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Application of nuclear data covariance matrices to representativity calculations

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Abstract. The neutronics design of new reactors has been historically relying on zero power research reactors for the simulation of the core irradiation conditions as well as for nuclear data and code validation. In this framework, a study on the possible MYRRHA representativity improvement coming from the loading of MOX fuel in VENUS-F zero power reactor is under investigation. This work analyses the effect of the nuclear data used in the sensitivity and representativity calculations, highlighting the need for a comprehensive set of nuclides and reactions to be further studied.

1 Introduction

VENUS-F [1] is the fast zero-power research reactor operated at SCK CEN to be representative of the neutronics of MYRRHA [2] evolving core design. Most of the nuclides foreseen in the MYRRHA fuel assembly are present in the VENUS-F fuel assemblies as well, meaning that for example Pb and Bi of the lead-bismuth eutectic (LBE) coolant of MYRRHA are simulated in VENUS-F via Pb and/or Bi rodlets or plates. MYRRHA will feature 30%w.t.-enriched MOX fuel, simulated in the VENUS-F cores loaded so far using 30%w.t.-enriched metallic uranium fuel and Al₂O₃.

The main representativity limitation of such VENUS-F assemblies to the MYRRHA ones comes from their different fuel composition. Therefore, the possibility to load MOX fuel in VENUS-F is under investigation. However, since no fast reactor MOX rodlet is available at SCK CEN, the only solution to insert Pu in the VENUS-F lattice is the use of existing PWR MOX fuels. Because of the strong difference in both Pu vector and content, a representativity study is performed on a number of proposed assembly designs to identify the most promising one before moving to a full core representativity assessment. In the following, the methodology for the representativity measure is summarized and the impact on that of the nuclear data choice is investigated.

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2 Methodology

2.1 Representativity

In this study, the representativity parameter r used in the design choice is defined to be the correlation of two models induced by the nuclear data, which is

$$r = \frac{S_V^t \Sigma_{nd} S_M}{\sqrt{S_V^t \Sigma_{nd} S_V} \sqrt{S_M^t \Sigma_{nd} S_M}}, \quad (1)$$

where S are the nuclide-reaction-energy sensitivity vectors (S_V : VENUS-F assemblies; S_M : MYRRHA assembly) and Σ_{nd} is the nuclear data covariance matrix associated with the evaluated nuclear data library. This equation was already used in the frame of nuclear reactor representativity study [3] and is in principle applicable to any parameter for which sensitivities can be computed (e.g.: k_∞ , β_{eff}).

2.2 Model design

Among several assembly models proposed in the frame of the VENUS-F MOX loading investigation [8], two were chosen for this study on the effect of the nuclear data evaluation. These feature the Bi coolant simulator only (no Pb is present in the presented models) and will be named *checkerboard* (left in Fig. 1) and *plates* (right in Fig. 1). Fig. 1 also reports the MYRRHA fuel assembly at beginning of irradiation to which the representativity was computed.

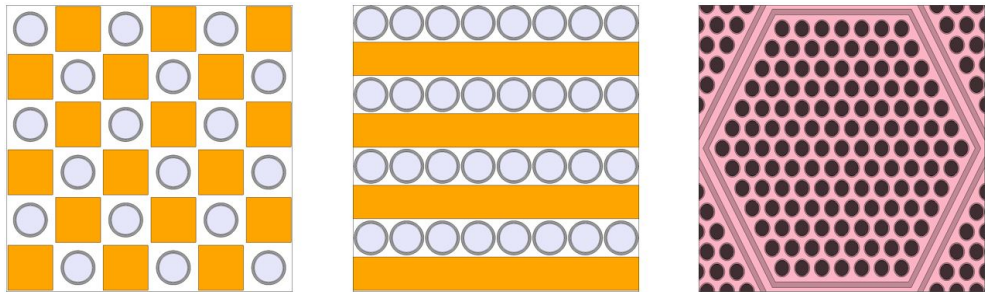


Figure 1. Proposed VENUS-F assembly designs and MYRRHA assembly (hexagonal). Yellow: Bi, light gray: VENUS-F MOX, gray: stainless steel, white: air, pink: LBE, black: MYRRHA MOX.

