

Critical review of CIELO evaluations of $n + {}^{235}\text{U}$, ${}^{238}\text{U}$ using differential experiments

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Abstract. Key reactions have been selected to compare JEFF-3.3 (CIELO 2) and IAEA CIELO (CIELO 1) evaluated nuclear data files for neutron induced reactions on ${}^{235}\text{U}$ and ${}^{238}\text{U}$ targets. IAEA CIELO evaluation uses reaction models to construct the evaluation prior, but strongly relied on differential data including all reaction cross sections fitted within the IAEA Neutron Standards project. The JEFF-3.3 evaluation relied on a mix of differential and integral data with strong contribution from nuclear reaction modelling. Differences in evaluations are discussed; a better reproduction of differential data for the IAEA CIELO evaluation is shown for key reaction channels.

1 Introduction

An international collaboration called CIELO (Collaborative International Evaluated Library Organisation) was initiated by the Nuclear Energy Agency of the OECD with the main goal to improve our understanding of neutron reactions on key isotopes that are important in nuclear applications [1–4]. A central role of this project is taken by ${}^{235}\text{U}$ and ${}^{238}\text{U}$, which are the major components of the reactor fuel in energy applications.

Existing evaluations ENDF/B-VII.1 [5] and JEFF-3.2 [6] perform very well for many applications. However, discrepancies have been pointed out between integral performance and differential data (e.g., for prompt fission neutron spectra of thermal ${}^{235}\text{U}$ (n,f) [7–9]), or between evaluated data from different libraries (e.g., between ${}^{235}\text{U}$ inelastic cross sections [10]). Those challenges led to new evaluations for ${}^{235}\text{U}$ and ${}^{238}\text{U}$ targets, in particular by the JEFF (JEFF-3.3) and by the IAEA CIELO [11,3] collaborations. Note that both evaluations have been released. The IAEA CIELO evaluation was adopted by the ENDF/B-VIII.0 library [12] that was released in February 2018. Authors were the lead authors of the IAEA CIELO evaluation. A brief comparison between the mean values of important differential quantities evaluated in these libraries is the subject of this short contribution. The integral performance of these libraries will be compared elsewhere.

2 Comparison of JEFF-3.3 and IAEA CIELO evaluations

Let's review some of relevant reaction channels.

2.1 Total cross sections

Neutron total cross sections from 20 keV to 30 MeV on ${}^{235}\text{U}$ and ${}^{238}\text{U}$ targets agree within experimental uncertainty (about 2%–3% including 1% systematic) for both JEFF-3.3 and IAEA CIELO evaluations. The agreement of $n + {}^{235}\text{U}$ cross section is shown in Figure 1. Note the uncertainty band (thin blue lines) shown around the JEFF-3.3 cross sections (bold blue line). The IAEA CIELO evaluation is shown in bold green line. Total cross sections in evaluated files are derived directly from the employed optical model, which are documented in reference [13] for the JEFF-3.3 evaluation and in references [14–16] for the IAEA CIELO evaluation on ${}^{235}\text{U}$ and ${}^{238}\text{U}$ targets, respectively.

2.2 Fission cross sections

Evaluated ${}^{235}\text{U}$ (n,f) and ${}^{238}\text{U}$ (n,f) cross sections in JEFF-3.3 correspond to the IAEA Neutron Standards 2006 [17,18], and are within 0.5% of the latest IAEA Standards 2017 [19] used in the IAEA CIELO file.

Despite this close agreement it should be noted that the evaluation methods differ significantly. The JEFF-3.3 evaluation team replaced their own calculated fission cross sections for both U isotopes (e.g., Ref. [13]) by the IAEA Standard 2006. It is expected that cross-section differences between calculated fission cross sections and Standards

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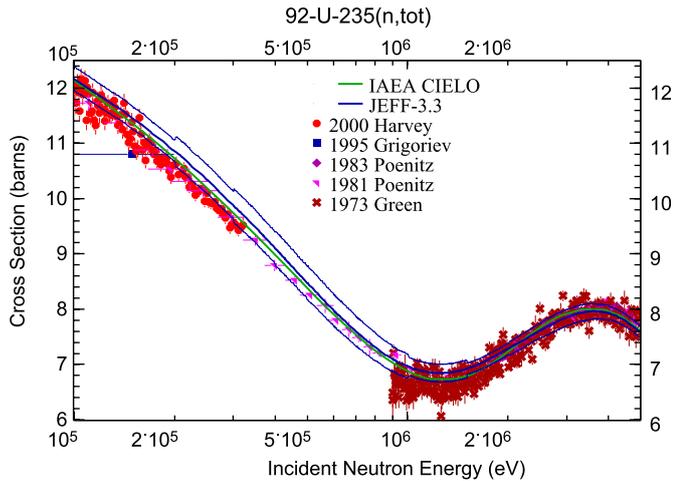


