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TSUNAMI-3D and SAMPLER/KENO comparison for sensitivity and uncertainty analysis in neutron multiplication factor for LWRs

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Abstract - *The use of Best-Estimate computer codes is one of the greatest concerns in the nuclear industry especially for licensing analysis. Of paramount importance is the estimation of the uncertainties of the whole system in order to establish the safety margins based on high reliable results. The estimation of these uncertainties should be performed by applying a methodology to propagate the uncertainties from the input parameters and the models implemented in the code to the output parameters.*

In this study, two different approaches have been used for the Sensitivity Analysis (SA) and Uncertainty Quantification (UQ), the adjoint-based perturbation theory of TSUNAMI-3D, and the stochastic sampling technique of SAMPLER/KENO.

Two models of Light Water Reactors were studied in the framework of the OECD/NEA UAM-LWR benchmark, a Boiling Water Reactor (BWR) and a Pressurized Water Reactor (PWR). Both of them at Hot Full Power (HFP) and Hot Zero Power (HZP) conditions, with and without control rod. The presentation of the k_{eff} results of all simulation and a comparison of both methods will be discussed.

I. INTRODUCTION

In neutron transport simulations, it is important to implement Best-Estimate models that give sensitivity and uncertainty information to increase the results reliability [1].

With currently code capability, it is possible to predict the k_{eff} and study the reactivity of a system with low computational time, by deterministic and stochastic approach. After transport calculation, it is recommended to compare obtained results with other simulations and reference values, in order to verify the apply methodology. Moreover, understanding uncertainties is important for introducing appropriate design margins and deciding where additional efforts should be undertaken to reduce these uncertainties.

In this study, the comparison of the multiplication factor is achieved for two assembly calculations under the OECD/NEA Benchmark for Uncertainty Analysis in Best-Estimate Modelling (UAM), for Design, Operation and Safety Analysis of LWRs [2].

Modern neutron transport codes, such as the KENO Monte Carlo approach [3] in the SCALE code system, can predict k_{eff} with a high degree of precision. For that reason, this study compares two modules of SCALE, TSUNAMI-3D and SAMPLER/KENO, both employing KENO-VI sequence, for BWR and PWR simulation. The resulting k_{eff} values are compared among the two module and with reference values.

Using these two different approach, TSUNAMI-3D and SAMPLER/KENO, it was possible to perform the Sensitivity Analysis (SA) with the aim to studying which input parameters are more influential in the predicted response, and Uncertainty Quantification (UQ) to analyzing the distribution of outputs and computed its standard deviation.

II. CODE DESCRIPTION

Calculations are carried out with the SCALE code in version 6.2.1. The two module employed are TSUNAMI-3D and SAMPLER/KENO, with the ENDF/B-VII.1 library. Moreover, the 56group library was used in the multigroup transport calculation and covariance matrices processing.

1. Uncertainty based on Sensitivity Coefficients

The general approach for the uncertainty quantification rely on sensitivity coefficients is based on the "sandwich formula" obtained with the propagation of moments [4]. A brief explanation of this methodology follows.

Being R the calculated response function of a system which depends on (α_1,...,α_n) parameters, R can be approximated by a linear function of (α_1,...,α_n) using the Taylor series approximation around a nominal value (α_1^0,..., α_n^0), where $\delta\alpha_1=\alpha_1 - \alpha_1^0$:

$$R(\alpha_1,\dots,\alpha_n) = R(\alpha_1^0,\dots,\alpha_n^0) + \sum_{i=1}^{n}\left(\frac{\partial R}{\partial \alpha_i}\right)_{(\alpha_1^0,\dots,\alpha_n^0)} \partial\alpha_i \qquad (1)$$

Then, taking the parameters of the system as random variables, R becomes a random variable for which its mean coincides with the response function at the nominal value, and its variance is calculated with the "sandwich rule":

$$var\,(R) = S V_\alpha S^T \qquad (2)$$

where $S=(\partial R/\partial\alpha_1,\dots,\partial R/\partial\alpha_n)$ is the vector of the sensitivity coefficients, and V_α is the covariance matrix of the system parameters.

