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Recommendations for MYRRHA relevant cross section data to the JEFF project

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2017

Joint
Research
Centre

EUR 28957 EN

JRC Science Hub
https://ec.europa.eu/jrc

JRC109182

EUR 28957 EN

PDF ISBN 978-92-79-77162-0 ISSN 1831-9424 doi:10.2760/485552

Luxembourg: Publications Office of the European Union, 2017

How to cite this report: G. Žerovnik, et al., *Recommendations for MYRRHA relevant cross section data to the JEFF project*, EUR 28957 EN, Publications Office of the European Union, Luxembourg, 2017, ISBN 978-92-79-77162-0, doi:10.2760/485552, JRC109182.

Recommendations for MYRRHA relevant cross section data to the JEFF project

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Contents

Abstract 4
1 Introduction 5
2 The MYRRHA concept 6
3 Nuclides and reactions relevant for MYRRHA 7
4 The CIELO project 8
5 Recommendations to JEFF 10
  5.1 ^{16}O 10
  5.2 ^{56}Fe 10
  5.3 ^{204,206,207,208}Pb 11
  5.4 ^{209}Bi 13
  5.5 ^{235,238}U 14
  5.6 Pu nuclides 18
6 Conclusion 20
References 21
List of abbreviations and definitions 25
List of figures 26
List of tables 27

Abstract

Within the framework of Work Package 10 of the EC FP7 CHANDA project, nuclear data of importance for the operation of MYRRHA, a lead-bismuth cooled accelerator driven reactor under development at SCK•CEN (BE), were studied. Based on data in the main nuclear data libraries, i.e. JEFF, JENDL, ENDF/B and BROND, and in the TENDL and CIELO libraries and on experimental data reported in the literature, recommendations to the JEFF project were made for several nuclides of interest to the MYRRHA reactor.

1 Introduction

Nuclear data uncertainties are one of the most important sources of uncertainty in reactor physics simulations [1]. Unfortunately, there is still a significant gap between the current uncertainties and the target uncertainties [2]. The EC FP7 CHANDA (solving CHAllenges in Nuclear DAta) project [3] aims at improvement of nuclear data used in simulations in order to improve the design and utilization of expensive nuclear systems. In particular, CHANDA Work Package 10 (WP10) [4] focuses on nuclear data required for the development, safety assessment and licensing of the MYRRHA experimental reactor [5], and on recommendations for data improvements to the JEFF project [6].

In previous years, a nuclear data Sensitivity and Uncertainty (S/U) analysis for the latest design of the MYRRHA reactor core [7] was carried out using various codes and methodologies. The aim was to identify the most relevant nuclear data parameters (nuclides and quantities) for some important response functions (i.e. the multiplication factor k_{eff} and the effective delayed neutron fraction β_{eff}) of the MYRRHA system.

For the S/U studies, the MYRRHA model was used with both the KENO-VI [8] and MCNP [9] radiation transport codes, the former one being used for the Monte Carlo neutron transport calculations in the SCALE system [8]. Additionally, a cylindrical geometry model of the MYRRHA critical configuration was constructed for the deterministic neutron transport calculations performed with the PARTISN [10] and SUSD3D [11] codes, both part of the XSUN-2013 system [12].

Sensitivity coefficients for k_{eff} in the critical MYRRHA model, calculated within Task 10.1 and presented in Deliverable D10.1 [13] of the CHANDA project WP10, were used to determine the list of nuclides and quantities important for MYRRHA from the aspect of nuclear criticality. This list was confirmed by a similar study of the delayed neutron fraction sensitivities on nuclear data [14].

In this report recommendations to the JEFF project for MYRRHA-relevant nuclear data are given. They result from a comparison of nuclear data from different nuclear data libraries starting from the list of materials and reactions/quantities that were defined in Ref. [13]. This comparison was presented as a part of Deliverable D10.2 [15]. The JEFF-3.2 library [16] was taken as a reference in the comparison. Other officially released libraries considered were ENDF/B-VII.1 [17], JENDL-4.0 [18], TENDL-2014 [19] and BROND-3.1 [20]. In addition data from the test library JEFF-3.3T and the one produced as part of the CIELO (Collaborative International Evaluated Library Organization) project [21] were included. The comparison was done both on the level of energy dependent microscopic data and on the level of results of integral benchmark experiments (shielding, criticality). The study was carried out in different stages, by substituting the entire library or by substituting parts of it (e.g. a single element, nuclide, quantity, reaction, or energy region). When necessary, the cross sections were pre-processed using the NJOY processing system [22]. For the substitution of the data for individual reactions from different libraries, the SANDY code [23] developed at SCK•CEN was used.

The CIELO pilot project [21] aims at combining the efforts of nuclear data experimentalists and evaluators towards the production of new generation neutron data files for the most important nuclides for reactor applications, including ^{16}O, ^{56}Fe, ^{235,238}U and ^{239}Pu. Therefore, to avoid an overlap with CIELO, the study within CHANDA WP10 focused as much as possible on the other quantities in the list mentioned above which are relevant for MYRRHA neutronic calculations. The main focus was on nuclear data for neutron induced reactions in bismuth and lead, which are important for neutron transport calculations and for an estimate of neutron activation of the coolant. This study was presented in Deliverable D10.3 [24].

Finally, as a main part of the study, recommendations to the JEFF project are given for neutron induced cross section data for ^{16}O, ^{56}Fe, ^{209}Bi, ^{204,206,207,208}Pb and ^{235,238}U.

2 The MYRRHA concept

MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications), a flexible experimental facility and a GEN-IV reactor system [25], is currently being designed at SCK•CEN, Mol, Belgium [5]. It is planned 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 Ref. [26]. A mixed-oxide (MOX) fuel core is planned as the primary design option. For the sensitivity study of nuclear data, a simplified model [7], homogenised on fuel assembly level, was used. The layout of the core for both the critical and sub-critical configurations is shown in Figure 1. The vertical layout of the model for the sub-critical core is given in Figure 2.

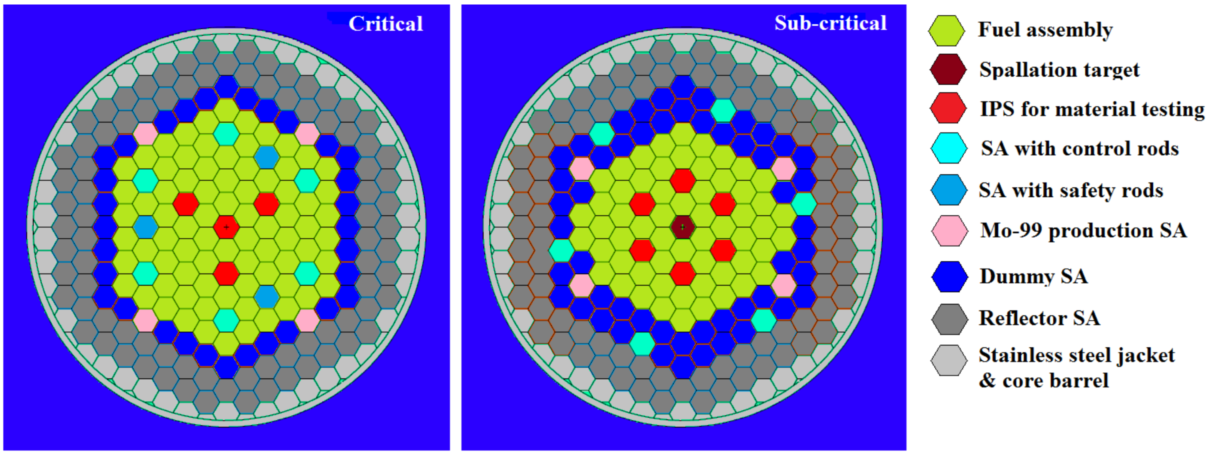

Figure 1: Critical (left) and sub-critical (right) MYRRHA MOX core layouts, showing the positions of different types of assemblies and sub-assemblies (IPS – In-Pile test Section, SA – Sub-Assembly).