Fig. 1. Evaluated cross sections from IAEA CIELO and JEFF-3.3 libraries for ^{235}U (n,tot) compared to selected experimental data from EXFOR [20].

(e.g., as shown in JEFF-3.2 [6]) were dumped into the elastic cross sections. However, those differences will also be shown in other calculated cross sections including inelastic scattering and capture due to the constrain to reproduce the well-known total cross section.

Meanwhile, the IAEA CIELO evaluation employed the optical model for fission [21–23] to describe Neutron Standards fission cross sections for both uranium targets within 3% as shown in references [11,24–26]. Such description allows minimizing the impact of fission modelling on competing neutron capture and neutron scattering channels (Fig. 2).

2.3 Inelastic cross sections

Inelastic scattering is the only reaction that changes the neutron energy without losing the neutrons below 5 MeV in the energy range where the fission neutron flux is the largest. As such the inelastic cross sections is extremely important for neutron transport in reactors.

Both evaluations for inelastic scattering cross sections are based on model calculations, and the observed agreement is generally good, in fact much better than differences discussed at 2011 IAEA meeting [10]. The largest difference between ^{238}U (n,n') cross sections reaches 4% at 3 MeV; the corresponding difference between ^{235}U (n,n') cross sections is larger reaching 13% at 4.4 MeV. However, evaluations agree within quoted uncertainties, even if the IAEA CIELO uncertainties are smaller (around 5% at the maximum) than those in the JEFF-3.3. library. It should be noted that IAEA CIELO evaluated inelastic cross sections were found in references [21,25] to be in good agreement with JENDL-4 evaluation [27].

2.4 ($n,2n$) and ($n,3n$) cross sections

($n,2n$) reaction is the main competition to fission in both uranium targets above 7–8 MeV of neutron incident energy. The agreement of evaluated ^{238}U ($n,2n$) cross

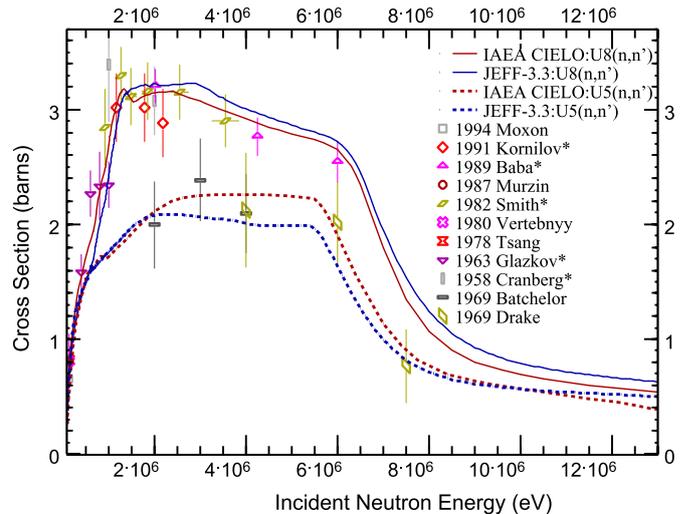


Fig. 2. Evaluated ^{238}U (n,n') and ^{235}U (n,n') cross sections from IAEA CIELO and JEFF-3.3 libraries compared to selected experimental data from EXFOR [20].