Usually the sensitivity coefficients are calculated as relative values (relative standard deviation):

$$S_i' = \frac{\partial R/R}{\partial \alpha_i/\alpha_i} \quad (3)$$

however, both values, the standard deviation and the relative standard deviation, are used as a measure of the uncertainty on the response function.

$$(rel.std.dev.(R))^2 = \frac{var\,(R)}{R^2} = S' V_\alpha' S'^T \quad (4)$$

Therefore, the sensitivity coefficients of the response function to the system parameters, S_i or S'_i, should be calculated and the covariance matrix (V_α) or the relative covariance matrix (V'_α) should be provided to reach a complete uncertainty quantification of the system.

2. TSUNAMI-3D sequence

The TSUNAMI-3D [5] sequence uses the KENO-VI Monte Carlo transport code that used the adjoint-based perturbation theory to address the sensitivity of k_{eff} to cross-section data. Moreover, it performs the problem-dependent resonance self-shielding calculations with BONAMI and CENTRM sequences to take into account the appropriate cross-section data and the sensitivity of the resonance-shielding region, considering all materials present in the model [6].

The sensitivity coefficients are obtained through direct perturbation of the input data and interpretation in changes of the output [7]. In direct perturbation, the k_{eff} is computed first with the nominal values of the input, and then with the selected values increased (and decreased) by a certain percentage. Therefore, in TSUNAMI-3D the sensitivity coefficient of k_{eff} to some input value α is computed as:

$$S_{k,\alpha} = \frac{\alpha}{k} \times \frac{dk}{d\alpha} = \frac{\alpha}{k} \times \frac{k_{\alpha^+} - k_{\alpha^-}}{\alpha^+ - \alpha^-} \quad (5)$$

where α^+ and α^- represent the increased and decreased values, respectively, of the input quantity α and $k_{\alpha+}$ and $k_{\alpha-}$ represent the corresponding values of k_{eff}.

Since direct perturbation calculations are performed using KENO, the Monte Carlo approach is applied to the k_{eff} error propagation.

Assuming all values are uncorrelated, the error propagation technique is applying as:

$$\sigma_S = \sqrt{\left(\frac{(\sigma_{k^+}^2 + \sigma_{k^-}^2)}{(k^+ - k^-)} + \frac{\sigma_k^2}{k^2}\right) \times \left(\frac{k^+ - k^-}{k}\right)^2} \times \frac{\alpha}{\alpha^+ - \alpha^-} \quad (6)$$

After the k_{eff} sensitivities propagation, the TSUNAMI-3D sequence determine the uncertainty in the computed k_{eff} due to the tabulated cross-section data. These uncertainties are stored in terms of energy-dependent covariance matrices in the ENDF/B-VII.1 comprehensive library of SCALE.

The covariance libraries had a great importance for uncertainties calculation. They were developed by processing all available covariance information from the respective library, which is limited to only few dozen nuclide. For all other nuclides, the integral uncertainty data [8] for thermal and intermediate energies were used to form the energy-dependent matrices.

TSUNAMI-3D computes the cumulative uncertainty in k_{eff} due to uncertainties in all nuclides and reactions, or to each specific nuclide and reaction. Thus, specific sources of uncertainty can be easily identified.

3. SAMPLER/KENO sequence

SAMPLER is a module for statistical uncertainty analysis that can be used with any sequences in SCALE code. In this study it was used coupled with KENO-VI module for a Monte Carlo approach where a large amount of calculations are performed sampling the problem parameters as random variables, and then carrying out a statistical analysis.

In SAMPLER/KENO, after the transport calculation, the probability density functions (PDF) defined by information in the SCALE multigroup covariance library was sampled. To do this, SAMPLER produces random perturbations for the input Computational Data Vector (CDV) that contains all nuclear cross-sections data. Then, statistical analysis are applied to the output parameters to evaluate responses distributions and quantify uncertainties [9]. The SCALE multigroup covariance data are given as relative values of the infinitely dilute cross-sections. Thus, a random perturbation sample for cross-sections $\sigma_{x,g}(\infty)$ corresponds to $\Delta\sigma_{x,g}(\infty)/\sigma_{x,g}(\infty)$. The GRS sampling based tool XSUSA converts these values to a set of multiplicative perturbation factors $Q_{x,g}$ that are applied to the reference data to obtain the altered values:

$$\sigma'_{x,g} = Q_{x,g}\sigma_{x,g}\,, \quad (7)$$

where

$$Q_{x,g} = 1 + \frac{\Delta\sigma_{x,g}(\infty)}{\sigma_{x,g}(\infty)} \quad (8)$$

