Use of integral experiments for the assessment of the ^{235}U capture cross section within the CIELO Project

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Abstract. A new ^{235}U capture cross-section evaluation, evaluated by ORNL and the CEA Bruyères-le-Châtel (BRC) has been proposed within the CIELO project. IRSN, who participates in the CIELO project, contributes with data testing and has carried out benchmark calculations using few benchmarks, extracted from the ICSBEP database, for testing the new ^{235}U evaluation. The benchmarks have been selected by privileging the experiments showing small experimental uncertainties and a significant sensitivity to ^{235}U capture cross-section. The k_{eff} calculations were performed with both the MCNP 6 code and the 5.C.1 release of the MORET 5 code, using the ENDF/B-VII.1 library for all isotopes except ^{235}U , for which both the ENDF/B-VII.1 and the new ^{235}U evaluation was used. The benchmark selection allowed highlighting a significant effect on k_{eff} of the new ^{235}U capture cross-section. The results of this data testing, provided as input for the evaluators, are presented here.

1 Introduction

The *Collaborative International Evaluated Library Organization* Pilot Project, known as the CIELO project, is an initiative aimed at improving data evaluation by combining efforts from several institutions around the world. Over the last couple of years, evaluation work has been done to improve data evaluation for six isotopes, namely ^1H , ^{16}O , ^{56}Fe , $^{235-238}\text{U}$, and ^{239}Pu . The Working Party on International Nuclear Data Evaluation Co-operation (WPEC) subgroup 29 (SG 29) was established to investigate an issue with the ^{235}U capture cross-section in the energy range from 0.1 to 2.25 keV.¹ The WPEC criticality calculation results indicated an overestimation of the ^{235}U capture cross-section of 10 % or more, starting around 100 eV. To understand and solve the problem, recommendation was made to perform new capture cross-section measurements followed by a resonance evaluation. Hence, time-of-flight capture cross-section measurements were done at the Rensselaer Polytechnic Institute (RPI)² and at the Los Alamos National Laboratory (LANL).³ Integral quantities, such as fission and capture resonance integral Westcott factors were also included in the evaluation. These new measurements were used together with the SAMMY computer code, developed by ORNL, to re-evaluate the ^{235}U resonance parameters in the energy range from thermal to 2.25 keV. The CEA/Bruyères-le-Châtel (BRC) was responsible to re-evaluate the ^{235}U resonance parameters in the fast energy region.

The Institut de Radioprotection et de Sûreté Nucléaire (IRSN) has carried out benchmark calculations, using few benchmarks extracted from the International Criticality Safety Benchmark Evaluation

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Project (ICSBEF) Handbook, 4 for testing the new ^{235}U capture cross-section evaluation over the whole energy range. The impact of the inclusion of the new evaluation was studied for selected critical benchmarks that give, when combining experiments, a sensitivity coverage to ^{235}U capture cross-section in each of the thermal, epithermal and fast energy range. The benchmark calculations, used to investigate the impact of the new ^{235}U evaluation, were performed using Monte-Carlo methods.

Table 1. Benchmarks integral sensitivities to the ^{235}U capture cross-section.

Series of experiments	Benchmark k_{eff}	Benchmark k_{eff} uncertainty	k_{eff} sensitivity ^{235}U capt. < 0.625 eV	k_{eff} sensitivity 0.625 eV < ^{235}U capt. < 100 keV	k_{eff} sensitivity ^{235}U capt. > 100 keV	k_{eff} sensitivity ^{235}U capt. total
HEU-SOL-THERM-004-006	1.00000	0.00590	-10.76%	-6.03%	-0.04%	-16.82%
HEU-SOL-THERM-049-012	1.00120	0.00210	-8.72%	-8.67%	-0.14%	-17.53%
HEU-SOL-THERM-004-003	1.00000	0.00390	-7.14%	-13.91%	-0.16%	-21.21%
HEU-SOL-INTER-001-001	1.00000	0.00330	-5.33%	-15.73%	-0.34%	-21.40%
HEU-COMP-INTER-004	1.00000	0.00400	-0.25%	-16.01%	-0.31%	-16.56%
HEU-MET-INTER-007-031	0.99960	0.00220	-2.20%	-12.77%	-1.42%	-16.39%
HEU-MET-FAST-007-010	0.99810	0.00120	-0.77%	-9.64%	-2.07%	-12.48%
HEU-MET-FAST-042-002	0.99960	0.00090	-0.01%	-7.47%	-2.86%	-10.34%
HEU-MET-FAST-038-001	0.99990	0.00070	-0.01%	-6.31%	-3.00%	-9.31%
HEU-MET-FAST-070-003	1.00130	0.00130	-0.22%	-6.57%	-3.43%	-10.22%
HEU-MET-INTER-006-002	1.00010	0.00080	N.A	N.A	N.A	N.A
HEU-MET-INTER-001-001	0.99660	0.00260	N.A	N.A	N.A	N.A
IEU-MET-FAST-007-001	1.00460	0.00020	0.00%	-1.82%	-2.97%	-4.79%
HEU-MET-FAST-007-032	0.99410	0.00120	0.00%	-1.09%	-3.51%	-4.60%
HEU-MET-FAST-001-001	1.00000	0.00100	0.00%	-0.78%	-3.19%	-3.97%