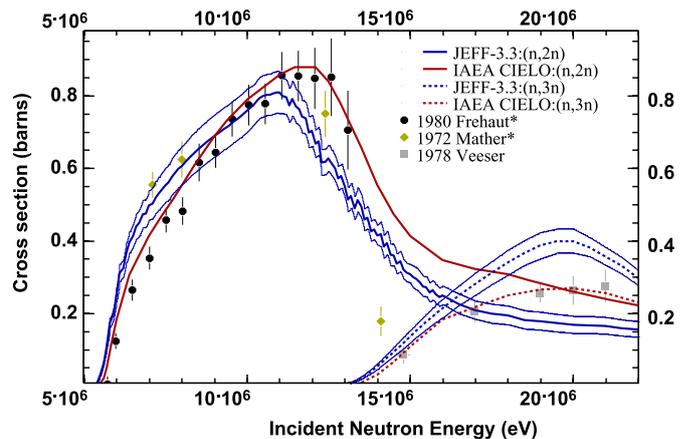


Fig. 3. Evaluated ^{235}U (n,xn) cross sections from IAEA CIELO and JEFF-3.3 libraries compared to selected experimental data [28–30].

sections is reasonable as discussed in reference [11]. However, larger differences are observed for evaluated ^{235}U ($n,2n$) and ^{235}U ($n,3n$) cross sections as shown in Figure 3, even if the shape of cross sections is similar. Evaluated uncertainties for the JEFF-3.3 library are also shown and differences between evaluations are larger than quoted uncertainties at the maximum of evaluated excitation functions both for the $2n$ and $3n$ emissions. Significant differences are also observed near threshold which imply large differences in the derived ^{235}U ($n,2n$) and ^{235}U ($n,3n$) spectrum averaged cross section (SACS) in $^{252}\text{Cf}(\text{sf})$ reference neutron spectrum. If we exclude Mather 1972 data, which are discrepant, then the IAEA CIELO evaluation is in significant better agreement with differential data than the JEFF-3.3 evaluation, especially for the ^{235}U ($n,3n$) cross section.

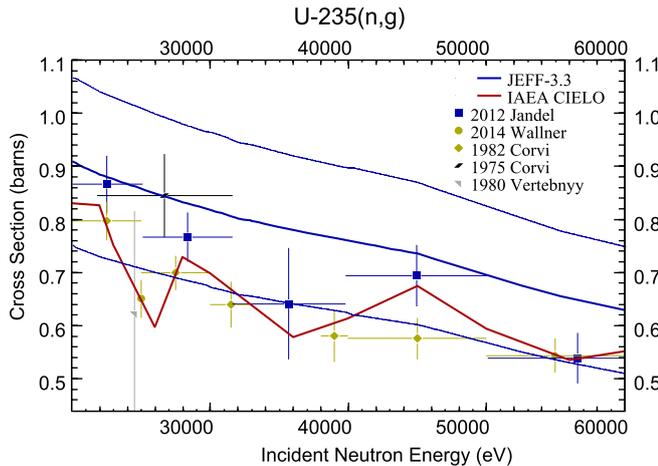
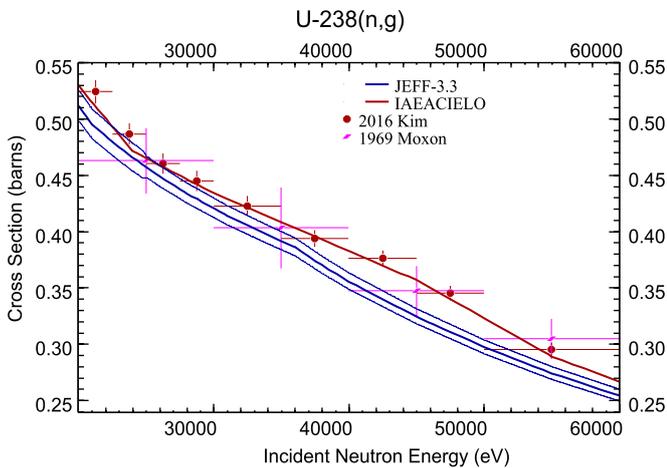
(a) $^{235}\text{U}(n,\gamma)$ from 20 keV up to 60 keV.(b) $^{238}\text{U}(n,\gamma)$ from 20 keV up to 60 keV.

Fig. 4. Evaluated capture cross sections on ^{235}U and ^{238}U targets in the region relevant to the calculation of the MACS at (30 keV) are compared to experimental data retrieved from EXFOR [20]. (a) $^{235}\text{U}(n,\gamma)$ from 20 keV to 60 keV, (b) $^{238}\text{U}(n,\gamma)$ from 20 keV to 60 keV.

