Nuclear Data Uncertainty Analysis to Meet the Target Accuracy Requirements on the MYRRHA k_{eff}

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Abstract. MYRRHA is a flexible experimental facility being designed at the SCK CEN, in Mol, Belgium. Cooled by lead-bismuth, it is conceived to operate both in sub-critical mode, as an accelerator driven system, and in critical mode, as a fast reactor. In order to comply with MYRRHA reactor design requirements, uncertainties due to nuclear data must be quantified. Significant gaps between the uncertainties and the target accuracies have been systematically shown in the past. In this paper, first, a Sensitivity and Uncertainty analysis with JEFF-3.3 nuclear data library of the effective neutron multiplication factor k_{eff} of the latest MYRRHA reactor design - v1.8 - is presented. Then, since target accuracy for k_{eff} of 300 pcm is exceeded, a Target Accuracy Requirement assessment is performed in order to find out the required accuracy on cross section data to meet the requested target accuracy. To reach the requested target accuracy, a reduction of the uncertainty in the fission and capture cross sections of ^{240}Pu JEFF-3.3 evaluation is needed.

1 Introduction

MYRRHA - Multi-purpose hYbrid Research Reactor for High-tech Applications - is a flexible experimental facility being designed at the Belgian Nuclear Research Centre (SCK CEN), Mol, Belgium [1]. Cooled by lead-bismuth, it is conceived to operate both in sub-critical mode, as an accelerator driven system, and in critical mode, as a fast reactor.

In order to comply with MYRRHA reactor design requirements, uncertainties must be quantified. In nuclear reactor design the major sources of uncertainty generally are the material properties, the fabrication tolerances, the operating conditions, the simulation tools and the nuclear data. The uncertainty in nuclear data is one of the most important sources of uncertainty in reactor physics simulations [2], and significant gaps between the uncertainties and the target accuracies (i.e., maximum acceptable uncertainties for a certain parameter) have been systematically shown in the past for advanced reactor systems parameters, such as k_{eff} [3,4]. Meeting the target accuracy is required not only to achieve the requested level of safety for MYRRHA, but also to minimize the increase in the costs due to additional safety measures.

Target Accuracy Requirements (TAR) assessments allow identifying nuclear data needs and requirements. Since the accuracy and priorities strongly depend on the assumed uncertainty data [3], and since numerous nuclear data libraries with updated uncertainty evaluations have been released in the recent years (i.e., JEFF-3.3 [5], ENDF/B-VIII.0 [6], JENDL-5 [7]) and new ones are currently being produced, such as JEFF-4 [8], it is necessary to provide updated target accuracies for advanced reactor design parameters and nuclear data.

In this paper, first, a Sensitivity and Uncertainty (S/U) analysis of the effective neutron multiplication factor k_{eff} of the latest MYRRHA reactor design - v1.8 [9] - is presented. Then, since the target accuracy for k_{eff} is still exceeded by ~300 pcm (1 pcm = 10^5) a TAR assessment is performed in order to find out the required accuracy on cross section data to meet the target accuracies defined by MYRRHA designers. Finally, recommendations on nuclear data needs and requirements for MYRRHA are given.

2 Sensitivity and Uncertainty Analysis

In nuclear data science and reactor physics simulations, sensitivity analyses study the variation of a physical parameter or reactor response when system parameters vary (e.g., how a k_{eff} changes when nuclear data change); and allow identifying the most important nuclear data for neutron-induced reactions and establishing a ranking of importance for the investigated response. Uncertainty analyses allow quantifying the uncertainty in the reactor response originating from the uncertainties in nuclear data.

S/U analyses have been conducted for previous MYRRHA designs [4,10-15]; nevertheless, an updated analysis was needed in order to take into account changes in core design revision v1.8 [9].

For the k_{eff} S/U analysis, the neutronics model of the MYRRHA v1.8 critical configuration homogenized at the fuel assembly level, developed in Ref. [16], was

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used. The model is presented in Fig. 1. The core is composed of 69 hexagonal MOX fuel elements (in salmon), six boron carbide B_4C control rod bundles (in red), three B_4C safety rod bundles (in yellow), one in-pile section for material testing and experiments with fast neutron fluxes (in light blue), six thermal in-pile sections (in pink), 36 dummy assemblies filled with lead-bismuth (in blue), 42 reflector assemblies with bundles of magnesium oxide MgO rods (in cream), steel (in brown) and the core barrel (in green).

