

# The CIELO Collaboration: Progress in International Evaluations of Neutron Reactions on Oxygen, Iron, Uranium and Plutonium

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**Abstract.** The CIELO collaboration has studied neutron cross sections on nuclides that significantly impact criticality in nuclear technologies -  $^{16}\text{O}$ ,  $^{56}\text{Fe}$ ,  $^{235,8}\text{U}$  and  $^{239}\text{Pu}$  - with the aim of reducing uncertainties and resolving previous discrepancies in our understanding. This multi-laboratory pilot project, coordinated via the OECD/NEA Working Party on Evaluation Cooperation (WPEC) Subgroup 40 with support also from the IAEA, has motivated experimental and theoretical work and led to suites of new evaluated libraries that accurately reflect measured data and also perform well in integral simulations of criticality.

## 1 Introduction

The Collaborative International Evaluated Library Organization (CIELO) [1], coordinated by the Nuclear Energy Agency (NEA) Working Party on Evaluation Cooperation (WPEC) Subgroup 40 since 2013, has stimulated advances to the neutron cross section evaluations of nuclides that significantly impact our nuclear technologies: oxygen,

iron, and uranium and plutonium isotopes. The benefits of a CIELO-coordinated effort between experts in nuclear science from around the world has led to the advances described in this paper.

Computational nuclear science and computing advances have played a key role in CIELO's progress. Fast computers have enabled large-scale nuclear criticality and transport simulations, mostly with the MCNP code, to

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assess the performance of proposed evaluation changes, with a feedback loop leading to the optimization of the data files. Nuclear reaction theory and modeling codes for coupled channels, statistical reactions and fission, and R-matrix, continue to be refined. The community is also starting to understand the benefits, and use of, sensitivity tools such as the NEA's Nuclear Data Sensitivity Tool (NDaST) to help focus research efforts. Also, various insights from the NEA/WPEC Subgroup 39 adjustment project have been useful.

Experimental work has always been the foundation of nuclear reaction data evaluations, and must remain so despite the costs and time involved in executing new measurement concepts to determine cross sections to unprecedented accuracy. The rallying of efforts behind CIELO has led to measurements over the course of this pilot project, most notably measurements at the Institute for Reference Materials and Measurements (IRMM)/Geel, CERN, Rensselaer Polytechnic Institute/Troy, Los Alamos, and Triangle University Nuclear Laboratory (TUNL), North Carolina.

The CIELO projects has worked with the IAEA standards project to stay abreast of standards cross section advances, and remain consistent with them. This pertains to recommendations on actinide fission and capture cross sections. A new standards evaluation will be released in 2017 [2], and will be domented in a Nuclear Data Sheets issue in January 2018.

## 2 CIELO evaluations created

The CIELO pilot project has a goal of resolving some previous discrepancies in the evaluated data, via peer review interactions together with new experiments, thoery, and simulation. But it is also recognized that – in some cases – differences of opinion persist, reflecting open unsolved problems and uncertainties. In these cases the goal is to document the differences (see Refs. [1, 3–5]) and reflect them in alternate data evaluations. We account for this diversity by creating and archiving two sets of files, CIELO-1 and CIELO-2, with each set of files designed to work together as a suite in criticality applications. Many of the cross section updates have compensating impacts on criticality. For example in thermal systems involving uranium and oxygen, the increased criticality from the lower average-energy  $^{235}\text{U}$  prompt fission neutron spectrum (PFNS) is partly compensated by the changes to oxygen that lower the criticality (increased  $(n,\alpha)$  leads to more neutron absorption; and a lower scattering cross section leads to more leakage and less moderation).

In practice, CIELO-1 is being considered for adoption in the ENDF community (for example, they are used in ENDF/B-VIII.0-beta2), and CIELO-2 in the JEFF community. These are illustrated in Table 1.

## 3 $^{235}\text{U}$ neutron reactions

Prior to CIELO, evaluation projects have been strongly influenced by the  $^{235}\text{U}$  resonance analyses by Derrien and

**Table 1.** Lead laboratories evaluating CIELO1,2 databases. CIELO-1 is being adopted by ENDF, CIELO-2 by JEFF. Many other labs contributed, including with data measurements.

Isotope	CIELO-1	CIELO-2
$^{16}\text{O}$ res.	LANL/IRMM	IRSN/IRMM
$^{16}\text{O}$ fast	LANL	LANL
$^{56}\text{Fe}$ res.	IRSN	IRSN
$^{56}\text{Fe}$ fast	BNL/IAEA/CIEA	JEFF
$^{235}\text{U}$ res.	ORNL/IRSN	IRSN/ORNL
$^{235}\text{U}$ fast	IAEA+LANL PFNS	CEA
$^{238}\text{U}$ res.	IRMM	IRMM
$^{238}\text{U}$ fast	IAEA +LANL PFNS	CEA
$^{239}\text{Pu}$ res.	ORNL/CEA	ORNL/CEA
$^{239}\text{Pu}$ fast	LANL	CEA

Leal, used in many of the world's various libraries. Previous higher energy neutron cross section evaluation work in the US was led by Young and Chadwick, and Madland for the PFNS, (LANL); in Europe by Romain, Morillon (CEA), and Vladuca and Tudora for PFNS, and in Japan by Iwamoto, Otuka, Chiba, Kawano, and Ohsawa for PFNS. The present CIELO evaluation work was done by Capote, Trkov, Leal, Pigni, Talou and Rising.

A new resonance analysis has been developed by Leal (IRNS and ORNL), described separately in these proceedings; Leal's work modified the resolved resonances to account for the new LANL and RPI capture data, and better model the standards fisison integral in the 7.8-11 eV range (the CIELO-2 file). Pigni (ORNL) and Trkov (IAEA) built on Leal's work with various modifications for the CIELO-1 evaluation, as described below.