2.5 Capture cross sections

IAEA CIELO $^{235}\text{U}(n,\gamma)$ cross sections were modified to follow fluctuations observed in Jandel's Los Alamos experiment [31], and are compared to the JEFF-3.3 cross section in Figure 4a. The JEFF-3.3 evaluation seems to be about 20% larger than the IAEA CIELO evaluation in the whole energy range shown in the picture. Note that the IAEA CIELO follow experimental fluctuations which can not be reproduced by statistical model calculations.

IAEA CIELO $^{238}\text{U}(n,\gamma)$ cross sections were adopted from Neutron Standards fit [19] and are shown in Figure 4b compared to evaluated JEFF-3.3 cross section. Evaluated reference $^{238}\text{U}(n,\gamma)$ cross sections within the Neutron Standards are in excellent agreement with newest high-accuracy measurement at JRC Geel [32,33], while the evaluated JEFF-3.3 cross sections are lower in the whole energy range. The difference between both evaluations reaches about 7% around 45 keV.

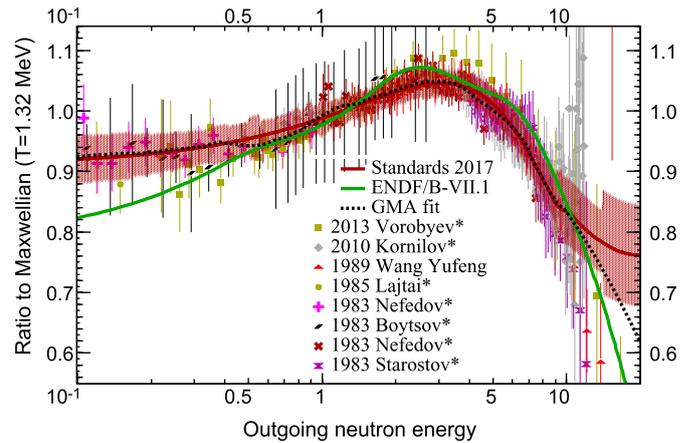


Fig. 5. $^{235}\text{U}(n_{th},f)$ PFNS experiments are compared with the Standards 2017 evaluation (bold red), the GMA fit (dashed black), and the ENDF/B-VII.1 evaluation (bold green). Above 9 MeV the Standards 2017 evaluation was fitted to the $^{90}\text{Zr}(n,2n)$ spectrum average cross sections.

Note that the overestimation in JEFF-3.3 evaluation of the $^{235}\text{U}(n,\gamma)$ measured data from 20 keV to 60 keV and the underestimation of the $^{238}\text{U}(n,\gamma)$ measured data led to a very strong underestimation of the measured Maxwellian Averaged Cross Sections (MACS) of the ratio $^{238}\text{U}(n,\gamma)/^{235}\text{U}(n,\gamma)$ near 25–30 keV by Wallner and collaborators [34]; the measured ratio is 0.60 ± 0.03 (5% uncertainty) while the derived ratio from the JEFF-3.3 evaluation is 0.49 which is 22% lower than the measured value! Such difference is outside the quoted uncertainties of IAEA CIELO evaluation, but it is within the much larger uncertainties given in the JEFF-3.3 file.

2.6 Thermal-neutron induced prompt fission neutron spectra

The ^{235}U thermal prompt neutron fission spectrum (PFNS) is one of the most important quantities for reactor applications as it represents the main source of reactor neutrons. A new evaluation of this spectrum was undertaken using a least-square code GMAP within the IAEA project, using shape data measured relative to the $^{252}\text{Cf}(sf)$ PFNS standard spectrum. The average energy of the ^{235}U thermal PFNS was determined to be 2.00 ± 0.01 MeV [7–9]. Such average energy was also adopted by the JEFF-3.3 in Figure 5 the results of the un-smoothed GMAP evaluation (black dashed line) are compared with the experimental input data [35–41] and with the ENDF/B-VII.1 evaluation, which is very similar to the JEFF-3.2 evaluation. The ENDF/B-VII.1 evaluation (bold green line, which was based on Madland–Nix model [42]) is lower than the GMAP fit below ≈ 1.2 MeV of outgoing neutron energy, but it is higher than the GMAP fit from 1.2 MeV to 9 MeV. The JEFF-3.3 evaluation shape is different from 1 to 9 MeV, but it is similar to the ENDF/B-VII.1 evaluation below 500 keV and above 10 MeV.

