Sensitivity analysis of the nuclear data for MYRRHA reactor modelling

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Abstract

A global sensitivity analysis of effective neutron multiplication factor k_{eff} to the change of nuclear data library revealed that JEFF-3.2T2 neutron-induced evaluated data library produces closer results to ENDF/B-VII.1 than does JEFF-3.1.2. The analysis of contributions of individual evaluations into k_{eff} sensitivity allowed establishing the priority list of nuclides for which uncertainties on nuclear data must be improved.

Detailed sensitivity analysis has been performed for two nuclides from this list, ^{56}Fe and ^{238}Pu. The analysis was based on a detailed survey of the evaluations and experimental data. To track the origin of the differences in the evaluations and their impact on k_{eff}, the reaction cross-sections and multiplicities in one evaluation have been substituted by the corresponding data from other evaluations.

Introduction

The Multi-Purpose Hybrid Research Reactor for High-Tech Applications (MYRRHA) research reactor is being designed at SCK•CEN, Belgium. This flexible facility will operate in both critical (at nominal power 100 MWth) and subcritical operation modes (at ~70 MWth). The latter one represents an accelerator-driven system (ADS), where neutrons driving the subcritical MOX-fuelled core are originated from the lead-bismuth eutectic (LBE) spallation target bombarded by a 600 MeV proton beam with intensity up to ~3 mA from a superconducting linear accelerator. The design characteristics of MYRRHA are determined by the international needs in terms of flexible fast spectrum irradiation capabilities, ADS demonstration and the targeted applications catalogue for this facility. As a direct consequence of the desired high flux levels [$\sim 3 \times 10^{15}$ n/(cm^{2}s)], and hence high-power density, a compact core is needed, and therefore the central hole in the core which houses the spallation target should be of limited dimensions. This required high cooling efficiency which is provided by the LBE, thanks to its low melting temperature which allows the primary systems to function at rather low temperatures. A pool-type system has been chosen to profit from the thermal inertia provided by a large coolant volume (OECD/NEA, 2009). The neutronics design of MYRRHA is a challenging task since the huge amount of heavy metal coolant, the highly enriched mixed-oxide (MOX) fuel and the presence of high-energy neutrons in the subcritical operation mode require accurate knowledge of safety parameters such as an effective neutron multiplication factor k_{eff}, reactivity coefficients, etc. The calculation of these characteristics heavily relies on the nuclear data which thus must be accurate enough to ensure acceptable uncertainties on calculated neutronic parameters. The Belgian licensing authorities require that safety-related neutronics calculations of MYRRHA must be performed with the selected, validated and approved nuclear data set. A primary step towards the creation and validation of such data set is the nuclear data sensitivity and uncertainty analysis with respect to MYRRHA. The sensitivity of effective neutron multiplication factor of MYRRHA critical core to the nuclear data has been thoroughly studied and the results are reported below. The priorities on the dedicated differential and integral experiments targeting to reduce key nuclear data uncertainties are discussed.

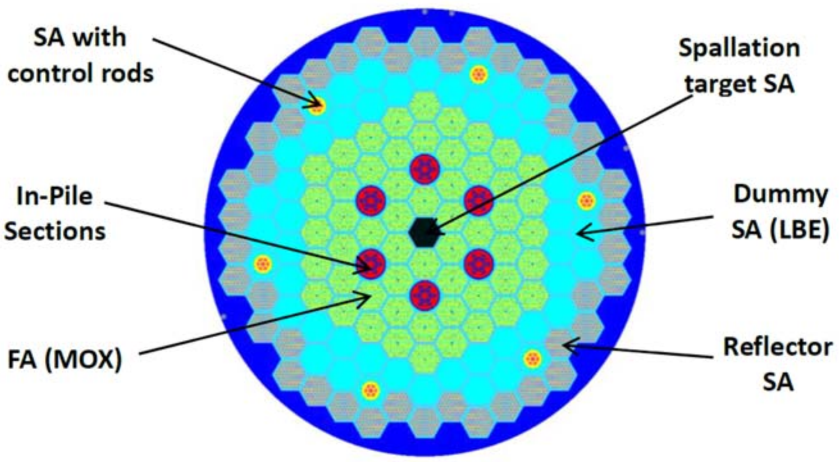
Sensitivity analysis of general purpose neutron induced data

