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INTERNATIONAL NUCLEAR DATA EVALUATION NETWORK (INDEN) ON THE EVALUATED DATA OF STRUCTURAL MATERIALS (6)

Summary Report of the IAEA Consultants Meeting
18 – 21 December 2023

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November 2024

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Contents

1. Introduction

A Consultancy Meeting was held from 18 to 21 December 2023 with the objective of bringing together the collaborators of the INDEN network to discuss the progress made and the issues identified in the evaluation of structural materials. The International Nuclear Data Evaluation Network (INDEN), managed by the IAEA, was initiated in 2018 as a platform for internationally recognized experts who, at regularly held meetings, exchange technical information and collaborate on nuclear data evaluation activities with the aim of improving upon the current quality of available nuclear data. The dual focus is convergence of evaluation input data and validation criteria as well as production of evaluated data files for testing, following best evaluation practices. The range of activities is broad and involves besides evaluation work also experimental campaigns, benchmarking to provide evaluation feedback, and methodological developments, in close exchange with national and international evaluation projects.

The particular focus of discussions at this meeting was to scrutinize INDEN evaluations, discuss their performance in various benchmarks, as many of these evaluations are considered for adoption in the upcoming ENDF/B-VIII.1 and JEFF-4 release. Several presentations were dedicated to novel evaluation methods based on the Monte Carlo approach, and therefore extensive discussions were dedicated to this topic.

The meeting was opened by Arjan Koning, Section Head of the IAEA Nuclear Data Section, followed by a brief introduction given by Roberto Capote and Georg Schnabel. Maria Diakaki agreed to serve as Rapporteur of the meeting. Gustavo Nobre agreed to take on the role of Chairperson to lead through the meeting program consisting of 13 presentations given by experts from seven Member States, OECD/NEA and the IAEA.

2. Presentation Summaries

Participants' presentations are available from the meeting webpage:

https://conferences.iaea.org/event/375/contributions/

2.1 The ENDF/B-VIII.1 release and future plans on structural materials, G. Nobre

Gustave Nobre summarized the ongoing preparatory work for the next release (version VIII.1) of the ENDF/B library foreseen for 2024. This included an overview of planned updates to the evaluations in the various sublibraries. Furthermore, the adoption of GitLab for coordinating the collaborative library update process was presented, providing examples which make the benefits tangible, such as improved traceability. Finally, the status of the draft of the ENDF/B-VIII.1 reference paper was presented.

2.2 Accounting for model uncertainty in Bayesian evaluation of nuclear data, E. Alhassan

Erwin Alhassan presented a Monte Carlo-based evaluation method that takes into account potential deficiencies of nuclear models. The method employs Bayesian Model Averaging (BMA) to sample in addition to model parameter values also from various nuclear models relevant for the prediction of cross sections, such as the optical model and level density models. The approach was implemented for the nuclear model code system TALYS and results of its application for proton-induced cross sections of ^{58}Ni were discussed. While the overall feasibility of the approach has been demonstrated, one open issue is the appearance of unphysical kinks in excitation functions due to applying the BMA locally at each incident energy without imposing any constraint on smoothness. The solution put forward in the presentation is to perform a post-processing of the obtained cross section curves by fitting splines through them. As the approach implements a Monte Carlo procedure, comprehensive uncertainty information can be extracted by calculating weighted averages from the obtained samples. The presentation also elaborated on how model uncertainties can be extracted from the evaluation procedure. In the future, the approach may be extended to include information from integral benchmarks, such as criticality benchmarks.

2.3 The nuclear data evaluation pipeline of Uppsala University (NEPU) - addressing model defects and data inconsistencies, A. Göök

The presentation titled "The Nuclear Data Evaluation Pipeline of Uppsala University (NEPU)" by Alf Göök, Henrik Sjöstrand, and Erik Andersson Sundén, addresses methods to handle model defects and data inconsistencies in nuclear data evaluations. The objective is to develop a pipeline that enhances methodologies to manage these issues, automates the evaluation process for reproducibility, and provides an intuitive framework for nuclear data evaluation. The pipeline integrates software packages and scripts to perform all nuclear data evaluation steps, e.g., utilizing EXFOR for data retrieval, the Levenberg-Marquardt algorithm for parameter optimization, and TALYS for nuclear reaction modelling. It operates on high performance clusters, which enables large-scale parallelization and efficient testing and validation. The workflow includes data retrieval, uncertainty correction, parameter sensitivity evaluation, Gaussian Process setup, and a Multivariate Normal (MVN) approximation for the posterior pdf. It addresses random uncertainties by estimating data distribution around a smooth energy-averaged cross-section using Gaussian Processes and corrects systematic uncertainties by identifying inconsistencies between datasets using linear splines and MVN priors. To account for model defects, Gaussian Processes are incorporated in the parameter domain, which allows the parameters to vary as a function of energy. This ensures a consistent physics description. The pipeline was applied to ^{52}Cr cross-sections and validated using cross-validation. The pipeline demonstrated good performance with a slight tendency to overestimate uncertainties. Future work involves refining the treatment of low-energy structures and ensuring the evaluation respects sum-rules.

2.4 Lowering the ENDF-6 entrance barrier for evaluators, G. Schnabel

The ENDF-6 format [1] is widely used for the storage and dissemination of nuclear data. Major nuclear data libraries, such as ENDF/B, JEFF, JENDL, CENDL, BROND, TENDL store nuclear data in this format. Despite the broad adoption of this format, software tools to interact with the data, especially regarding the creation of ENDF-6 files, are scarce. This circumstance motivated the development of a Python package at the IAEA Nuclear Data Section called *endf-parserpy* [2] whose purpose is to remove the technical barrier between data and users imposed by the ENDF-6 format. Users should be empowered to work with the data at a higher abstraction level than position-based access of numerical fields in an ASCII text file. The requirements that guided the development of the package were:

1) To support reading and writing of the entire ENDF-6 format standard
2) Convenient access to all data in a data science-centric language, such as Python and R
3) Provably correct implementation of the ENDF-6 format

These requirements were addressed by extending the formal notation used in the ENDF-6 formats manual to a formal language that also supports the specification of nested sections, repetitions, and conditional presence of ENDF-6 records [3]. The format description of the manual was subsequently translated into this formal language. The Python package endf-parserpy interprets the formal format description for the purpose of reading, writing, and validating nuclear data stored in the ENDF-6 format. More precisely, it maps the nuclear data from the ENDF-6 format into a nested dictionary in Python where all data is accessible under variable names. In addition, data organized in such dictionaries can also be written out as ENDF-6 formatted files. Therefore, users can approach these tasks on a higher logical level involving variable names and frees them from formatting data at a low-level involving position-based storage of numerical fields. The package is open-source, well-documented and available at [2].

References:

[1] https://www.nndc.bnl.gov/endfdocs/ENDF-102-2023.pdf
[2] https://github.com/iaea-nds/endf-parserpy
[3] https://arxiv.org/abs/2312.08249

2.5 New integral experiments in Rez - focus on PFGS of ^{252}Cf(s.f) and ^{235}U(n_{th},f), M. Kostal

Michal Kostal presented new integral experiments performed in Rez. He gave a brief description of the research infrastructure used by Rez experts, which are the LR-0, LVR-15 (Si filtered beam for stilbene calibrations) and VR-1 reactor as well as a ^{252}Cf source and various spheres including metallic spheres and water spheres to study gamma production. He further described the experimental methods available at Rez, which are neutron spectrometry (excellent agreement – PTB monolines and Si filtered beam), gamma spectrometry using stilbene up to 15 MeV, and gamma spectrometry using HPGe. Furthermore, activation measurements of activated samples (RR determination) and flux measurements (prompt gamma production experiments) can be performed.