On the other side, the IAEA CIELO PFNS evaluation for $E > 9$ MeV was based on the evaluated SACS for the $^{90}\text{Zr}(n,2n)$ dosimetry reaction [43] and on the linear

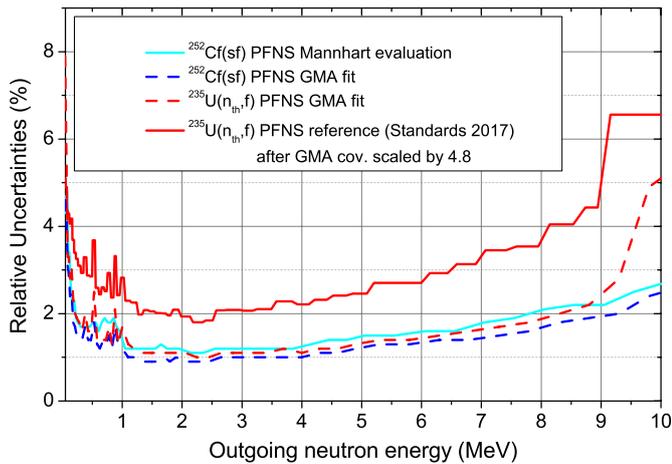


Fig. 6. Uncertainties of the $^{235}\text{U}(n_{th},f)$ (bold red) and $^{252}\text{Cf}(sf)$ (cyan) PFNS evaluations are compared with the corresponding ones obtained in the GMA fit (dashed lines).

dependence of the SACS on E as tested in references [7–9]. The PFNS uncertainty from 9 to 14 MeV was estimated to be 7% from the uncertainty of the SACS for the $^{90}\text{Zr}(n,2n)$. The suggested PFNS energy dependence above 9 MeV significantly improves the agreement with measured SACS for $(n, 2n)$ dosimetry reactions when IRDFF cross-section evaluations [44,45] are used to calculate the corresponding SACS. However, the extrapolated PFNS above 10 MeV is significantly larger than JEFF-3.2 and JEFF-3.3 evaluations based on Madland–Nix model [42].

The GMAP derived uncertainties for both $^{252}\text{Cf}(sf)$ and $^{235}\text{U}(n_{th},f)$ PFNS are represented by dashed lines in Figure 6; the GMAP $^{235}\text{U}(n_{th},f)$ PFNS uncertainty is always larger than the GMA $^{252}\text{Cf}(sf)$ PFNS uncertainty as expected. The later is close, but slightly smaller than the uncertainty of $^{252}\text{Cf}(sf)$ Mannhart evaluation (cyan line); the fitted $^{252}\text{Cf}(sf)$ PFNS shape was practically unchanged. Therefore, Mannhart evaluation [46] as listed in reference [18] was kept as the $^{252}\text{Cf}(sf)$ PFNS standard.

However, the GMAP derived uncertainty of the $^{235}\text{U}(n_{th},f)$ PFNS average energy was 5 keV, which was considered underestimated. An estimated 10 keV uncertainty was quoted based on expert assessment in references [7–9]. That uncertainty assessment is confirmed by the observed spread in measured PFNS as shown in Figure 5; the additional 5 keV uncertainty could be assigned to the unrecognized shape uncertainty in the existing experimental data¹. By scaling the PFNS covariance matrix the minimum PFNS uncertainty in the region of 2–3 MeV was increased approximately by factor of 2 to reach about 2%; the scaled uncertainty reached 4.5% at 9 MeV.

Final $^{235}\text{U}(n_{th},f)$ PFNS uncertainty is shown in Figure 6 by a bold red line, and corresponds to the red uncertainty band shown in Figure 5.

¹ The increase of the uncertainty of the PFNS average energy from 5 keV to 10 keV was achieved by rescaling the GMAP PFNS covariance matrix by a factor of 4.8.

3 Conclusions

Significant differences between the IAEA CIELO and JEFF-3.3 (CIELO 2) evaluations are shown for neutron capture on ^{235}U and ^{238}U targets, $^{235}\text{U}(n,2n)$ and $^{235}\text{U}(n,3n)$ cross sections and the ^{235}U thermal-neutron induced prompt fission neutron spectrum. Differences in evaluations are tracked to differences in evaluation methods, but also to differences between measured differential data and model-based JEFF-3.3 evaluation; the IAEA CIELO evaluation reproduces the differential cross section and PFNS data.

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