SIMILARITY AND UNCERTAINTY ANALYSIS OF THE ALLEGRO MOX CORE

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1. Introduction

In the Gas Fast Reactor development plan, ALLEGRO is the first necessary step towards the electricity generating prototype GFR. This paper presents the first stage of study for the ESNII+ 75 MW_{th} ALLEGRO reactor conceptual design [1]. Several studies on conventional metal-clad MOX core are presented, covering similarity and uncertainty analyses. Detailed SCALE [2] KENO VI models have been developed and numerous calculations were performed to determine neutronic parameters, such ask_{eff}, neutron flux spatial distribution, fission source distribution, local multiplicative factors, sensitivity profiles and response uncertainties.The main principles of fast reactor systems are rather well understood, however, their optimization, in order to comply more effectively with requirements and their timely deployment, requires the research in nuclear data. Although most nuclear data are by and large available in modern data files, their accuracy and validation is still a major concern. The main source of uncertainty in the calculated response is due to uncertainties in evaluated nuclear data such as microscopic cross sections (XS), fission spectra, neutron yield, and scattering distributions that are contained in cross section evaluations. These uncertainties are governed by probability distributions which are unknown, but the evaluated data values are assumed to represent the mean of the distribution, and the evaluated variance represents a measure of the distribution width. Correlations as well as uncertainties in nuclear data may have a significant impact on the overall uncertainty in the calculated response; thus, it is important to include them in the uncertainty analyses. By application of TSUSANAMI-IP utility available in SCALE system the neutronic similarity of ALLEGRO MOX core to the specific set of benchmarks was calculated and evaluated.

2. Theory

TSUNAMI-IP utility uses sensitivity data generated by TSUNAMI-1D and/or TSUNAMI-3D [3]sequences and cross section-covariance data stored in the 44GRPCOV library. TSUNAMI-1D/3D are sequences that execute modules to determine response sensitivities and uncertainties. The linked computations perform the cross section self-shielding operations, forward and transport calculations, computation of sensitivity coefficients and calculation of the response uncertainty. The whole application system - ALLEGRO MOX sensitivity calculation in 238 and 44 energy group structures is described elsewhere in detail [4]. The SCALE covariance library [5] is based on several different uncertainty approximations with varying degrees of fidelity to the actual nuclear data evaluation. The library includes evaluated covariances obtained from ENDF/B-VII, ENDF/B-VI, and JENDL3.3 for more than 50 materials. It is assumed that covariances taken from one data evaluation such as ENDF/B-VI or JENDL-3.3, can also be applied to other evaluations of the same data, such as ENDF/B-VII. If this is done judiciously for cases in which the nuclear data evaluations are similar, then the covariances taken from one source should be a reasonable representation of uncertainties for the other evaluations [6].

ORNL has a database of pre-calculated sensitivity profiles for several hundred critical benchmark experiments specified in the ICSBEP Handbook [7]. These sensitivities may be input to TSUNAMI-IP utility, along with calculated sensitivity profile of application system. In our case 494 benchmark experiments with various energy group structures were used.

Three global integral indices [2] are used in the analysis to assess the similarity of ALLEGRO MOX neutronic core design (hereinafter application – index *a*) and a single experiment (*e*) on a system-wide basis for all nuclides and reactions. Each integral index is normalized such that a value of 1.0 represents complete similarity between ALLEGRO MOX core design and specific benchmark experiment and the value of 0.0 indicates no similarity. The uncertainty of the integral response ΔR (for instance k_{eff}) on the target integral parameter by the use of XS sensitivity coefficients denoted by symbol *S* and XS covariance matrix *M* can be evaluated by the well-known sandwich formula:

$$\Delta R^2 = S_R M S_R^T . \tag{1}$$

where the impact of the individual reactions and energy groups can be evaluated separately. The diagonal elements of the resulting matrix, defined as the solution of Eq.(1), represent the relative variance values for each of the system under consideration, and the off-diagonal elements are the relative covariances between given experiments. Following the SCALE methodology, these covariances transformed to correlation coefficients (*ck*) describe the degree of correlation (coupling) in the uncertainties between the two specific systems. This correlation (coupling) demonstrates the level of similarity in predicted response biases between various systems in the frame of XS induced uncertainties. The *E* parameter given by Eq. (2) assesses similarity between two systems based on the magnitude and shape of all sensitivity profiles.