After the description of available infrastructure and measurement possibilities, a summary of selected experimental results was given. Results associated with the newly published ICSPBEP benchmarks were presented:

- ALARM-CF-SST-SHIELD-001: The benchmarked quantity is neutron leakage flux and the spatial distribution of reaction rates.
- ALARM-CF-FE-SHIELD-002.
- ALARM-CF-NI-SHIELD-002: The benchmarked quantities are neutron leakage flux and reaction rates on surface.

Leakage benchmarks for aluminium, Teflon and tungsten are planned, with the benchmarked quantity being the neutron leakage flux and the reaction rates distribution in various depths of the material. It was emphasized that integral experiments, such as neutron leakage from simple mono material arrangements combined with reaction rates, are of great interest because they provide complementary information.

The presentation continued by summarizing a variety of performed measurement campaigns, which are briefly described in the following paragraphs.

Gamma production experiments using various neutron sources ^{252}Cf(s.f) and various solutions (NaCl, $FeSO_4$, $MnSO_4$) were performed, enabling the validation of capture gammas and gammas from inelastic scattering. This validation can also provide information on whether the data in nuclear libraries allows for the accurate calculation of gamma heating.

Measurements of Total Fission Gamma Spectra (TFGS) from ^{252}Cf(s.f) were realized with results being consistent with previous measurements. The comparison of these measurements with the ^{252}Cf(s.f.) prompt fission gamma spectrum (PFGS) above 2 MeV (where the contribution of the delayed gammas had not yet been definitely experimentally established) revealed a notable excess of TFGS over PFGS values. This finding indicates that the delayed γ-rays could extend from 2 MeV to even higher energies, but further study is needed.

Measurements of gamma spectra in the special core of LR-0 up to 13 MeV were performed. The comparison with the ENDF/B-VIII.0 evaluation showed good agreement. It was also shown that in the special core of LR-0, the gamma spectrum is undistinguishable from ^{235}U PFGS in the region above 10.5 MeV.

Furthermore, an experiment has been performed to determine the effect of iron blocks in the reactor core on criticality. In this experiment, a reference neutron field has been identified in the driver core used. The experimentally determined water level is used in the calculation with ENDF/B/VIII.0 in combination with various evaluations (Fe from INDEN, being a candidate for ENDF/B-VIII.1, O from ENDF/B-VII.1). The underestimation of k_{eff} using ENDF/B-VIII.0 becomes larger with an increasing amount of iron in the core. When 12 iron blocks are around the core and one large block is placed in the center (each block has 170 kg), the calculation underestimates the measurement by about 460 pcm.

During three large experiments, a large collection of various foils has been placed in the LR-0 reference field, benchmarking 30 evaluated reaction rates. In general, a good agreement with IRDF-II has been confirmed. Noteworthy, also a foil using the ^{58}Ni(n,x)^{57}Co reaction has been tested, which is not a dosimetrical reaction. However, measurements showed good agreement with ENDF/B-VIII, indicating that this reaction may be considered as a dosimetrical reaction in the future.

In another experimental campaign, a characterization of neutron spectra from ^{18}F producing accelerators was undertaken, which revealed a large discrepancy between measured and calculated spectra. This mismatch becomes worse for larger angles.

A characterization of neutron spectra from DT generators has also been performed using scintillation neutron spectrometry and semiconductor gamma spectrometry. These techniques have proven to be suitable methods for this purpose.

It has also been experimentally confirmed that the INDEN manganese evaluation is an improvement, which seems to be more reliable than other evaluations. The lower energy peaks (for example the DD reaction) were also evaluated by means of the ^{115}In(n,n') reaction because the cross section in the low energy region is much higher than for higher energies. The results are also consistent with results obtained by the stilbene detector.

Drawing from the experiences made in these and other experiments, the presentation also included useful suggestions and comments for consideration by meeting participants, which are summarized in the following paragraphs.

Integral experiments using a ^{252}Cf neutron source and well-defined material slabs or spheres of various materials and dimensions are excellent tools for the validation of cross sections. One reason for this statement is the fact that the ^{252}Cf(s.f) neutron spectrum is a standard with low uncertainties compared to the typical uncertainties in the reactions that need to be folded with it for the evaluation of the experiment. Therefore, it is justified to neglect the uncertainties in the ^{252}Cf(s.f) neutron spectrum. Furthermore, the evaluation of the pure ^{252}Cf(s.f) neutron spectrum allows for the realistic estimation of deconvolution method uncertainty. Because the spectrum is well known with very low uncertainties, the discrepancy between tabulated and evaluated spectra reflects the systematic uncertainty. One pertinent benchmark design is given by a sphere with ^{252}Cf(s.f.) neutron source in its centre. The simple geometry and good material characterization possible for this design helps perform reliable calculations, and hence promotes meaningful comparisons between calculated and measured values. Water can be used as solvent to thermalize the neutrons so that most gammas are produced by thermal neutron capture.

There are also other experiment types that have been identified as tools for giving valuable feedback to nuclear data evaluators. The silicon filtered neutron field is an essential tool for the verification of the neutron response matrix used in the evaluation of benchmark measurements. Furthermore, integral benchmarks using the small DT generators provide valuable validation of data needed for fusion research. In this regard, the methodology used in the LR-0 lab seems to be pertinent. Finally, the driver core used in the LR-0 benchmark refence neutron field is a valuable instrument for the validation of various structural component cross sections. For instance, this benchmark already helped reveal discrepancies in k_{eff} hinting at inaccuracies in the neutronic description of steel. As another example, it allowed to identify a trend: With an increasing amount of iron acting as reflector, the underestimation of the measurement by the calculation becomes larger.

Finally, the next paragraphs describe experimental possibilities that can be implemented in the future.

Activation experiments can also be realized with "small sources" with a Q=1E8 n/s. In this case, however, large foils must be used. In addition, if detectors are well-characterized and computational models available for them, even measurements of large foils on cap are feasible.

Complementary experiments, namely experiments using independent methods, such as the proton recoil method and activation method, are of great interest because results can be cross-validated.

The presented benchmarks have been demonstrated to be useful for the identification of issues in differential nuclear data. However, for the identification of issues in the description of gamma production, there is a strong need of well-defined integral experiments focusing on gamma production.

2.6 JEFF-4T3 status and NEA pipeline developments, D. Foligno

JEFF-3.3, a milestone in nuclear data evaluations, was released in 2017, with the highly anticipated JEFF-4.0 slated for 2024. During the interim, annual test library releases were issued to support continuous development and refinement efforts.

A significant aspect of this period was the thorough reassessment of fission yields for thermal neutron induced fission of ^{235}U and ^{239}Pu. However, this endeavor faced challenges due to discrepancies among experimental datasets. To tackle this issue, two evaluation methods were proposed: "conservative sorting" and "strict sorting." Despite yielding similar mean values, these methods displayed differences in uncertainties. After rigorous testing, the conservative approach was selected, involving the addition of a 2.5% independent uncertainty to reconcile the varying datasets.

Throughout the evaluation process, a minor normalization error was identified by Charles Wemple from Studsvik, underscoring the importance of meticulous verification and testing procedures. This error was swiftly addressed, ensuring the accuracy and reliability of the data.

In the latest JEFF-4T3 iteration, several INDEN files were integrated, and Cédric Jouanne from CEA completed gamma decay cascade reconstructions for inelastic scattering and neutron capture. Additionally, updates were made to neutron evaluations, including the restoration of eight groups of delayed neutron data and adjustments to major actinides such as U-235 and Pu isotopes. Two datasets for Pu were generated: unadjusted and adjusted, with further testing required to determine their suitability for inclusion in the final JEFF-4.0 release.

JEFF-4T3 also witnessed the transition from TENDL-2021 to TENDL-2023 files and from JENDL-4 to JENDL-5. However, ongoing work on ^{238}U necessitated a delay in the official JEFF-4T3 release to ensure thorough verifications.