The neutronics calculations of the MYRRHA critical and subcritical cores are carried out at SCK•CEN with the general purpose radiation transport code MCNPX (Pelowitz, 2008) which has nowadays almost no alternates when dealing with ADS-related problems. Since this code relies heavily on the general and special purpose neutron data, several evaluated neutron-induced data libraries of last generation have been processed at SCK•CEN for various nuclear temperatures, including neutron-induced data from ENDF/B-VII.1 (Chadwick, *et al.*, 2011) and JEFF-3.1.2 (Santamarina, *et al.*, 2009). The test version of the JEFF-3.2 library, JEFF-3.2T2, has been added to this list (OECD/NEA, 2012). The libraries have been processed by the ALEPH-DLG code (Haeck and Verboomen, 2005) which automatises evaluated data processing with the NJOY code (MacFarlane and Muir, 1994) and performs quality assurance of produced transport libraries suitable for MCNPX.

As a result, three neutron-induced data libraries in ACE format have been generated for the set of 22 nuclear temperatures from 300 to 2 100 K (Stankovskiy, 2012).

The subcritical core configuration has been chosen for this study. It is targeted to operate at k_{eff} ~0.95 and is composed of 58 MOX-fuelled assemblies surrounding LBE spallation target subassembly (SA). The core also hosts several in-pile sections dedicated for the materials testing. The MCNPX geometry model is shown in Figure 1.

Figure 1: Subcritical core layout



To identify the most problematic nuclides from the viewpoint of nuclear data quality, nuclear data sensitivity analysis has been performed. It has become customary in nuclear data sensitivity studies to calculate the sensitivity of integral parameters to the arbitrary variation of nuclear data. Prior to this, the sensitivity of effective neutron multiplication factor k_{eff} to the choice of nuclear data library has been investigated.

Table 1 lists the effective neutron multiplication factors calculated for subcritical core with three neutron-induced point-wise data libraries: ENDF/B-VII.1, JEFF-3.1.2 and JEFF-3.2T2. ENDF/B-VII.1 was treated as a reference library so that the deviations of results obtained with the JEFF libraries were calculated as:

$$\Delta = \frac{k_{endfb} - k_{jeff}}{k_{endfb}} \ (\%) \qquad (1)$$

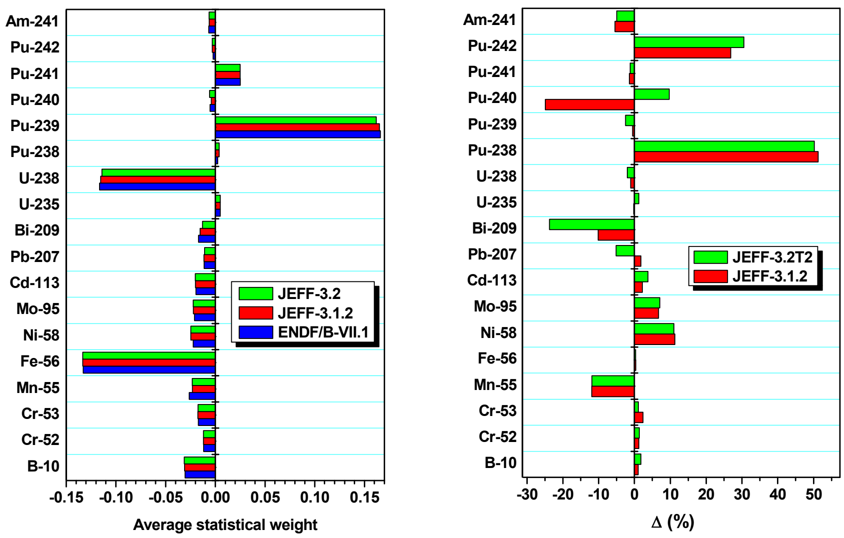
where k is the neutronics parameter under investigation (k_{eff} in Table 1).