$$E = \frac{S_a S_e^T}{|S_a||S_e|} . \tag{2}$$

If the qroup-wise sensitivity data for all nuclides and reactions for each system are considered as a vector, the index *E* is the cosine of the angle between the two sensitivity vectors. If theses vectors are parallel (*E*=1), the systems are proportional. The next *G* index assesses the similarity of two systems based on normalized differences in the energy dependent sensitivity data for fission, capture and scatter. A physical interpretation of the *G* index is the ratio of the sum of the sensitivity coefficients of the application that are covered by the experiment to the sum of the sensitivity coefficients for the application. The *G* index is defined as follows:

$$G = 1 - \frac{\sum_n \sum_x \sum_j \left(S_{x,j}^{a,n} - S_{x,j}^{e',n} \right)}{\sum_n \sum_x \sum_j \left(S_{x,j}^{a,n} \right)} . \tag{3}$$

where the symbol *n* stands for the number of application system nuclides, *x* represents the reaction and *j* summation is performed over all energy groups. As can be seen from Eq. (3), a *G* of 1 indicates complete similarity and a *G* value of 0 indicates no similarity. The nuclide-reaction specific partial integral index based on the same coverage criteria as *G* is denoted *g*.

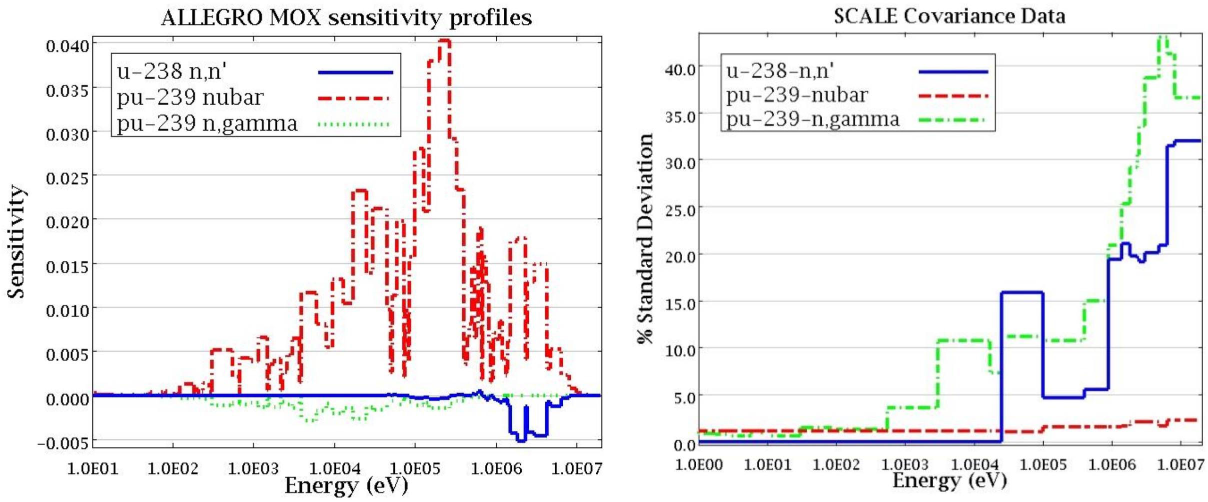
3. Results

Mentioned above, the TSUNAMI sequence computes the contributors to the application response uncertainty due to the XS covariance data. The relative standard deviation of ALLEGRO MOX k_{eff} due to XS covariance data is 1.0404%. Tab.1 lists the top 16 covariance matrices that contribute to the k_{eff} uncertainty. These contributors represent more that 98% of the total uncertainty induced by XS data. The k_{eff} in the case of 238 energy group calculation with control and safety rods reaches 1.02534 ± 0.00019.