The  $^{235}\text{U}$  resolved resonance CIELO-1 evaluation recently released within the ENDF/B-VIII.0 $\beta$ 2 nuclear data library has been developed on the basis of newly evaluated thermal neutron constants [2] as well as of new thermal Prompt Fission Neutron Spectra (PFNS) [6]. The softer thermal PFNS adopted in CIELO-1 increases criticality, especially for high-leakage benchmarks (and thus introduces a strong positive slope for  $k_{\text{eff}}$  v. ALTF (Above Thermal Leakage Fration) for HST benchmarks unless other changes are made). For energies below 100 eV, this work restores benchmark performance for  $^{235}\text{U}$  solutions by combining changes to the prompt resonance  $\bar{\nu}$  and the resonance parameters. In achieving this, the present set of resonance parameters yields cross sections still in reasonable agreement with the suite of experimental data included in the previous resonance evaluations. Additionally, the set of  $\eta$  measurements performed by Brooks [7] in the mid-sixties at the Atomic Energy Research Establishment (Harwell) were analyzed and included in the fit for incident neutron energies up to 20 eV. Figure 1 displays multiple measurements of Brooks [7] in the incident neutron energy range up to 5 eV but also measured data of Wartena and Weigmann [8] in the low energy range between 0–0.5 eV. All measurements normalized to the reported  $\nu$  value. The comparison of ENDF/B-VII.1 (in red) and ENDF/B-VIII.0 $\beta$ 2 (in blue)  $\eta$  values is also shown. Although the large uncertainties above 2 eV, the CIELO

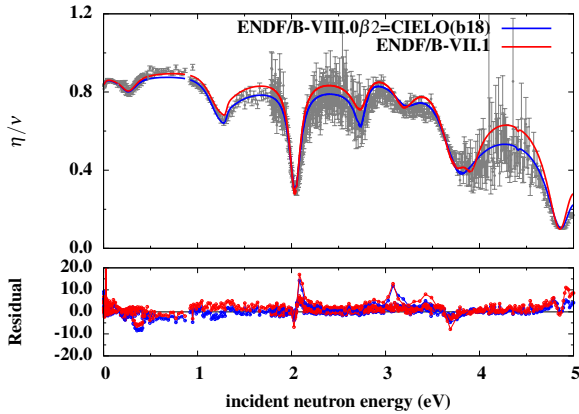
$\eta$  (decreased) values are on average in better agreement with the experimental data than ENDF/B-VII.1 values. This was achieved by increasing the capture cross sections mostly in the valley of the resonances while keeping their peak values unchanged. The resonance at  $E_n=2$  eV is clearly an example.

The sensitivity of the resonance parameters to fission cross sections seems to be more relevant than to capture cross sections at neutron energies  $\geq 4$  eV. This effect is evident in the fission cross sections shown in blue continuous line in the Fig. 2 where Gwin's fission cross section measurements are displayed along with ENDF/B-VII.1 and ENDF/B-VIII.0 $\beta 2$  values.

The decreased neutron production suggested by Brooks' data also seemed consistent with the use of a softer PFNS and the newly fitted thermal neutron constants in order to compensate the decreased criticality. Moreover, the values of the resonance parameters were constrained by cross section integrals, e.g. the fission integral in the incident energy range between 7.8–11 eV,

$$I_f = \int_{7.8\text{eV}}^{11\text{eV}} \sigma_f(E; \mathbf{a}) dE = 247.0 \text{ b} \cdot \text{eV} \text{ (current value)}, \quad (1)$$

recommended by the standards and by recent nTOF data.

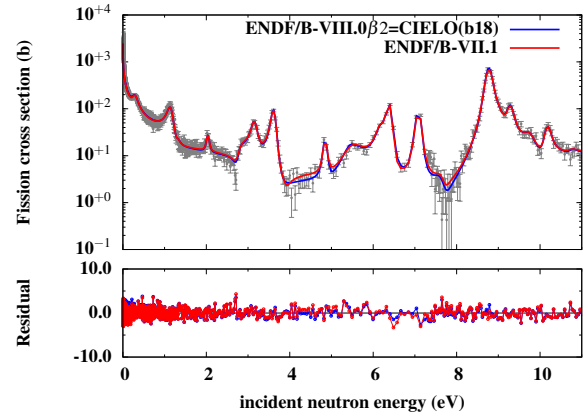


**Figure 1.**  $n+^{235}\text{U}$   $\eta$  measurements of Brooks, Wartena, and Weigmann compared to ENDF/B-VII.1 and CIELO-1 values.

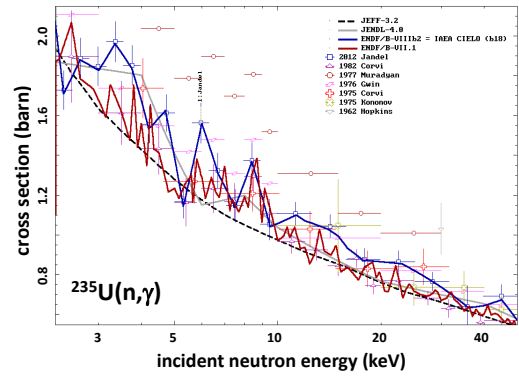
The CIELO  $^{235}\text{U}$  capture cross section above a keV is shown in Fig. 3. It follows the recent Jandel Los Alamos measurement, lying significantly below ENDF/B-VII.1 below 2 keV and above it for energies up to 50 keV.