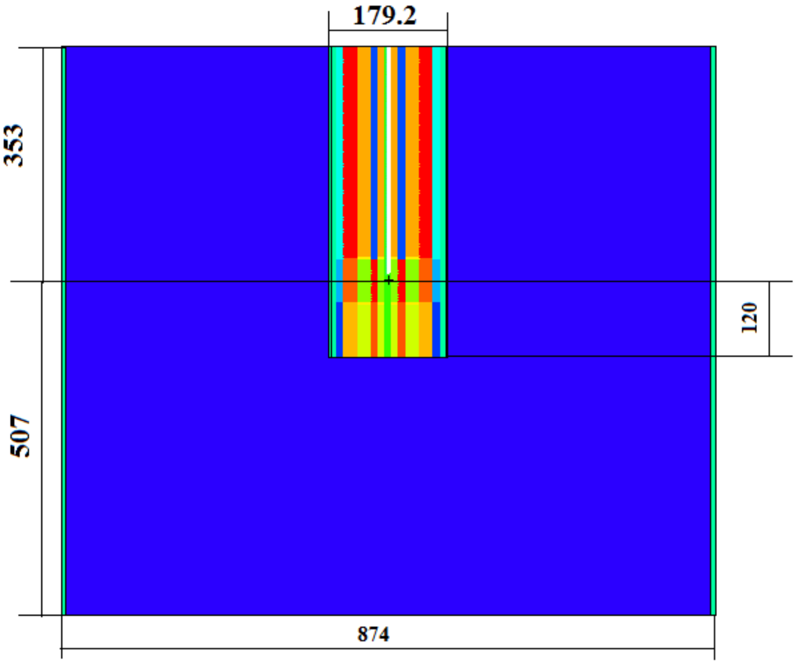

Figure 2: Vertical layout of the MYRRHA sub-critical MOX core model (dimensions given in cm).

3 Nuclides and reactions relevant for MYRRHA

The sensitivity coefficients for k_{eff} in the critical MYRRHA model, calculated within Task 10.1 and presented in Deliverable D10.1 of CHANDA [13], were used to determine the list of nuclides and quantities important for MYRRHA from neutronic point of view. The list is given in Table 1. The nuclides which influence k_{eff} the most are ^{56}Fe, ^{238}U and ^{238,239,240}Pu. Taking into account the flexibility of the MYRRHA facility in providing various irradiation environments, ^{208}Pb, ^{209}Bi, ^{235}U and ^{241,242}Pu were also considered. Due to the importance of ^{16}O as part of the fuel, this nuclide was added to the list. In Table 1, only ^{208}Pb is listed as important for the MYRRHA system. However, due to the importance as part of the coolant, other stable lead isotopes, i.e. ^{204,206,207}Pb, were also considered. The list was confirmed by a similar study of the delayed neutron fraction sensitivities on nuclear data [14].

Table 1: List of nuclides, quantities and reactions, most relevant for MYRRHA: σ denotes the reaction cross section, $\bar{\nu}$ the fission neutron multiplicity and χ the fission neutron spectrum.

Nuclide	Quantity/reaction	Energy region
^{16}O	σ(n,n)	continuum (fast)
^{56}Fe	σ(n,n) σ(n,n') σ(n,γ)	resonance and continuum continuum resonance and continuum
^{208}Pb	σ(n,n) σ(n,n')	resonance and continuum resonance and continuum
^{209}Bi	σ(n,n') σ(n,γ)	resonance and continuum resonance and continuum
^{235}U	$\bar{\nu}$ σ(n,f) σ(n,γ)	resonance and continuum resonance and continuum resonance and continuum
^{238}U	σ(n,n) σ(n,n') σ(n,γ)	continuum resonance and continuum resonance and continuum
^{238}Pu	σ(n,f)	resonance and continuum
^{239}Pu	$\bar{\nu}$ χ σ(n,f) σ(n,γ)	continuum continuum continuum resonance and continuum
^{240}Pu	$\bar{\nu}$	continuum
^{241}Pu	σ(n,f)	resonance and continuum
^{242}Pu	σ(n,f)	continuum

4 The CIELO project

CIELO is an international pilot project [21] which aims at improving evaluations of neutron induced interaction cross sections for nuclides of major importance for nuclear industry: ^{16}O, ^{56}Fe, ^{235,238}U and ^{239}Pu. Some of these improvements are also of importance for MYRRHA.

In order to improve the nuclear data libraries for these nuclides, an international collaboration was established, coordinating experimental, theoretical and simulation efforts. The aim of the collaboration was to make an inventory of open issues, to solve these issues and to create improved evaluated nuclear data files incorporating the advances made within the project. These new evaluated data files are to be available for adoption by the main nuclear data libraries.

The CIELO project is coordinated by the Nuclear Energy Agency (NEA) Working Party on Evaluation Cooperation (WPEC) Subgroup 40. JRC Geel is actively involved in the improvement of evaluations for ^{16}O and ^{238}U, and also partly contributes to the validation of the ^{56}Fe evaluation.

One of the important aims of the CIELO project, i.e. to create evaluations of nuclear data for the chosen nuclides which would be universally accepted, was fulfilled only partially. Due to differences in opinions of some directly involved institutions, it was finally decided to create two separate evaluations: CIELO-1 and CIELO-2 [27]. The CIELO-1 evaluation is strongly based on work co-ordinated by the Nuclear Data Section of the International Atomic Energy Agency (IAEA). This evaluation will be taken over in ENDF/B-VIII.0. The CIELO-2 evaluation is a combination of work at different institutes and organisations, strongly based on work done by CEA (Commissariat à l'Énergie Atomique et aux énergies alternatives) and IRSN (Institut de Radioprotection et de Sûreté Nucléaire). It will be partly taken over in JEFF-3.3.

Two evaluations for ^{16}**O** were presented in CIELO, one from LANL (Los Alamos National Laboratory) using the R-Matrix code EDA [28], the other one done at IRSN with the code SAMMY [29]. The differences caused by the choice of theoretical framework are much smaller than the impact of the experimental data sets chosen for fitting the model parameter, e.g. the total cross section at thermal energy differs by approximately 1%, as two different values for the coherent scattering length were assumed. But in this energy region both evaluations reproduce the experimental data much better than e.g. ENDF/B-VII.1. At higher energies the difference between the two evaluations becomes more pronounced, especially for the (n,α) cross section, in which differences as high as 30% can be observed. The LANL evaluation will be adopted in the new ENDF/B-VIII.0 library. The IRNS evaluation was considered in the JEFF-3.3T3 test library. However, the following version, JEFF-3.3T4, reverted back to the ENDF/B-VII.1 evaluation.

The resolved resonance parameters for ^{56}**Fe** in the CIELO-1 evaluation [30] were adopted from JENDL-4.0. This evaluation is mainly based on the original JEF-2.2 evaluation by F. Fröhner. In JENDL-4.0 minor modifications were implemented, e.g. the resonance at 59.5 keV was removed. In the CIELO-1 file a background capture cross section was added to produce a $1/v$ dependence of the cross section due to external contributions. In the continuum energy region, a new evaluation of the inelastic scattering cross section was performed based on data from Negret et al. [31] (with adjusted energy calibration) and renormalized data from Dupont et al. [32]. The total cross section was adopted from JEFF-3.2. CIELO-1 will be adopted in the new ENDF/B-VIII.0 library. For CIELO-2, the resonance region was extended to 2 MeV and combined with the continuum region from JEFF-3.2. Unlike CIELO-1, CIELO-2 does not contain any additional background contribution for the capture cross section.

The CIELO-1 evaluation for ^{235,238}**U** is described by Capote et al. [33]. The parameters in the resolved resonance region (RRR) for ^{238}U are taken from Kim et al. [34]. This file was constructed starting from the resonance parameters proposed by Derrien et al.