Table 1: Effective neutron multiplication factor calculated with different libraries

Library	k_{eff} (std. dev.)	Difference (pcm)	Δ(%)
ENDF/B-VII.1	0.95911 (0.00004)	–	–
JEFF-3.1.2	0.96301 (0.00005)	390	0.41
JEFF-3.2T2	0.96091 (0.00004)	180	0.19

The deviation of JEFF-3.1.2 from ENDF/B-VII.1 does not exceed 0.5% and is even less for the test version of the JEFF-3.2 library. Both the ENDF/B and JEFF libraries tend to converge, however, JEFF libraries overestimate k_{eff} compared to ENDF/B-VII.1. The net neutron production by each nuclide calculated as differences between neutron statistical weights of production [by fission and (n,xn) reactions] and loss (capture) is plotted in Figure 2. This figure helps to identify the main contributors to the general neutronic behaviour of the reactor.

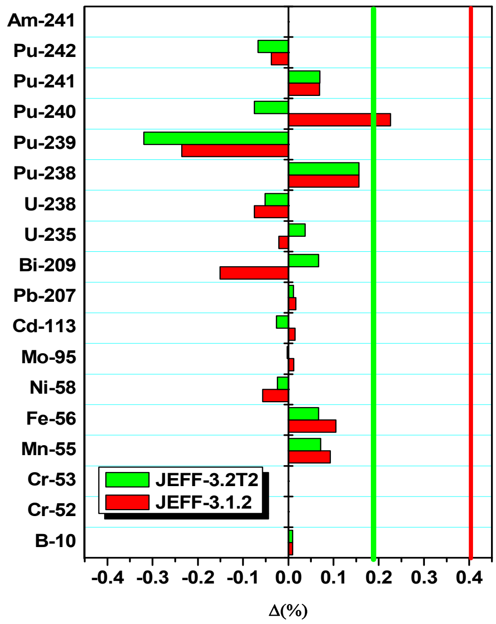
Figure 2: Net neutron production on selected nuclides (a) and deviations of JEFF libraries from ENDF/B-VII.1 (b)



As it is seen from Figure 2(a) the majority of neutrons is generated by fissions of ^{239}Pu. The positive contributions into the net neutron production are also given by ^{238,241}Pu and ^{235}U. Major neutron absorbers are ^{238}U, ^{56}Fe and other nuclides composing structural steels. LBE nuclides do not significantly change the net neutron production. However, Figure 2(b), which shows the deviations of JEFF-3.1.2 and JEFF-3.2T2 from ENDF/BVII.1, indicates that data for ^{239}Pu, ^{238}U and ^{56}Fe are less uncertain than even plutonium isotopes and ^{209}Bi. For instance, net neutron production on ^{238}Pu is rather small (but positive). However, the differences between the JEFF and ENDF/B-VII.1 libraries reach 50%. The sensitivity of the effective neutron multiplication factor to the evaluated data file choice for a particular nuclide has been studied by substituting the reference ENDF/B-VII.1 data for this nuclide with data taken from JEFF-3.1.2 or JEFF-3.2T2. The differences in k_{eff} caused by this data substitution are shown in Figure 3. The strong underestimation of k_{eff} (compared to the reference ENDF/B-VII.1 case) is observed for ^{239}Pu with both JEFF-3.1.2 and JEFF-3.2T2. The new evaluated file proposed for JEFF-3.2 has an even higher impact due to reduced fission cross-section, because, as is seen from Figure 2, the net neutron production is lower than in other evaluations. However, this 0.3% underestimation does not change the global picture when ENDF/B-VII.1 is substituted by JEFF libraries. This global difference, as demonstrated by Figures 2 and 3, is governed by the combined effect of other plutonium isotopes, ^{56}Fe and ^{55}Mn. For instance, the JEFF-3.2T2 evaluation results in higher neutron absorption by ^{240}Pu than JEFF-3.1.2 with ENDF/B-VII.1 data in between. As a result, k_{eff} is highly sensitive to this, even small, difference.