The inelastic scattering cross section has been reevaluated as part of a new optical and statistical model analysis of direct and compound reactions. CIELO's total inelastic scattering is reduced compared to ENDF/B-VII.1, see Fig. 4. At higher incident energies above 10 MeV, pre-equilibrium processes become important. These, together with inelastic scattering reactions involving the excitation of collective states, are included in EMPIRE model calculations, allowing for the modeling of 14 MeV secondary neutron emission data measured by Kammerdiener at Livermore shown in Fig. 5

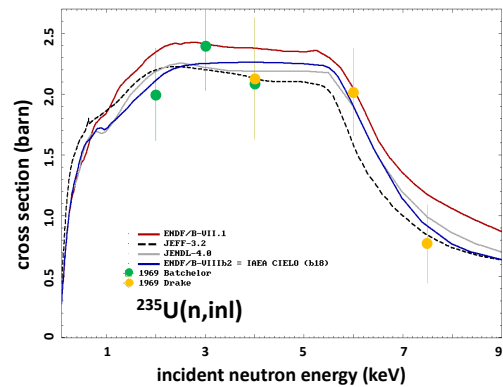
The importance of the need for a better understanding of the prompt fission neutron spectra (PFNS) from ac-



**Figure 2.**  $n+^{235}\text{U}$  Gwin's fission measurement compared to ENDF/B-VII.1 and ENDF/B-VIII.0 $\beta 2$  values.

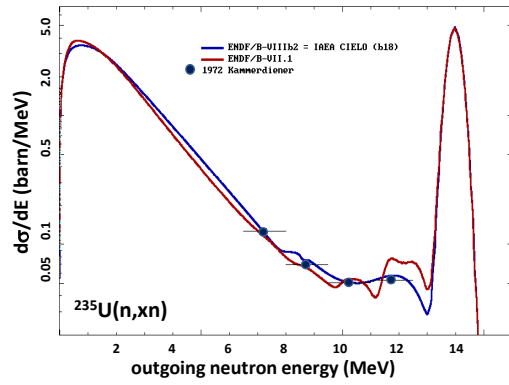


**Figure 3.**  $^{235}\text{U}(n,\gamma)$  neutron capture. CIELO-1 follows the Jandel data up to 50 keV.



**Figure 4.**  $^{235}\text{U}(n,\text{inelastic})$  total inelastic cross section.

tinides, owing to its large impact on criticality calculations, led to a multi-year IAEA Coordinated Research Project, the results of which are now documented in a major article [6]. An important conclusion was that the PFNS from thermal neutrons on  $^{235}\text{U}$  should have a lower average energy, 2.00 MeV, versus the previous 2.03 MeV, based on



**Figure 5.**  $^{235}\text{U}(n,xn)$ . CIELO-1 secondary neutron spectra for 14 MeV incident energy, compared to ENDF/B-VII.1.

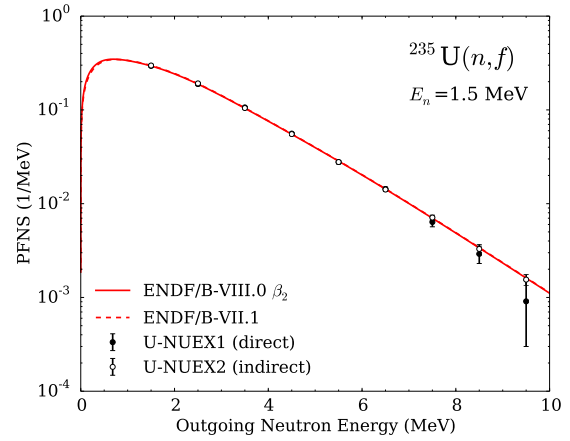
an IAEA analysis of spectra and dosimetry activation measurements<sup>1</sup>. At higher neutron energies - 0.5 up to 5 MeV incident energy - CIELO adopts the calculated values by Rising and Talou which were based on an extension of the Madland-Nix type approach, calibrated to measured data. This spectrum is seen to agree fairly well with the NUX data of Lestone and Shores in Figs. 6 for incident neutrons with an average energy of about 1.5 MeV. It is evident from the average PFNS energies shown in Fig. 7 that the Talou-Rising PFNS data above 0.5 MeV incident energy matches the new IAEA spectrum average energy at thermal, and removes the previous ENDF/B-VII.1 unphysical kink in the neutron average energy near 3 MeV (which was based on matching one particular data set, that of Boykov). Above 5 MeV the ENDF/B-VII.1 PFNS is maintained, although it is recognized that an upgrade is eventually needed to properly account for preequilibrium processes above 10 MeV incident energy.

#### 4 $^{238}\text{U}$ neutron reactions

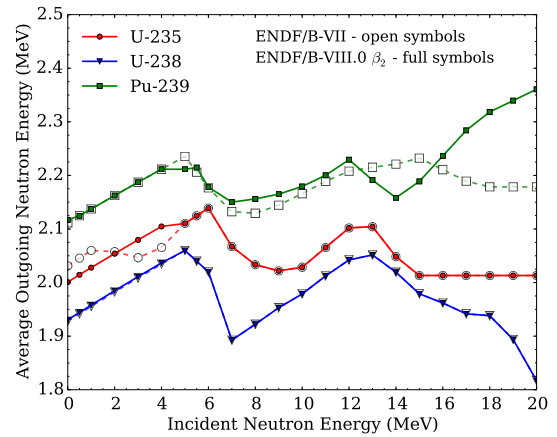
Prior to CIELO, evaluation projects have been strongly influenced by the  $^{238}\text{U}$  resonance analyses by Derrien, Courcelle, Leal, and Froehner, used in many of the world's various libraries. Previous higher energy neutron cross section evaluation work in the US was led by Young and Chadwick, and Madland for PRNS (LANL); in Europe by Romain, Morillon (CEA), and Vladuca and Tudora for PFNS, and in Japan by Iwamoto, Otuka, Chiba, Kawano, and Oh-sawa for PFNS. The present CIELO evaluation work was done by Capote, Trkov, Schillebeeckx, Kopecky, Talou and Rising.

A new evaluation for neutron induced reaction on  $^{238}\text{U}$  in the resonance region was carried out considering well documented experimental data in the literature. Resonance parameters of individual resonances below 1200 eV were adjusted from a simultaneous resonance shape analysis of capture data obtained at GELINA [9] and trans-

<sup>1</sup>This is a flashback to the past. Watt's seminal 1952 Physical Review paper parameterized the data of the time with a functional form that had an average energy of 2.00 MeV!



