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: $^{239}\text{Pu}(n,\gamma)$ both in resonance and fast energy region, (n,f) fast, χ and ν fast; $^{238}\text{U}(n,n')$ fast, (n,γ) resonance and fast, (n,n) resonance and fast; ^{240}Pu ν fast; $^{238}\text{Pu}(n,f)$ both resonance and fast; $^{56}\text{Fe}(n,\gamma)$ both resonance and fast. Differences of less than 4% between codes were obtained for these quantities, with few exceptions ($^{238}\text{Pu}(n,f)$, $^{238}\text{U}(n,n)$ and $^{56}\text{Fe}(n,\gamma)$ reactions). Nuclear data covariance matrices of different libraries (SCALE 6, COMMARA 2 and JENDL 4.0m) were used to derive the uncertainty in k_{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 ^{239}Pu , in the ^{238}U inelastic scattering cross section and ^{239}Pu fission cross section, using the covariances from SCALE 6, COMMARA 2 and JENDL 4.0m, respectively.

Keywords:

MYRRHA

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Sensitivity and uncertainty

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ADS

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

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_{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 (Kodali, 2001) codes, both part of the XSUN 2013 system (Kodali 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, δk , 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 Σ is expressed as:

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

where δA and δB 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_{eff} due to the uncertainty in nuclear data can be deduced. The uncertainty in the system k_{eff} value is given as:

$$\frac{\Delta k_{eff}}{k_{eff}} = \sqrt{CS^T}, \quad (2)$$

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 Σ , expressed in relative terms.

3.2. MCNP

The Differential Operator Technique (Hall, 1982; Rief, 1984) which calculates the change in k_{eff} (Δk_{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 σ_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:

$$\Delta k_{eff} = k_{eff}(\sigma_x) - k_{eff}(\sigma_{x,0}) = \left. \frac{\partial k}{\partial \sigma} \right|_{\sigma_{x,0}} \Delta \sigma + \left(\frac{1}{2} \frac{\partial^2 k}{\partial \sigma^2} \right)_{\sigma_{x,0}} (\Delta \sigma)^2 + \dots$$

$$[\Delta k_{eff}]_{PERT,1^{st}} + [\Delta k_{eff}]_{PERT,2^{nd}} + \dots, \quad (3)$$

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.

¹ 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.

Fig. 1. Critical (left) and sub-critical (right) MYRRHA Sub-Assembly (SA) distributions.

Fig. 2. Vertical layout of the MYRRHA model (dimensions given in cm).

The MCNP/KSEN card can compute the sensitivity coefficients of the k_{eff} to nuclear data. A method based on linear perturbation theory using adjoint weighting, the same method as used by TSU NAMI, is employed for this purpose. The adjoint weighting is performed in a single forward calculation using the Iterated Fission Probability method (Kiedrowski and Brown, 2013, 2009). An important limitation of the adjoint based methods as implemented in MCNP is that they do not consider perturbations that may arise from scattering laws or from fission emission spectra. This limitation has been shown to lead to spurious results (Pelowitz, 2014).

3.3. SUS3D

An updated version of the Windows interface package XSUN 2013 was used for the MYRRHA deterministic sensitivity and uncertainty analysis. The package was developed at JSI to facilitate the deterministic radiation transport and cross section sensitivity uncertainty calculation, and in particular to help users in the preparation of input cards, rapid modification and execution of the complete chain of codes including TRANSX (cross section preparation), PARTISN (neutron/gamma transport) and SUS3D (sensitivity and uncertainty analysis).

SUSD3D (Kodeli, 2001) is based on the first order generalised perturbation theory. The code calculates the sensitivity coefficients and the standard deviation in the calculated detector responses or design parameters of interest due to the input cross sections and their uncertainties. Either relative or absolute sensitivities of the response R (such as reaction rates, fluxes, k_{eff} and the effective delayed neutron fraction, β_{eff}) to the perturbation of cross section σ can be calculated. Nuclear data uncertainties are propagated using Eq. (2). Contribution of the uncertainties in the secondary energy and angular distribution (SED/SAD) of the emitted particles can be estimated as well. Integral parameter uncertainties due to fission spectra uncertainties can be calculated either using the classical or the constrained sensitivity method (Kodeli et al., 2009), particularly useful in case when the fission spectra covariance matrices do not comply exactly with the ENDF 6 Format Manual rules. S/U calculations of β_{eff} can also be carried out using a method based on the derivation of Bretscher's k ratio formula, as described in reference (Kodeli, 2013).