Mathematically, the uncertainty in an individual output parameter k is determined as:

$$\Delta k^{exp}(i) = \hat{\mu}_i = \sqrt{\frac{1}{n-1}\sum_{a=1}^{n}\left((k_{calc}^{MC}(i))_a - \overline{k_{calc}^{MC}(i)}\right)^2}\,, \quad (9)$$

where $\Delta k^{exp}(i)$ is the uncertainty in system i due to uncertainties in the input parameters. $(k_{calc}^{MC}(i))_a$ is the ath Monte Carlo (MC) sample of system i, where all uncertain input parameters have been randomly varied within a specified distribution [10].

In SAMPLER, the covariance between two systems, i and j, is determined as:

$$\hat{\Sigma}_{ij} = \sqrt{\frac{1}{n-1}\sum_{a=1}^{n}\left((k_{calc}^{MC}(i))_a - \overline{k_{calc}^{MC}(i)}\right)\left((k_{calc}^{MC}(j))_a - \overline{k_{calc}^{MC}(j)}\right)}\,, \quad (10)$$

and the correlation coefficient between systems i and j can be determined from Eq. (5) and (6) as:

$$c_{ij} = \frac{\hat{\Sigma}_{ij}}{\hat{\mu}_i \hat{\mu}_j}, \qquad (11)$$

Moreover, in SAMPLER it is assumed that the PDF of input parameters is normal distributed and is completely defined by the expected values and covariance matrices, but this does not mean that the output response will have a normal distribution too. In this study, the size of perturbation generated for input parameters was 1000 samples that ensure the 95% of uncertainty and 95% of statistical confidence of the k_{eff} results.

The distribution of output parameters from SAMPLER can be analyzed to obtain the standard deviations for all responses.

III. MODEL DESCRIPTION

This study take part into the OECD/NEA UAM-LWR benchmark which aims to prepare a work program with steps (exercises) that will develop the uncertainty analysis methodologies, for multi-physics and multi-scale simulation. Reference systems and scenarios for coupled code analysis are defined to study the uncertainty effects for all aspect of the system calculations. To achieve these targets, measured data from plant operation and experimental reference data are available for all participants to the benchmark.

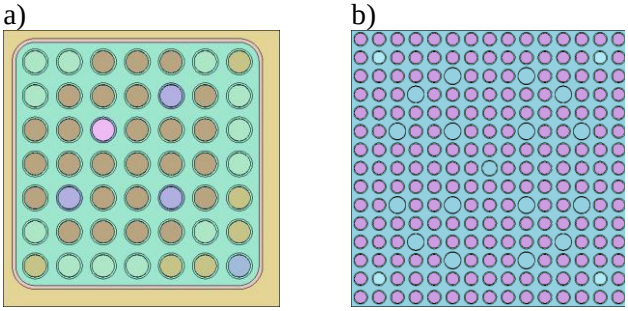

Fig. 1. a) BWR and b) PWR unrodded fuel assemblies.

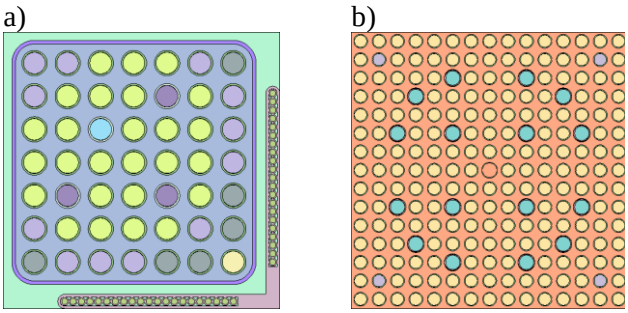

Fig. 2. a) BWR and b) PWR rodded fuel assemblies.

Two main LWR types have been selected for this study, based on the available data:

- Pressurized Water Reactor (PWR) Three Mile Island 1.

- Boiling Water Reactor (BWR) Peach Bottom 2.

Both models have been analyzed at Hot Full Power (HFP) and Hot Zero Power (HZP) conditions. Additionally, the two models have been designed with and without control rod. With a total of eight configurations.
The two fuel assembly geometries are shown in Figure 1 and 2, while Table I and Table II presents the fuel assemblies reference configurations.