**Figure 6.**  $^{235}\text{U}(n,\text{PFNS})$ . CIELO's prompt fission neutron spectra compared to NUX data and to ENDF/B-VII.1, for 1.5 MeV incident energy. The "indirect" NUX data converts the (more accurate) plutonium NUX data to uranium using ratio measurements from Sugimoto [6].

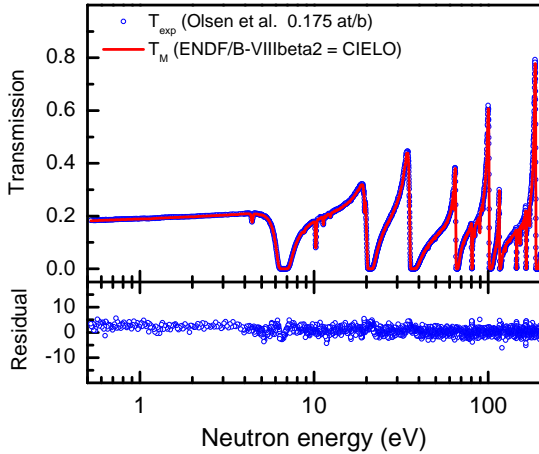


**Figure 7.** Acinide averaged prompt fission neutron energy in CIELO-1 versus ENDF/B-VII.1.

mission data obtained at a 42 m and 175 m station of Refs. [10], [11]. The contribution of the bound states was adjusted to produce a parameter file that is fully consistent with these data. This is illustrated in Fig. 8 which compares the experimental Texp and theoretical transmission TM for the uranium sample with a 0.175 at/b areal density. Using the parameters of ENDF/B-VII.1, which are adopted from Derrien et al. [12], the theoretical and experimental transmission are not consistent. This suggests that Derrien et al. [12] applied a normalization correction to the experimental transmission to get a consistent fit.

In the unresolved resonance region average capture and total cross sections were derived from a least squares analysis of experimental data reported in the literature using the GMA code. These capture data are shown in Fig. 9. The generalised ENDF-6 model together with the standard

boundary conditions was used to parameterise these average cross sections in terms of average parameters following a procedure described in Ref. [13]. The neutron strength functions and hard sphere scattering radius were adjusted to reproduce results of optical model calculations using the DCCOM potential of Quesada et al. [14] and the inelastic neutron scattering data of Capote et al. [15], which include compound-direct interference effects, were adopted.



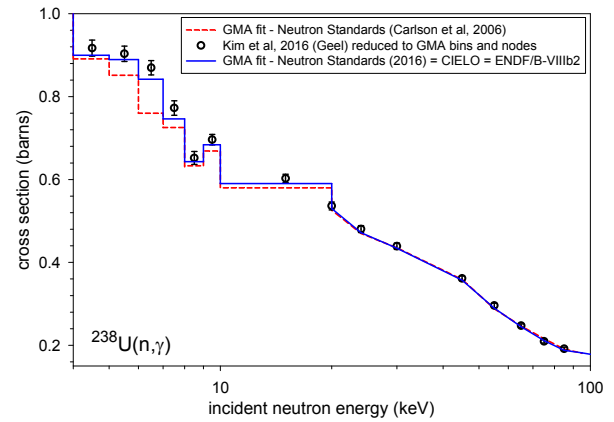
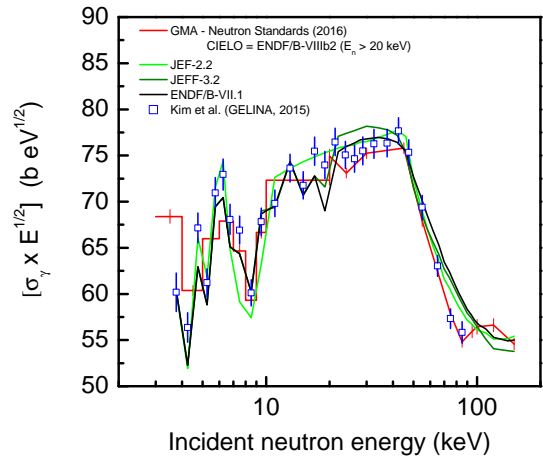
**Figure 8.** Resonance analysis of  $^{238}\text{U}$  transmission data.

The  $^{238}\text{U}$  inelastic scattering cross section has been a focus of attention in the CIELO collaboration, owing to its large impact on simulations of fast reactor criticality. The new evaluation shown in Fig. 10 is based on advanced nuclear reaction theory predictions, which include improved nuclear structure treatments and fission competition modeling (since accurate measurements of inelastic scattering are challenging).

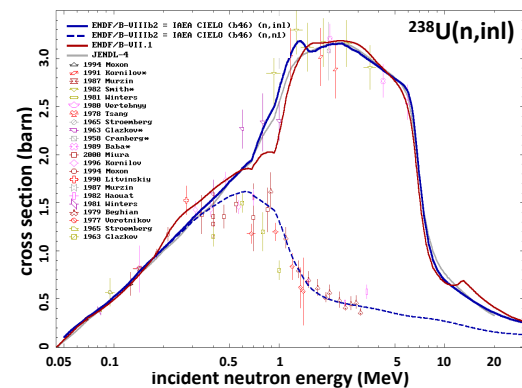
The evaluated  $^{238}\text{U}(n,2n)$  cross section is shown in Fig. 11, compared to ENDF/B-VII.1 and to data. The earlier ENDF/B-VII.1 evaluation rose to higher values in the 6-8 MeV region above the threshold compared to some of the other evaluations, and this same behavior is seen in the new CIELO evaluation, informed in part by new Krishichayan measurements from TUNL. The previous VII.1 evaluation was motivated by old LANL Knight data, together with integral measurements of  $(n, 2n)$  reaction rates in critical assemblies, and this behavior is corroborated by the TUNL and other measurements, which guided the model calculations used in the present analysis.