[35]. These parameters were adopted in the main nuclear data libraries ENDF/B-VII.1, JEFF-3.2 and JENDL-4.0. Kim et al. [34] replaced the parameters for energies below 1200 eV by parameters derived from a combined analysis of transmission and capture data obtained at ORELA and GELINA, respectively. They also changed the parameters of the bound states. The CIELO-1 evaluation in the unresolved resonance region (URR) is taken from Sirakov et al. [36]. The EMPIRE-3.2 code [37] was used to produce cross sections in the continuum region up to 30 MeV. The results of the CIELO-1 evaluation are fully consistent with all relevant neutron cross section standards. For the CIELO-2 evaluation, adjustments were done to ensure consistency with a set of integral benchmark experiments. The average capture cross section for ^{238}U in CIELO-2 is reduced by about 7% compared to the one in CIELO-1. Hence, it is in disagreement with the one derived within the neutron standards project and the average capture cross section of Kim et al. [34]. In addition, the $R = \sigma_\gamma(^{238}\mathrm{U})/\sigma_\gamma(^{235}\mathrm{U})$ capture cross section ratio, averaged over a Maxwellian neutron spectrum with thermal energy 25 keV, in CIELO-2 ($R_{CIELO\text{-}2}$ = 0.49) is about 20% smaller compared to the one (R_{exp} = 0.60 ± 0.03) determined with atomic mass spectrometry measurements by Wallner et al. [38]. The ratio derived from the cross sections in CIELO-1 ($R_{CIELO\text{-}1}$ = 0.57) is within the uncertainty in agreement with this experimental value. The lower ratio for CIELO-2 is due to the lower capture cross section of ^{238}U(n,γ) which is compensated by a higher capture cross section of ^{235}U(n,γ) to maintain results of integral benchmark experiments. For ^{235,238}U, the CIELO-1 and CIELO-2 evaluations will be adopted in the new ENDF/B-VIII.0 and JEFF-3.3 libraries, respectively.

For **^{239}Pu**, the fission cross section in CIELO-1 increased by almost 0.5% in the continuum energy region with respect to the ENDF/B-VII.1 library. CIELO-1 adopted the cross section from the latest update of the standards project [39]. In the continuum energy region, a new evaluation of the capture cross section was made in CIELO-1. For CIELO-2, a new evaluation of the URR and continuum region was made, and the RRR was extended from 2.5 keV to 4 keV. The prompt fission neutron multiplicities $\overline{\nu_p}$ in CIELO-1 and CIELO-2 differ by about 1% following adjustments to improve the agreement between calculations and experimental data from a series of criticality benchmarks. Compared to CIELO-2, the fission cross section and the fission neutron multiplicity in CIELO-1 are closer to the available energy dependent experimental data. The CIELO-1 and CIELO-2 evaluations will be adopted in the new ENDF/B-VIII.0 and JEFF-3.3 libraries, respectively.

5 Recommendations to JEFF

For most of the materials given in Table 1 (^{56}Fe, ^{204,206,207,208}Pb, ^{209}Bi, ^{235,238}U and ^{238,239,240,241,242}Pu), a detailed study of the available experimental data in the EXFOR database [40] and other sources was performed for the quantities (cross sections, prompt, delayed and total fission neutron multiplicities) and reactions (capture, fission, elastic and inelastic scattering) of interest for MYRRHA. The data in some evaluated nuclear data libraries (JEFF-3.2, ENDF/B-VII.1, JENDL-4.0 and TENDL-2014) were compared with each other and with experimental data. Details of this comparative study were presented in the CHANDA WP10 Deliverables D10.2 [15] and D10.3 [24]. In this section recommendations to JEFF, based on these studies, are given for ^{16}O, ^{56}Fe, ^{204,206,207,208}Pb, ^{209}Bi, ^{235,238}U and ^{239}Pu.

5.1 ^{16}O

At the moment the ENDF/B-VII.1 evaluation, especially at low energies, is not agreeing with the experimentally derived total cross section data. This will be improved with the release of ENDF/B-VIII.0, as the new file will be based on the LANL evaluation performed with the code EDA. For the test library JEFF3.3T3, the IRSN evaluation done with the code SAMMY was included. However, in the latest JEFF3.3T4 library the file from the ENDF/B-VII.1 library was chosen.

At present the LANL evaluation is recommended. Nevertheless, any new release of either library should include a new evaluation of the RRR with better and clearer justified choices of the experimental data used for deriving the model parameters.

5.2 ^{56}Fe

Within the framework of both the CIELO and CHANDA project, the ^{56}Fe cross sections proposed in the CIELO-1, JEFF-3.3T2 and ENDF/B-VII.1 libraries were validated using results of shielding benchmarks from the SINBAD database [41], i.e. the ASPIS-Fe88, JANUS, NESDIP and EURACOS Fe benchmarks. This study reveals that the agreement between the experimental data and results of calculations using different libraries depends on the benchmark and the observed quantity. This is partly due to different sensitivity profiles of the benchmarks under consideration. However, it may also be due to possible deficiencies in the benchmark models.

For example, as shown in Figure 3, the computational model of the ASPIS-Fe88 system is able to predict the ^{103}Rh(n,n′) reaction rate at different depths of the iron shield better when using the CIELO-1 library rather than the JEFF-3.3T2 or ENDF/B-VII.1 library. The inelastic scattering reaction on rhodium has a relatively low neutron threshold energy of ~40 keV. This might indicate that the contribution of the additional background cross section in the CIELO-1 ^{56}Fe evaluation improves the capture cross section in the RRR above 50 keV. This additional background cross section is not present in JEFF-3.3T2 or ENDF/B-VII.1. On the other hand, for some reactions with a higher energy threshold, e.g. ^{32}S(n,p), the agreement between experimental and calculated reaction rates is worse for reaction rates derived with CIELO-1 compared to JEFF-3.3T2 or ENDF/B-VII.1.

No definite overall conclusions on the quality of the test libraries can be drawn based on a validation with integral benchmark experiments. However, the CIELO-2 library fails to reproduce the Negret et al. [31] and renormalized Dupont et al. [32] inelastic cross sections measurements from GELINA. Therefore, the CIELO-1 evaluation is recommended for ^{56}Fe.

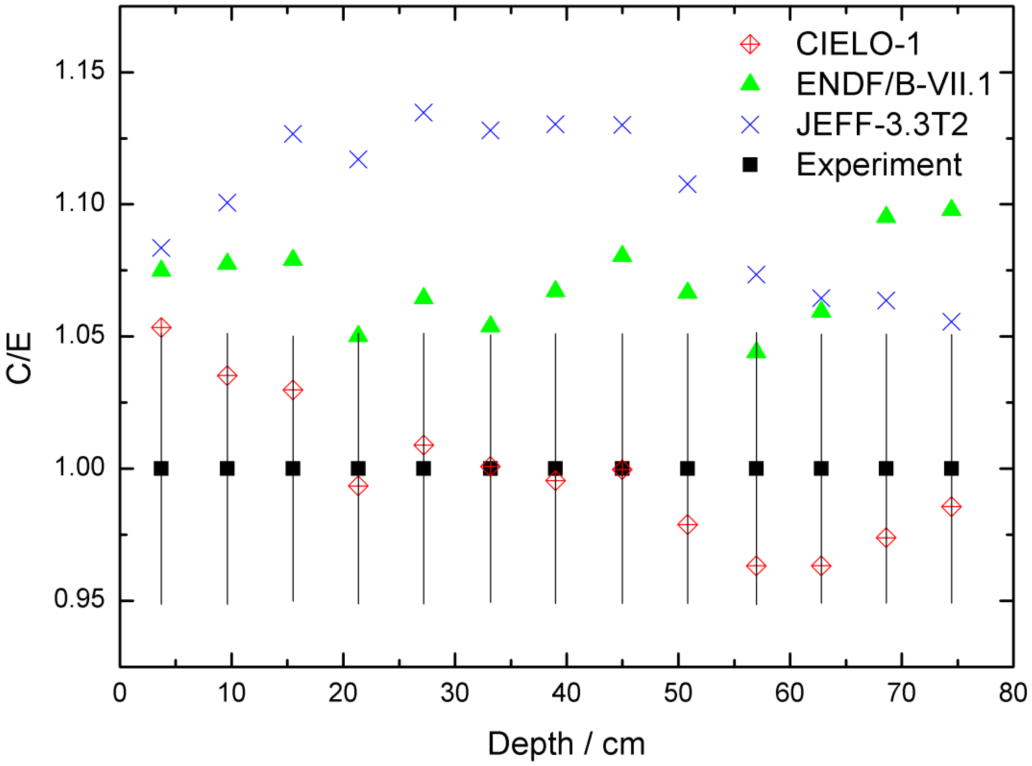

Figure 3: Comparison of the calculated ^{103}Rh(n,n’) reaction rates (C), relative to the experimental value (E), as a function of depth of the iron shield of the ASPIS-Fe88 system. Monte Carlo calculations were performed using the ENDF/B-VII.1, CIELO-1 and JEFF-3.3T2 nuclear data libraries.