4. Results

4.1. Criticality calculations

The criticality calculations for the MYRRHA core design have been performed with the codes and methodologies described above, applying one or more different sets of nuclear data libraries in each case. Results for the critical and sub critical configurations are presented in Tables 1 and 2 respectively. The following considerations are worth mentioning:

Table 1

Criticality calculations results for the critical configuration of MYRRHA. Deterministic XSUN/PARTISN k_{eff} results have no statistical uncertainty (5×10^{-7} convergence criterion was used).

Library	Code	k_{eff}
JEFF-3.1.2	MCNP	1.00754 ± 0.00003
	SCALE-CE	1.00657 ± 0.00009
	SCALE-MG	1.00944 ± 0.00006
ENDF/B-VII.0	MCNP	1.00408 ± 0.00003
	MCNP	1.00400 ± 0.00003
	XSUN	1.00541
ENDF/B-VII.1	XSUN ¹	1.00590

¹ Obtained using finer space mesh grid. Note that there is a non-linear relation between k_{eff} and the mesh size.

Table 2

Criticality calculations results for the sub-critical configuration of MYRRHA.

Library	Code	k_{eff}
JEFF-3.1.2	MCNP	0.95410 ± 0.00003
ENDF/B-VII.0	SCALE-CE	0.95357 ± 0.00008
	MCNP	0.95090 ± 0.00003
ENDF/B-VII.1	MCNP	0.95106 ± 0.00003

Using the SCALE code, both multi group, MG, and continuous energy, CE, methodologies were assessed (Romojaro et al., 2015). For the MG calculations, the SCALE 238 energy groups criticality safety library was used. This library was processed using a standard weighting function suitable for thermal systems, which is not the most accurate for fast reactor applications. Consequently, significant differences were expected in MYRRHA criticality calculations, although no impact was observed in the sensitivity and uncertainty calculations.

It was not possible to match exactly some temperatures of the MYRRHA design in the SCALE CE simulations, since the modular code AMPX for the production of the cross sections was not available. 293 K, 565 K and 900 K were used instead of the 300 K average temperature of the thermal in pile sections, the 550 K average temperature of the lead bismuth eutectic LBE pool and the 800 K average temperature of the homogenized mixture of the fuel, clad and LBE. This may produce biases between codes.

The discrete ordinates code PARTISN was employed for the critical core k_{eff} calculations using the cylindrical model and P_5/S_{16} approximation (5th Legendre order, 16 angles quadrature). A neutron cross section library based on ENDF/B VII.1 and processed using NJOY 99 (MacFarlane and Muir, 1999) into 33 energy groups (ECCO 33 group structure (Kodeli, 2015)) for the different model temperatures was used. The grid size was varied in order to estimate its impact and to optimise the space mesh used in the simulations. The difference between the direct and adjoint calculation for k_{eff} are circa 50 pcm, which is slightly larger than usually observed using the PARTISN code, probably due to a difficult convergence of the thermal neutron adjoint flux requiring a very fine space mesh (note that the adjoint calculation starts with the thermal group).

The following differences are observed in Table 1:

A difference of ~550 pcm can be found due to the use of different codes/models employing the ENDF/B VII.0 or ENDF/B VII.1 library. This difference is comparable with the results usually attributed to other fast reactors (Bortot et al., 2015). A slightly lower difference (up to ~350 pcm) can be found in results between different cross section libraries JEFF 3.1.2 and ENDF/B VII.0 (or ENDF/B VII.1), comparable with reference (Stankovskiy et al., 2014). This difference in k_{eff} between JEFF 3.1.2 and ENDF/B VII.0 can be mainly attributed to the differences in the cross sections of the following quantities: $^{209}\text{Bi}(n, \gamma)$, $^{238}\text{U}(n, n)$ and (n, n') , $^{238}\text{Pu}(n, \gamma)$ and (n, f) , ^{239}Pu $\bar{\nu}$, $^{241}\text{Pu}(n, f)$ and $^{242}\text{Pu}(n, \gamma)$, (n, f) , (n, n) and (n, n') .