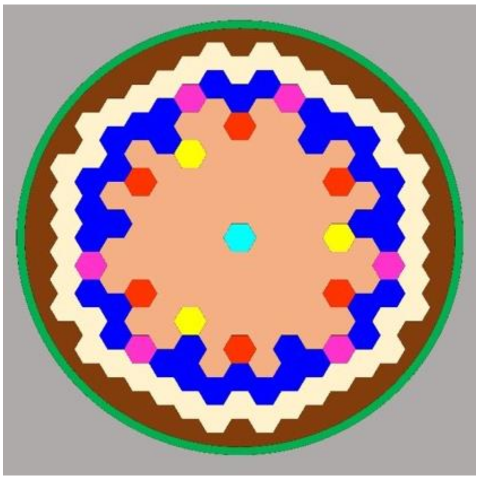

Fig. 1. Critical MYRRHA v1.8 homogenized model [16].

A S/U analysis was carried out using the JEFF-3.3 evaluated nuclear data library. Sensitivity calculations were performed with the Serpent 2 reactor physics Monte Carlo code [17] and the ECCO 33 energy group structure [18]. The uncertainty quantification was conducted using the OECD/NEA NDaST tool [19].

In Fig. 2, the energy and region integrated sensitivity coefficients to the ten most important nuclides and reactions (quantities) for MYRRHA's effective multiplication factor are presented. Values are in very good agreement with those reported for previous MYRRHA version - v1.6 - in Ref. [10].

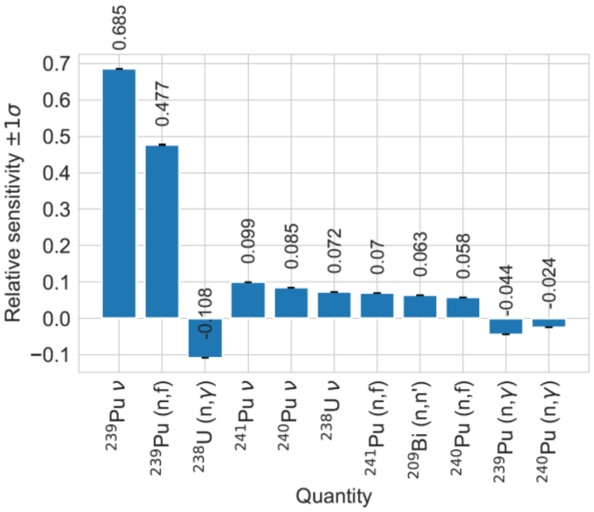

Fig. 2. k_{eff} integrated sensitivity coefficients for MYRRHA.

The results from the uncertainty quantification are presented in Table 1. Uncertainties in the average number of emitted neutrons from fission ν and in the average fission spectrum χ were not propagated, since covariances are not available in NDaST. This explains the underestimation of the total uncertainty by ~200 pcm compared to Ref. [10]. Strong effect of the negative cross correlation in the fast energy range between ^{240}Pu(n,f) and ^{240}Pu(n,γ) in JEFF-3.3 can be observed. Second highest contribution to the uncertainty comes from ^{240}Pu(n,f), while ^{239}Pu(n,f) is the third major contributor due to its small uncertainty, in spite of its high sensitivity. It can also be concluded that main S/Us for k_{eff} did not change from MYRRHA v1.6 to revision v1.8.

From the designer's point of view, the determination of the k_{eff} target accuracy is a rather complex issue due to the number of factors to take into account, such as reactor criticality, rods' safety margins, safety parameters, etc. The estimated reactivity worth of the safety rods in MYRRHA's critical configuration is ~5000 pcm [4]. The combined uncertainty from all sources, nuclear data among them, should not exceed this value. On the other hand, a possible underestimation of k_{eff} will require loading of additional fuel assemblies in the core periphery to reach the criticality. Following the MYRRHA core rotational symmetry, 3 or 6 fuel assemblies would have to be added. Taking into account that preliminary studies have shown that the reactivity worth of a peripheral fuel assembly is ~50 pcm [20], a k_{eff} target accuracy of 300 pcm is deemed to be satisfactory in order to minimize the increase in the costs of additional fuel assemblies.

It can be seen in Table 1 that the target accuracy for k_{eff} is exceeded. Thus, a TAR assessment to identify the accuracy on cross section data needed to satisfy MYRRHA requirements is needed.

Table 1. k_{eff} nuclear data uncertainty quantification for MYRRHA. Uncertainties due to Monte Carlo counting statistics are negligible, thus they are omitted.