The 2D fuel assemblies in Fig. 1 were modeled in Serpent [4] with reflective boundary conditions. The sensitivity of k_∞ to the capture, fission, elastic and inelastic reaction cross sections as well as to the neutron multiplicity ($\bar{\nu}_p$, $\bar{\nu}_d$) — according to the standard ENDF-6 nomenclature [9], MT: 102, 18, 2, 4, 456, 455 — of the nuclides in the simulation — ^{238}U , ^{235}U , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu , ^{241}Am , ^{56}Fe , ^{16}O , ^{209}Bi — was computed using the sensitivity module of Serpent considering 15 latent generations. The results of simulations performed with ENDF/B-VIII.0 [7], JEFF-4T2.2 [5] and JENDL-4.0u [6] data are compared in the following.

Because of the fuel availability at VENUS-F, 14%w.t.-enriched MOX was modeled in the VENUS-F assembly designs. The 40 year decay of such a fuel, computed assuming a loading in December 2023, leads to the production of ^{241}Am . The reference actinide vector

of the MYRRHA MOX fuel considered for preliminary design against the one modeled in the VENUS-F assemblies is reported in Tab. 1, where the lower enrichment and the longer decay time are visible¹.

Table 1. MOX fuel actinide array mass density ratio: VENUS-F over MYRRHA

²³⁵ U	²³⁸ U	²³⁸ Pu	²³⁹ Pu	²⁴⁰ Pu	²⁴¹ Pu	²⁴² Pu	²⁴¹ Am
0.71	1.23	0.19	0.53	0.42	0.11	0.28	2.34

3 Results

The impact of nuclear data on the representativity parameter has two main sources: on the one hand it comes from the differences in the sensitivity profiles computed using different nuclear data, on the other hand it lies in the use of evaluated covariance matrices in Eq. 1. In this section those results are analysed for the two assembly models proposed for VENUS-F.

3.1 Sensitivity profiles

Fig. 2 reports the k_∞ relative sensitivity computed with Serpent for the four most relevant nuclear data in the analyzed systems. The lower relevance of ²³⁸U in MYRRHA compared to VENUS-F is attributable to the higher plutonium enrichment of the MYRRHA fuel. This also explains the larger importance of $\bar{\nu}_p$ of ²³⁹Pu in MYRRHA when compared to the proposed VENUS-F assembly designs. Overall, the sensitivities computed for the proposed checkerboard and plate designs practically overlap, being the two designs fairly similar as in a fast system the nuclide share is more relevant than the location of the components. All the presented sensitivity results are affected by minimal statistical error, of the order of 10^{-4} tops in absolute terms, as reported in Fig. 2 (dashed line in the plots; values in relative terms on the right axis). Fig. 2 shows a negligible effect of the nuclear data library choice on the computed sensitivity profiles. This is consistent with the literature [10] and comes from the global nature of k_∞ .

To complement the study with a measure of the change in the sensitivity of k_∞ to less relevant reactions too, the similarity was calculated with two libraries p and q for each design as

$$e_{p,q} = \frac{S_p^t \cdot S_q}{|S_p||S_q|}. \quad (2)$$

This approach is analogous to what is proposed in Eq. 1, not weighting the sensitivity over the covariance matrix. This is the same as considering an identity covariance matrix and has the advantage of not requiring the choice of an evaluated covariance matrix in the calculation, making e suitable for library comparison. Eq. 2 is symmetric with respect to p and q , meaning $e_{p,q} = e_{q,p}$. The computed similarities are above 0.99 for each nuclear data library couple on any of the assembly designs. The complement to 1 of e is attributable both to actual sensitivity differences coming from the library choice (orthogonality) and to statistical fluctuation.

¹The MOX composition of the current design of MYRRHA as well as the one of the fuel available at VENUS-F is confidential. Indicative values of the MYRRHA MOX fuel concentration can be found in Ref. [11].