In spite of a relatively coarse ECCO 33 energy group structure used in the PARTISN calculations as compared to the 238 group SCALE and pointwise MCNP libraries, the results are consistent with the results by other codes, which implies that the energy group structure chosen and the method of self shielding treatment were suitable for this application.

For the sub critical configuration, differences between SCALE and MCNP using the ENDF/B library are ~260 pcm, while there is

Table 3

Bias effects in MYRRHA.

Bias effect	Reactivity (pcm)
PARTISN ¹ – MCNP	141
SCALE – MCNP	330
Detailed model – Simplified model	460
3D model – Cylindrical model	125
JEFF-3.1.2 – ENDF/B-VII.0	350

¹ Model and MG effects are also included in this bias.

a difference of 16 pcm between ENDF/B VII.0 and ENDF/B VII.1. A difference of ~300 pcm can be found between JEFF 3.1.2 and both versions of ENDF/B VII. These differences between codes and libraries are consistent with the ones obtained for the critical configuration (Table 1).

It should be noticed that the use of different models, libraries, codes and methodologies (by different users) might introduce bias effects in the criticality results. In order to assure the reproducibility of this work, the biases have been identified for the MYRRHA neutronic model and are provided in Table 3. These biases give an estimation of the impact in MYRRHA's k_{eff} when performing a simulation with different tools. The bias introduced by the combination of these effects has not been studied in this work.

4.2. Sensitivity analysis

The Integrated Sensitivity Coefficients, ISC, obtained by SCALE and MCNP, using the ENDF/B VII.0 library, and by SUS3D, using the ENDF/B VII.1 library, for the 10 major contributors to the uncertainty in k_{eff} for the MYRRHA critical core are shown in Table 4. It can be highlighted that:

- $^{238}\text{Pu}(n, f)$ (Fig. 3), obtained by MCNP/PERT card, has an 25% difference regarding the SCALE result. If the KSEN card is used (Table 4), the difference increases to 83%;
- $^{238}\text{U}(n, n)$ (Fig. 4), obtained by SUS3D, has a difference of 51% to the value provided by SCALE, which can be mainly attributed to omitting the implicit sensitivity contribution (not taking into account the effects associated with changes in resonance shielded MG data) in SUS3D. An assessment with the SCALE code revealed that the contribution of the implicit term to the total sensitivity for this quantity is 30%. The rest of the difference can be attributed to differences in the group structure and in the model;
- $^{56}\text{Fe}(n, \gamma)$ (Fig. 5) has a difference of 11% (active zone only) between MCNP and SCALE and 20% (whole core) between SUS3D and SCALE. The differences obtained for this quantity between SUS3D and SCALE are mostly due to different models used in SUS3D (2D cylindrical) and SCALE (3D). Note that in the active zone SUS3D and SCALE results differ by less than 2%;
- other ISC values are very close between codes, most of them with a difference smaller than 4%. Sensitivity profiles of the most relevant quantities are given in Figs. 6–8

For the subcritical core, the main sensitivity coefficients (Table 5) and sensitivity profiles of the top 5 contributors (Fig. 9) were obtained with SCALE. These results were compared with the sensitivity coefficients calculated using the direct perturbation method (Radulescu et al., 2008), which employs variations of nuclide density that result in small k_{eff} variations consistent with the linear perturbation approximation and allows determining the total sensitivity coefficients. Relative differences of less than 3% between TSUNAMI and the direct perturbation total sensitivity coefficients were obtained, which ensures the consistency of the calculations.

Table 4

ISC of the major contributors for the critical core obtained by the different codes.