Table I. BWR Assemblies data

Parameter	**BWR**
FA pitch (mm)	152.4
Unit cell pitch (mm)	18.75
Fuel pellet diameter (mm)	12.1158
Fuel density (g/cm^3)	10.42
Cladding outside diameter (mm)	14.3002
Cladding thickness (mm)	0.9398
Cladding material	Zirc-2
Cladding density (g/cm^3)	6.55
Gap material	He
Moderator material	H_2O

Table II. PWR Assemblies data

Parameter	**PWR**
FA pitch (mm)	218.11
Unit cell pitch (mm)	14.427
Fuel pellet diameter (mm)	9.391
Fuel density (g/cm^3)	10.283
Cladding outside diameter (mm)	10.928
Cladding thickness (mm)	0.673
Cladding material	Zirc-4
Cladding density (g/cm^3)	6.55
Gap material	He
Moderator material	H_2O

IV. RESULTS AND ANALYSIS

In this section, the results of transport calculation are presented, as well as the sensitivity analysis and propagation of uncertainties results with TSUNAMI-3D and SAMPLER/KENO simulations. Moreover, the neutron multiplication factor results, with their standard deviation, of the two different codes are presented and compared.

In the first place, it is possible to visualize the input of the TSUNAMI-3D simulations with the KENO3D visualization tool for check the accuracy of the models, like it is shown in Figure 3, as an example, for the BWR and PWR unrodded configurations.

The primary objective of this study is to compare the obtained multiplication factor with reference values and between the two employed modules of SCALE. Table III reports this information.

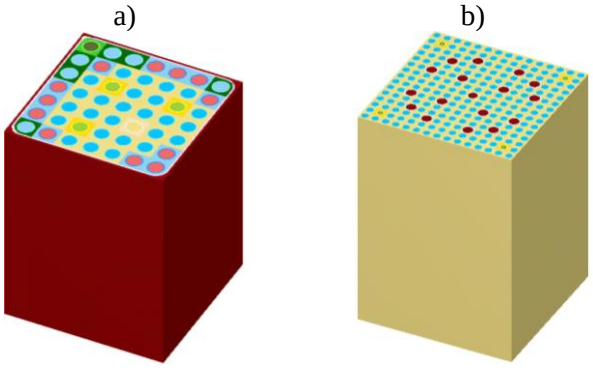

Fig. 3. a) BWR and b) PWR geometry model.

In Table III, the first column shows the case to compare, the second one contains the reference values found in UAM-Benchmark results. The third and fourth columns represent TSUNAMI-3D calculations (k_{eff} result with its uncertainty) while the fifth column shown TSUNAMI-3D error with UAM-Benchmark reference values. Subsequently, the results of SAMPLER/KENO calculations (k_{inf} result with its uncertainty) and their comparison with reference values are shown from columns sixth to eighth. Then, last column in Table III shows a comparison of SAMPLER/KENO and TSUNAMI-3D calculations.

Looking at this table it is possible to see that in TSUNAMI-3D the total uncertainty of the k_{eff} have been evaluated with ranging from 0.036% to 0.068% for all test cases. Moreover, the k_{eff} results are in good agreement with Benchmark values. The calculate errors were lower for the unrodded configurations than rodded ones. But, in general, all error varying between 0.18% and 0.53% for the BWR simulations, and between 0.03% and 0.38% for the PWR simulations.

For SAMPLER/KENO simulations the results were quite different. The standars deviations ranging from 0. 018% to 0.038% for BWR cases and from 0.025% to 0.031% for PWR cases. Regarding k_{eff} results, they have been compared with Benchmark values and TSUNAMI-3D results. In the first case, the k_{eff} of SAMPLER/KENO were very close to the Benchmark values, with errors ranging from 0.05% to 0.18% for all cases, except the BWR_HFP_unrodded and PWR_HZP_rodded cases that presents errors of 0.51% and 0.65% respectively.

For these two cases the differences were probably due to some inconsistency in reference values. Taking into account that the reference values adopted in these tables have been calculated as the average of all submitted results of all benchmark participants, referring to the last submission of year 2016. These values do not take into account the different codes employed by the participant, the different methodologies, the Multigroup or Continuous Energy approach, and so on. For this reason, in some cases differences can be noted.