Efforts were also dedicated to streamlining data processing procedures, with the NEA developing a dedicated pipeline on GitLab. This pipeline, tailored for the JEFF community, facilitates the automatic and consistent processing of JEFF files. Notably, it enables the provision of processed files for various codes, including TRIPOLI-4, FISPACT-II, MCNP, Serpent, SCALE, and OpenMC. Recent enhancements have further expanded its capabilities, including the implementation of processing routines for Thermal Scattering Law files, thereby enhancing the utility and accessibility of the data.

2.7 Neutron inelastic cross section derived from gamma-production cross section (n,n'γ) reactions and Pygmy dipole resonance, V. Pronyaev

Vladimir Pronyaev discussed the origin of the differences between the total inelastic cross section and the sum of the cross sections of gamma transitions to the ground state measured in inelastic scattering. It was shown that the main contribution to the missed gamma transitions in some nuclei can be made by the isoscalar component of the pygmy-dipole resonance, lying between 5 – 7 MeV of excitation energy with a direct gamma transition to the ground state. New measurements can be carried out by paying more attention to the registration of gamma rays with energies up to 8 MeV.

2.8 Updates on the study of the Fe isotopes, M. Diakaki

Maria Diakaki's presentation focused on both theoretical and experimental work on iron. During the CIELO project [1], issues in the description of the $^{56}Fe(n,\gamma)$ reaction were identified, which were addressed by adding an artificial background between 10 eV and 100 keV in the ENDF/B-VIII.0 evaluation. M. Diakaki and collaborators investigated possible physical interpretations of this additional background and hypothesized that it may correspond to a direct radiation capture (DRC) process. Results including the theoretical modeling of the DRC using the pdix code [2–4] were shown and compared with JEFF3.3, ENDF/B-VIII.0 and the INDEN candidate evaluation. One important finding was that the calculation results are sensitive to changes in optical model parameters. It was also recognized that negative resonances need to be added to be able to describe the cross section simultaneously correctly at the thermal point and to align with the INDEN 2022 / JENDL-5 evaluation in the energy region where the artificial background needed to be added. The treatment of the direct capture components still needs to be included in the evaluation process using the CONRAD code. The functionality for testing and adjusting the resolved resonance parameters (RRP) is already available in CONRAD. The investigations summarized indicate that the direct capture process is important and needs to be considered in the modeling for a correct description.

Regarding experimental work, preliminary results, and details of two experimental campaigns at GELINA were presented.

Neutron induced scattering (including both elastic and inelastic) on iron isotopes was measured at GELINA using highly enriched ^{56}Fe and ^{54}Fe targets. It is the first time that enriched targets are used. The analysis of ^{56}Fe still needs to be finalized. A new experimental campaign to measure neutron scattering on ^{63,65}Cu with enriched samples will be performed within the APRENDE project using the ELISA setup. This work will be done within a PhD thesis supervised jointly by NTUA and CEA. Improvements of the ELISA setup are also considered and discussions in this regard with the local staff at JRC-Geel are ongoing.

Transmission measurements using natural Fe samples of different thicknesses are performed at GELINA. Two natural iron samples of two thicknesses have already been measured and the analysis is ongoing. A thick natural iron sample (with a thickness of about 9 cm) will also be measured once GELINA is functional again.

References:
[1] M. Herman et al., Nucl. Data Sheets **148** (2018) 214-253.
[2] A. Mengoni, et al., Phys. Rev. C (rapid) **52**, No 5 (1995).
[3] T. Kikuchi, et al., Phys. Rev. C **57** (1998) 2724.
[4] Y. Nagai, et al., Phys. Rev. C **102** (2020) 044616.

2.9 Measurements and evaluation of structural materials at RPI, Y. Danon

Yaron Danon presented some recent experimental, validation, and evaluation results for ^{54}Fe, Pb, Zr, F and Ta.

^{54}Fe measurements and evaluation

Measurements of a 96% enriched ^{54}Fe sample were performed for neutron capture using an array of C_6D_6 detectors at a flight path distance of 45m, and transmission at a flight path distance of 30m. The experimental data were reduced to capture yield and transmission including covariances. These data and other data available in EXFOR [1] were used to evaluate resonance parameters by fitting the experimental data using SAMMY [2]. Current results for both transmission and capture were shown. The new data and evaluation will mostly impact parameters below 300 keV.

Pb isotope evaluations

Results for Pb isotopes were shown during the INDEN meeting in 2022. In the 2023 meeting it was reported that the evaluations for ^{206,207,208}Pb had been completed and submitted to ENDF/B-8.1b3.

Zr isotope evaluations

The presentation showed a sensitivity analysis quantifying the contribution of different Zr isotopes and reactions to criticality. Based on this information and new available experimental data, RPI is focusing on evaluation of the RRR and URR for ^{90,91}Zr isotopes. SAMMY fits for ^{90}Zr were presented extending the RRR to 500 keV.

F and Ta Quasi differential measurements

New quasi-differential measurements for TEFLON ($(C_2F_4)_n$) and Ta samples were performed to validate new ENDF/B-8.1b2 evaluations. The experimental results for different angles were compared with MCNP simulations of the experiments. A carbon sample was also measured and used for normalization of the simulations and for validation of the experimental processing and the simulations' accuracy.

The results for Ta shown in Fig. 1 indicate that the new evaluation ENDF/B-8.1b2 is an improvement over the previous ENDF evaluation, especially at back angles.

A TEFLON sample was measured to validate the ENDF/B-8.1b2 evaluation for fluorine which was adopted from an INDEN evaluation. Overall, the new ENDF/B-8.1 b2 evaluation is an improvement over ENDF/B-8.0 [3]. An example is shown in Fig. 2 for 150 deg demonstrating that the new INDEN evaluation has the best agreement with the experimental data.

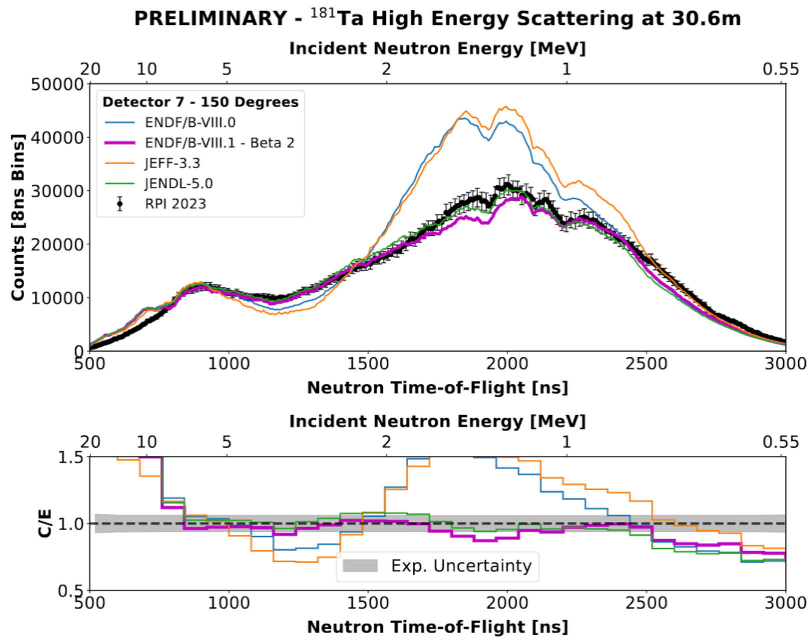


FIG. 1. Neutron time of flight spectrum for neutrons scattered from Ta to a back scattering angle of 150 deg, comparing the experiments with simulations using different evaluations. Both ENDF/B-8.1b2 and JENDL 5.0 agree best with the experiment compared to ENDF/B-8.0 and JEFF-3.3 evaluations.