5.3 ^{204,206,207,208}Pb

For ^{204,206,207,208}Pb the cross sections that are recommended in the main libraries JEFF-3.2, ENDF/B-VII.1 and JENDL-4.0 can be improved based on available experimental data. This is illustrated in Figure 4 for ^{208}Pb, with a natural abundance varying between 51.28% and 56.21% [42]. This figure compares the experimental transmission of Carlton et al. [43] and the one obtained with the total cross section of ENDF/B-VII.1, JENDL-4.0, JEFF-3.2 and JEFF-3.3T1. The data of Carlton et al. [43] result from TOF measurements at a 200 m transmission station of ORELA using Pb samples enriched in ^{208}Pb. In the RRR, which for ^{208}Pb extends up to 1 MeV, all evaluations are mostly consistent with the experimental data of Carlton et al. [43]. Above 1 MeV, the JENDL-4.0 library is evidently better than other considered libraries. In JEFF-3.3T1, the background cross section proposed in JEFF-3.2 was changed for ^{206,207,208}Pb. This resulted in larger differences between the experimental and calculated transmission at incident neutron energies between the energies of resonance peaks. This effect is especially important for ^{206,207}Pb. In general, the best agreement between experimental and calculated transmission is obtained when the total cross section is taken from JENDL-4.0. More detailed results of this study were already reported in Deliverable D10.3 [24]. These problems were already reported to the JEFF committee [44] and fixed for the test version JEFF-3.3T2. In this version the JENDL-4.0 evaluation was taken as a basis with some modifications in the inelastic scattering cross section. For the inelastic cross section the results of TOF measurements at GELINA carried out by Mihailescu et al. [45] were included. Therefore, the JEFF-3.3T2 evaluation is recommended for ^{204,206,207,208}Pb.

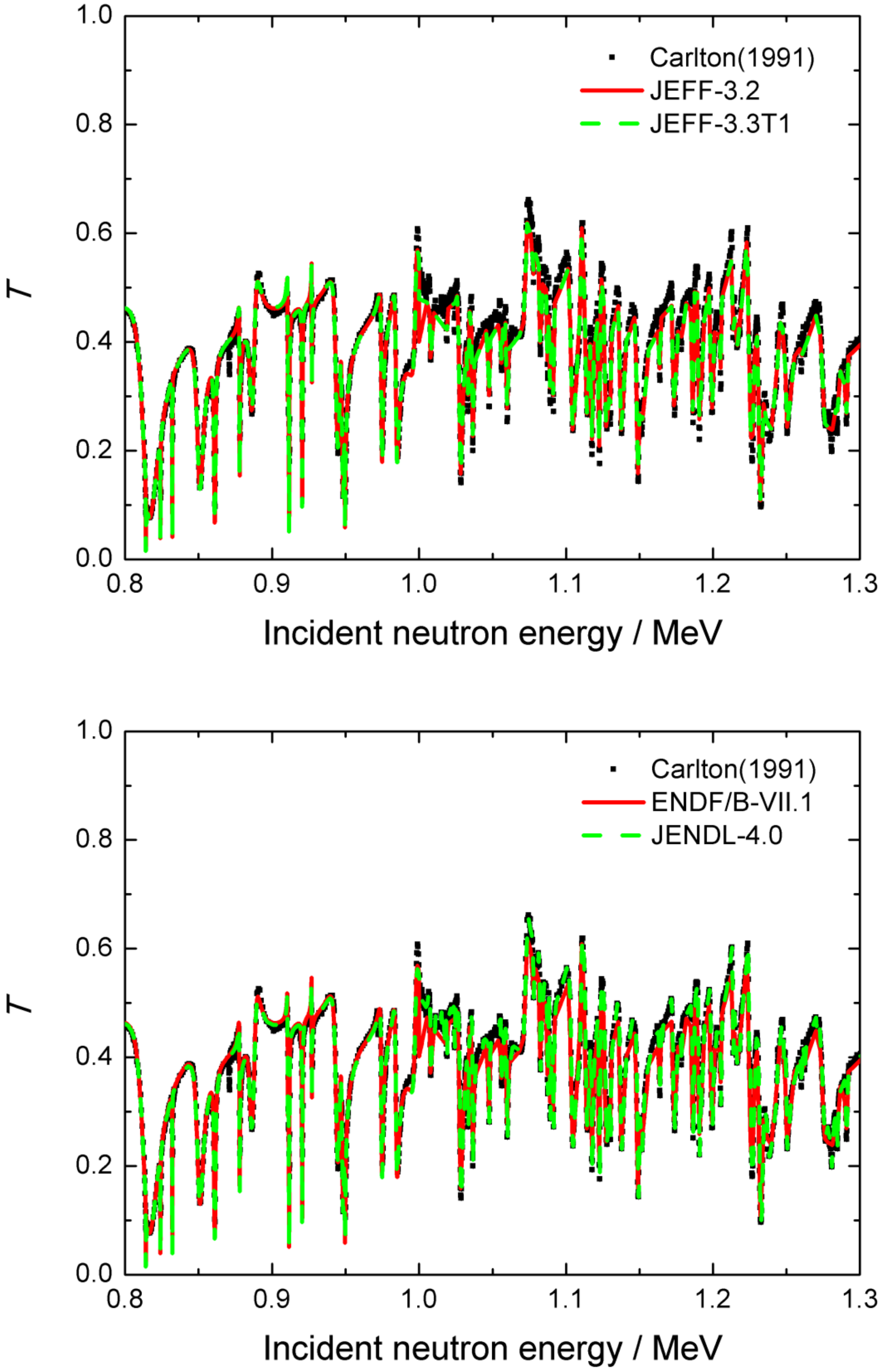

Figure 4: Transmission T as a function of incident neutron energy. The transmission is through an enriched ^{208}Pb sample with an areal density of 0.18594 at/b. Results of the ^{208}Pb transmission measurement from Carlton et al. (1991) are compared with transmission calculated using cross sections from the JEFF-3.2 and JEFF-3.3T1 (top) and ENDF/B-VII.1 and JENDL-4.0 (bottom) libraries.

5.4 ^{209}Bi

Similar to the case of the stable Pb isotopes, problems with the background cross section and the boundary between RRR and URR in JEFF-3.2 and JEFF-3.3T1 were also noticed for ^{209}Bi. They were already reported in Deliverable D10.3 [24] and recommendations were given to the JEFF committee [44]. Also for ^{209}Bi a JEFF-3.3T2 version was created by using the JENDL-4.0 evaluation as a basis combined with results of inelastic scattering cross section measurements by Mihailescu et al. [46] performed at GELINA.

The branching ratio (BR = σ_g/σ_m) for the ^{209}Bi(n,γ) cross section, i.e. the ratio of the cross section σ_g for production of the ground state ^{210g}Bi to the cross section σ_m for production of the isomeric state ^{210m}Bi, is very important for coolant activation in MYRRHA. This BR is required to determine the production of ^{210}Po, which is produced through the decay of ^{210m}Bi. Unfortunately, the energy dependence of this BR is difficult to measure. Experimental data that can be used to evaluate this ratio above thermal energy are limited to the results of activation measurements at 30 keV and 534 keV by Saito et al. [47], and measurements by Borella et al. [48] at GELINA. The BR derived from these experimental data together with the one derived from measurements at the cold neutron beam of the research reactor in Budapest [49] are plotted as a function of energy in Figure 5. The BR derived from the cross sections in the JENDL-4.0, JEFF-3.2, BROND-3.1, JENDL/A-96 and RUSFOND-2010 libraries are also shown.

