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Use of integral experiments for the assessment of a new ^{235}U IRSN-CEA evaluation

Raphaëlle Ichou[1,a], Nicolas Leclaire[1], Luiz Leal[1], Wim Haeck[1], Benjamin Morillon[2], Pascal Romain[2], and Helder Duarte[2]

[1] IRSN, PSN-EXP/SNC/LNR-LNC, 92250 Fontenay-aux-Roses, France
[2] CEA DAM, DIF, 91297 Arpajon, France

Abstract. 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, due to a possible overestimation of 10% or more. To improve the ^{235}U capture crosssection, a new ^{235}U evaluation has been proposed by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) and the CEA, mainly based on new time-of-flight ^{235}U capture cross-section measurements and recent fission cross-section measurements performed at the n_TOF facility from CERN. IRSN and CEA Cadarache were in charge of the thermal to 2.25 keV energy range, whereas the CEA DIF was responsible of the high energy region. Integral experiments showing a strong ^{235}U sensitivity are used to assess the new evaluation, using Monte-Carlo methods. The k_{eff} calculations were performed with the 5.D.1 beta version of the MORET 5 code, using the JEFF-3.2 library and the new ^{235}U evaluation, as well as the JEFF-3.3T1 library in which the new ^{235}U has been included. The benchmark selection allowed highlighting a significant improvement on k_{eff} due to the new ^{235}U evaluation. The results of this data testing 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 ^{1}H, ^{16}O, ^{56}Fe, $^{235-238}$U, and ^{239}Pu. The Working Party on International Nuclear Data Evaluation Co-operation SG 29 was established to investigate an issue with the ^{235}U capture cross-section in the energy range from 0.1 keV 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]. Furthermore, recent fission cross-section measurements have been performed at the n_TOF facility from CERN [4], which provided strong support to the fission standard values. Indeed, the normalization of these experimental data in the [7.8–11] eV energy range supported the standard value in this energy region and also reinforced the standard averaged fission cross-section values in the resonance region. These new measurements were used together with the SAMMY [5] computer code, developed by ORNL, to re-evaluate the capture and fission ^{235}U resonance parameters in the energy range from thermal to 2.25 keV. Integral quantities, such as fission and capture resonance integral and Westcott factors were also included in the evaluation. The CEA DIF was in charge of the evaluation at high energy and recommendations done by the CIELO organization [6,7] concerning the ^{235}U PFNS (prompt fission neutron spectrum) among others, were followed. Finally, a common IRSN-CEA evaluation called "u235_irsncea_1" was released. IRSN has carried out benchmark calculations, using few-selected benchmarks extracted from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [8] for testing the new ^{235}U evaluation over the whole energy range. The impact of the inclusion of the new evaluation was studied for selected critical benchmarks sensitive to the ^{235}U capture cross-section in the thermal, epithermal and fast energy ranges. The benchmark calculations were performed using Monte-Carlo codes.

2. Benchmark selection

The DICE database, associated with the ICSBEP Handbook, was used to select the experiments sensitive to ^{235}U cross-sections. The available integral sensitivities, mainly calculated with the TSUNAMI-3D module of SCALE, were extracted from the database in the thermal ($E < 0.625$ eV), epithermal ($0.625\ \text{eV} < E < 100$ keV), and fast ($E > 100$ keV) energy ranges, for both the ^{235}U capture and fission cross-sections. Experiments showing too high measurement uncertainty were discarded. When possible, benchmarks showing the highest integral sensitivity to ^{235}U capture have been selected with the smallest value for the sensitivity to the other isotopes (H, O,..etc) cross-sections to focus on ^{235}U capture. Table 1 shows the integral sensitivities

[a] e-mail: raphaelle.ichou@irsn.fr

Table 1. Integral sensitivity of k_{eff} to ^{235}U capture and fission cross-sections.

