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## Nuclear data sensitivity and uncertainty analysis of effective neutron multiplication factor in various MYRRHA core configurations



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#### ABSTRACT

A sensitivity and uncertainty analysis was carried out to estimate the uncertainty in the neutron multiplication factor  $k_{eff}$  and to identify the most important nuclear data for neutron induced reactions for criticality calculations of the latest MYRRHA designs. Sensitivity profiles, i.e. sensitivity to the nuclear data as a function of incoming neutron energy, were derived for both a critical and sub-critical core. They were calculated using codes that are based on different methodologies including stochastic and deterministic calculations (i.e. SCALE, MCNP and XSUN). The neutron induced nuclear data sensitivity analysis outlined the following quantities to be of special importance for the MYRRHA reactor concept:  $^{239}$ Pu(n, $\gamma$ ) both in resonance and fast energy region, (n,f) fast,  $\chi$  and  $\nu$  fast; <sup>238</sup>U(n,n') fast, (n, $\gamma$ ) resonance and fast, (n,n) resonance and fast;  $^{240}$ Pu v fast;  $^{238}$ Pu(n,f) both resonance and fast;  $^{56}$ Fe(n, $\gamma$ ) both resonance and fast. Differences of less than 4% between codes were obtained for these quantities, with few exceptions  $(^{238}Pu(n,f),\ ^{238}U(n,n)$  and  $^{56}Fe(n,\gamma)$  reactions). Nuclear data covariance matrices of different libraries (SCALE-6, COMMARA-2 and JENDL-4.0m) were used to derive the uncertainty in  $k_{\it eff}$  based on the calculated sensitivities. This study reveals that the largest contributions to  $k_{eff}$  uncertainty result from the uncertainty in the average prompt neutron fission multiplicity of <sup>239</sup>Pu, in the <sup>238</sup>U inelastic scattering cross section and <sup>239</sup>Pu fission cross section, using the covariances from SCALE-6, COMMARA-2 and JENDL-4.0m, respectively.

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#### 1. Introduction

Various projects and workshops have been set up in recent years to address the increasing demand from nuclear research, industry and regulators to support neutronic calculations of best-estimate predictions with their confidence bounds (Ivanov et al., 2013) and to address the nuclear data needs for the design and safety analysis of Advanced Fast Reactors and Advanced Fuel Cycle Scenarios. The uncertainty in nuclear data is one of the most important sources of uncertainty in reactor physics simulations (Kodeli, 2007), however, significant gaps between the current uncertainties and the target accuracies have been systematically

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shown (Harada and Plompen, 2014). The EC FP7 CHANDA project (CHANDA, 2013), whose acronym stands for "solving CHAllenges in Nuclear DAta", addresses the challenges in the field of nuclear data for nuclear applications. This project will allow European scientists and institutions to improve the nuclear data needed for simulation tools in order to increase the accuracy of code assessments and consequently to better focus the design of expensive experimental validations.

In particular, a part of CHANDA is focused on studying the nuclear data required for the development, safety assessment and licensing of the MYRRHA experimental reactor (Engelen et al., 2015), and on giving recommendations for data improvements. Additionally, support to the JEFF project (Koning, 2007) will be provided by identifying issues in nuclear data files for MYRRHA-relevant elements and isotopes (CHANDA DOW, 2013). Therefore, a nuclear data sensitivity and uncertainty (S/U) analysis of the latest

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design of the MYRRHA cores (Stankovskiy and Van den Eynde, 2014) has been carried out using various codes and methodologies. Sensitivity and uncertainty analyses have been conducted for previous MYRRHA designs (Díez et al., 2014; Stankovskiy et al., 2014; Sugawara et al., 2011); nevertheless, an updated analysis was needed in order to take into account new nuclear data libraries and changes in core design (Van den Eynde et al., 2015).

In this paper, main results of the analysis are presented, providing a list of the most relevant isotopes and reactions from the criticality safety point of view. A comparison between the sensitivity coefficients obtained with different codes has also been performed and the uncertainty in the effective neutron multiplication factor,  $k_{\it eff}$ , due to the uncertainty in nuclear data has been calculated using covariance matrices from different databases. The results of this study will be used in forthcoming CHANDA tasks to analyse the nuclear data libraries and to identify experimental data that can be used to improve the present evaluations, with the objective of reducing the nuclear data uncertainties of MYRRHA-key elements.

#### 2. MYRRHA core model

MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications), a flexible experimental facility is being designed at SCK-CEN, Mol, Belgium (Engelen et al., 2015). It is conceived to operate both in sub-critical, or Accelerator Driven System (ADS) mode, driven by a 600-MeV linear proton accelerator, and in critical mode, as a lead-bismuth cooled fast reactor. The updated core design is described in detail in reference (Van den Eynde et al., 2015). For this study a simplified model (Stankovskiy and Van den Eynde, 2014), homogenised on fuel assembly level, has been used. The layout of the core is shown in Fig. 1 for both critical and sub-critical configurations, while the model vertical layout (for sub-critical core) is given in Fig. 2.