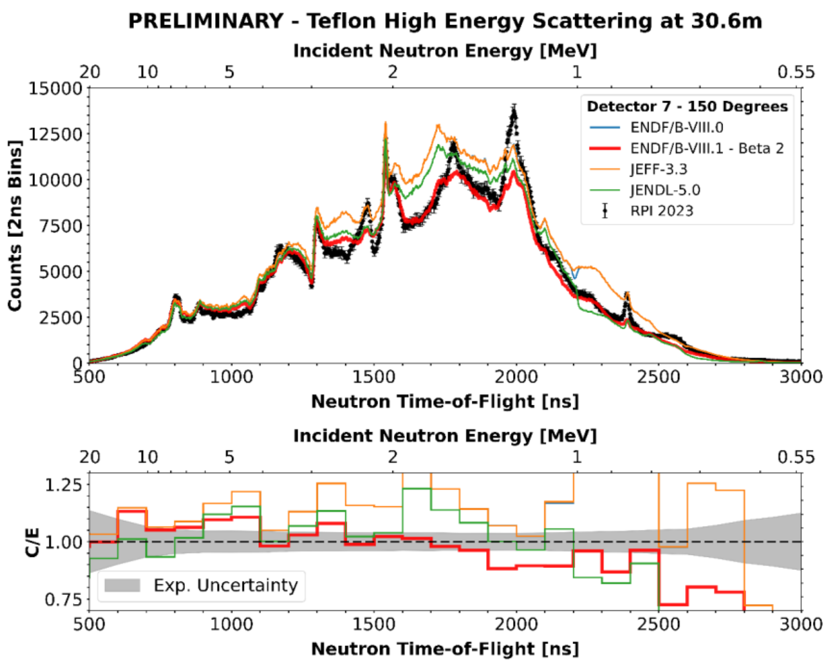


FIG. 2. Neutron time of flight spectrum for neutrons scattered from TEFLON to a forward scattering angle of 150 deg, comparing the experiments with simulations using different evaluations. The ENDF/B-8.1b2 (INDEN) evaluation shows very good agreement with the experimental results compared to other evaluations.

References :
[1] N. Otuka, E. Dupont, V. Semkova, et al., Towards a More Complete and Accurate Experimental Nuclear Reaction Data Library (EXFOR): International Collaboration Between Nuclear Reaction Data Centers (NRDC), Nucl. Data Sheets **120** (2014) 242.
[2] N.M Larson, Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations, Report ORNL/TM-9179/R8, Oak Ridge National Laboratory (2008).
[3] D.A. Brown, M.B. Chadwick, R. Capote, et al., ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data, Nucl. Data Sheets **148** (2018) 1 – 142.

2.10 Some issues with the INDEN structural material evaluations, A. Trkov

Andrej Trkov summarized the performance of the ^{56}Fe, ^{57}Fe, ^{63}Cu and ^{65}Cu INDEN candidate evaluations in various benchmarks and identified open issues. Overall, the ^{56}Fe and ^{57}Fe evaluations show good performance and no changes to the cross sections are needed. For the copper evaluations, it was found that the performance of the INDEN copper evaluations is generally good. However, the angular distributions included in the evaluation seem to be in contradiction with data measured by Popov below 0.3 MeV. For this comparison, the angular distribution data was reconstructed based on resonance parameters, including some smoothing. It was noted that potentially a factor (2l+1) had been erroneously included in the Legendre coefficients, potentially making the comparison invalid. The simple solution attempt to integrate Popov data below 0.3 MeV into the evaluation seems, unfortunately, to degrade the performance in benchmarks, particularly in the case of IMF020 and IMF022. These findings hint at the copper evaluations being affected by unidentified compensating errors or that the IMF020 and IMF022 benchmarks are wrong. At present, no adequate solution regarding the angular distribution is available.

2.11 Nuclear data feedback on structural, moderating and absorbing materials through the MAESTRO experimental programme in MINERVE, P. Leconte (presented by D. Bernard)

Several experimental programmes have been carried out for validating nuclear data for LWR reactors over the past 30 years (Burn-up credit programme 1992-2000, OSMOSE 2005-2010, OCEAN 2005-2010, HTC 2004-2011). However, a lack of validation remained for important structural materials (e.g. zircaloy, Inconel, stainless steel), moderator materials (e.g. light and heavy water, carbon, beryllium), detection materials (e.g. cobalt, vanadium, rhodium) and absorbing materials (Ag, In, Cd, natural Dy, Er, Eu, Gd, Hf).

The aim of the MAESTRO programme launched in 2011 is the experimental validation of capture cross sections for structural, detection and absorbing materials for GEN-III+ applications, as well as the validation of scattering reactivity worth of moderators. The materials considered in the experiments are water, natural beryllium and carbon and methylene for moderators, natural Mg, Al, Cl, Ca, Ti, Cr, Fe, Ni, Cu, Zn, Zr, Mo and Sn for structural materials, natural V, Mn, Co, Nb, Rh for detection materials, natural Ag, In, Cd, Eu, Gd, Dy, Er, Hf, Eu, Ag and Cs for absorber elements and several industrial alloys, i.e. Zy4, M5, SS304, SS315, Inconel-800. Within the MAESTRO programme, these materials are studied in pile-oscillation and activation experiments.

The experimental campaigns in the MAESTRO programme have been carried out in four phases. In the first phase taking place in 2011, a R1UO2 core configuration (see diagram in presentation) was employed. Pile-oscillation of Rh, Co, Mn, V, Au rods and B, Li and Gd solutions was studied, and neutron activation measurements were performed for Co and Mn. Further details are provided in JEF/DOC-1486 [1]. In the second phase running from 2012 to 2012, the MAESTRO core configuration was adopted, and neutron activation measurements performed for ^{109}Ag, ^{133}Cs, ^{51}V, ^{115}In, ^{151,153}Eu, ^{64,68}Zn, ^{94,96}Zr, ^{98,100}Mo and ^{112,117,122}Sn and ^{197}Au, documented in the WONDER2015 proceedings [2]. In the third phase from 2013 to 2014, using again the MAESTRO core configuration, spectral indices, cadmium ratio and CU_8/F_{tot} were assessed, and dosimetry performed. Pile-oscillation measurements were undertaken for many materials (Au, B, Li, Ag, Cd, Cl, Ca, V, Co, Cr, Cs, Dy, Er, Eu, Gd, In, Mn, D2O, H2O, Be, CH2 , Cu, Fe, Mo, Nb, Ni, Ti , Zn, V, Al2O3 , Al, C, Mg, Si, Sn, Inconel-718, SS304, SS316, Al-5754, M5TM, Zy4). Finally, in the fourth phase that started in 2016, a core configuration labeled as MAESTRO SL-core was adopted and pile-oscillation measurements carried out for Hf, ^{107}Ag, Rh and ^{153}Eu. The samples used were available as either pure rods, liquid solutions or powder mix and have been carefully calibrated and assessed. In particular, reactive impurities were evaluated, and masses and dimensions of samples accurately determined at a level of 0.1 mg and 10 μm, respectively.

Accompanying simulations were performed with TRIPOLI using a model of the MINERVE core. The model was simplified by using a homogenized driver zone and a simplified description of the graphite reflector. Validation studies have been undertaken to gauge the impact of these simplifications on simulation results. Rigorous uncertainty quantification was undertaken to consider three types of uncertainty: measurement uncertainty, technological uncertainties (e.g. related to sample characteristics) and the Monte Carlo error. The APOLLO/P_{ij} model for uncertainty analysis was employed as it was deemed accurate enough and features comparatively short computation times.

In the following, important findings of the analysis of spectral characterization, neutron activation and pile-oscillation experiments are provided. The simulations used as nuclear data library the test library JEFF-T4 as well as JEFF-3.2 and 3.1.1.