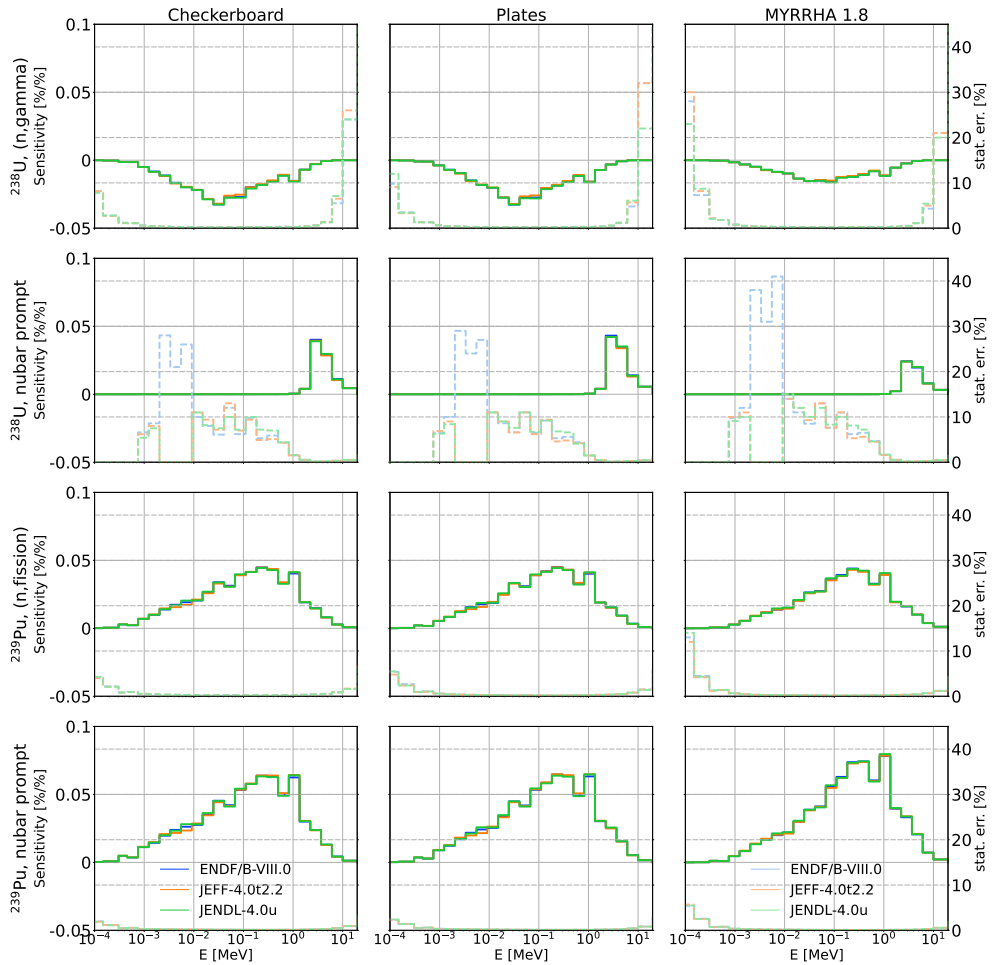


Figure 2. Relative k_{∞} sensitivity profiles to the most relevant nuclear data in the analysed systems (left axis, full line) and corresponding relative statistical error (right axis, dotted line).

3.2 Representativity

Tab. 2 reports the k_{∞} representativity values computed with ENDF/B-VIII.0, JEFF-4T2.2² and JENDL-4.0u. Good (0.90 - 0.95) to very good (0.95 - 1.00) representativities of the proposed VENUS-F fuel assembly designs to MYRRHA were computed for all the nuclear data libraries. The standard error from the Serpent counting statistics of the sensitivity profiles was propagated to the representativity values and is always lower than 0.1%.

Varying the nuclear data library, the plates design consistently performs better than the checkerboard one in terms of representativity; this seems to be a consequence of a slightly better match of the sensitivities computed in the plate design to the ones of the MYRRHA fuel assembly, especially for the reactions of ^{238}U (see Fig. 3). This is a consequence of a more MYRRHA-representative fuel-to-other-elements ratio in the plates design than in the

²The representativity calculation with JEFF-4T2.2 was performed using JEFF-4T2.2 sensitivity profiles and JEFF-3.3 covariance matrices because of partial unavailability of the JEFF-4T2.2 covariance matrices at the time of the calculation.

checkerboard one. JEFF-4T2.2 gives slightly larger representativity values than the other libraries for both the studied designs, JENDL-4.0u and ENDF/B-VIII.0 follow.