Moreover, they have been compared the k_{eff} results with both module of SCALE. In general, this comparison gave better results for the BWR cases, for which errors ranging from 0.09% to 0.35%. While, for the PWR cases these errors varying between 0.24% and 0.62%. The error of the PWR_HZP_rodded case highlights that TSUNAMI-3D simulation was closer to reference values, in contrast with SAMPLER/KENO simulation. Thus, this specific case will be further investigate.

Table III. TSUNAMI-3D – SAMPLER/KENO multiplication factor comparison.

Assembly multiplication factor	Benchmark	TSUNAMI		Error	SAMPLER		Error	TSUNAMI-3D – SAMPLER/KENO
	Average	**Value**	**Stddev**	**(%)**	**Average**	**Stddev**	**(%)**	**Error (%)**
BWR_HFP unrodded	1.076E+00	1.08007	6.80E-04	0.38	1.08147	3.09E-04	0.51	0.13
BWR_HZP unrodded	1.108E+00	1.10597	6.50E-04	0.18	1.10697	2.40E-04	0.09	0.09
BWR_HFP rodded	7.870E-01	0.78970	5.40E-04	0.34	0.78785	3.81E-04	0.11	0.23
BWR_HZP rodded	8.620E-01	0.85741	4.90E-04	0.53	0.86044	1.86E-04	0.18	0.35
PWR_HFP unrodded	1.398E+00	1.40031	3.60E-04	0.17	1.39584	2.58E-04	0.15	0.32
PWR_HZP unrodded	1.412E+00	1.41584	4.40E-04	0.29	1.41241	2.53E-04	0.05	0.24
PWR_HFP rodded	1.025E+00	1.02114	5.70E-04	0.38	1.02634	3.18E-04	0.13	0.51
PWR_HZP rodded	1.035E+00	1.03528	4.70E-04	0.03	1.04170	3.16E-04	0.65	0.62

In addition, TSUNAMI-3D simulation gave the sensitivity coefficients integrated by energy, region and mixture. Table IV and Table V shown these results for the BWRs and PWRs cases, respectively.

These sensitivities coefficient resulted after applying the sandwich rule and shown which reaction cross-section is involved in the uncertainty of the neutron multiplication factor calculation. The list of reaction cross-section is similar in both tables. Moreover, the difference in sensitivity between HFP and HZP configuration can be explained because the variance-covariance matrices used in the sandwich rule do not change between cases.

Table IV. Sensitivity Coefficients results for BWR cases.

System	Energy, Region and Mixture Integrated Sensitivity Coefficients		System	Energy, Region and Mixture Integrated Sensitivity Coefficients	
BWR_HFP unrodded	$^{235}U_{nubar}$	9.2719E-01	BWR_HFP rodded	$^{235}U_{chi}$	5.0058E-10
	$^{238}U_{n,gamma}$	-2.2819E-01		$^{235}U_{nubar}$	8.8982E-01
	$^{235}U_{chi}$	-5.0181E-10		$^{238}U_{n,gamma}$	-2.2771E-01
	$^{238}U_{n,n'}$	-8.9920E-03		$^{238}U_{n,n'}$	-1.5632E-02
	$^{235}U_{n,gamma}$	-1.0405E-01		$^{235}U_{fission}$	7.7719E-02
	$^{235}U_{fission}$	4.2169E-01		$^{238}U_{nubar}$	1.1015E-01
BWR_HZP unrodded	$^{235}U_{nubar}$	9.3945E-01	BWR_HZP rodded	$^{235}U_{nubar}$	9.2189E-01
	$^{238}U_{n,gamma}$	-2.0553E-01		$^{238}U_{n,gamma}$	-1.9169E-01
	$^{235}U_{chi}$	-1.1995E-09		$^{235}U_{chi}$	-9.6646E-10
	$^{235}U_{fission}$	4.2349E-01		$^{235}U_{fission}$	4.5927E-01
	$^{235}U_{n,gamma}$	-1.0252E-01		$^{238}U_{n,n'}$	-6.5970E-03
	$^{238}U_{n,n'}$	-6.1720E-03		$^{235}U_{n,gamma}$	-9.4584E-02

Table V. Sensitivity Coefficients results for PWR cases.