	EALF (eV)	^{235}U capture	^{235}U fission
HST-004-006	2.00E-01	−16.8%	26.3%
HST-049-012	6.22E-01	−17.5%	31.8%
HST-004-003	2.77E+00	−21.2%	29.4%
HSI-001-001	1.38E+01	−21.4%	32.2%
HECTOR	1.41E+02	−16.6%	65.2%
HMI-007-031	1.41E+03	−16.4%	42.4%
ZEUS-001	4.94E+03	−18.5%	45.8%
ZEUS-002	9.71E+03	−17.4%	47.1%
HMF-007-010	2.24E+04	−12.5%	51,1%
ZEUS-003	2.32E+04	−15.7%	48.6%
HMI-001-001	2.95E+04	−13.2%	55.7%
HMF-070-003	5.29E+04	−10.2%	57.6%
ZEUS-004	7.74E+04	−12.4%	51.8%
HMF-038-001	2.03E+05	−9.3%	52.3%
BIGTEN	4.19E+05	−4.8%	49.7%
HMF-007-032	7.01E+05	−4.6%	62.9%
GODIVA	7.93E+05	−4.0%	64.4%
FLATTOP	8.38E+05	−4.8%	57.6%

of k_{eff} to the ^{235}U capture and fission cross-sections, for the selected benchmarks. The selection covers a large range of experiments characteristics available in the ICSBEP Handbook: Highly (HEU) and Intermediate (IEU) Enriched Uranium benchmarks, for different systems (metal and solution) and neutron energy range where the majority of the fissions occur (fast, intermediate, thermal spectra systems). The selection is ordered according to their EALF value.

3. Results

3.1. JEFF-3.2 library

The impact of the new preliminary ^{235}U resonance evaluation in benchmark calculations was investigated using the selected benchmarks. The new set of ^{235}U resonance parameters was converted into the ENDF format and included in the JEFF-3.2 ^{235}U library, where it replaced the existing JEFF-3.2 resonance parameters. The new ^{235}U library was processed with the GAIA 1.1 code [9] (using NJOY 99 [10]) to generate MCNP formatted cross-section. The k_{eff} calculations were performed, for the selected benchmarks, with the 5.D.1 beta version of the MORET 5 [11] code, using JEFF-3.2. In addition, k_{eff} calculations were performed using JEFF3.2, together with the new ^{235}U evaluation. The MORET 5 k_{eff} results, obtained using JEFF-3.2 library, together with the k_{eff} results obtained for the new ^{235}U version in JEFF-3.2, are shown in Fig. 1, and compared to the benchmark k_{eff} values.

The results of the new ^{235}U cross-section evaluation highlight a clear difference compared to JEFF-3.2 results, depending on the sensitivity to ^{235}U capture and according to the benchmarks characteristics (composition, energy spectrum, uranium enrichment, etc.). Except for a few cases, the new ^{235}U evaluation tends to improve the results. The calculation results tend to get closer to the experimental points inside the 3σ experimental uncertainty using the modified ^{235}U. The impact of the new ^{235}U evaluation varies from −1100 pcm (HMF-070-003)

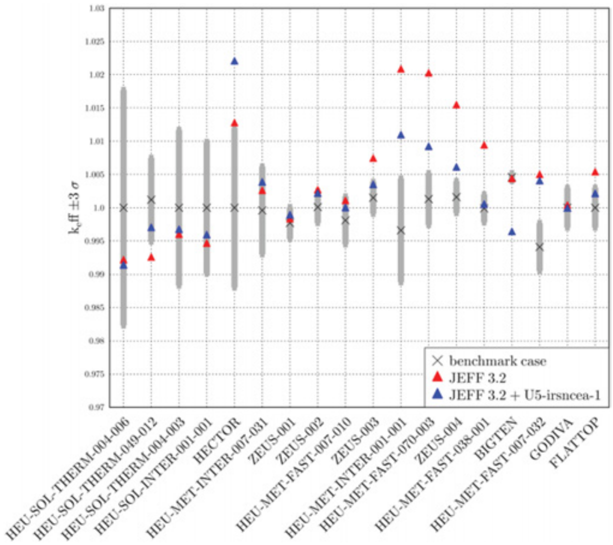

Figure 1. k_{eff} results obtained with MORET 5 using JEFF-3.2 library (red), and using JEFF3.2 library with new ^{235}U evaluation (blue), together with the benchmark k_{eff} (experimental uncertainty in 3σ).