Quantity	Integrated Sensitivity Coefficients (%/%)		
	SCALE ENDF/B-VII.0	MCNP/KSEN ENDF/B-VII.0	SUSD3D ENDF/B-VII.1
$^{239}\text{Pu } \nu$	$6.9794 \times 10^{-1} \pm 2 \times 10^{-5}$	$7.06160 \times 10^{-1} \pm 3 \times 10^{-6}$	6.99×10^{-1}
$^{238}\text{Pu}(n,f)$	$4.830 \times 10^{-1} \pm 2 \times 10^{-4}$	$4.92730 \times 10^{-1} \pm 4 \times 10^{-6}$	4.88×10^{-1}
$^{238}\text{U}(n,\gamma)$	$-1.1939 \times 10^{-1} \pm 6 \times 10^{-5}$	$-1.16880 \times 10^{-1} \pm 2 \times 10^{-6}$	-1.20×10^{-1}
$^{240}\text{Pu } \nu$	$7.910 \times 10^{-2} \pm 3 \times 10^{-5}$	$8.0206 \times 10^{-2} \pm 2 \times 10^{-6}$	7.83×10^{-2}
$^{239}\text{Pu}(n,\gamma)$	$-5.80 \times 10^{-2} \pm 3 \times 10^{-4}$	$-5.58540 \times 10^{-2} \pm 2 \times 10^{-7}$	-5.71×10^{-2}
$^{238}\text{U}(n,n')$	$-1.84 \times 10^{-2} \pm 4 \times 10^{-4}$	$-1.900 \times 10^{-2} \pm 2 \times 10^{-5}$	-1.87×10^{-2}
$^{56}\text{Fe}(n,\gamma)$ – whole core	$-1.8138 \times 10^{-2} \pm 9 \times 10^{-6}$	–	-1.45×10^{-2}
$^{238}\text{U}(n,n)$	$1.67 \times 10^{-2} \pm 2 \times 10^{-4}$	$1.544 \times 10^{-2} \pm 3 \times 10^{-5}$	8.09×10^{-3}
$^{238}\text{Pu}(n,f)$	$1.3000 \times 10^{-2} \pm 3 \times 10^{-6}$	$2.2224 \times 10^{-3} \pm 6 \times 10^{-7}$	1.26×10^{-2}
$^{56}\text{Fe}(n,\gamma)$ – active zone	$-8.498 \times 10^{-3} \pm 5 \times 10^{-6}$	$-7.5713 \times 10^{-3} \pm 4 \times 10^{-7}$	-8.65×10^{-3}
$^{239}\text{Pu } \chi$	$0.00000 \pm 3 \times 10^{-5}$	$0.000000 \pm 5 \times 10^{-6}$	0.00

Fig. 3. Sensitivity coefficients of $^{238}\text{Pu}(n,f)$ provided by the different codes, for the critical core and whole energy interval. MCNP results using the PERT card are presented.

Fig. 5. Sensitivity coefficients of $^{56}\text{Fe}(n,\gamma)$ provided by the different codes for the active zone of the critical core and whole energy interval. MCNP results using the KSEN card are presented.

Fig. 4. Sensitivity coefficients of $^{238}\text{U}(n,n)$ provided by the different codes for the critical core and whole energy interval. MCNP results using the KSEN card are presented.

4.3. Uncertainty analysis

The determination of the k_{eff} target accuracy is a rather complex issue. The estimated reactivity worth of the safety rods in MYR

Fig. 6. Sensitivity coefficients of $^{239}\text{Pu } \nu$ provided by the different codes for the critical core and whole energy interval. MCNP results using the KSEN card are presented.

RHA's critical configuration is ~ 5000 pcm. Regarding the safety aspect, the combined uncertainty from all sources, nuclear data among them, should not exceed this value. On the other hand, a

Fig. 7. Sensitivity coefficients of $^{238}\text{U}(n,n')$ provided by the different codes for the critical core. MCNP results using the KSEN card are presented.

Fig. 8. Sensitivity coefficients of $^{238}\text{U}(n,\gamma)$ provided by the different codes for the critical core and whole energy interval. MCNP results using the KSEN card are presented.

Table 5
Main sensitivity coefficients for the sub-critical core obtained with SCALE/Tsunami.