Tab.1. *Uncertainty contribution in ALLEGRO MOX k_{eff}.*

No.	Covariance Matrix		Contributions to Uncertainty in k_{eff} (% Δk/k)	No.	Covariance Matrix		Contributions to Uncertainty in k_{eff} (% Δk/k)
	Nuclide-Reaction	**Nuclide-Reaction**	**Due to the Matrix**		**Nuclide-Reaction**	**Nuclide-Reaction**	**Due to the Matrix**
1	^{239}Pu nubar	^{239}Pu nubar	6.7999E-01	9	^{238}U n,gamma	^{238}U n,gamma	1.5155E-01
2	^{238}U n,n'	^{238}U n,n'	5.0948E-01	10	^{238}U nubar	^{238}U nubar	1.1712E-01
3	^{240}Pu nubar	^{240}Pu nubar	2.3377E-01	11	^{56}Fe elastic	^{56}Fe elastic	9.6235E-02
4	^{239}Pu n,gamma	^{239}Pu n,gamma	2.3310E-01	12	^{56}Fe n,gamma	^{56}Fe n,gamma	7.5133E-02
5	^{239}Pu chi	^{239}Pu chi	2.1225E-01	13	^{241}Pu fission	^{241}Pu fission	6.7164E-02
6	^{238}Pu fission	^{238}Pu fission	2.0489E-01	14	^{240}Pu fission	^{239}Pu fission	5.8365E-02
7	^{238}U elastic	^{238}U n,n'	1.9741E-01	15	^{52}Cr elastic	^{52}Cr elastic	5.4093E-02
8	^{239}Pu fission	^{239}Pu fission	1.8240E-01	16	^{239}Pu n,n'	^{239}Pu n,n'	5.4073E-02

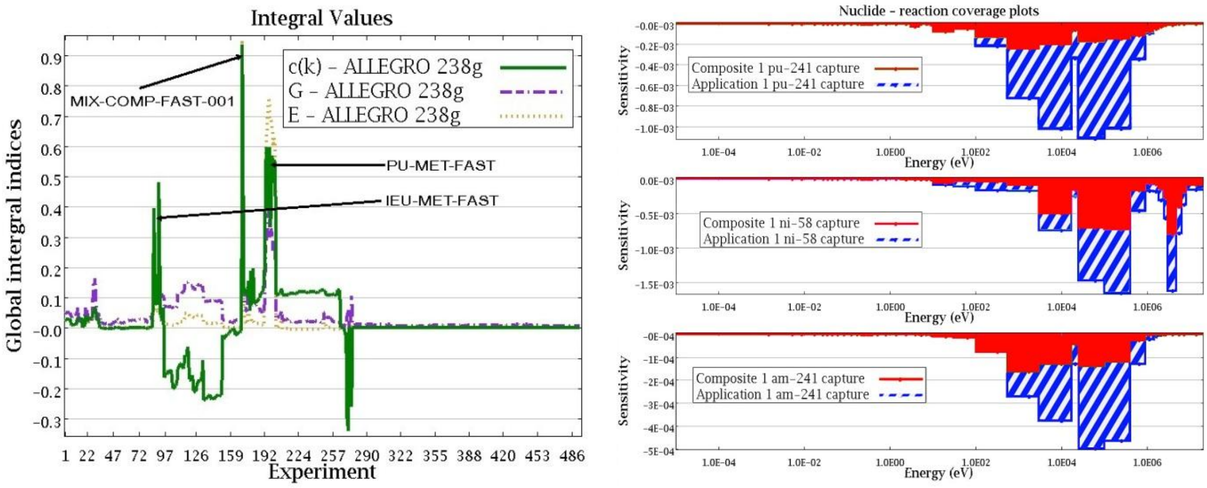
The top contributor to application k_{eff} uncertainty is the ^{239}Punubar. This is due to the large PuO_2volume fraction (25.5%) in the MOX fuel and as can be seen in Fig.1, alsodue to the high sensitivities above 100 keV threshold. In case of ^{238}U n,n’ there are large negative sensitivities in the energy range above 1 MeV burdened with significant relative standard deviation of XS data (20 ÷ 35%). Although k_{eff} sensitivities to ^{239}Pu n, gamma are in magnitude much smaller than ^{238}U n,n’ and ^{239}Pu nubar, the uncertainty associated to XS data is large and varies between 5 to 45% in the relevant energy range.



a) b)

Fig.1: *Application sensitivity profiles and covariance data.*

Similarity assessment procedure identified three groups of potential experiments, where *ck*coefficients got over 0.4. However, only one experiment (MIX-COMP-FAST-001-001)reached *ck* greater than 0.9, as can be seen in Fig. 1-a).



a) b)

Fig.2: *Integral indices and coverage plots.*

The good similarity results are mainly driven by the type of fuel (MOX) and fuel cladding material used in the ALLEGRO model and in theMIX-COMP-FAST-001-001 experiment. Although the *E* coefficient reaches a quite high value (0.95), the big portion (25%) of ALLEGRO sensitivity profiles is uncovered (*G*) by this experiment. This is mainly caused by different construction materials and coolants (helium vs sodium) used in adopted models resulting to the dissimilar neutron spectra.The short characteristics of other identified experiments are shown in following Tab. 2.