This model has been used by both KENO-VI and MCNP¹ (Pelowitz, 2014) radiation transport codes, the former one being used for the Monte Carlo transport calculations in the SCALE system (Rearden and Jessee, 2016). Additionally, a cylindrical geometry model of MYRRHA critical configuration was constructed to be used in the neutron transport calculations performed by the PARTISN (Alcouffe et al., 2008) and SUSD3D (Kodeli, 2001) codes, both part of the XSUN-2013 system (Kodeli and Slavic, 2013). This model was developed using equivalent concentric cylinders conserving the total mass of each material. Hence, no further homogenization was required. Additionally, an adjustment of the arrangement of the cylinders was necessary in order to represent MYRRHA critical core configuration with high-fidelity.

#### 3. Codes and methodologies

The basic principles to perform a sensitivity analysis are well understood. For the S/U analysis of the MYRRHA reactor core, the procedures included in some of the state-of-the-art computer codes dedicated to reactor core analyses have been used in this work. In particular, the calculations have been performed with the SCALE6.2 system, in its third beta release, the MCNP code, and the XSUN-2013 system. In this section the methodologies used by each of the codes to perform the sensitivity and uncertainty calculations are summarized.

#### 3.1. SCALE

SCALE performs the nuclear data S/U analysis using the TSU-NAMI control module. The methodology used by TSUNAMI to produce the sensitivity coefficients (Rearden, 2004) is based on 1st order perturbation theory. The sensitivity coefficients, S, are calculated as the sum of implicit and explicit terms. The implicit sensitivity is needed to take into account the effect on  $k_{eff}$  of perturbing one cross section that affects the resonance shielded values of other cross sections. The explicit sensitivity coefficients are calculated using the Adjoint Weighted Technique, based on the perturbation,  $\delta k$ , of the  $k_{eff}$ . Two calculations are performed, one forward and one adjoint, to solve the Boltzmann transport equation. Ignoring the second order perturbation term, the sensitivity of  $k_{eff}$  to a perturbation in the macroscopic cross section  $\Sigma$  is expressed as:

$$S_{k,\Sigma(\vec{r})} = \frac{\Sigma(\vec{r})}{k} \frac{\delta k}{\delta \Sigma(\vec{r})} = -\frac{\Sigma(\vec{r})}{\delta \Sigma(\vec{r})} \frac{\langle \phi^{\dagger} \left( \delta A - \frac{1}{k} \delta B \right) \phi \rangle}{\langle \phi^{\dagger} \left( \frac{1}{k} B \right) \phi \rangle}, \tag{1}$$

where  $\delta A$  and  $\delta B$  represent small linear perturbations in the operators of the neutron transport equation (A is the operator that represents the scattering and total interactions terms, while the operator B represents the fission term) due to perturbations in the macroscopic cross sections.

Once the sensitivity coefficients are obtained, the uncertainty in the  $k_{\rm eff}$  due to the uncertainty in nuclear data can be deduced. The uncertainty in the system  $k_{\rm eff}$  value is given as:

$$\frac{\Delta k_{eff}}{k_{eff}} = \sqrt{SCS^T},\tag{2}$$

where C is the symmetric  $M \times M$  matrix (M is the number of nuclide-reaction pairs times the number of energy groups) containing the relative covariance elements in the nuclear data and S is the vector of length M containing the above defined relative sensitivities of the calculated  $k_{eff}$  to cross sections  $\Sigma$ , expressed in relative terms.

#### 3.2. MCNP

The Differential Operator Technique (Hall, 1982; Rief, 1984) which calculates the change in  $k_{eff}$  ( $\Delta k_{eff}$ ) due to perturbation in the microscopic cross section,  $\Delta \sigma$ , is implemented in the MCNP/ PERT card. It is based on a Taylor series expansion presented as follows, where  $\sigma_x$  is the perturbed microscopic cross section,  $\sigma_{x,0}$  is its nominal value and  $\Delta \sigma = \sigma_x - \sigma_{x,0}$  is the perturbation:

$$\Delta k_{eff} = k_{eff}(\sigma_{x}) - k_{eff}(\sigma_{x,0}) 
= \left(\frac{\delta k}{\delta \sigma}\Big|_{\sigma_{x,0}} \Delta \sigma\right)_{1^{st}} + \left(\frac{1}{2} \frac{\delta^{2} k}{\delta \sigma^{2}}\Big|_{\sigma_{x,0}} (\Delta \sigma)^{2}\right)_{2^{nd}} + \dots 
= \left[\Delta k_{eff}\right]_{PERT,1^{st}} + \left[\Delta k_{eff}\right]_{PERT,2^{nd}} + \dots,$$
(3)

Only the first derivative, which derives the probability of the random walk occurring, is required for sensitivity coefficients since the second derivative considers the changes in the fission source distribution, which is approximated as unperturbed by the Differential Operator method. As used in reference (Favorite, 2009) to compare SCALE and MCNP/PERT card sensitivity results, only the first term should be considered in PERT card for a proper comparison. It has been pointed out in the bibliography (Kiedrowski and Brown, 2011; Pelowitz, 2014) that this method for calculating sensitivities to scattering cross sections could be wrong because the scattering affects the fission source spatial distribution, so a first order approximation could not be sufficient.

<sup>&</sup>lt;sup>1</sup> MCNPX 2.7.0, MCNP 6.1 and MCNP 6.1.1beta were used in this work. The obtained results were the same (between one sigma), consequently, no specification of the code version is mentioned from this point forward.

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