Nuclide	Region	Reaction	Total sensitivity (%/%)
^{239}Pu	Fuel assembly active part	Total	$4.369 \times 10^{-1} \pm 2 \times 10^{-4}$
^{238}U	Fuel assembly active part	Total	$-6.73 \times 10^{-2} \pm 5 \times 10^{-4}$
^{241}Pu	Fuel assembly active part	Total	$5.898 \times 10^{-2} \pm 3 \times 10^{-5}$
^{240}Pu	Fuel assembly active part	Total	$3.323 \times 10^{-2} \pm 6 \times 10^{-5}$
^{209}Bi	Dummy sub-assembly middle	Total	$2.54 \times 10^{-2} \pm 2 \times 10^{-4}$
^{209}Bi	Fuel assembly active part	Total	$1.10 \times 10^{-2} \pm 3 \times 10^{-4}$
^{238}Pu	Fuel assembly active part	Total	$1.0307 \times 10^{-2} \pm 6 \times 10^{-6}$
^{208}Pb	Dummy sub-assembly middle	Total	$1.008 \times 10^{-2} \pm 8 \times 10^{-5}$
^{235}U	Fuel assembly active part	Total	$9.851 \times 10^{-3} \pm 6 \times 10^{-6}$
^{56}Fe	Fuel assembly active part	Total	$-9.2 \times 10^{-3} \pm 7 \times 10^{-4}$

possible underestimation of k_{eff} will require loading of additional fuel assemblies in the core periphery to reach the criticality. Given that MYRRHA has a certain rotational symmetry, 3 or 6 fuel assemblies would have to be added. Taking into account that the

Fig. 9. SCALE/Tsunami calculated sensitivity coefficients of main contributors to k_{eff} uncertainty for the sub-critical core.

reactivity weight of a peripheral fuel assembly is ~ 50 pcm (Malambu and Stankovskiy, 2014), 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.

4.3.1. SCALE

The SCALE/Tsunami code is able to decompose the k_{eff} uncertainty in the main contributing quantities, as it is demonstrated in Table 6. It can be ascertained, by the similarity of the major contributors, that the most relevant quantities are nearly identical for the critical and sub critical configurations for what concerns k_{eff} calculations.

It is important to note that the source of cross section uncertainties for the SCALE 6.2b3 system is the SCALE covariance library, whose data has been assembled from covariance evaluations from ENDF/B VII.0, ENDF/B VI and JENDL 3.3. In particular, for plutonium isotopes and $\bar{\nu}$ reaction in general, uncertainties in ENDF/B VII.1 are very different from the uncertainties in the SCALE library (Díez et al., 2015). This has a very large impact when the uncertainty in the k_{eff} is propagated, as can be observed in the results obtained by SUS3D3D (Table 7).

4.3.2. SUS3D3D

The cross section covariance matrices needed for SUS3D3D uncertainty calculation were taken from the SCALE 6.0m (NEA DB, 2011), JENDL 4.0m (Iwamoto et al., 2011) and COMMARA 2

Table 6
 k_{eff} uncertainty and main contributors obtained with SCALE/Tsunami-MG. Statistical uncertainty of calculations not shown due to being negligible.

Quantity	$\Delta k_{\text{eff}}/k_{\text{eff}} (\%)$	
	Critical core	Sub-critical core
$^{239}\text{Pu } \nu$	0.705	0.709
$^{238}\text{U}(n,n')$	0.319	0.310
$^{239}\text{Pu}(n,\gamma)$	0.270	0.251
$^{240}\text{Pu } \nu$	0.235	0.242
$^{239}\text{Pu}(n,f)$	0.188	0.192
$^{239}\text{Pu } \chi$	0.182	0.175
$^{238}\text{Pu}(n,f)$	0.161	0.170
$^{238}\text{U}(n,\gamma)$	0.156	0.143
$^{238}\text{U}(n,n)$	0.122	0.122
$^{56}\text{Fe}(n,\gamma)$	0.094	0.100
Other reactions	0.216	0.232
Total	0.957	0.957

Table 7
 k_{eff} uncertainty and main contributors for the critical core obtained using SUSD3D and different cross section covariance evaluations.