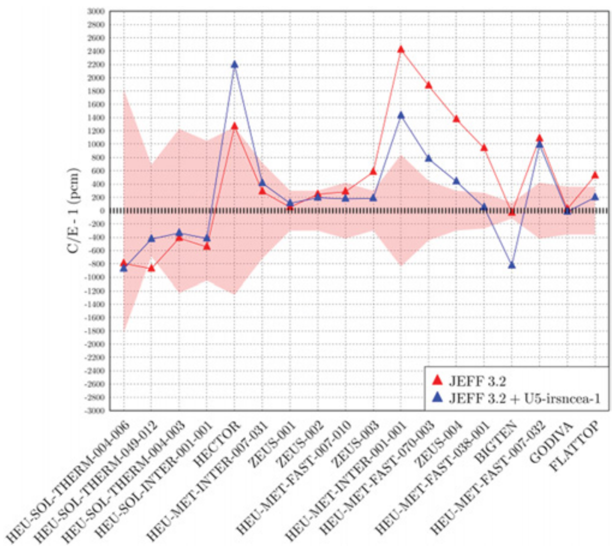

Figure 2. C/E results obtained with MORET 5 using full JEFF3.2 library (red), and using JEFF-3.2 library with new ^{235}U evaluation (blue), with the C/E uncertainty in 3σ (red band).

to about +900 pcm (HECTOR) for all the selected benchmarks.

The C/E results, obtained with MORET 5, using full JEFF-3.2 library together with the new ^{235}U evaluation are shown in Fig. 2. The JEFF-3.2 C/E results (in red) for solutions sensitive to the thermal energy range are rather low but in a good agreement, within the 3σ uncertainty. But for cases sensitive to higher energies, the results are mainly overestimated. The C/E results, except for a few cases, are located at a upper limit of the uncertainty range or even higher. The two exceptions are BIGTEN and GODIVA results which perfectly match the experimental data with the JEFF-3.2 library. The C/E results obtained with the new ^{235}U in a JEFF-3.2 environment tend to be on average improved, compared to the full JEFF-3.2 results, especially in the intermediate energy range where a bias reduction is observed. For the benchmarks

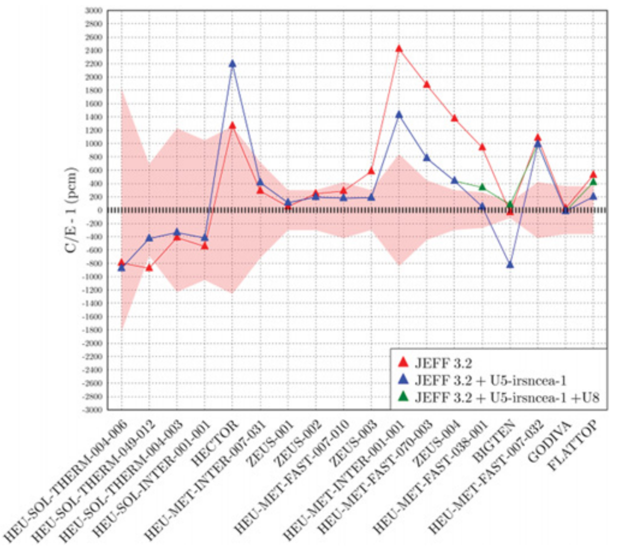

Figure 3. C/E results obtained with MORET 5 using full JEFF3.2 library (red), JEFF-3.2 library with new ^{235}U (blue), and with both new ^{235}U and ^{238}U (green) evaluations.