Quantity				**$\Delta k_{eff}/k_{eff}$ (%)**
^{240}Pu	(n,f)	^{240}Pu	(n,γ)	-0.614
^{240}Pu	(n,f)	^{240}Pu	(n,f)	0.558
^{239}Pu	(n,f)	^{239}Pu	(n,f)	0.276
^{239}Pu	(n,f)	^{239}Pu	(n,γ)	0.259
^{240}Pu	(n,γ)	^{240}Pu	(n,γ)	0.202
^{238}U	(n,γ)	^{238}U	(n,γ)	0.172
^{238}U	(n,f)	^{238}U	(n,γ)	0.171
^{239}Pu	(n,γ)	^{239}Pu	(n,γ)	0.126
^{238}U	(n,f)	^{238}U	(n,f)	0.113
Total uncertainty in k_{eff}				**0.588**

3 Target Accuracy Requirements

The TAR analysis can be considered as the inverse problem of the uncertainty quantification. Details about the methodology can be found in Ref. [21]. The uncertainty data requirements can be obtained by solving the following minimization problem:

$$Q = \sum_i \frac{\lambda_i}{d_i^2} \quad i = 1, \dots, I \tag{1}$$

$$\sum_i S_{ni}^2 d_i^2 + \sum_{ii'} S_{ni} d_i Corr_{ii'} d_{i'} S_{ni'} + \sum_i S_{ni} d_i Corr_{ij} d_j S_{nj} + P \le (R_n^T)^2 \tag{2}$$

$$n = 1, \dots, N \quad j = 1, \dots, K$$

$$0 \le d_i \le d_0 \tag{3}$$

Where Q is the function to minimize, composed by d_i, which represents the unknown uncertainty data requirements and λ_i, which denotes cost parameters related to each cross section and should give a relative figure of merit of the difficulty of improving that parameter, i.e., the difficulty of reducing uncertainties with an appropriate experiment. d_0 are the initial data uncertainties, i.e., uncertainties in JEFF-3.3 covariance files. S_{ni} are the sensitivity coefficients for the integral parameter and R_n are the target accuracies of the N integral parameters. $Corr_{ii'}$ are the correlations between variable i and variable i'. To be able to solve the problem, the number of variables I is obtained by selecting the variables based on their contribution to the uncertainties; for instance, by selecting only those that globally account at least for a fixed quantity. P represents the constant residual uncertainty for integral parameter R_n due to the unselected variables and K is the total number of constant terms that are correlated to variable j through $Corr_{ij}$.

This methodology has been implemented using the Sequential Least Square Programming (SLSQP) algorithm and the Trust-region method [22] to solve the minimisation problem. Similar algorithms have been used to perform a TAR analysis for ALFRED reactor in Ref. [23], although no correlation between nuclear data was taken into account. However, as shown in Ref. [21], the impact of nuclear data correlation terms is very significant in target accuracy assessment evaluation and produces very stringent requirements on nuclear data.

In the present TAR analysis for MYRRHA, the ten most important quantities presented in Fig. 2 were selected as input variables, contributing to more than 90% of the total uncertainty in *k_{eff}*. Nuclear data correlations and uncertainties from JEFF-3.3 were used in the calculations. A constant cost function $\lambda_i = 1$ was selected. The impact of the residual uncertainty and the correlations with unselected variables, i.e., 3rd and 4th terms of Eq. 2, were neglected. The 7 energy group structure proposed in Ref. [21], based on physical considerations, was utilized to reduce the number of variables of the minimization problem.

A summary of the most important results from the TAR analysis are shown in Fig. 3 and Fig. 4, including initial uncertainties d_0 (prior uncertainties) and nuclear data accuracy requirements d_i (posterior uncertainties) for MYRRHA.

Since a constant cost function has been used, it should be noted that a greater reduction in the uncertainty is obtained for quantities with a significant prior uncertainty. That is the case for ^{240}Pu(n,f), which is ranked 9th in Fig. 2, but is the major contributor to the uncertainty in k_{eff} for MYRRHA using JEFF-3.3 nuclear data library (Table 1) due to the significant uncertainty in the ^{240}Pu(n,f) evaluation, as can be seen in Fig. 3.