At low energies, the BR derived from the data in JENDL-4.0, JEFF-3.2 and BROND-3.1 are consistent with the experimental value determined in Ref. [49]. The ones derived from the JENDL/A-96 and RUSFOND-2010 libraries are larger by a factor 6.7 and 1.8, respectively. In general the best agreement between experimental and evaluated BR is obtained with the ones derived from the BROND-3.1 library. Therefore, this BR is recommended. Nevertheless, to reduce the uncertainty on the estimated production of ^{210}Po additional experimental data of the energy dependent BR are required. In addition, the status of both the total and capture cross section of ^{209}Bi can be improved by new TOF cross section measurements.

The JEFF-3.3T2 evaluation together with the branching ratio (BR) from the BROND-3.1 library are recommended for ^{209}Bi.

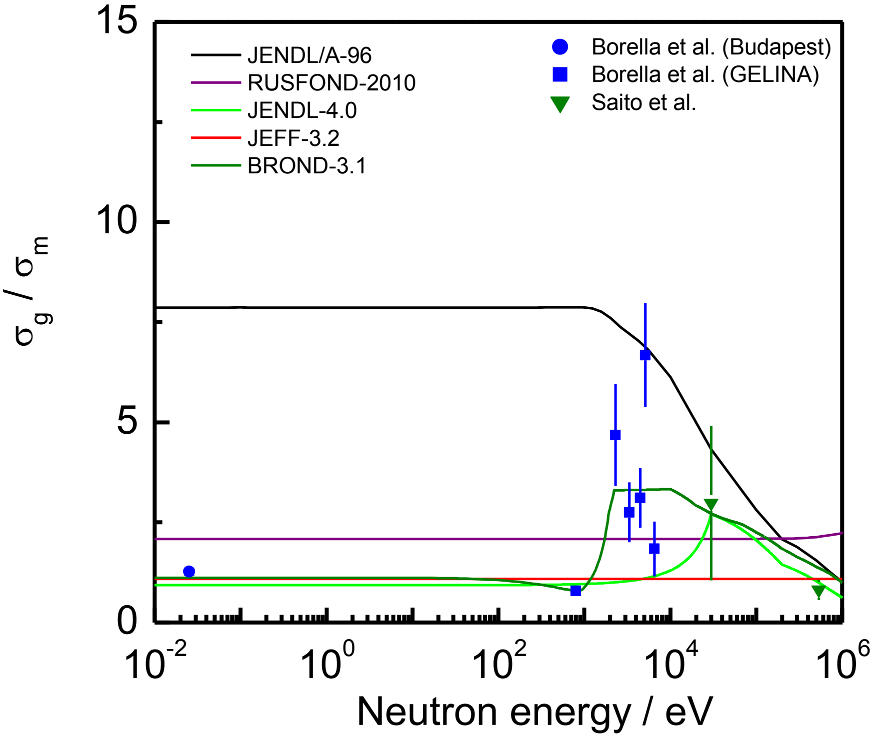

Figure 5: Comparison of the branching ratio BR = σ_g/σ_m of the capture cross section to the ground state ^{209}Bi(n,γ)^{210g}Bi and to the isomeric state ^{209}Bi(n,γ)^{210m}Bi as a function of incident neutron energy. The ratios resulting from measurements of Refs. [47]-[49] are compared with the ratios derived from the evaluated cross sections in the JENDL-4.0, JEFF-3.2, BROND-3.1, JENDL/A-96 and RUSFOND-2010 libraries.

5.5 ^{235,238}U

As discussed in section 4 there is a substantial difference between the cross sections for ^{235,238}U in CIELO-1 and CIELO-2. Therefore, the performance of these libraries was compared based on the BigTen criticality benchmark (ICSBEP identifier IMF-007). The main objective of this exercise was to verify the impact of the differences in the ^{238}U(n,γ) and ^{235}U(n,γ) cross sections between the two files. To exclude that the change in bound state parameters for CIELO-1 would influence this comparison, the impact of this change was verified using the criticality benchmark series LMT-006 from ICSBEP. This benchmark is very sensitive to cross section data in the thermal energy region. Unfortunately, an MCNP input file for this benchmark was not available. Therefore, a MCNP6 model of the benchmark was produced [50]. A dedicated library CIELO51 was created by changing only the parameters of the bound states in ENDF/B-VII.1. The results in Figure 6 illustrate that the modification of the parameters of the bound states does not causes significant differences in the calculation of the k_{eff}.

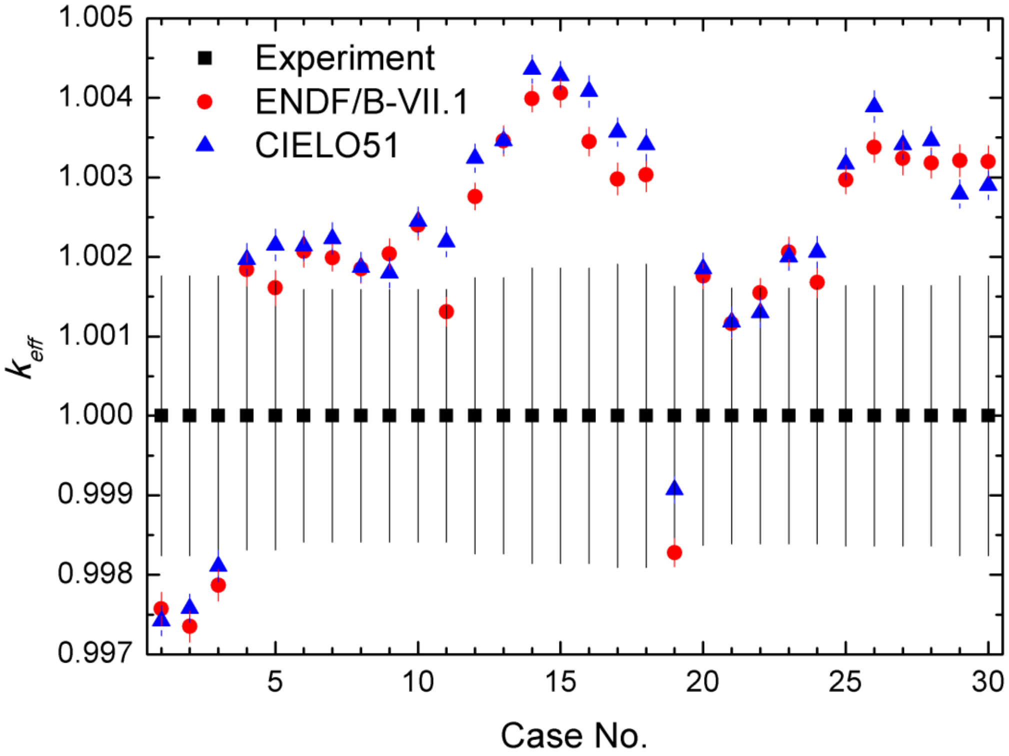

Figure 6: Comparison of the measured and calculated multiplication factor k_{eff} for different cases of the benchmark LMT-006. The calculated multiplication factors are derived with ENDF/B-VII.1 and a modified version of ENDF/B-VII.1, which is referred to as CIELO51. The latter was created to verify the effect of changing only the parameters of the bound states.