System	Energy, Region and Mixture Integrated Sensitivity Coefficients		System	Energy, Region and Mixture Integrated Sensitivity Coefficients	
PWR_HFP unrodded	$^{235}U_{nubar}$	9.4449E-01	PWR_HFP rodded	$^{235}U_{nubar}$	9.2489E-01
	$^{238}U_{n,gamma}$	-1.9942E-01		$^{238}U_{n,gamma}$	-1.8851E-01
	$^{235}U_{n,gamma}$	-1.4856E-01		$^{235}U_{chi}$	1.0501E-09
	$^{235}U_{chi}$	5.0347E-10		$^{238}U_{n,n'}$	-9.1201E-03
	$^{235}U_{fission}$	2.7327E-01		$^{235}U_{n,gamma}$	-1.2712E-01
	$^{238}U_{n,n'}$	-5.1767E-03		$^{235}U_{fission}$	3.7797E-01
PWR_HZP unrodded	$^{235}U_{nubar}$	9.4582E-01	PWR_HZP rodded	$^{235}U_{nubar}$	9.2687E-01
	$^{238}U_{n,gamma}$	-1.9388E-01		$^{238}U_{n,gamma}$	-1.8334E-01
	$^{235}U_{n,gamma}$	-1.4795E-01		$^{235}U_{chi}$	-6.2371E-10
	$^{235}U_{chi}$	-4.5228E-10		$^{238}U_{n,n'}$	-8.6500E-03
	$^{235}U_{fission}$	2.7240E-01		$^{235}U_{n,gamma}$	-1.2715E-01
	$^{238}U_{n,n'}$	-4.9003E-03		$^{235}U_{fission}$	3.7507E-01

A list of the uncertainty contributors to the k_{eff} of each variance-covariance matrix of the reaction pair were presented Figure 4 for the BWR cases and Figure 5 for the PWR cases. It can be see that 235U-nubar and 238U-n,gamma are the most influential reactions for both cases, BWR and PWR. Moreover, the given rel.std.dev.(%) for these two reactions have resulted in 0.035% as a maximum value

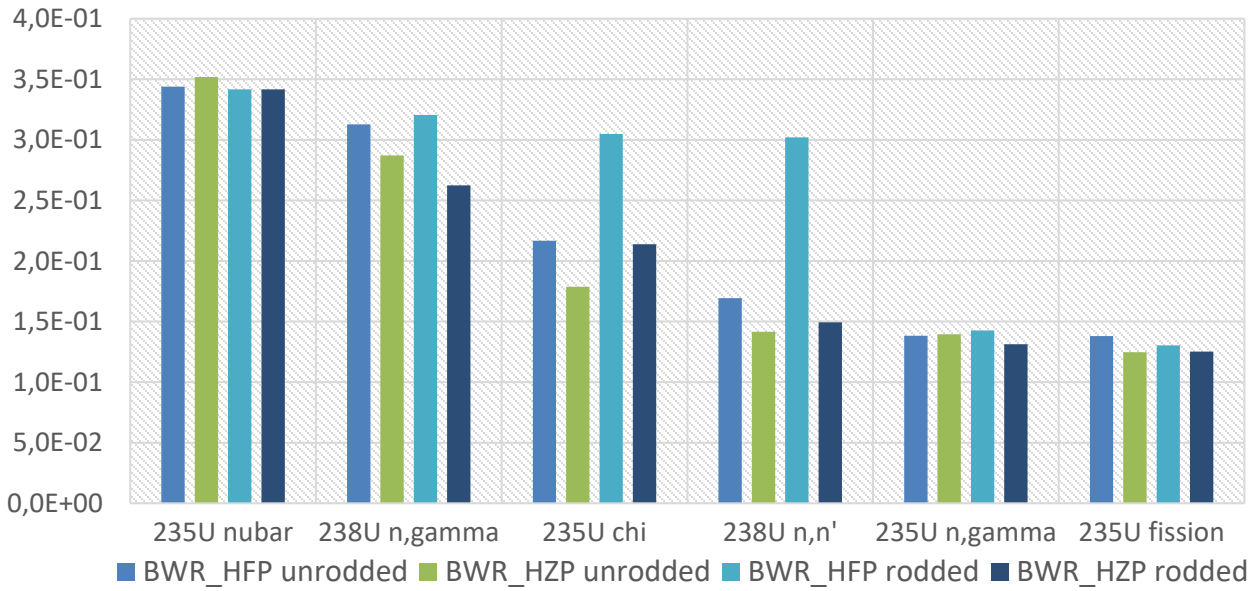

Fig. 4. Uncertainty contributors to the k_{eff} of each variance-covariance matrix of the reaction pair. BWR cases.