The microscopic fission ratio was measured with micro fission chambers relying on thermal (^{235}U, ^{239}Pu) and threshold reactions (^{240}Pu, ^{242}Pu). The simulation results for the ratios of these reactions were compatible with the measurements considering uncertainties. Likewise, simulation results of the activation rate ratio ^{58}Ni(n,p)/^{197}Au(n,γ), and capture rate on ^{238}U and total fission rate of ^{235}U+^{238}U using UO_2 samples were compatible with measurements.

However, the analysis of cadmium ratio experiments revealed discrepancies between measurements and simulations pointing at issues in the evaluated nuclear data. These discrepancies were observed for ^{115}In(n,γ)^{Cd}/^{115}In(n,γ), ^{109}Ag(n,γ)$_{Cd}$/^{109}Ag(n,γ) and ^{133}Cs(n, γ)$_{Cd}$/^{133}Cs(n,γ) with simulation results being multiples of the experimental uncertainty away from the measured values. For indium, it was discovered that the description of the isomeric ratios is missing in the investigated JEFF-3.x libraries, which may be related to the observed discrepancy.

Neutron activation experiments were performed with irradiation times between one and three hours at 80 W, followed by a cooling time of a few hours. Acquisition times for γ-spectrum measurements were minutes to hours. Correction factors were computed to account for self-absorption inside the sample as well as the spatial distribution of the γ-source. Relevant radioactive decay data comprised half-lives, γ-emission probabilities as well as the isomeric rate for metastable nuclides. Measurements were made relative to gold capture rates, employing three pure gold rods and one aluminum alloy of gold. The measurements confirmed the adequateness of JEFF-3.2 capture cross section evaluations for ^{98,100}Mo, ^{115}In, ^{109}Ag, ^{133}Cs, ^{96}Zr, ^{64,68}Zn. Going from JEFF-3.1.1 to JEF-3.2, improvements for ^{94}Zr and ^{122}Sn could be confirmed. However, improvements are still required for ^{151,153}Eu, ^{113}In, ^{94}Zr and ^{112}Sn. An underestimation of ^{153}Eu capture is consistent with BUC programme results.

Pile-oscillation experiments relied on a servo-driven calibrated pilot rod. At least five measurements of ten cycle oscillations per sample were carried out. Reactivity worth measurements were normalized by using the gold standard (implemented as pure rods of gold (99.995% purity) with 1.0, 1.6, and 2.0mm diameters). Regarding, uncertainty quantification, several uncertainties could be reduced compared to older programmes. Using 10 cm long rod type examples, it could be confirmed that JEFF-3.2 capture cross section evaluations for Fe, Cr, Ni, Mo, Cu are adequate and a good consistency for stainless steel was also observed. Also, the JEFF-3.2 scattering cross section evaluation for CH_2 and Be turn out to perform well. Improvements, however, are required for Zn, Ti and Nb and odd results were observed for Inconel-718 alloy, which consists mostly of nickel. Discrepancies for 30 cm long rod-type samples were more pronounced affecting most studied samples, in particular the graphite results, which is relevant as the elastic scattering cross section of ^{nat}C is a neutron data standard. Several causes of errors were investigated, such as a bias in the IFP (= perturbation approach introduced in TRIPOLI4-DEV) calculation method, missing impurities of the material certificate and photonuclear reactions. The consistency for liquid type samples was overall much better. However, results of D_2O are dubious with a C/E-1 value of -32% and the investigation of possible causes did not yield an indication of the reason. Also, improvements and/or new measurements are required for Er and In. On the positive side, reactivity worth for Cd, Cl, Gd, Ag, Cs, Dy and Mn could be well predicted using JEFF-3.2, and Cd clearly improved from JEF-3.1.1 to JEFF-3.2. Finally, regarding the measurements using powder type samples, a slight underestimation was observed for ^{107}Ag, which, however, is acceptable considering the low impact in fuel cycle studies. An underestimation, consistent with neutron activation experiments, was confirmed for ^{153}Eu. The capture cross section evaluations of ^{103}Rh and ^{nat}Hf seem to be adequate based on the pile-oscillation results.

In summary, the spectral characterization experiments showed very good consistency for all measurements. Nuclear structure data may be improved by identifying a possible energy dependent behavior of the isomeric ratio of ^{115}In and ^{133}Cs capture. Furthermore, many materials could be validated by demonstrating a difference of experiment and simulation below a 2σ threshold (scattering materials: H_2O, CH_2; capturing materials: Rh, Hf, Cd, Cl, Gd, Ag, Cs, Dy, Mn, Fe, Cr, Ni, Mo, Cu; and consistency with stainless steel 304L and 316L). However, evaluation improvements and/or additional measurements are required for the scattering materials D_2O, C, Al, Mg and for the capturing materials Nb, Ti, Zn, Zr, Si, Sn, Er, In, ^{107}Ag and ^{151,153}Eu. In addition, some clear inconsistencies, probably due to issues with sample characterization, were discovered for Inconel-718 (inconsistent with Ni) and Al5754 (inconsistent with Al). Comparing JEFF-3.1.1 to JEFF-3.2 performance, the new evaluations of capturing materials ^{122}Sn, Zn and ^{113}Cd clearly improve performance. In the future, sensitivity coefficients provided by the EGPT method implemented in APOLLO2 could be leveraged by the CONRAD code to derive trends and associated covariance for nuclear data.

References:

[1] P. Leconte, "MAESTRO: Measurement of the thermal capture cross section of Mn55, Co59, Vnat and Rh103", November 2012, JEF/DOC-1486

[2] P. Leconte, B. Geslot, et al., EPJ Web Conf. 111 (2016) 07001

2.12 Halfway Monte Carlo for integral adjustment, E.A. Sunden

We have developed a method to include integral data while being constrained by differential measurements. The Half Monte Carlo (HMC) method has been implemented and is ready to be integrated into the pipeline at Uppsala University. The inclusion of integral data does not affect the central values of the cross-sections by more than 2% in a bin. However, it affects the correlation between reaction channels. Future use of the HMC framework includes work on shielding experiments (SINBAD).

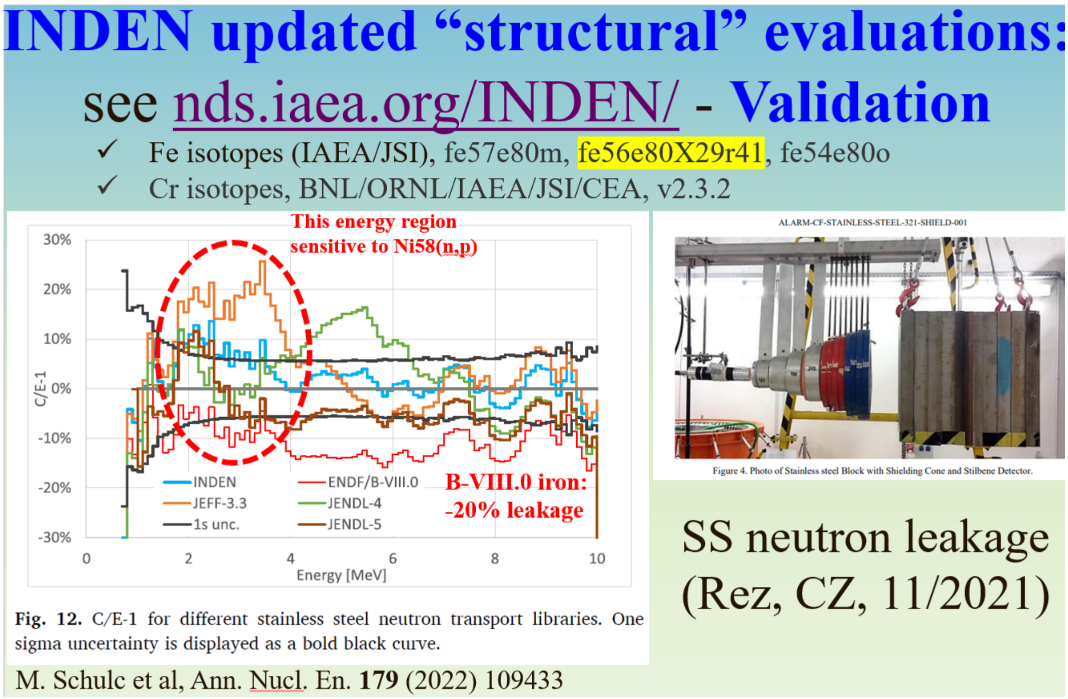
2.13 Overview of selected INDEN evaluations ^{56,57}Fe, ^{63,65}Cu, and ^{19}F, R. Capote

A comprehensive summary on modifications of the IAEA INDEN evaluations of iron, copper and fluorine isotopes was presented and discussed.