To compare the CIELO-1 and JEFF-3.3T evaluations of the main uranium nuclides ^{235,238}U, a sensitivity study was performed. The results of this study were already presented to the JEFF committee [51]. The test versions of CIELO-1 and JEFF-3.3T3, which is representative for CIELO-2, were compared for the BigTen criticality benchmark with IMF-007 as ICSBEP identifier. This benchmark is sensitive to both ^{235}U and ^{238}U in the energy region covering the RRR, URR and continuum region up to about 10 MeV. In all considered libraries the URR lies between 2.25 keV and 25 keV for ^{235}U, and between 20 keV and 149 keV for ^{238}U. The impact of specific nuclear data, i.e. cross sections and fission neutron multiplicities, was verified using the JEFF-3.2 library as a starting file. The SANDY code was used to replace specific data in a specific energy region in the starting file. The results of this exercise, presented in Figure 8, confirm the high sensitivity of this benchmark to the ^{235}U(n,γ) and ^{238}U(n,γ) cross section in the energy region above 20 keV. They also illustrate that a decrease in ^{238}U(n,γ) cross section can be compensated by an increase in ^{235}U(n,γ) cross section to approach the experimental k_{eff}.

Unfortunately, the data in Figure 8 do not provide a clear evidence to favour one of the two libraries. Nevertheless, there are several arguments in favour of the CIELO-1 library. The cross sections in the CIELO-1 library are more consistent with the neutron standards, which are the basis of the majority of energy dependent microscopic cross section data. The capture cross section in CIELO-1 is fully consistent with the experimental data of Kim et al. [34], which were determined with an uncertainty of less than 2%. The capture cross section ratio $R = \sigma_\gamma(^{238}\mathrm{U})/\sigma_\gamma(^{235}\mathrm{U})$ derived from CIELO-1 is fully consistent with the experimental value of Wallner et al. [38]. The one derived from CIELO-2 is 20% smaller. The increase in the ^{235}U(n,γ) cross section to compensate for the decrease in ^{238}U(n,γ) is also not supported by energy dependent microscopic cross section data for ^{235}U(n,γ) that are reported in the literature. This is shown in Figure 7 which compares experimental data for the ^{235}U(n,γ) cross section with the ^{235}U(n,γ) cross section in JEFF-3.2, CIELO-1 and CIELO-2. In the energy region between 30 keV and 100 keV the ^{235}U(n,γ) cross section in CIELO-2 is systematically larger than the experimental data reported in the literature. All these arguments justify the recommendation for CIELO-1, especially when neutron transport calculations are required for the development of a new system for which no dedicated integral benchmark data are available.

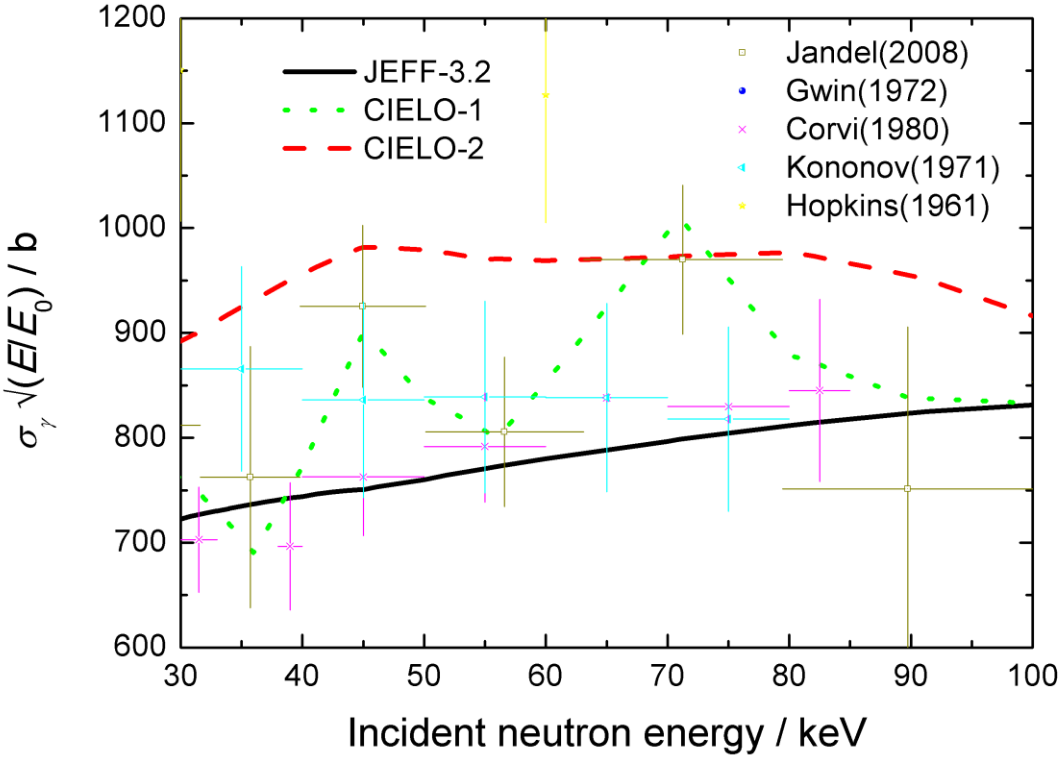

Figure 7: Comparison of the ^{235}U(n,γ) cross section, multiplied by $\sqrt{E/E_0}$, as a function of incident neutron energy E from different nuclear data libraries with energy dependent experimental data for neutron energies between 30 keV and 100 keV. The constant $E_0 = 0.253\ \mathrm{eV}$ represents the thermal energy.