Tab. 2.*Integral indices for similar experiments in relation to ALLEGRO MOX.*

ID	ICSBEPID	Fissile material	Moderator	Average Fission Group Energy	Neutron Flux > 100 keV	Capture > 100 keV	Cladding	Reflector	*ck*	*E*	*G*
171	MIX-COMP-FAST-001-001	MOX	Na	99.8keV	57%	22%	SS	Depl.U	0.93	0.95	0.75
197	PU-MET-FAST-008-001	Pu Metal	-	1.08 MeV	95%	80%	-	Th	0.60	0.68	0.30
194	PU-MET-FAST-002-001	Pu Metal	-	1.28 MeV	97%	85%	-	-	0.60	0.62	0.30
199	PU-MET-FAST-018-001	Pu Metal	-	913keV	92%	57%	-	Be	0.57	0.67	0.30
201	PU-MET-FAST-023-001	Pu Metal	-	1.17 MeV	97%	83%	-	Gr	0.56	0.63	0.26
202	PU-MET-FAST-024-001	Pu Metal	-	647 keV	95%	45%	-	PE	0.54	0.62	0.27
193	PU-MET-FAST-001-001	Pu Metal	-	1.28 MeV	97%	86%	-	-	0.54	0.60	0.26
200	PU-MET-FAST-022-001	Pu Metal	-	1.26 MeV	97%	86%	-	-	0.54	0.60	0.26
196	PU-MET-FAST-006-001	Pu Metal	-	1.11 MeV	94%	75%	-	Nat. U	0.47	0.77	0.42

From Tab.2 we can conclude that the majority of identified experiments,with exception of MIX-COMP-FAST-001-001, are simple plutonium metal systems. The average fission group energy in these systems is quite high due to the absence of moderator and structural materials (over 1 MeV). Because of their simplicity, the*G* value gets very low for all cases. The values of*g*indices for the nuclide – reaction pairs,having the great impact to active core neutron balance, are given in Tab. 3.

Tab. 3.The results of nuclide-reaction specific partial integral index g.

ID	^{238}U capture	^{238}U total	^{239}Pu capture	^{238}U n,n'	^{240}Pu capture	^{56}Fe capture	^{58}Ni capture	^{238}U scatter	^{241}Pu capture	^{16}O capture	^{241}Am capture
171	1.00	0.99	0.98	0.99	0.46	0.90	0.47	0.96	0.20	1.00	0.35

The data presented in Tab.3 highlight thenuclide – reaction pairs which are not sufficiently covered by the MIX-COMP-FAST-001-001 experiment. Fig. 2-b) shows the coverage of the most problematic nuclide – reaction sensitivity profiles by the use of all experiments involved in calculation. The hashed area of sensitivity profiles highlights the importance of experimental verification of used nuclear data in energies in the interval between 100 keV and 1 MeV.

4. Conclusion

The similarity and uncertainty analysis of the ESNII+ ALLEGRO MOX core has identified specific problems and challenges in the field of neutronic calculations. Similarity assessment identified 9 partly comparable experiments where only one reached *ck* and *E* values over 0.9. However the Global Integral Index G remains still low (0.75) and cannot be judgedas sufficient. The total uncertainty of calculated k_{eff} induced by XS data is according to our calculation 1.04%. The main contributors to this uncertainty are ^{239}Pu nubar and ^{238}U inelastic scattering. The additional margin from uncovered sensitivities was determined to be0.28%. The identified low number of similar experiments prevents the use of advanced XS adjustment and bias estimation methods. More experimental data are needed and presented results may serve as a basic step in development of necessary critical assemblies. Although exact data are not presented in the paper, faster 44 energy group calculation gives almost the same results in similarity analysis in comparison to more complex 238 group calculation.

Finally, it was demonstrated that TSUNAMI-IP utility can play a significant role in the future fast reactor development in Slovakia and in the Visegrad region. Clearly a further R&D and strong effort should be carried out in order to receive more complex methodology consisting of more plausible covariance data and related quantities.

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