2 Benchmark selection

2.1 Description of the method based on sensitivities

The DICE database, associated with the ICSBEF Handbook, was used to select the experiments sensitive to the ^{235}U capture. The available integral sensitivities, mainly calculated with the TSUNAMI-3D module of SCALE, were extracted from the database in each of the thermal ($E < 0.625$ eV), epithermal ($0.625 \text{ eV} < E < 100 \text{ keV}$), and fast ($E > 100 \text{ keV}$) energy ranges, for both the ^{235}U capture cross-section and the ^{235}U fission cross-section, which is considered as the main background. The selection was based on several criteria: experiments showing too high uncertainty in the measured k_{eff} were discarded and, when possible, benchmarks showing the highest possible integral sensitivity to ^{235}U capture in each of the energy ranges and, at the same time, the lowest background cross-sections (^{235}U fission cross-section, H, O, .. etc.) sensitivity, have been selected. Table 1 shows the integral sensitivities to the ^{235}U capture cross-section in each energy range, as well as the total integral sensitivity to the ^{235}U capture, for the selected benchmarks. The DICE 2014 data also provide with the differential sensitivities of benchmarks to the different parameters as for instance nuclide, type of cross-section, etc. Figure 1 shows the sensitivity of k_{eff} to the ^{235}U capture and to the ^{235}U fission cross-section for the six most sensitive benchmarks (HST-004-006, HST-049-012, HCI-004, HMI-006-002, HMI-001 and HMF-007-032) among the selection.

2.2 Benchmark description

The experiments available in the ICSBEP Handbook are categorized by fissile media: Highly (HEU), Intermediate (IEU), or Low Enriched (LEU) Uranium; physical form of the fissile material (metal, solution and miscellaneous systems); and neutron energy range where the majority of the fissions occur (fast, intermediate, thermal spectra systems). The description of the selected benchmarks is presented in Table 2.

Figure 1. Sensitivity of k_{eff} to the ^{235}U capture (left) and to the ^{235}U fission (right) cross-section for the six most sensitive benchmarks, computed with the MORET 5 Monte Carlo code.

Table 2. Selected benchmarks description.

HEU-SOL-THERM-004-(003 and 006)	UO ₂ F ₂ solution – U (93.6% ²³⁵ U) – Spherical tank – Heavy water reflection
HEU-SOL-THERM-049-012	Uranyl Nitrate solution – U (85% ²³⁵ U) – Spherical tank – Water reflection
HEU-SOL-INTER-001-001	UO ₂ F ₂ solution – U (93.6% ²³⁵ U) – Spherical tank – Heavy water reflection
HEU-COMP-INTER-004-001 (HECTOR)	Uranium/Boron/Graphite powder – U (92% ²³⁵ U)
HEU-MET-INTER-007-031	Metallic Uranium plates (93.15% ²³⁵ U) – Polyethylene moderated – No reflection
HEU-MET-FAST-007-(010 and 032)	Metallic Uranium plates (93.15% ²³⁵ U) – Polyethylene (010), Teflon (032) moderated – No reflection
HEU-MET-FAST-042-002	Heterogeneous HEU cylinder – Vanadium diluted and Beryllium Oxide moderated
HEU-MET-FAST-038-001	Heterogeneous cylindrical assembly – (96% ²³⁵ U), Beryllium and Beryllium Oxide disks – Depleted Uranium reflection
HEU-MET-FAST-070-003	Highly enriched Uranium, Tungsten, Aluminum Oxide plates – U (93% ²³⁵ U) – Al ₂ O ₃ reflected
HEU-MET-INTER-006-002 (ZEUS-002)	Cylindrical disks assemblies – metallic U (96% ²³⁵ U) – Graphite moderated and Cu reflected
HEU-MET-INTER-001-001	Uranium/Iron cylinder – U (93% ²³⁵ U) – Stainless steel reflected
IEU-MET-FAST-007-001 (BIGTEN)	Uranium (10% ²³⁵ U) cylinders reflected by 15 cm depleted Uranium
HEU-MET-FAST-001-001 (GODIVA)	Metallic Uranium sphere Godiva – U (93.7% ²³⁵ U) – No reflection