Quantity	$\Delta k_{eff}/k_{eff}$ (%)		
	SCALE-6.0m	COMMARA-2	JENDL-4.0m
$^{239}\text{Pu } \nu$	0.701	0.056	0.112
$^{238}\text{U}(n,n')$	0.324	0.331	0.148
$^{239}\text{Pu}(n,\gamma)$	0.265	0.273	0.194
$^{240}\text{Pu } \nu$	0.227	–	0.016
$^{239}\text{Pu}(n,f)$	0.188	0.185	0.266
$^{239}\text{Pu } \chi$	0.183	–	0.206
$^{238}\text{Pu}(n,f)$	0.160	–	–
$^{238}\text{U}(n,\gamma)$	0.152	0.157	0.196
$^{238}\text{U}(n,n)$	0.085	0.087	0.024
$^{238}\text{U } \nu$	0.083	0.085	0.044
$^{56}\text{Fe}(n,\gamma)$	0.073	–	0.085
$^{56}\text{Fe}(n,n)$	0.049	–	0.137
$^{56}\text{Fe}(n,n')$	0.032	–	0.098
Total XS	0.922	0.511	0.512
Total PFNS ¹	0.210	–	0.210
Total	0.945	~0.5	0.553

¹ Prompt fission neutron spectra.

(Herman et al., 2011) libraries. The SCALE 6.0m library contains 44 group covariances from the SCALE 6 package released by the ORNL team for the purpose of the UAM project. The 33 group COMMARA 2 covariance data, developed at BNL to be used together with the ENDF/B VII.0, has been made available for the WPEC Subgroup 33 (Salvatores et al., 2014). JENDL 4.0m covariances were processed using the NJOY 99 code.

The principal contributors and the total uncertainty estimations based on the above covariance data are listed in Table 7. No uncertainty value is given for some quantities due to the covariance matrix not being processed for them in this work. Relatively large differences can be observed between different data. The total uncertainty in k_{eff} ranges between ~0.5% (COMMARA 2 and JENDL 4.0m) and ~1% (SCALE 6.0m). SCALE 6.0m has in particular more conservative uncertainties in $\bar{\nu}$ for ^{239}Pu and ^{240}Pu . On the

other hand, JENDL 4.0m predicts slightly larger uncertainties due to the cross sections of iron.

4.3.3. Additional MCNP calculations

In addition to the uncertainty evaluation methods discussed and applied, the k_{eff} uncertainty resulting from a series of MCNP calculations with random data files has been evaluated. Since ^{239}Pu and ^{238}U , due to their high content in MYRRHA MOX fuel, are major contributors into the neutron balance of the system, and have largest ISC of k_{eff} to nuclear data (Section 4.2), the study was limited to the nuclear data uncertainty propagation of these two nuclides. The JEFF 3.1.2, which has been a reference library for MYRRHA neutronic calculations, does not possess the covariance information for ^{239}Pu and ^{238}U data. In contrast, ENDF/B VII.1 evaluations include the covariance matrices for the cross sections, fission neutron multiplicity $\bar{\nu}$ and fission spectrum χ . In the framework of the joint collaborative project (SCK-CEN, 2014), AREVA GmbH has generated a set of 100 random files based on the ENDF/B VII.1 evaluation for each of these two nuclides using the NUDUNA code (Buss et al., 2011). The overall uncertainty propagation due to complete covariance data has been studied for these two nuclides together. The results are summarized in Table 8 and Fig. 10.

The first trial set of calculations was performed with 500,000 neutrons, which resulted in an average k_{eff} statistical uncertainty of 67 pcm. The second set of calculations was performed with a 20 fold increased number of neutrons decreasing the statistical uncertainty to 18 pcm. In the case of the calculations set with randomly sampled files, the value of k_{eff} averaged over 100 samples remains underestimating nominal k_{eff} while the statistical error (18 pcm) is lower than the difference between k_{eff} (32 pcm).

The uncertainty of 413 pcm obtained due to covariance information for ^{239}Pu and ^{238}U is found to be nearly half the total uncertainty of 957 pcm calculated by SCALE (Table 6). However, it agrees quite well with the uncertainty due to ^{239}Pu and ^{238}U predicted by COMMARA 2 and JENDL 4.0m (Table 7), 511 pcm and 476 pcm respectively, which confirms that SCALE gives more conservative estimations of the uncertainty.

Table 8
Nominal and average k_{eff} values and resulting statistical uncertainties for two sets of calculations with different number of source particles. Reference $k_{eff} = 1.00400 \pm 0.00003$ (Table 1).