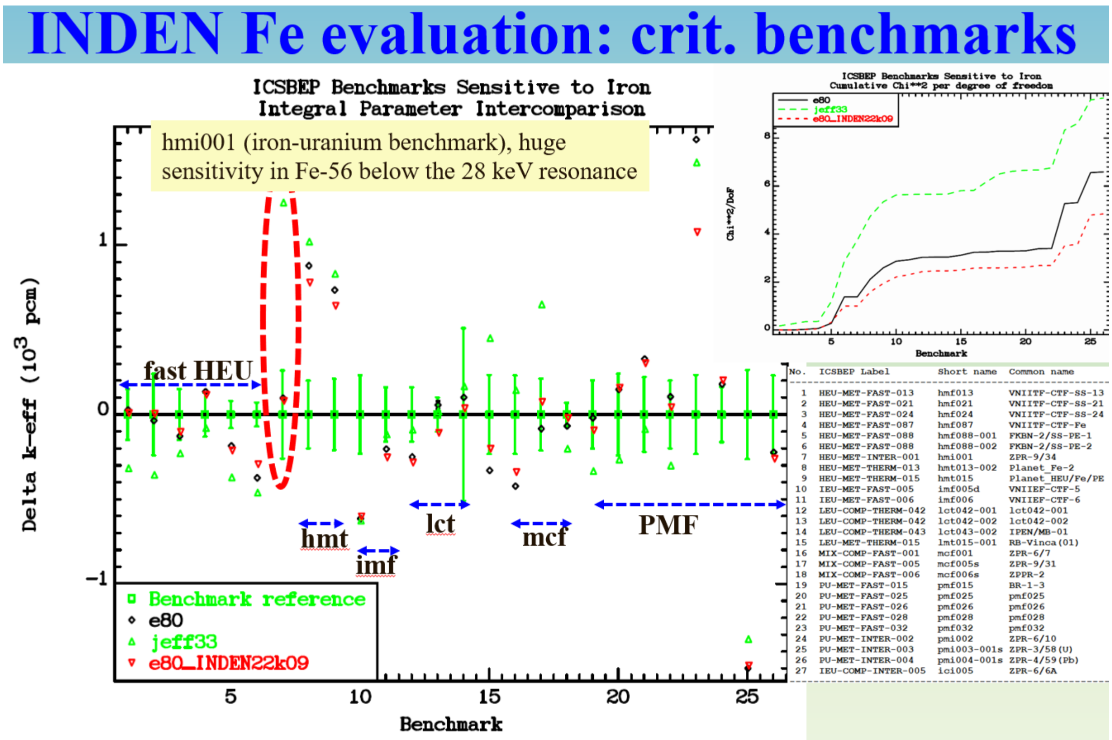
Updated evaluated files are available from the INDEN webpage (INDEN - International Nuclear Data Evaluation Network (iaea.org)): tab: Fe isotopes, tab: Cu isotopes, and F-19.

Fe isotopes:

Improvements in iron addressed deficiencies in neutron transmission through very thick shielding in the resonance region. Both changes in ^{57}Fe total cross sections and small changes in ^{56}Fe elastic cross sections were responsible for improved performance. Capture on iron isotopes was fixed by RPI experiments in the fast region above 400 keV. A 1/v background contribution likely coming from direct capture was confirmed for ^{56}Fe below 100 keV of neutron incident energy, which is in good agreement with the JENDL-5 evaluation. RPI (quasi-differential) and Rez (Cf-neutron leakage) experiments confirmed superior performance of the INDEN Fe evaluation compared to the JEFF-3.3 for neutron incident energies from 400 keV up to 3 MeV.



Iron criticality performance of the ENDF/B-VIII.0 evaluation was maintained as shown in the figure below.



Criticality as a function of the stainless steel reflector thickness is also preserved compared to ENDF/B-VIII.0 and improved compared to the JEFF-3.3 evaluation as shown in the figure below.

INDEN Fe/Cr evaluation: SS reflectors

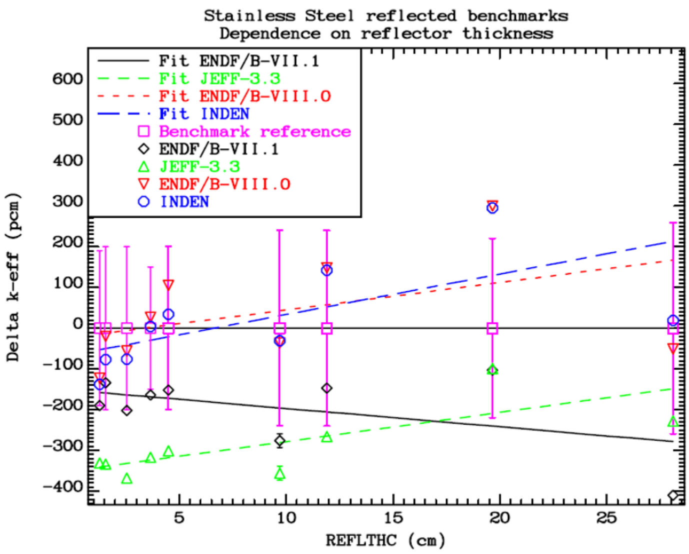


Table 2. Short list of ICSBEP criticality fast benchmarks with different thicknesses of stainless steel reflectors.

ICSBEP Label	Short name	Common name	Reflector thickness [cm]
HEU-MET-FAST-084	hmf084-019	Comet-Fe	1.27
PU-MET-FAST-025	pmf025	pmf025	1.55
HEU-MET-FAST-084	hmf084-007	Comet-Fe	2.54
HEU-MET-FAST-013	hmf013	VNIITF-CTF-SS-13	3.65
PU-MET-FAST-032	pmf032	pmf032	4.49
HEU-MET-FAST-021	hmf021	VNIITF-CTF-SS-21	9.70
PU-MET-FAST-026	pmf026	pmf026	11.9
PU-MET-FAST-028	pmf028	pmf028	19.7
PU-MET-FAST-015	pmf015s	BR-1-3	28.1

A. Trkov et al, EPJ Web of Conferences **284**, 12002 (2023)

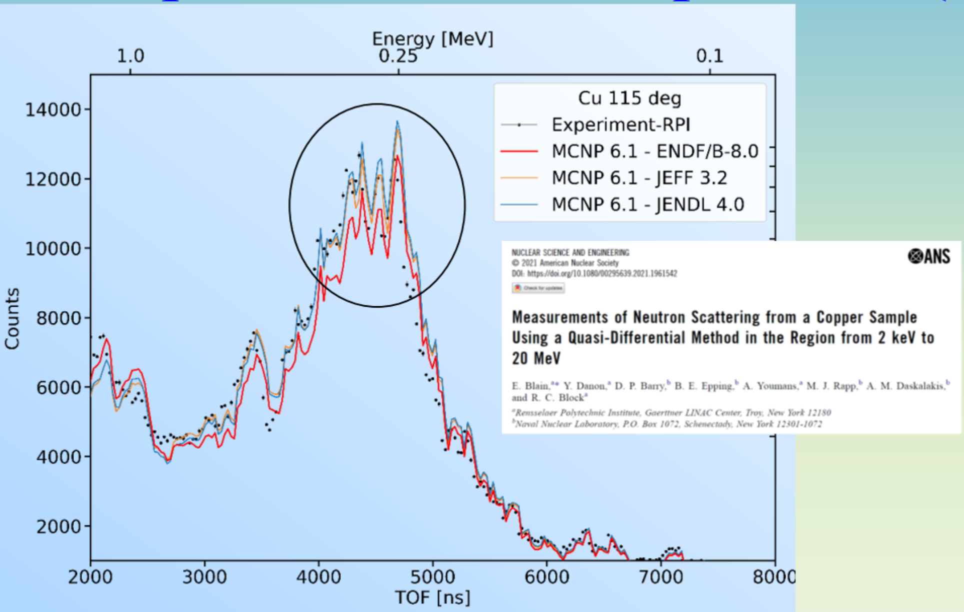
The PETALE experiment broadly confirmed the better performance of the Fe INDEN evaluation as shown by Ligonnet et al at the JEFF meeting in 2023.