## 5 $^{239}\text{Pu}$ neutron reactions

Prior to CIELO, evaluation projects have been strongly influenced by the plutonium resonance analyses by Derrien, Leal, Larson, de Saussure, Fort, and Nakagawa. Higher energy neutron cross section plutonium evaluation work in the US was led by Young, Arthur, Chadwick, Talou, and MacFarlane, and Madland for PFNS (LANL); in Europe by Romain, Morillon, and Delaroche (CEA); and in Japan by Iwamoto, Otuka, Chiba, and Kawano.

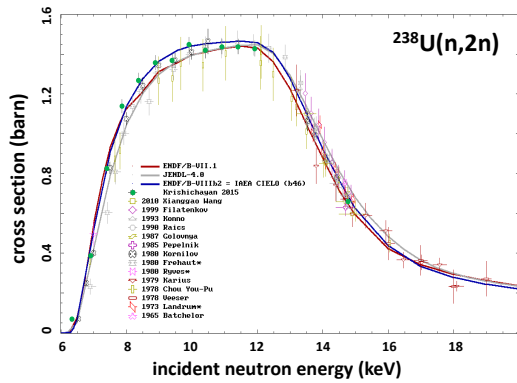


**Figure 9.**  $^{238}\text{U}$  neutron capture for CIELO (upper figure), and the updated grouped standards cross section (lower figure).



**Figure 10.**  $^{238}\text{U}(n,\text{inel.})$  in CIELO-1 versus ENDF/B-VII.1.

In the last three years CIELO collaboration made only modest advances to  $^{239}\text{Pu}$ , adopting the earlier WPEC Subgroup 34 work on resonances by de Saint Jean, Noguere, Penelieu, Bernard, Serot, Leal, Derrien, Kahler, and McKnight, and by updating the ENDF capture cross sections in the fast range between 30 keV and 2 MeV.



**Figure 11.**  $^{238}\text{U}(n,2n)$  excitation function in CIELO, compared to data that include the recent TUNL measurements.

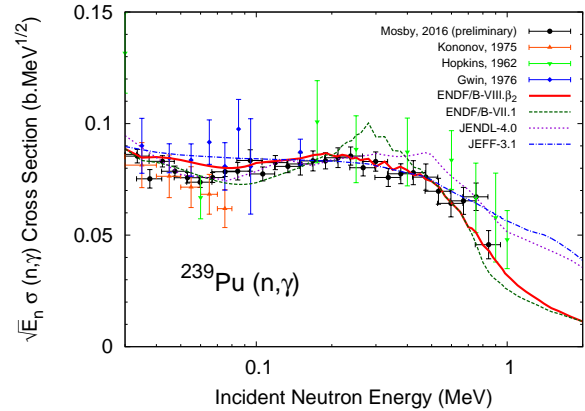
Earlier evaluations, such as ENDF/B-VII and JEFF-3.1, JENDL suffered from a longstanding deficiency: an overprediction of plutonium solution criticality in transport simulations by approximately 500 pcm (0.5% in  $k_{\text{eff}}$ ) [16]. The proposed resonance and prompt nuclide updates by Subgroup 34 remove approximately half of this over-prediction. The further influence of our  $^{16}\text{O}$  CIELO evaluation changes, and the new scattering kernels recommended by WPEC/Subgroup 41, now lead to much-improved thermal plutonium solution criticality predictions as discussed below in Sec. 8.

Additional improvements must follow this pilot project. In the coming years we expect to see new plutonium prompt fission spectra (PFNS) and fission cross section data from the Los Alamos Chi-nu and TPC experiments; as an interim step we included the Neudecker PFNS spectrum for incident energies above 5 MeV, which provide an improved treatment of the effects of multi-chance fission and preequilibrium processes. Also, the recent Mosby *et al.* DANCE capture data should impact a future plutonium resonance analysis in the unresolved and resolved resonance regions, analogous to how DANCE data influenced the  $^{235}\text{U}$  CIELO evaluation described above. In the fast region above 30 keV, these data motivated the capture cross section change shown in Fig. 12.

## 6 $^{56}\text{Fe}$ neutron reactions

A new effort by the CIELO collaboration to improve iron cross sections was deemed important based on sensitivity studies of nuclear criticality and shielding, and thermal and fast reactor design work. For example, uncertainty assessments performed by WPEC Subgroup 26 for innovative reactor systems shows that the knowledge of the inelastic scattering cross section of  $^{56}\text{Fe}$  should be improved to meet the target accuracy requirements for these systems.

The previous  $^{56}\text{Fe}$  evaluations in the various libraries from different regions are largely independent, with some exceptions such as the resolved resonance parameters. They rely on the optical model and statistical model calcu-



**Figure 12.**  $^{239}\text{Pu}(n,\gamma)$  in CIELO-1 versus ENDF/B-VII.1, showing the influence of the new Los Alamos DANCE data.

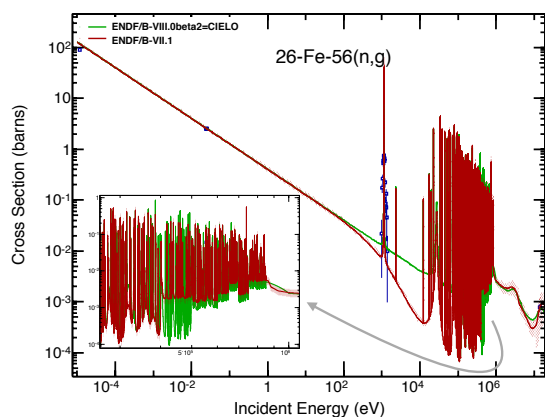
lations, where the secondary particle energy and angular distributions play an important role in radiation shielding calculations. The evaluations can be separated into four energy ranges: (a) the resolved resonance region up to 850 keV, (b) from 850 keV to about 7 MeV where fluctuation still persists in the measured total cross section, (c) from about 7 MeV to 20 MeV, and (d) above 20 MeV. F. Perey and C. Perey of ORNL evaluated the resolved resonance parameters for ENDF/B-VI, and ENDF/B-VII.1 and CENDL have the same resonance parameter set. Other evaluations (JENDL, JEFF, and ROSFOND) adopt a modified version of the resolved resonances by Fröhner, performed for the JEF-2.2 evaluation.

