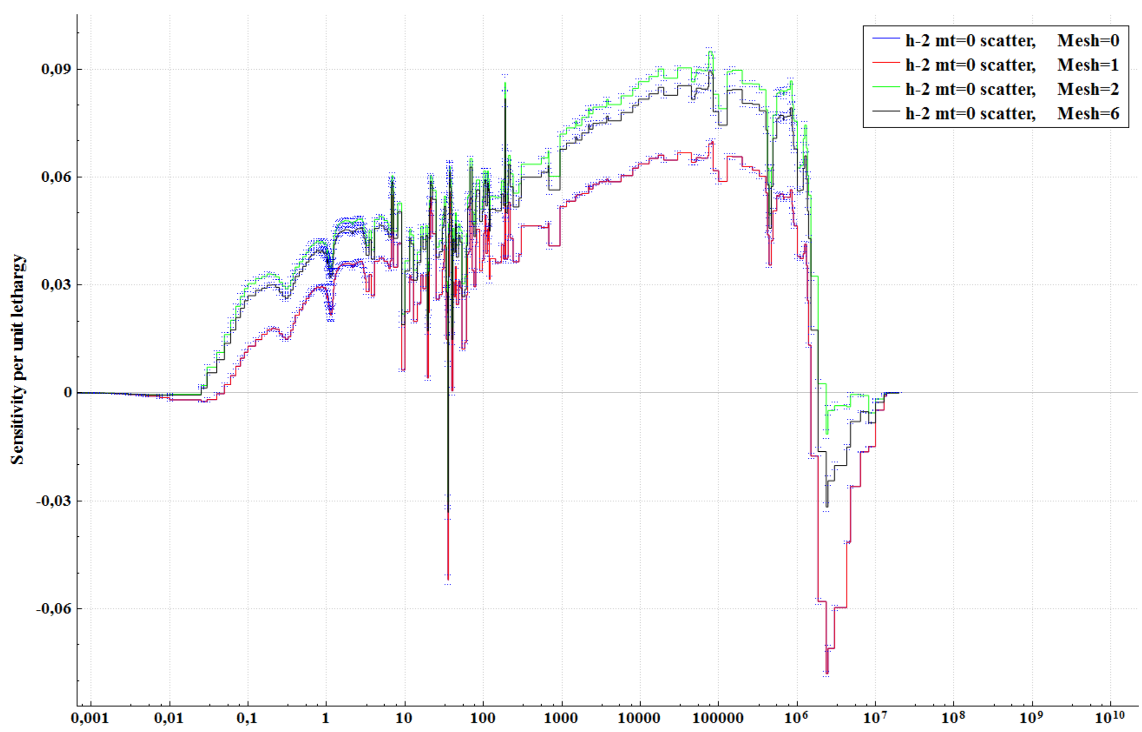

Fig 4. Spacial meshing effect on ^{2}H sensitivity coefficients

In Fig 4 we can see the effect of the spatial meshing on the sensitivity coefficients of ^{2}H nuclide. There is no difference in case of mesh 0 and 1, and a sligth difference between mesh 2 and 6. The sensitivity of k_{eff} to nuclear data is higher when the meshing is incresed and it is pronounced and positive in intermedites energies regions while it is negative in the high-energies regions.

5. Conclusion

The sensitivity study of k_{eff} performed with the SCALE 6.2.3 for Es salam fuel assembly allowed the identification of ^{235}U, ^{238}U and ^{2}H as the main contributors to sensitivity of this parameter. This result was expected because those nuclides are the most efficient isotopes in the fuel assembly.

The use of the multigroup ENDF/B-VII.1 library with 56 group covariance data reveal better results for ^{235}U isotope because the cross sections covariance data were improved in this library.

Moreover, the use of the spacial meshing technique, implemented in the SCALE 6.2 code, for isotopes with high scattering cross section, improved the number of standard deviation when the sensitivity coefficients were compared to the direct perturbation coefficients. Subdividing the geometry provides better resolution of the variation of the flux across the system and produces more accurate results.

The sensitivity analysis applied in this study is the first step, which is the reference for Es-Salam reactor core safety analyses. A further study will be carried out to determine the sensitivity of physical parameters to nuclear data uncertainty in the reactor core and quantify the uncertainty of those parameters with the identification of the most contributors to the k_{eff} uncertainty.

Conflict of Interest

The authors declare that they have no conflict of interest

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