It is noted that the ^{54}Fe evaluation should be improved, especially the inelastic and elastic reactions using the latest measured data in Geel.

Cu isotopes:

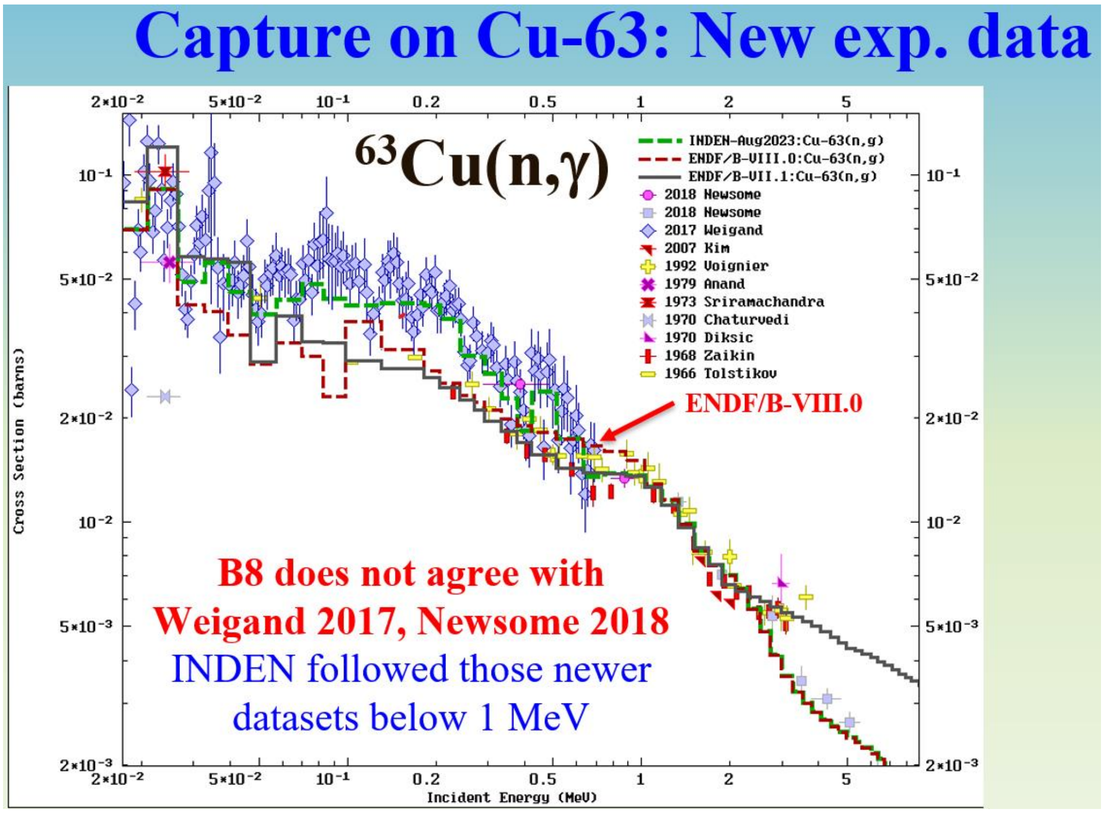
Neutron reaction data for the copper isotopes were re-evaluated within the INDEN project. Further work is needed to improve the agreement with discrepant data for the elastic and inelastic cross sections below 3 MeV. It was shown at RPI that the ENDF/B-VIII.0 evaluation around 300 keV disagreed with the measured neutron yield, see the figure below.

RPI quasi-differential experiment (2021)



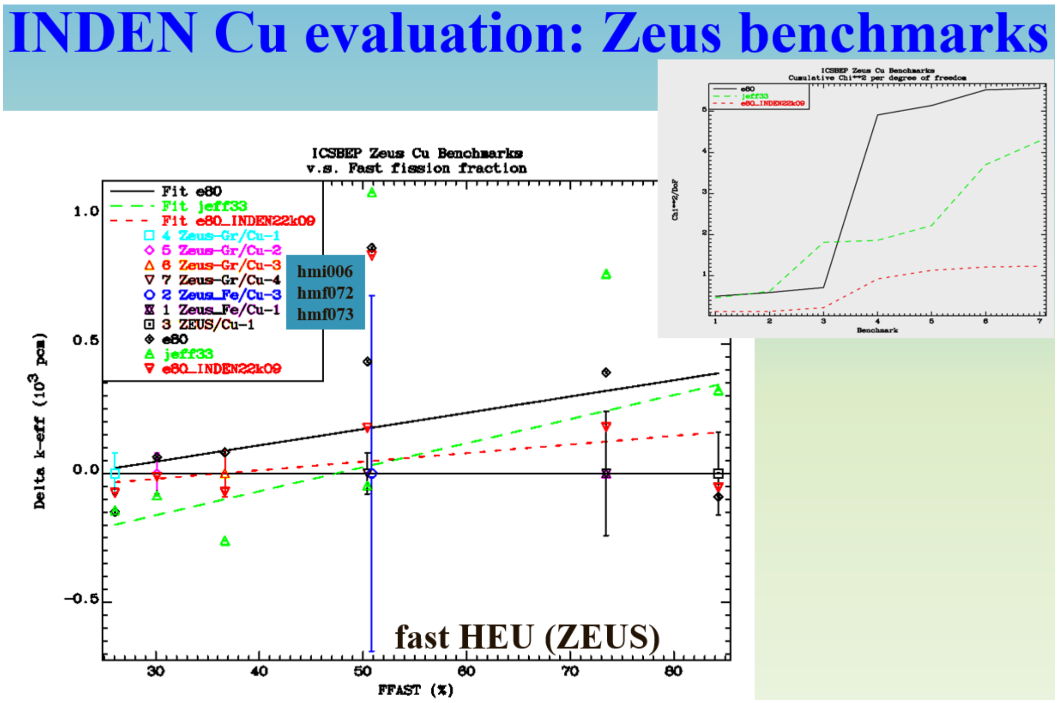
Y. Danon, presented at INDEN-SM meeting, 2022

The capture cross section was changed in the RRR and in the fast region both for ^{63}Cu (the dominant element) and ^{65}Cu. See the new evaluation compared to the previous one below.