In the MeV energy region, the fluctuation behavior seen in the experimental total cross sections, which an optical model cannot reproduce, should exist in the evaluated files, as this can be important in neutron transport and shielding calculations. Usually the total cross sections in this energy region are obtained by tracing the experimental data available. For the other reaction channels, the Hauser-Feshbach model calculations are used for the evaluation, though the model codes employed are different.

The CIELO evaluation is based on a new resonance analysis from Leal up to an energy of 850 keV, together with guidance on angular distributions from RPI “quasi-differential” scattering data, and simulations of iron-reflected critical assembly data. Up to 4 MeV, the evaluated data for total, elastic, and inelastic scattering is based on measured data. At higher energies, EMPIRE nuclear model calculations played an important role, including the use of a soft-rotor optical model potential. The present CIELO work was performed by Herman, Nobre, Brown, Arcilla, Trkov, Capote, Leal, Plompen, Danon, Qian, Ge, Liu, Hanlin, Ruan, and Sin.

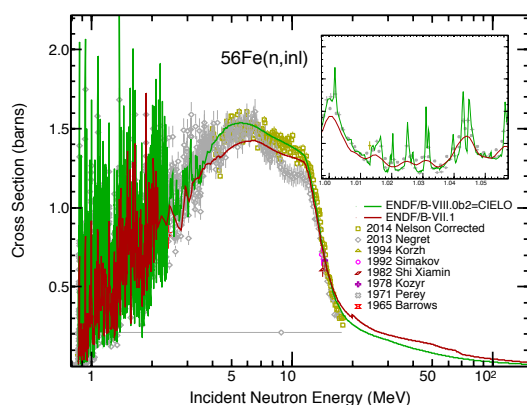
Leal’s INRS-v2 resolved resonance analysis was adopted up to the first inelastic scattering level (850 keV). This analysis included the use of new RPI data. As in previous evaluations, “background” modifications to the cross sections above 500 keV were added, to account for hypothesized missing p- and d-wave resonances and to avoid an unphysically-low neutron capture cross section.

In addition, a background was added in the 10 eV – 100 keV region was added to extend the “1/v” dependence (see Fig. 13, motivated in part by a desire to better model the ZPR-34/9 critical assembly.



**Figure 13.**  $^{56}\text{Fe}(n,\text{capture})$  in CIELO-1 versus ENDF/B-VII.1

The inelastic scattering in CIELO up to 4 MeV follows experimental data from Geel (Negret) and from Dupont (unpublished; corrected by Trkov); the latter data having a higher resolution, which is reflected in CIELO versus the earlier VII.1 evaluation. Above 4 MeV, EMPIRE model calculations are used, which were validated against the Negret and the Nelson (Los Alamos) measurements of inelastic scattering followed by gamma-ray emission. Compared to ENDF/B-VII.1, the inelastic scattering cross section in CIELO is larger, for the energy range from threshold up to 14 MeV (Fig. 14). (We note that this is in contradiction to feedback from the WPEC adjustment project, Subgroup 39, which suggests an inelastic scattering reduction near threshold; future testing of our evaluation will help resolve this seeming discrepancy).



**Figure 14.**  $^{56}\text{Fe}(n,\text{inelastic})$  in CIELO versus ENDF/B-VII.1

## 7 $^{16}\text{O}$ neutron reactions

The existing ENDF database comes from a merging of R-matrix analyses by Hale of LANL above 3.4 MeV, and by Lubitz and Caro of KAPL below 3.4 MeV, together with higher energy data from measurements and model calculations by Young and Chadwick. This evaluation has been adopted by (or at least strongly influenced) many other evaluation projects, for example JEFF3.2, CENDL, and ROSFOND. But the CIELO researchers recognized that some significant modifications are now warranted; for example, a previous renormalization of the  $(n,\alpha)$  cross section downwards by 32% going from ENDF/B-VI.8 to ENDF/B-VII is now removed, as described below. We note that this conclusion differs from that summarized in our CIELO document at the beginning of the project three years ago [1]. CIELO evaluation work for oxygen has been performed by Hale, Leal, Lubitz, Kunieda, Plompen, Kopecky, Kawano, Quaglion and others. Two sets of evaluations were created for testing: Hale’s (CIELO-1), and Leal’s (CIELO-2), the latter having two options for the  $(n,\alpha)$  cross section that can be studied.

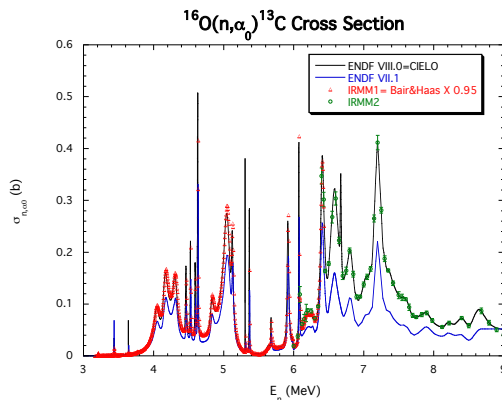
The  $^{16}\text{O}(n,\alpha)$  reaction is important in nuclear criticality applications involving oxide fuels, and water, and its inverse – the  $^{13}\text{C}(n,\alpha)$  reaction – plays an essential role in nucleosynthesis studies, being a major source of neutrons in the s-process responsible for many of the elements produced above the iron peak.

Hale, Paris and Kunieda have been making the point, for over a decade, that R matrix calculations constrained by unitarity, together with  $^{16}\text{O}$  total and elastic scattering data, point to the need for a significantly higher  $(n,\alpha)$  cross section in the 3-6 MeV range compared to ENDF/B-VII.1. This view was adopted for the CIELO evaluation, where the cross section was increased by  $\sim 40\%$  over this range, with further increases as the incident energy extends to 9 MeV. Even though the Nuclear Energy Agency NDaST sensitivity calculations of Hill show a very small sensitivity of the most-sensitive benchmarks to this cross section (about 3 pcm per % change in  $(n,\alpha)$ ), the very large change in the cross section leads to significant increases in calculated criticality.