Figure 3: Sensitivity Δ_i of k_{eff} to the change of nuclear data for a particular nuclide

Horizontal lines show the differences in k_{eff} obtained with global library change: from ENDF/B-VII.1 to JEFF-3.1.2 (red line) and to JEFF-3.2T2 (green line)



It is also interesting to note that differences in net neutron behaviour of ^{56}Fe between evaluations are rather small, while k_{eff} has a remarkable increase when substituting the ENDF/B-VII.1 evaluation with JEFF. This immediately shows that elastic and inelastic scattering cross-sections of ^{56}Fe together play a more important role than neutron capture. Figures 2 and 3 give an indication of which data has higher integrated sensitivity coefficients without performing separate calculations of these coefficients. The uncertainty levels on the data can also be predicted when analysing these figures. Indeed, rather large positive differences in neutron production on ^{238}Pu provoke a significant increase in k_{eff} (by 0.15%). This means that fission cross-section and average neutron release per fission event are rather uncertain.

Sensitivity and uncertainty analysis performed for a previous model of MYRRHA, XT-ADS (Sugawara, *et al.*, 2011) resulted in the priority list of uncertainties which have to be improved by setting up dedicated integral and differential experiments. For the current design, which differs from XT-ADS by fuel enrichment, fuel assembly design, etc., the neutron spectrum remains almost the same; the priority list has not been changed significantly. One can only add ^{55}Mn neutron capture cross-section, ^{56}Fe elastic and inelastic scattering cross-sections and change the sequence in descending order of importance:

- ^{239}Pu neutron capture and fission neutron yields;
- ^{238}Pu fission, capture and (n,2n) cross-sections;
- ^{240}Pu fission neutron yield;
- ^{241}Pu fission and elastic scattering cross-sections;
- ^{56}Fe neutron capture, elastic and inelastic scattering cross-sections;
- ^{55}Mn neutron capture cross-section;
- ^{209}Bi neutron capture and (n,2n) cross-sections.

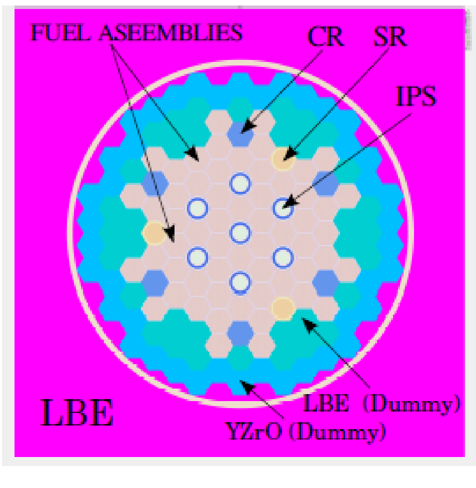
To confirm the results of this sensitivity analysis, detailed sensitivity and uncertainty analysis for the current MYRRHA design has been launched in the framework of the EC FP7 CHANDA project. Some preliminary results are reported below.

Sensitivity profiles

A detailed sensitivity analysis of k_{eff} to the neutron cross-section data has been performed using the SCALE-6.1 code suite (ORNL, 2011). The calculation sequence included KENO-VI Monte Carlo forward and adjoint transport calculations followed by the calculation of sensitivity coefficients by the SAMS module. SAMS calculates the sensitivity coefficients to every cross-section involved in the transport calculations as well as to the fission neutron multiplicity ($\bar{\nu}$) and the fission spectrum (χ).

A model of a critical MYRRHA core with 57 fresh fuel assemblies has been used for KENO-VI calculations. The number of assemblies in this case is less than for the subcritical core reported in the previous section because higher Pu content in MOX has been used here. The core layout is shown in Figure 4. The fuel assemblies are modelled in detail, while the rest of the elements (in-pile sections for material testing, subassemblies with control and safety rods, dummy assemblies and reflector assemblies) is represented as homogenised hexagonal cells. The control rods are extracted from the core giving an initial reactivity excess of ~5 000 pcm.