Table 2. Computed representativities of the proposed checkerboard and plates VENUS-F assembly proposed designs to the one of MYRRHA.

	checkerboard	plates
ENDF/B-VIII.0	0.91	0.94
JEFF-4T2.2	0.95	0.96
JENDL-4.0u	0.93	0.94

Fig. 3 reports how the representativity cumulates to the values in Tab. 2 including more nuclides in the analysis. Comparing the two designs, consistent trends are noticed. ^{239}Pu and ^{238}U are the main contributors to the total representativity for every design because of the large sensitivity of k_{∞} to their data. The different contribution of these nuclides to the total representativity noticed for the calculations performed with different nuclear data libraries is explained by the differences in the evaluated uncertainties. As a matter of fact, ENDF/B-VIII.0 evaluates larger uncertainties for the reactions of ^{239}Pu and JENDL-4.0u evaluates larger uncertainties for the reactions of ^{238}U , which is consistent with Fig. 3.

The covariance matrices of the cross sections of ^{241}Am are stored in JEFF-3.3 in the MF32 file, which was not processed in this study. Finally, JEFF-3.3 and JENDL-4.0u do not provide any covariance evaluation for the elastic scattering and capture cross sections of ^{209}Bi . One should consider that the contribution to the cumulated representativity is positive for any nuclide as its sign depends on the alignment of the sign of the product of the sensitivity vectors (and the sensitivity of k_{∞} will be positive to σ_f and negative to σ_c no matter the considered nuclide). Despite this, the JEFF calculation results in larger representativity. This is because the contribution of those nuclides to the cumulated representativity is small, as visible in Fig. 3 for ENDF/B-VIII.0 and JENDL-4.0u. Indeed, the lack of covariance information (or a not complete sensitivity vector) makes the analysis blind to some characteristics of the analysed system.

Despite some nuclides in Fig.3 being not relevant to the cumulated sensitivity, those should not be excluded from the analysis as their negligible contribution does not necessarily come from low sensitivity or covariance evaluation. Their low contribution to the representativity might be negligible because of an orthogonality of the two systems compared, which would make it information-bearing.

4 Conclusion

Two MOX assembly designs were proposed for the VENUS-F reactor to make it more similar to MYRRHA. For the sake of this study, assemblies with a bismuth coolant simulator were considered only. The representativity of the proposed designs to MYRRHA fuel assembly was assessed to identify the most promising VENUS-F proposed design, which resulted to be the one where the bismuth coolant simulator is included in the form of plates.

The impact of the nuclear data library choice on the sensitivity and representativity calculation was assessed. The k_{∞} sensitivity calculation resulted to be practically independent on the nuclear data library employed in the simulation, with similarities above 0.99 among the sensitivities of any design to itself computed with any library. The difference on the representativity obtained using different nuclear data libraries (up to about 4%) is then likely to be attributed to the different covariance evaluations. This differs both in the evaluated data and in

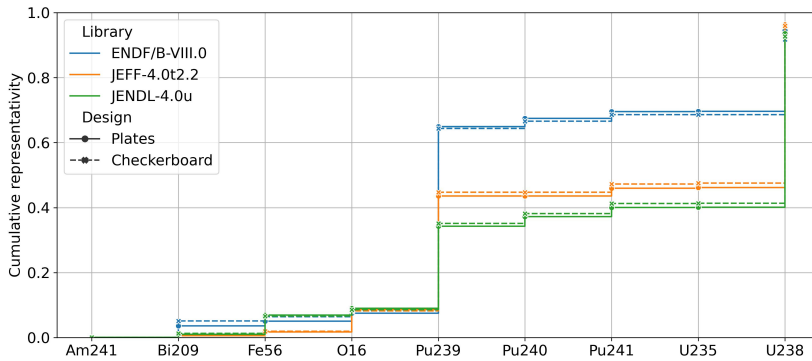


Figure 3. Nuclide contribution to the cumulated representativity.

their availability, highlighting the importance of considering a most complete set of nuclides and reactions in the sensitivity-representativity calculation to get more holistic results.

This work represents a first study in this sense, to be further investigated especially moving to a 3D MOX assembly design and to a full core design, where changes in the sensitivity profiles are expected as a consequence of the softer spectrum and therefore some of the conclusions of this work shall be checked again. Moreover, speaking of a full VENUS-F core design featuring some MOX fuel assemblies, one shall consider that the available MOX fuel at VENUS-F would likely be enough for a central zone of the core, which would require a driver with the current metallic U fuel. Based on their experience, the authors expect the representativity of k_{eff} would be reduced in such a U-MOX hybrid configuration. Yet, analyses will be carried out to assess the representativity of local observables (such as reaction rate ratios), which could still prove satisfactory in the MOX area.

ACKNOWLEDGEMENTS

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