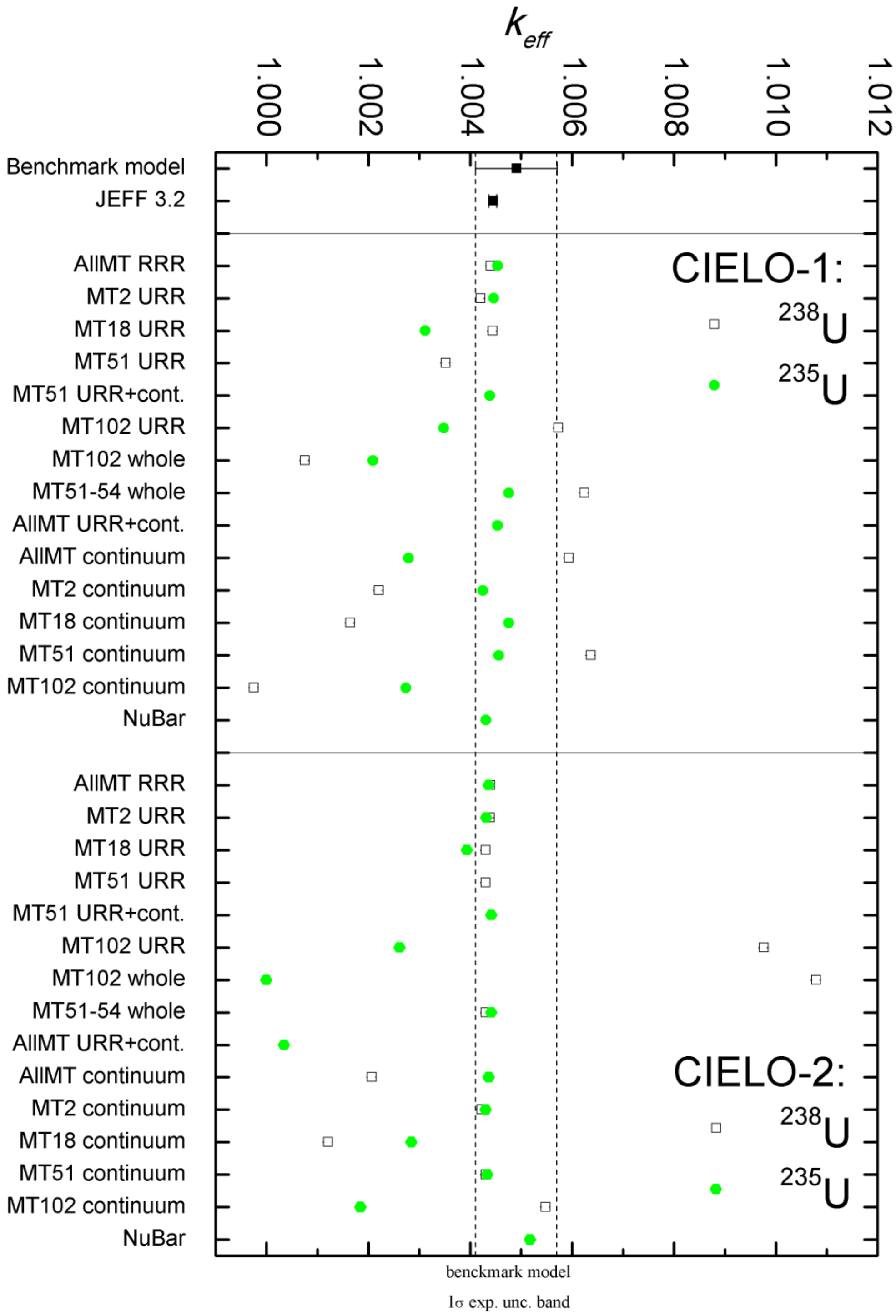

Figure 8: Comparison of the BigTen (IMF-007) multiplication factor k_{eff} calculated with different nuclear data libraries. The first two lines are the experimental value and the value calculated with the starting file (i.e. JEFF-3.2), respectively. At the top, the results obtained by substituting the JEFF-3.2 cross sections for different reactions and energy regions by the CIELO-1 cross sections, are shown. At the bottom, a similar comparison is made for CIELO-2. The standard ENDF-6 convention for neutron induced reactions is used: MT2 – elastic scattering, MT18 – fission, MT51,52, … – inelastic scattering to the first, second, … excited level, MT102 – capture. NuBar represents the fission neutron multiplicity ($\bar{\upsilon}$).

5.6 Pu nuclides

For ^{239}Pu, the nuclear data in the CIELO-1 and JEFF-3.3T4 test libraries were compared with the corresponding data in the main nuclear data libraries and with energy dependent experimental data. The JEFF-3.3T4 evaluation is representative for CIELO-2. Significant differences between the cross sections and other quantities in CIELO-1 and CIELO-2 exist, as already discussed in section 4. There are notable differences in the fission cross section σ_f and the fission neutron multiplicity $\bar{\nu}$. As an example, the fission cross section in CIELO-2 below 10 eV is higher than the one in CIELO-1 and ENDF/B-VII.1 and is also systematically higher than most energy dependent experimental data. As seen in Figure 9, this effect is most pronounced between 0.5 eV and 1 eV. The energy dependent prompt fission neutron multiplicity $\overline{\nu_p}$ in CIELO-1 is in better agreement with experimental data compared to $\overline{\nu_p}$ in CIELO-2. In addition, the CIELO-1 evaluation also adopted the fission cross section from the standards project [39]. All these arguments justify the recommendation for CIELO-1, especially when neutron transport calculations are required for the development of a new system for which no dedicated integral benchmark data are available.

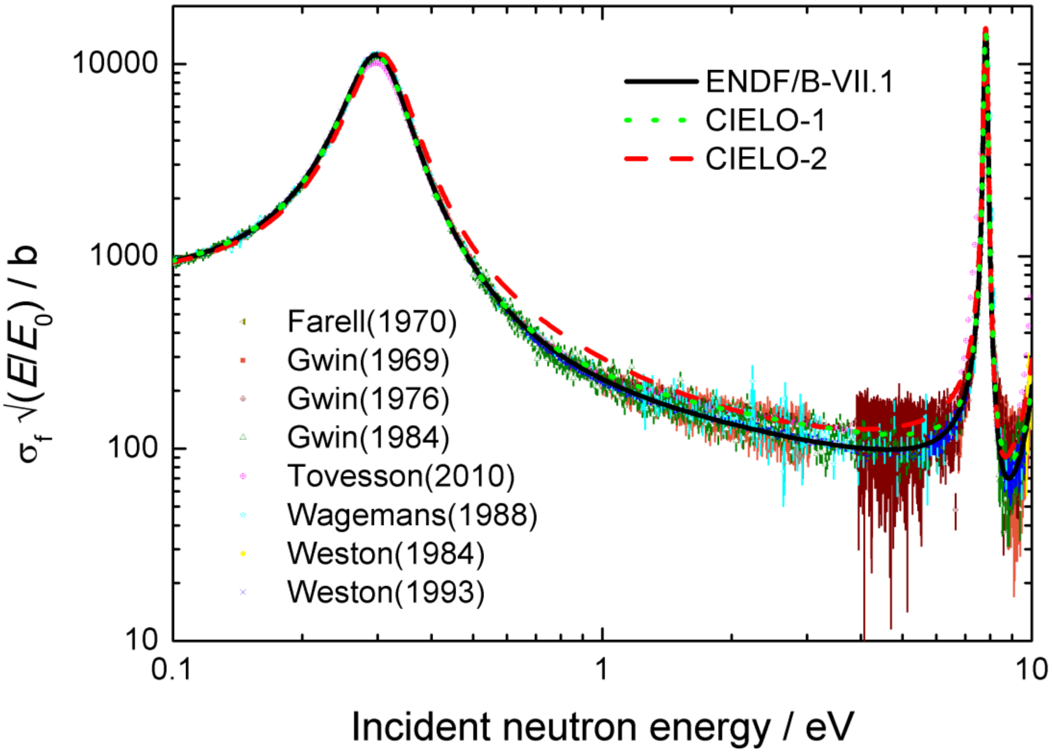

Figure 9: Comparison of the ^{239}Pu(n,f) cross section, multiplied by $\sqrt{E/E_0}$, as a function of incident neutron energy E from different evaluated nuclear data libraries and energy dependent experimental data for neutron energies between 0.1 eV and 10 eV. The constant $E_0 = 0.253\ \mathrm{eV}$ represents the thermal energy.

For other important plutonium isotopes (^{238,240,241,242}Pu), the cross sections from the fully released versions of the main nuclear data libraries were compared with available experimental data. Such a detailed exercise was not repeated with the current test libraries. However, some deficiencies in the libraries of these isotopes were revealed. A more detailed quality assessment of available evaluations is presented in the CHANDA WP10 Deliverables D10.2 [15] and D10.3 [24]. As an example, the ^{241}Pu(n,f) cross section from the current main evaluated nuclear data libraries is shown in Figure 10 in comparison with the results of the energy dependent measurement by Tovesson and Hill

[52] and with the results of the surrogate-ratio measurement by Desai et al. [53]. For the ^{241}Pu(n,f) reaction in the energy region below 1 MeV, cross sections from all current evaluated libraries are clearly too low. No recommendation is given for ^{238,240,241,242}Pu.

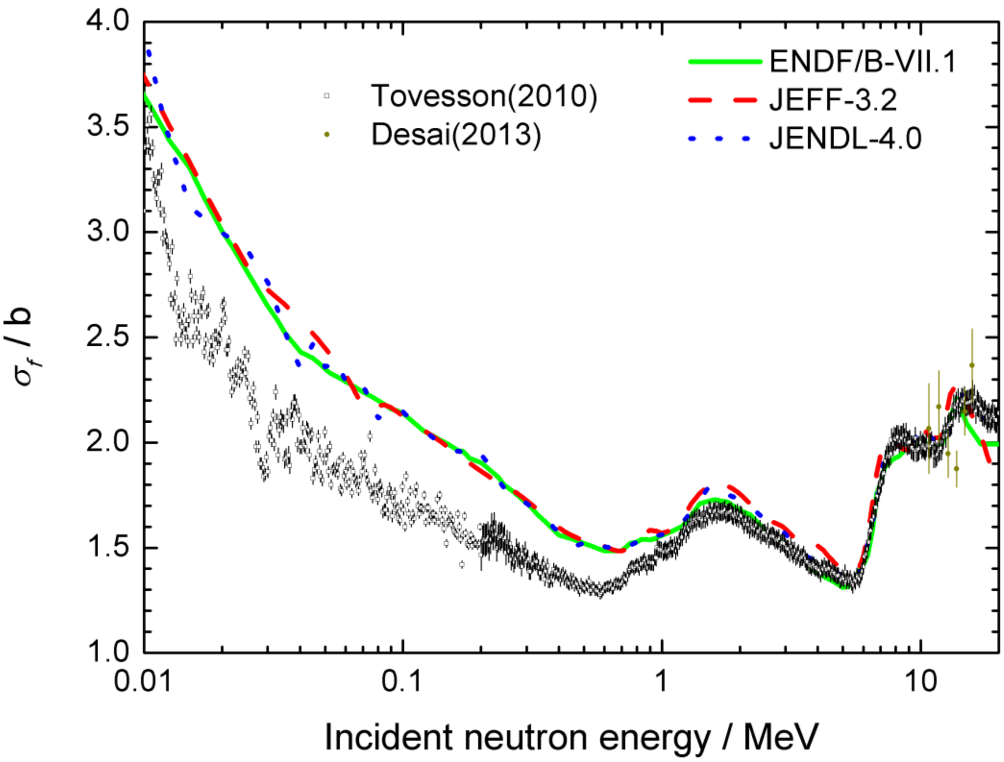

Figure 10: Comparison of the ^{241}Pu(n,f) cross section as a function of incident neutron energy from different evaluated nuclear data libraries and recent experimental data above 10 keV.