Figure 4: Model of MYRRHA critical core with 57 fresh fuel assemblies implemented in the KENO-VI code of the SCALE-6.1 package



In this sensitivity analysis the following values have been obtained:

- Sensitivity coefficients, $\frac{\partial k_{eff}}{k_{eff}} \Big/ \frac{\partial \sigma_i}{\sigma_i}$ which reflect the changes in k_{eff} with the variation of the energy group cross-section. The energy dependence of the sensitivity coefficients of the same reaction forms the sensitivity profile.
- Integrated sensitivity coefficients (ISC) as results of sensitivity profiles integration over energy. They are used to rank the reactions according to their importance for k_{eff}.

Table 2 lists the reactions influencing the criticality calculations of the MYRRHA core. Besides reactions on Pu and U isotopes, the elastic scattering of neutrons on ^{209}Bi could have a significant impact on k_{eff}. In general, this list of the 12 most important reactions corresponds to the list drawn up in the previous section. The exceptions are ^{56}Fe and ^{238}Pu, which certainly influence the criticality calculations but the integrated sensitivity coefficients on these isotopes are rather small. Hence, a deeper investigation of nuclear data for these isotopes is required. That is why these coefficients, three most important for each isotope, are also listed in Table 2 (highlighted in grey).

The comparison of nuclear data evaluations for ^{56}Fe and ^{238}Pu is presented below.

Table 2: Integrated sensitivity coefficients (ISC) sorted in decreasing order of ISC absolute value

The three largest ISC of ^{56}Fe and ^{238}Pu are highlighted in light and dark grey, accordingly

Isotope	Reaction	ISC	Std. dev. (1σ), %
^{239}Pu	$\bar{\nu}$	0.6969	0.01
^{239}Pu	(n,f)	0.4779	0.01
^{241}Pu	$\bar{\nu}$	0.1035	0.01
^{238}U	(n,γ)	-0.1023	0.02
^{240}Pu	$\bar{\nu}$	0.08256	0.01
^{241}Pu	(n,f)	0.07122	0.01
^{238}U	$\bar{\nu}$	0.06128	0.02
^{239}Pu	(n,γ)	-0.05764	0.03
^{240}Pu	(n,f)	0.05577	0.02
^{209}Bi	(n,n)	0.05039	0.30
^{238}U	(n,f)	0.03767	0.04
^{240}Pu	(n,γ)	-0.02564	0.03
^{56}Fe	(n,n)	0.02215	1.28
^{56}Fe	(n,γ)	-0.01409	0.02
^{56}Fe	(n,n′)	-0.00733	0.96
^{238}Pu	$\bar{\nu}$	0.01961	0.01
^{238}Pu	(n,f)	0.01347	0.01
^{238}Pu	(n,γ)	-0.00351	0.04

Impact of nuclear data evaluations for ^{56}Fe on MYRRHA criticality calculations

Evaluations from three major nuclear data libraries have been compared:

- The ENDF/B-VII.1 evaluation is based on the older data taken from ENDF/B-VI.1 (Chadwick, *et al.*, 1999).
- JENDL-4.0 data (Shibata, *et al.*, 2011) were taken from JENDL-3.3 (Shibata, *et al.*, 2002) with some reaction cross-sections recalculated for JENDL-4.0.
- The JEFF-3.1.2 evaluation was copied from EFF-3.1 (Hogenbirk, *et al.*, 1995).

Below 850 eV neutron capture and elastic scattering cross-sections are written by means of resonance parameters in all three evaluations. But ENDF/B-VI.1 and JENDL-4.0 provide a background cross-section for (n,γ) which is added to the cross-section calculated with the resonance parameters. On the other hand, EFF-3.1 provides more resonances for which at least two, at 423.1 and 446.0 keV, are not referred in the literature. The inelastic scattering cross-section is given with more detail in the EFF-3.1 evaluation, where more excited levels are represented compared to JENDL-4.0 and ENDF/B-VI.1. The impact of the above differences is shown in Table 3. The JEFF-3.1.2 and ENDF/B-VII.1 evaluations have been compared. Taking the JEFF-3.1.2 file for ^{56}Fe as reference (and using the JEFF-3.1.2 library for other nuclides), the inelastic scattering and neutron capture cross-sections were replaced in this file by the corresponding cross-section data from ENDF/B-VII.1 evaluation, and the impact on k_{eff} was studied.