3 Results

The impact of the new preliminary ^{235}U resonance evaluation in benchmark calculations was investigated using the identified benchmarks listed in the ICSBEP compilation. The new set of ^{235}U resonance parameters was converted into the ENDF format and, for testing purpose, included in the ENDF/B-VII.1 ^{235}U library, where it replaced the existing ENDF/B-VII.1 resonance parameters. The new ^{235}U -v4 library, also labelled “u235o4brc2”, was processed with the GAIA-NJOY 99 5 code to generate MCNP formatted cross-section. The k_{eff} calculations were performed, for the selected benchmarks, with both the MCNP 6 6 code and the 5.C.1 release of the MORET 5 7 code, using the ENDF/B-VII.1. In addition, k_{eff} calculations were also performed using ENDF/B-VII.1, together with the new ^{235}U evaluation. The MCNP and the MORET 5 k_{eff} results, obtained using the ENDF/B-VII.1 library, are shown in Figure 2, and compared to the benchmark k_{eff} . Except for a few cases, the calculation results are overall in good agreement with the experimental results, within the 3σ experimental uncertainty. The MCNP and MORET results are in good agreement, within 60 pcm (1 pcm = 10^{-5}), with a Monte-Carlo standard deviation of 10 pcm with the MORET code and varying from 5 to 25 pcm with the MCNP results.

Figure 2. k_{eff} results obtained with MCNP 6 (purple) and MORET 5 (red), using ENDF/B-VII.1 library, together with the benchmark k_{eff} (experimental uncertainty in 3σ).

The C/E results, obtained with MORET 5, using the ENDF/B-VII.1 library, together with the new ^{235}U evaluation, are shown in Figure 3. The results of the new ^{235}U cross-section evaluation highlight a discrepancy compared to the previous evaluation results. It varies, as expected, as a function of the ratio in sensitivity ^{235}U capture/background reactions and according to the benchmarks characteristics (composition, energy spectrum, uranium enrichment, etc...). The impact of the new ^{235}U evaluation varies from about +370 pcm (HST-049-012) to about -1000 pcm (BIGTEN) for all the selected benchmarks. For the BIGTEN benchmark, which is an intermediate-enriched uranium benchmark with fast spectrum containing a large amount of ^{238}U , the new evaluation leads to a significant under-prediction of about 1000 pcm, whereas the previous one showed a good C/E. This phenomenon is due to compensations effects and the fact that ^{238}U and ^{235}U cross-sections are correlated, and highlights

the fact that it would be necessary to re-evaluate ^{238}U together with ^{235}U . One can notice that, for the benchmarks sensitive to the intermediate energy range (HMF-038-001, HMF-070-003 and HMI-001), the k_{eff} tends to decrease compared to the old evaluation result and a trend in the C/E results can be observed. The impact of the new evaluation is smaller in the fast energy region (HMF-007-032 and GODIVA), except for BIGTEN, which involves intermediate-enriched uranium. Nevertheless, the benchmark selection allowed highlighting a significant effect on k_{eff} of the new ^{235}U capture cross-section, and the C/E results stay overall in good agreement, with, in some cases, a small improvement. It should be noted however that the results could be impacted by the nuclear data of other materials present in the ENDF/B-VII library. The C/E trend observed here may not be the same, if the ^{235}U evaluation is used with other cross section libraries for the other nuclides. Analysis work is ongoing to extract a tendency of the C/E results, which is important for the evaluation improvement.

Figure 3. C/E results obtained with MORET 5 using ENDF/B-VII.1 library, for the ENDF/B-VII.1 ^{235}U (red) and the new ^{235}U -v4 (blue).

4 Conclusion

IRSN and ORNL have been working in collaboration with the CEA/BRC to produce a complete evaluation for ^{235}U . Under reserve of data testing and validation, the evaluation will be made available for possible inclusion in the Joint European Fusion and Fission (JEFF) cross-section library. IRSN, which is involved in the CIELO project in the data testing, especially for the new ^{235}U capture cross-section, has carried out key critical benchmarks selection, regarding the sensitivities to the ^{235}U capture cross-section, in each of the energy ranges, and performed MCNP and MORET calculations for the selected benchmarks, using the new evaluation. The benchmark selection allowed highlighting a significant effect on k_{eff} and C/E results with the new ^{235}U evaluation.

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