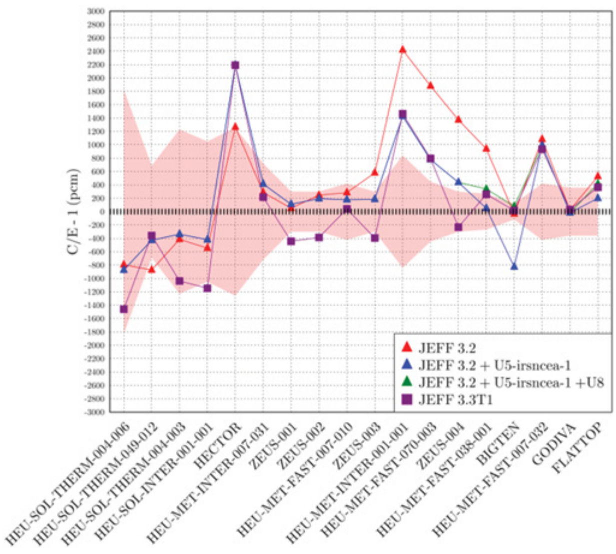

Figure 4. C/E results obtained with MORET 5 using full JEFF3.2 library (red), JEFF-3.2 library with new ^{235}U (blue) and with both new ^{235}U and ^{238}U (green), and with the full JEFF3.3T1 results (purple).

sensitive to the thermal energy range, the k_{eff} results, which were a bit underestimated with JEFF-3.2, are increased and the C/E results are improved. Concerning the benchmarks sensitive to the intermediate and fast energy ranges, the averaged C/E tends to be decreased, so that the agreement becomes better. The k_{eff} values of the ZEUS cases, for which the new ^{235}U resonance parameters have a strong impact in the intermediate energy range, become in good agreement and show a clear bias reduction. However, there remain some cases for which the C/E is improved but still stand outside or at the limit of the experimental uncertainty range: the HMF-070-003 and HMI-001 benchmarks. The HMI-001 benchmark, which is a ^{235}U (93%)/Fe cylinder reflected by stainless steel, sensitive to iron and aluminium, still shows a C/E result well above the uncertainty range. This could indicate that there could be a problem for iron and aluminium evaluations. The two exceptions, where the C/E gets worse, are the HECTOR and BIGTEN cases. The HECTOR experiment, which is an homogeneous fuel mixture of uranium oxide (92% enriched ^{235}U) and graphite, is very sensitive to graphite. This could be an indication that a more detailed study is necessary to understand the HECTOR benchmark results. For BIGTEN, which is an intermediate-enriched uranium benchmark with fast spectrum containing a large amount of ^{238}U, the new file leads to a strong decrease of 700 pcm, whereas JEFF-3.2 showed an excellent C/E result. In this case, including the new ^{238}U evaluation, proposed by CEA and IRMM, together with the new ^{235}U, is relevant. The C/E results obtained using JEFF3.2 library, together with the new ^{235}U and ^{238}U evaluations are shown in Fig. 3 and compared to the previous results. The new BIGTEN result, using both ^{235}U and ^{238}U resonance parameters, perfectly matches the experimental data. This points out the importance of evaluating the isotopes all together as they are strongly affected by each other.

Finally, the C/E results obtained with the new modified ^{235}U in a JEFF-3.2 environment, are overall in good agreement, and clearly tend to improve the results. The results tend to be even more improved when using the new ^{238}U evaluation. These results indicated that the new evaluations seemed to be going in the right direction. Consequently, both the new ^{235}U and ^{238}U evaluations were included in the JEFF-3.3T1 library.

3.2. JEFF-3.3T1 library

In order to evaluate the impact of these new ^{235}U and ^{238}U resonance parameters inclusion in JEFF-3.3T1 library, IRSN has performed data testing using JEFF3.3T1 library. The full JEFF-3.3T1 library was processed with GAIA 1.1 and the k_{eff} calculations were performed for the same benchmark selection with the 5.D.1 beta version of the MORET 5 [11] code. The C/E results obtained using full JEFF-3.3T1 library are shown in Fig. 4. The results clearly indicate a discrepancy compared to full JEFF-3.2 results with a strong improvement in the intermediate energy range. Regarding the considerable amount of modified isotopes between JEFF-3.2 and JEFF-3.3T1 libraries, it is not clear how to achieve a final conclusion. However, these modified files tend to either unchange or decrease the k_{eff} compared to the results using the new ^{235}U added in JEFF-3.2. The most notable results are the ZEUS cases whose k_{eff} values are clearly decreased and fall nearby the 3σ uncertainty. The ZEUS benchmark is a graphite moderated and Cu reflected assembly, very sensitive to Cu that has been modified between JEFF-3.2 and JEFF3.3T1, which can explain the new ZEUS results. It could also be explained by the new carbon graphite in JEFF-3.3T1 coming from JENDL4 library. The HECTOR benchmark is neither improved. Nevertheless, JEFF-3.3T1 results are showing an averaged improvement for the selected benchmarks compared to JEFF-3.2 and work is going on to understand and improve the results.