Table 3: Impact of modifications in the ^{56}Fe file

^{56}Fe file	Modified part	k_{eff}	Δk_{eff} (pcm)
JEFF-3.1.2	–	1.05374±0.00008	–
ENDF/B-VII.1	–	1.05224±0.00008	-150
JEFF-3.1.2	(n,n′)	1.05343±0.00007	-31
JEFF-3.1.2	(n,γ)	1.05275±0.00008	-99

The difference in neutron capture cross-section covers almost two-thirds of the difference observed in the results of criticality calculations done with two ^{56}Fe evaluations. The background cross-section provided in ENDF/B-VII.1 is responsible for this effect.

Impact of nuclear data evaluations for ^{238}Pu on MYRRHA criticality calculations

The analysis of three evaluations for ^{238}Pu reveals that:

- For ENDF/B-VII.1, a new evaluation was performed in September 2010. It takes the resonance parameters from JENDL-4.0.
- For JENDL-4.0, a completely new evaluation was released in January 2010.
- JEFF-3.1.2 takes the evaluation from JENDL-3.2 (Nakagawa, *et al.*, 1995), but in the unresolved resonance region the BROND-2.2 (Blokhin, *et al.*, 1994) evaluation is used.

The main differences in neutron capture and fission cross-sections are observed in the unresolved resonance region (URR), where the BROND-2.2 evaluation uses the resonance parameters to calculate the cross-section, while JENDL-4.0 provides cross-section values stored in MF=3, MT=18 and MT=102 (Trkov, *et al.*, 2012). The differences in fission neutron multiplicities can be grouped as less than 1% at the energies up to 1 MeV, and less than 5% from 1 to 20 MeV. The impact of these differences on the criticality calculations is shown in Table 4. The same methodology as for ^{56}Fe was applied.

Table 4: Impact of modifications in the ^{238}Pu file

^{238}Pu file	Modified part	k_{eff}	Δk_{eff} (pcm)
JEFF-3.1.2	–	1.05363±0.00008	–
ENDF/B-VII.1	–	1.05178±0.00008	-185
JEFF-3.1.2	$\bar{\nu}$	1.05378±0.00007	+15
JEFF-3.1.2	(n,f)	1.05201±0.00008	-162
JEFF-3.1.2	(n,γ)	1.05319±0.00008	-44

The difference in the fission cross-section is the most important for the MYRRHA criticality calculations. In the energy range between 0.5 and 150 keV, where BROND-2.2 data is used in JEFF-3.1.2, the cross-section runs higher than in the JENDL-4.0 evaluation.

Conclusions

Detailed sensitivity analysis of effective neutron multiplication factor to the change of nuclear data evaluation has been performed. It allowed creating a priority list of nuclides for further, deeper analysis. It has been shown that the test version of the JEFF-3.2 library gives closer results to ENDF/B-VII.1 than JEFF-3.1.2. With this tendency of libraries to converge, however, the open issue is to assess the uncertainties on the cross-sections and fission multiplicities.

The importance of the ^{56}Fe and ^{238}Pu reactions has been demonstrated. The main differences between evaluations and their impact on the criticality calculations for the MYRRHA neutronic model have been studied. For ^{56}Fe, the most relevant difference between evaluations comes from the background cross-section for radiative neutron capture reaction. It is given in the ENDF/B-VII.1 evaluation and is omitted in JEFF-3.1.2. A better description of the resonance range would improve the ENDF/B-VII.1 or JENDL-4.0 evaluations. For ^{238}Pu, the JEFF-3.1.2 file takes the unresolved resonance parameters from BROND-2.2, which overestimates neutron-induced fission cross-section and causes a large difference in the criticality calculations. A new evaluation for ^{238}Pu is highly recommended for future releases of the JEFF library. The comparison of nuclear data evaluations reported here for ^{56}Fe and ^{238}Pu will be extended in the framework of the EC FP7 CHANDA project on the other nuclides and reactions identified in this study.

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