The  $(n,\alpha)$  experimental data (and its inverse) supporting this change have been analyzed by Giorginis. Some progress has been made on clarifying what can only be said to be a messy state of affairs. The normalization of this reaction has been poorly understood in many experiments, and data have often been revised over the years. For example, the important Bair and Haas ORNL data are viewed by Giorginis as attractive owing to the use of a thin target, but to still need a renormalization – close to the originally-published values (he recommends 0.95) instead of the larger 0.80 renormalization down that was recommended by Bair and Haas. Giorginis recommends renormalizing the Harissopoulos data by 1.42. These assessments were based on a procedure to first determine the relative scale of these two measurements based on the thick-target yield over the narrow resonance at 1.056 MeV, and subsequently to correct for issues associated with the characterization of the  $^{13}\text{C}$  targets used in the experiments. He

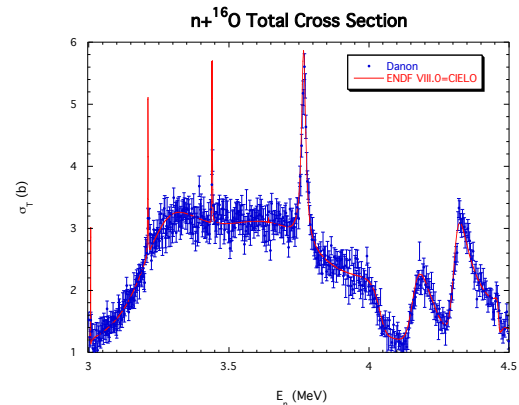
recommends renormalizing his own IRMM data, first published at the Trieste ND2007 conference, up to be consistent with the 0.95-normalized Bair and Haas data, though so far Goerginis has distributed IRMM data only in the 6.3–9 MeV range. (We assume that the Obninsk IPPE data remain in contradiction with the scale of new recommendation).

So although progress has perhaps been made, it is recognized that future experiments are needed to corroborate the large approximately 40% changes being made in CIELO-1 (Fig. 15). Indeed, new experimental efforts have been initiated by Los Alamos (Hye Young Lee *et al.*) using the LENS detector, and by astrophysical groups pursuing low-background underground measurements (Wiescher *et al.*), and we look forward to the publication of these data.



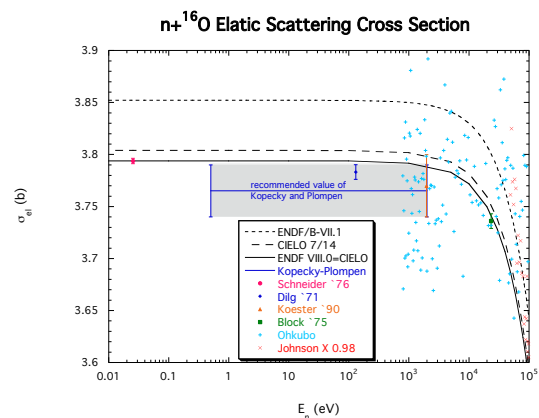
**Figure 15.**  $^{16}\text{O}(n,\alpha)$  in CIELO versus ENDF/B-VII.1, showing the higher cross section in the new evaluation.

The total  $^{16}\text{O}(n,\text{tot})$  cross section plays an important role in our understanding of neutron reactions in oxygen, in part because of its influence on the  $(n,\alpha)$  reaction via unitarity. Historically there have been questions at the 3–4% level regarding the absolute normalization of this cross section: for example the Cierjacks 1968 data being discrepant with the high-resolution Cierjacks 1980 data. Danon *et al.* have advanced our understanding here with a novel method in which the normalization of a measurement using a water target was made at 2.3 MeV, where the oxygen “window” (where the total cross section falls to almost zero owing to a destructive interference effect) allows the normalization to be made to the very well known hydrogen standard value. These new RPI data agree with Cierjacks 1968 to about 0.04%. These measurements were also treated as blind validation data, and Fig. 16 shows they support the new Hale evaluation, which was done *prior* to the measurement. Remarkably, the Hale evaluation agrees with the Danon RPI total cross section data to better than 1% over the energy range from 0.2–9 MeV. It is now thought that the Cierjacks 1980 total cross section data need to be renormalized up by approximately 3.2–3.8%.



**Figure 16.**  $^{16}\text{O}(n,\text{tot})$  total cross section in CIELO, calculated prior to the measured RPI data from Danon.

The other important change for oxygen is the lower total elastic scattering cross section adopted, from thermal to 10s of keV energies. An assessment by Kopecky and Plompen led to a recommendation of a low-energy value of 3.765 b (CIELO-2); Hale’s latest value of just under 3.8 barns in the CIELO-1 file - which was influenced also by the Schneider (1976) measurement - is about 1.5% lower than the previous ENDF/B-VII.1 evaluation (3.852b ), Fig. 17. This seemingly-modest decrease has a significant impact on criticality applications (for example, the NDaST sensitivity tools indicate HST benchmarks are sensitive at the 100pcm per % change in the elastic scattering cross section between 1 eV and 100 keV). Kozier, Roubtsov, Plompen and Kopecky [17] have noted that some heavy-water criticality benchmarks also suggest a lower thermal scattering cross section.



**Figure 17.**  $^{16}\text{O}(n,\text{elastic})$  total elastic scattering cross section in CIELO at low energies.

## 8 Criticality validation testing

Validation testing of CIELO files was done throughout the evaluation process, providing feedback on the data libraries and how they perform, in concert together, for thousands of criticality and neutron transmission benchmarks. The MCNP transport code was used, after the data were processed by NJOY. Most of the testing was done by Kahler (Los Alamos), Trkov (IAEA), Hill (NEA), Brown, Arcilla (BNL), Noguerre (CEA), Benjamin (CEA), Kodeli (Ljubljana), Haicheng (CIEA) and Palmiotti (INL).