6 Conclusion

In the framework of the EC FP7 CHANDA project WP10, efforts were made to improve evaluated nuclear data relevant for the design of the MYRRHA reactor. Previously, experimental and evaluated data were compared for nuclides and quantities most important for MYRRHA. Based on the study including both energy dependent and integral quantities, recommendations to the JEFF working group are given. In some cases, the recommendations are based on work resulting from the CIELO project. Recommendations are given for ^{16}O, ^{56}Fe, ^{204,206,207,208}Pb, ^{209}Bi, ^{235,238}U and ^{239}Pu. For ^{204,206,207,208}Pb and ^{209}Bi, the JEFF-3.3T2 evaluations are recommended, except for the ^{209}Bi(n,γ) cross section branching ratio, where the BROND-3.1 evaluation is preferred. For ^{16}O, ^{56}Fe, ^{235,238}U and ^{239}Pu, the CIELO-1 evaluations are recommended.

There are several ways to further improve nuclear data. In some cases, evaluated data do not reflect the quality of the available experimental data. In such cases, new evaluations are needed. Such examples are the ^{16}O(n,α) and ^{241}Pu cross sections. For other materials, experimental data can be improved. For ^{209}Bi, new time-of-flight experiments were performed. The analysis of the results of those measurements is ongoing. Additionally, measurements for the ^{209}Bi(n,γ) cross section branching ratio to the ground state ^{210g}Bi and to the isomeric state ^{210m}Bi are needed. Finally, new time-of-flight measurements of the neutron induced capture cross section in ^{56}Fe are recommended.

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List of abbreviations and definitions

ADS	Accelerator-Driven System
BR	Branching Ratio
BROND	Russian evaluated neutron data library
CIELO	Collaborative International Evaluated Library Organization
CHANDA	solving CHAllenges in Nuclear DAta
EC	European Commission
ENDF/B	Evaluated Nuclear Data File/B-version
GELINA	Geel Electron LINear Accelerator
IAEA	International Atomic Energy Agency
ICSBEP	International Criticality Safety Benchmark Evaluation Project
JEFF	Joint Evaluated Fission and Fusion file
JENDL	Japan Evaluated Nuclear Data Library
JRC	Joint Research Centre
KENO	a multigroup Monte Carlo code, part of SCALE package
MCNP	Monte Carlo N-Particle transport code
MOX	Mixed OXide
MYRRHA	Multi-purpose hYbrid Research Reactor for High-tech Applications
NEA	Nuclear Energy Agency (of the OECD)
ORELA	Oak Ridge Electron Linear Accelerator
PARTISN	PARallel, TIme-Dependent SN transport code system
RRR	Resolved Resonance Region
RUSFOND	RUSsian File Of evaluated Neutron Data
SANDY	SAmpler of Nuclear Data and uncertaintY
SCALE	Standardized Computer Analyses for Licensing Evaluation
SCK•CEN	Belgian Nuclear Research Centre
SINBAD	Shielding INtegral Benchmark Archive and Database
SUSD3D	1-, 2-, 3-Dimensional Cross Section Sensitivity and Uncertainty Code
TENDL	TALYS-based Evaluated Nuclear Data Library
TOF	Time-Of-Flight
URR	Unresolved Resonance Region
XSUN-2013	Windows interface environment for transport and sensitivity-uncertainty software TRANSX-2, PARTISN and SUSD3D
WP10	Work Package 10

List of figures

Figure 1: Critical (left) and sub-critical (right) MYRRHA MOX core layouts, showing the positions of different types of assemblies and sub-assemblies (IPS – In-Pile test Section, SA – Sub-Assembly). 6

Figure 2: Vertical layout of the MYRRHA sub-critical MOX core model (dimensions given in cm). 6

Figure 3: Comparison of the calculated ^{103}Rh(n,n′) reaction rates (C), relative to the experimental value (E), as a function of depth of the iron shield of the ASPIS-Fe88 system. Monte Carlo calculations were performed using the ENDF/B-VII.1, CIELO-1 and JEFF-3.3T2 nuclear data libraries. 11

Figure 4: Transmission T as a function of incident neutron energy. The transmission is through an enriched ^{208}Pb sample with an areal density of 0.18594 at/b. Results of the ^{208}Pb transmission measurement from Carlton et al. (1991) are compared with transmission calculated using cross sections from the JEFF-3.2 and JEFF-3.3T1 (top) and ENDF/B-VII.1 and JENDL-4.0 (bottom) libraries. 12

Figure 5: Comparison of the branching ratio BR = σ_g/σ_m of the capture cross section to the ground state ^{209}Bi(n,γ)^{210g}Bi and to the isomeric state ^{209}Bi(n,γ)^{210m}Bi as a function of incident neutron energy. The ratios resulting from measurements of Refs. [47]-[49] are compared with the ratios derived from the evaluated cross sections in the JENDL-4.0, JEFF-3.2, BROND-3.1, JENDL/A-96 and RUSFOND-2010 libraries. 14

Figure 6: Comparison of the measured and calculated multiplication factor k_{eff} for different cases of the benchmark LMT-006. The calculated multiplication factors are derived with ENDF/B-VII.1 and a modified version of ENDF/B-VII.1, which is referred to as CIELO51. The latter was created to verify the effect of changing only the parameters of the bound states. 15

Figure 7: Comparison of the ^{235}U(n,γ) cross section, multiplied by $E/E0$, as a function of incident neutron energy E from different nuclear data libraries with energy dependent experimental data for neutron energies between 30 keV and 100 keV. The constant $E0 = 0.253\ \mathrm{eV}$ represents the thermal energy. 16

Figure 8: Comparison of the BigTen (IMF-007) multiplication factor k_{eff} calculated with different nuclear data libraries. The first two lines are the experimental value and the value calculated with the starting file (i.e. JEFF-3.2), respectively. At the top, the results obtained by substituting the JEFF-3.2 cross sections for different reactions and energy regions by the CIELO-1 cross sections, are shown. At the bottom, a similar comparison is made for CIELO-2. The standard ENDF-6 convention for neutron induced reactions is used: MT2 – elastic scattering, MT18 – fission, MT51,52, … – inelastic scattering to the first, second, … excited level, MT102 – capture. NuBar represents the fission neutron multiplicity (υ). 17

Figure 9: Comparison of the ^{239}Pu(n,f) cross section, multiplied by $E/E0$, as a function of incident neutron energy E from different evaluated nuclear data libraries and energy dependent experimental data for neutron energies between 0.1 eV and 10 eV. The constant $E0 = 0.253\ \mathrm{eV}$ represents the thermal energy. 18

Figure 10: Comparison of the ^{241}Pu(n,f) cross section as a function of incident neutron energy from different evaluated nuclear data libraries and recent experimental data above 10 keV. 19

List of tables

Table 1: List of nuclides, quantities and reactions, most relevant for MYRRHA: σ denotes the reaction cross section, ν the fission neutron multiplicity and χ the fission neutron spectrum. 7

KJ-NA-28957-EN-N

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Publications Office

doi:10.2760/485552

ISBN 978-92-79-77162-0