3.3. k_{eff} contributions

In order to explain the impact of the new evaluations on the benchmark k_{eff} results, especially the impact of

Table 2. k_{eff} reaction rates contributions (in reaction/s) using JEFF-3.2 library for the FLATTOP case.

	P	**A**	**Fission**	**Capture**
JEFF-3.2 k_{eff} =1.0050 ± 9 pcm	1.786E-05	8.037E-06	7.007E-06	9.737E-07
JEFF-3.2 +U235 k_{eff} = 1.0026 ± 9 pcm	1.787E-05	8.053E-06	6.975E-06	1.034E-06
JEFF-3.2 +U235 +U238 k_{eff} =1.0041 ± 9 pcm	1.786E-05	8.051E-06	6.972E-06	1.036E-06

the different isotopes and reaction cross-sections, it is interesting to look more into detail at each component of the k_{eff}calculation. Here is presented an example of the reaction rates calculation in a few energy bins for the FLATTOP benchmark, using JEFF-3.2 library and adding the new ^{235}U and ^{238}U evaluations.

The k_{eff} definition can be written as:

$$k_{\text{eff}} = \frac{P}{A+L} \tag{1}$$

with:
P = Production, A = Absorption, L = Leakage
And if the leakage term is neglected:

$$k_{\infty} = \frac{P}{A} \tag{2}$$

with:

$$P = \tau_{Production} = \int \nu \Sigma_{fission}(E)\,\Phi(E)\,dE \tag{3}$$

$$A = \tau_{Absorption} = \int \Sigma_{Absorption}(E)\,\Phi(E)\,dE \tag{4}$$

And the macroscopic absorption cross section is:

$$\Sigma_{Absorption} = \Sigma_{fission} + \Sigma_{(n,2n)} + \Sigma_{(n,3n)} + \Sigma_{(n,\gamma)} \tag{5}$$

Table 2 shows the integrated reaction rates over all energy bins for the FLATTOP benchmark, obtained using MCNP6 [12] and both full JEFF-3.2, JEFF-3.2 with new ^{235}U and with both new ^{235}U and ^{238}U. It emphasizes the fact that a small variation of a reaction rate has a strong impact on k_{eff}. Using the new ^{235}U in JEFF-3.2 increases the total capture rate of around 6% and decreases the fission rate by 0.5%; this affects the k_{eff} by a decrease of around 250 pcm. When adding the new ^{238}U file, production and absorption rates are almost unchanged but k_{eff} value is increased by around 150 pcm. The indicated changes may be related to the leakage term in connection with the ^{238}U (elastic and inelastic) scattering cross-section.

4. Conclusions

IRSN and CEA have produced a new evaluation for ^{235}U in the thermal to fast energy range. IRSN, which is involved in the data testing, has carried out key critical benchmarks selection, regarding the sensitivities to the ^{235}U cross-section. MORET calculations have been performed for the selected benchmarks, using new evaluation in JEFF-3.2 library. The benchmark selection allowed highlighting a significant effect on k_{eff} and on C/E results, with an observed improvement when using the new ^{235}U resonance parameters compared to full JEFF-3.2. An even better improvement with the new resonance parameters ^{238}U has been noted. The new ^{235}U evaluation was made available for inclusion in the JEFF cross-section library and has been included in the JEFF3.3T1 version. A collaboration work between IRSN, CEA Cadarache and CEA DIF is ongoing to keep improving the results via benchmark testing.

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