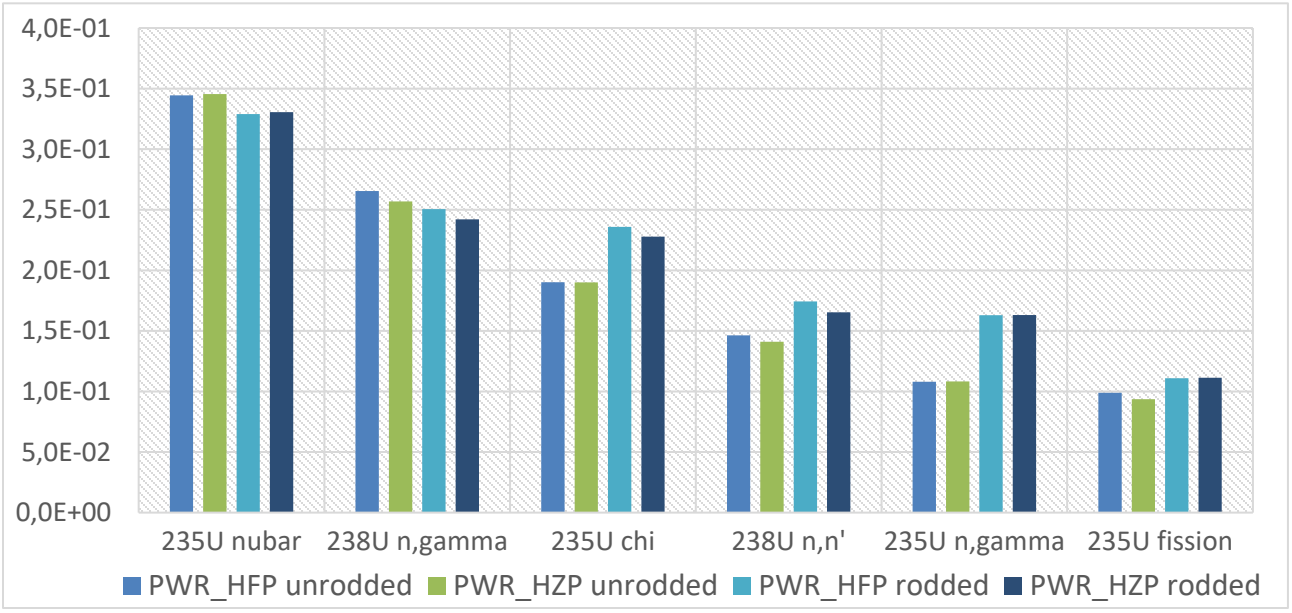

Fig. 5. Uncertainty contributors to the k_{eff} of each variance-covariance matrix of the reaction pair. PWR cases

V. CONCLUSIONS

This study achieves a cross-sections calculation with two 3D transport codes and provides confidence bounds with other statistical information. They could be very useful for the development of Best-Estimate codes, reduce the uncertainties in calculations and increase the results reliability.

The calculations and analysis are carried out in the framework of UAM-LWR-Benchmark with two test cases: PB-2 BWR and TMI-1 PWR fuel assembly. Following Benchmark specifications, eight different configurations have been performed.

In the first place, it has been possible to compare the results of k_{eff} and main cross-sections, between the two modules employed in SCALE, and with reference values.

It was found a good agreement in cross-section calculation, with both simulations, used in TSUNAMI-3D and SAMPLER/KENO calculation.

The uncertainties obtained in TSUNAMI-3D have been found to be ≈0.035% in all cases. Moreover, the most important contributors to the uncertainty in k_{eff} were found

$^{235}U_{nubar}$, $^{238}U_{n,\gamma}$, $^{235}U_{chi,}$ $^{238}U_{n,n,}$ $^{235}U_{n,\gamma}$, for almost all simulations.

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