Nominal k_{eff}	σ_{stat} (pcm)	Averaged over samples	Difference (pcm)	Uncertainty (pcm)
1.00411	67	1.00368	–43	433
1.00412	18	1.00380	–32	413

Fig. 10. k_{eff} and uncertainty convergence.

5. Conclusions

A model of the MYRRHA core has been developed for the critical and sub critical configurations and nuclear data sensitivity and uncertainty analyses have been performed in multi group and continuous energy using the KENO code included in SCALE6.2b3, in continuous energy using MCNP and with SUS3D using a multi group solver. The best estimate criticality calculations result in some differences in k_{eff} due to use of different nuclear data libraries and different codes.

A sensitivity and uncertainty analysis has been carried out with the TSUNAMI 3D module for both core configurations, identifying the major sensitivity coefficients, the uncertainty in k_{eff} , and the contribution of the most relevant quantities to the k_{eff} uncertainty. This set of results has been taken as a reference for the comparison with other codes.

Considerable differences have been observed between the k_{eff} uncertainties calculated using different covariance matrix evaluations. SCALE 6.0m covariance data have been found to be the most conservative resulting in the total uncertainty of $\sim 1\%$ (0.96% using TSUNAMI and 0.95% using SUS3D). Using COMMARA 2 (official ENDF/B VII.0 covariance library) and JENDL 4.0m the SUS3D code predicts the k_{eff} uncertainty of $\sim 0.5\%$ and 0.55%, respectively. SCALE 6.0m includes in particular more conservative uncertainties in ^{239}Pu , ^{240}Pu $\bar{\nu}$ and $^{238}\text{U}(n,n')$. On the other hand, JENDL 4.0m predicts slightly larger uncertainties due to the cross sections of iron. Main difference between the SCALE 6.0m and COMMARA 2 based uncertainties is in the predicted contribution of the uncertainties in ^{239}Pu $\bar{\nu}$. In the relevant energy range below ~ 100 eV the corresponding standard deviations are estimated to be 1%, $\sim 0.2\%$ and $\sim 0.1\%$ in SCALE 6.0m, COMMARA 2 and JENDL 4.0m, respectively.

Even slightly lower k_{eff} uncertainty of 413 pcm has been obtained from a series of MCNP calculations with randomly perturbed ^{239}Pu and ^{238}U data files using ENDF/B VII.1 cross sections and the corresponding covariances. Thus, the uncertainty due to nuclear data predicted by the different libraries and methods is from 413 to 957 pcm. This range of uncertainty surpasses the k_{eff} accuracy desired from the economic aspect. In order to provide a realistic estimation of k_{eff} uncertainty and reach the target accuracy, the evaluated data available for ^{239}Pu and ^{238}U should be improved.

Regarding the sensitivity analysis, the methodologies included in SCALE (TSUNAMI 3D), MCNP (PERT and KSEN cards) and SUS3D have been used to compare the integrated sensitivity coefficients and the energy dependent sensitivity coefficients of the major contributors to the k_{eff} uncertainty, observing differences of less than 4% between codes, with a few exceptions ($^{238}\text{Pu}(n,f)$, $^{238}\text{U}(n,n)$ and $^{56}\text{Fe}(n,\gamma)$). The following list of quantities has been outlined to be of special importance for the MYRRHA reactor concept:

- ^{239}Pu : (n,γ) both in resonance and fast energy region, (n,f) fast, χ and $\bar{\nu}$ fast;
- ^{238}U : (n,n') fast, (n,γ) resonance and fast, (n,n) resonance and fast;
- ^{240}Pu : $\bar{\nu}$ fast;
- ^{238}Pu : (n,f) both resonance and fast;
- ^{56}Fe : (n,γ) both resonance and fast.

Additionally, due to the flexibility of the MYRRHA facility in providing various irradiation environments, $^{209}\text{Bi}(n,\gamma)$ and (n,n') , $^{208}\text{Pb}(n,n)$ and (n,n') and ^{235}U $\bar{\nu}$, (n,f) and (n,γ) should also be considered in the resonance and fast energy regions.

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