Owing to space limitations, we do not report here in detail on the results, but instead point the reader to companion papers in these proceedings (see, for example, Kahler's paper). Compared to ENDF/B-VII.1 the CIELO-1 files used in EBDF/B-VIII.0-beta2 perform as follows: For fast Pu and U critical assemblies, they perform equally well, with some improved performance for reflected assemblies; for intermediate and thermal energy assemblies the performance is also comparable, though for plutonium thermal solutions (PST) the previous large ( $\sim 500$  pcm) overprediction is removed in the CIELO-1 evaluations, as discussed further below. The CIELO evaluations also appear to fix the problems noted by Japanese researchers on modeling sodium void reactivity in fast FCA assemblies.

We have used the NEA's NDaST sensitivity tools to assess the impact of some of the CIELO-1 cross section changes, relative to ENDF/B-VII.1. Below we use the changes to  $^{16}\text{O}$  ( $n,\alpha$ ) and ( $n,\text{elastic}$ ) as an illustrative example. Hill has analyzed over 3000 criticality benchmarks to characterize the effects.

The role of the increased CIELO-1  $^{16}\text{O}$  ( $n,\alpha$ ) reaction in absorbing neutrons and reducing criticality was found to be of order -100 pcm on LCT experiments, and about -50 pcm for HST experiments. The reduced low energy elastic scattering in CIELO, on the other hand, was found to be about -50 pcm on LCTs (but a higher value, -150-200 pcm on heavy water benchmarks), while for HST experiments the reduction is about -100 pcm for low-leakage systems (owing to reduced moderation), but as high as -300 pcm for high-leakage systems (where reduced scattering increases the leakage). The overall effects is that simulations of HST highly-enriched solution thermal critical assemblies typically change by -100-200 pcm, whereas LCT low-enriched uranium thermal assemblies change by -150-200 pcm. Some heavy water benchmarks change by almost -300 pcm. As noted earlier, compared to ENDFB-VII.1, these reductions in criticality are compensated (in part at least) by other changes to the  $^{235}\text{U}$  resonance and nubar data and the thermal PFNS.

For plutonium solution thermal (PST) critical assemblies, previous ENDF/B-VII and earlier JEFF and JENDL libraries largely overcalculated the criticality, by  $\sim 500$  pcm on average. The adoption of Subgroup 34's plutonium resonances and nubar removed about one half of this discrepancy. The aforementioned changes to oxygen further reduced the overprediction by 100-200 pcm with an average effect of about 150 pcm (of which about 3/5 was due to the reduced elastic channel, and 2/5 to the increased

( $n,\alpha$ )). Further small reductions came from the adoption of the new scattering kernel for water, and from the use of a slightly harder thermal PFNS for plutonium.

## 9 Future work

The CIELO pilot project ends in 2017. The progress made – including covariances – will be documented in a WPEC summary report, and the CIELO-1, CIELO-2 data libraries will be archived at the NEA and IAEA. Additional documentation will be provided in papers to be published in the January 2018 issue of Nuclear Data Sheets, edited by Pavel Obložinský.

We feel that the CIELO collaboration has stimulated much progress in nuclear experiments, theory, evaluation, and simulation. Many of the results will be adopted by regional evaluation efforts, such as ENDF and JEFF. In the long term, the community is considering the best way to continue such collaborative efforts in nuclear science, under the auspices of the IAEA and NEA.

## References

- [1] M.B. Chadwick, E. Dupont, E. Bauge *et al.*, Nucl. Data Sheets **118**, 1 (2014).
- [2] V. G. Pronyaev *et al.*, abstract 703, ND2016 International Conference on Nuclear Data and Technology.
- [3] E. Bauge *et al.*, Eur. Phys. J. A **48**, 113 (2012).
- [4] A. Plompen *et al.*, International Atomic Energy Agency Report INDC(NDS)-0597 (2012).
- [5] M.B. Chadwick, M.W. Herman, P. Obložinský *et al.*, *et al.* Nucl. Data Sheets **112**, 2887 (2011).
- [6] R. Capote *et al.*, Nuclear Data Sheets **131** 1 (2016).
- [7] F.D. Brooks *et al.*, Harwell report AERE-M1670.
- [8] H. Weigmann *et al.*, Int. Conf. on the Physics of Reactors, Marseille 1990, Vol.3 p.33 (1990), France
- [9] H.I. Kim, C. Paradela, I. Sirakov, B. Becker, R. Capote, F. Gunsing, G.N. Kim, S. Kopecky, C. Lampoudis, Y.-O. Lee, R. Massarczyk, A. Moens, M. Moxon, V.G. Pronyaev, P. Schillebeeckx and R. Wynants, Eur. Phys. J. A **52**, 170 (2016).
- [10] D.K. Olsen, *et al.*, Nucl. Sci. Eng. **62**, 479 (1977).
- [11] D.K. Olsen, *et al.*, Nucl. Sci. Eng. **66**, 141 (1978).
- [12] H. Derrien, L.C. Leal, N.M. Larson, A. Courcelle, ORNL/TM-2005/241, Oak Ridge National Laboratory (2005).
- [13] I. Sirakov, R. Capote, F. Gunsing, P. Schillebeeckx, A. Trkov, Ann. Nucl. Energy **35**, 1223 (2008).
- [14] J.M. Quesada, R. Capote, E.Sh. Soukhovitskii, S. Chiba, Nucl. Data Sheets **118**, 270 (2014).
- [15] R. Capote, A. Trkov, M. Sin, M. Herman, A. Daskalakis, Y. Danon, Nucl. Data Sheets **118**, 26 (2014).
- [16] A. Kahler *et al.*, Nucl. Data Sheets **112**, 2997 (2011).
- [17] K. Kozier, D. Roubtsov, A. Plompen, S. Kopecky, Proc. PHYSOR 2012 - Advances in Reactor Physics, April 15-20 (2012).