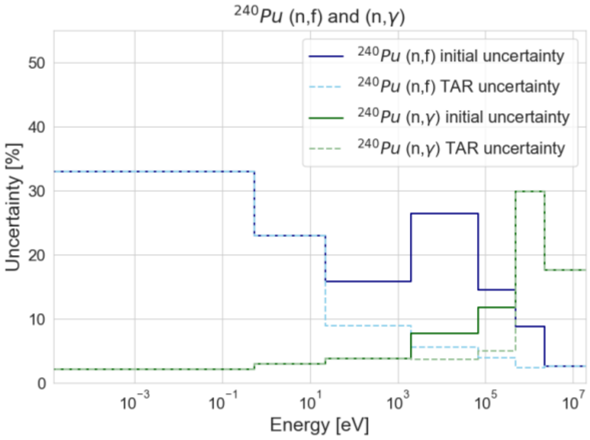

Fig. 3. ^{240}Pu(n,f) and (n,γ) prior and posterior uncertainty.

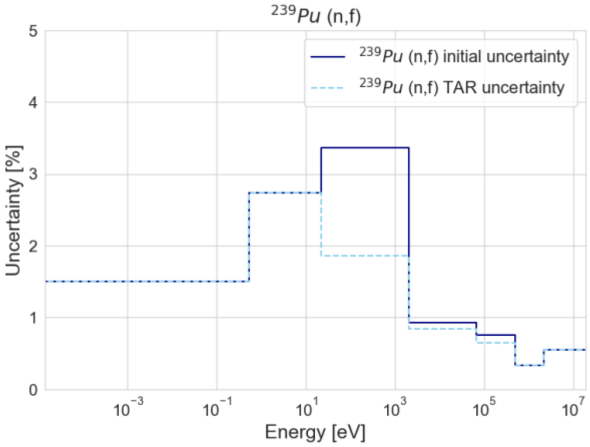

Fig. 4. ^{239}Pu(n,f) prior and posterior uncertainty.

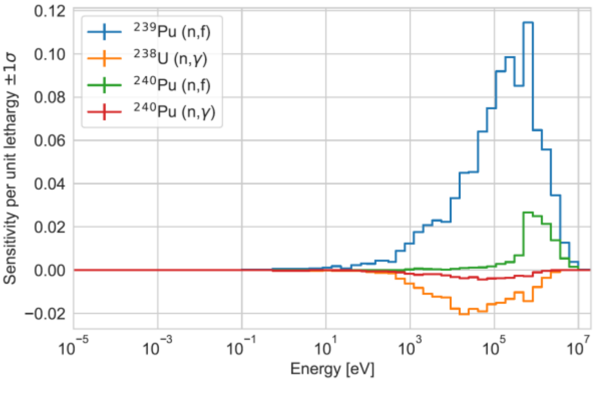

Fig. 5. ^{239}Pu(n,f), ^{238}U(n,γ), ^{240}Pu(n,f) and ^{240}Pu(n,γ) energy dependent sensitivity coefficients.

On the other hand, uncertainty in reactions with small d_0 values, in spite of their sensitivity, won't be reduced, such as ^{239}Pu(n,f) in Fig. 4.

There is no reduction in the uncertainty in the thermal energy range, since MYRRHA is a fast reactor and k_{eff} sensitivity coefficients bellow energies in the order of keV are practically 0, as reflected in Fig. 5.

A posterior total uncertainty of 300 pcm in k_{eff}, equal to the R_n target accuracy in k_{eff}, was obtained propagating the posterior uncertainties in the considered nuclear data. To reach the requested target accuracy for MYRRHA, a reduction of the uncertainty in the fission and capture cross sections of ^{240}Pu JEFF-3.3 evaluation is needed.

4 Conclusions

A Sensitivity and Uncertainty analysis of the effective neutron multiplication factor k_{eff} of the latest MYRRHA reactor design, v1.8 has been presented. A ranking of the most important isotopes and reactions for MYRRHA's k_{eff} has been derived. A total uncertainty in k_{eff} due to uncertainties in nuclear data of 588 pcm has been obtained, exceeding the target accuracy of 300 pcm based on fuel management considerations.

A Target Accuracy Requirement assessment has been performed in order to find out the required accuracy on the cross section data. In previous assessments, correlation terms have been neglected. The correlation terms introduce very stringent requirements on nuclear data and have been considered in this study. Since a constant cost function has been used, it should be noted that a greater reduction in the uncertainty is obtained for quantities with a significant initial uncertainty. After the TAR, the target accuracy in k_{eff} was reached. A reduction of the uncertainty in the fission and capture cross sections of ^{240}Pu JEFF-3.3 evaluation is needed to meet MYRRHA target accuracy requirements.

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