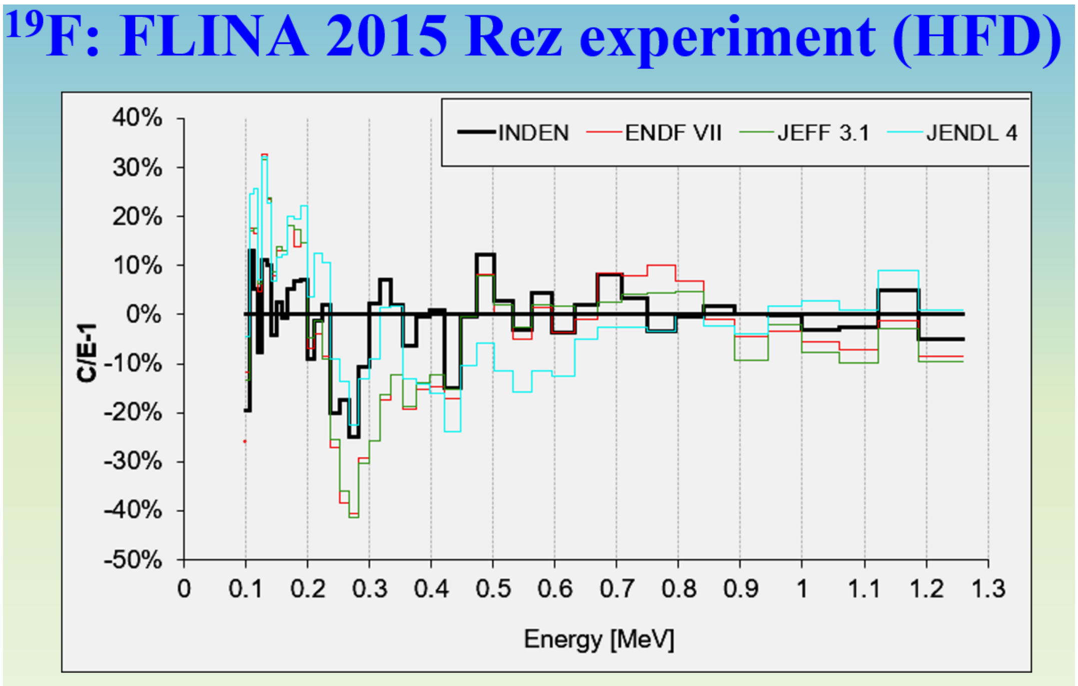
Criticality as a function of the fraction of fission induced by fast neutrons (FFAST%) in copper reflectors is shown in the figure below.

The INDEN copper evaluation improves the K_{eff} trend as a function of FFAST% as shown in the figure below.



^{19}F:

Improvement in fluorine evaluations was related to identified deficiencies in inelastic cross sections. Morgan (n,n'γ) data were used to derive the inelastic scattering cross sections on the first and second excited levels of fluorine. Elwyn elastic angular distributions were used for the evaluated file to define MF4 MT2 below 1.2 MeV. The impact of those cross-section changes on integral performance was dramatic and resulted in significant improvements of both criticality and shielding benchmarks, see the FLiNa leakage reactor experiment compared with the latest INDEN evaluation in the figure below.



Summarizing, the IAEA INDEN collaboration is addressing data issues with the following strategy:

- Identify data problems through integral validation and feedback;
- Identify underlying data issues in differential data evaluation (using sensitivity tools, among others).
- Assess available experimental differential data to find alternative solutions to improve integral benchmarks.
- Update selected experimental data to the latest standards/references.
- A GLSQ fit of available comprehensive datasets is the preferred solution.

3. Recommendations, Actions and Comments

Recommendations obtained during the meeting as well as planned actions are listed in the following. Remarks made during the meeting related to the recommendations and actions are also included.

First, recommendations for specific nuclides are given. Afterwards, general recommendations applying to more than one structural material are listed.

3.1 Individual nuclides

Iron:

- On-going experimental work related to elastic and inelastic scattering on iron isotopes will need to be considered in future evaluations.

- Current INDEN evaluations have been extensively validated with positive feedback including preliminary PETALE results, PCA (Westinghouse), Rez neutron leakage, 14 MeV benchmarks, ASPIS shielding and criticality benchmarks.
- Fe-54 inelastic deserves additional work. A new Resolved Resonance Region (RRR) evaluation for Fe-54 is on-going at RPI using new data from RPI, n_TOF and other collaborations and institutions.
- Measurements of prompt inelastic gammas from iron using a Cf source are planned.
- Measurement of capture for nat-Fe and Fe-56 from 1 keV and 2 MeV had been performed at RPI and were used above 400 keV for the CIELO (B8) evaluation. Recently, similar measurements of capture and fission in the thermal and resonance range have been performed for Fe, Mn, Co. Measurements for Cd, Cs are planned.

Lead:

- It is recommended to consider updated evaluations of Pb for ENDFB81.
- Additional technical work to further improve the performance of lead, especially regarding the performance for thermal benchmarks, is recommended. There is a documented improvement of lead fast critical assemblies. However, thermal benchmarks remain a challenge.

Zirconium:

- Work will be started on Zr-90 and Zr-91 within a collaboration of RPI, ORNL, and BNL with the IAEA contributing to these efforts.

Nickel:

- Lead slowing down spectrometer measurements show deficiencies in Ni RRR evaluations.
- There is a Cf neutron leakage measurement at Rez accepted as benchmark, which will be distributed on the INDEN website.
- These new measurements will be used as a basis to review the current INDEN evaluation.

F-19:

- The INDEN evaluation represents an improvement over previous evaluations (as indicated by the quasi-differential data of RPI, and criticality benchmarks) but further work is needed to address identified issues in quasi-differential measurements.
- It was recommended to use Teflon without additives for measurements (known under the name of Virgin Teflon).
- Neutron leakage measurements of fluorine containing materials both in Cf and 14 MeV sources are very much encouraged.
- Also, LPS (Livermore Pulsed Sphere) benchmarks with fluorine may be considered for validation.

Chromium:

- Validation for Cr (within the PETALE programme) is ongoing.
- The INDEN chromium evaluation was validated in criticality benchmarks and 14 MeV leakage experiments, and indirectly also validated by stainless steel (20% Cr) neutron leakage measurements at Rez.

Copper:

- New capture high-resolution measurements on Cu isotopes are required.
- Weigand 2017 data for Cu-63 and Prokop 2019 data for ^{65}Cu measurements are low resolution data and cannot be used to improve the RRR.
- New scattering measurements are planned at GELINA using the ELISA setup.
- The evaluation work for Cu within INDEN is ongoing, addressing differences to differential data that includes 1) angular distributions below 300 keV, 2) double-differential cross sections

from 10 to 20 MeV (to improve fusion performance in INDEN files, e.g. FNG benchmark), and 3) total cross sections and accordingly elastic and inelastic cross sections below 3 MeV. Options are explored to do an additional 14 MeV validation of copper blocks (e.g. at CV Rez).

- Weigand measurement for ^{63}Cu using TOF/Linac must be used carefully. The TOF setup seems not to be well characterized, such as the thickness of the Cu specimen, which is even a concern if the cross section is very low, e.g. tens of millibarn. Furthermore, information regarding whether a multiple scattering correction has been performed is missing, which is important in the resolved resonance region.

3.2 General

This section is subdivided into three groups with information pertaining to evaluation, validation, and the use of angular distributions.

Evaluation

- The direct capture contribution needs to be considered in the resonance evaluation up to a certain energy. For example, the s-wave contribution is important below the 28 keV resonance in ^{56}Fe, and the d-wave contribution seems to be important in ^{56}Fe somewhere between 500 keV and 2 MeV. Similar considerations are valid for Pb and Si isotopes.
- Evaluations should respect microscopic experimental data including cross sections, angular distributions, and spectra (differential data), also considering uncertainties. This is especially important if integral feedback is considered because there are several changes in nuclear data possible to improve benchmark performance. For example, fitting the angular distribution to Popov data worsens performance for the IMF20,22 benchmarks.
- The Nomenclature of TSL files should be standardized to facilitate their correct use. Persons from the nuclear data centers, such as Daniela Foligno from OECD-NEA and David Brown and Gustavo Nobre from BNL as well as TSL producers should be involved in this effort.
- A New Python tool is available for creating, updating, reading, writing, verifying, and translating ENDF-6 files. Especially, the ability to create ENDF-6 files from scratch is anticipated to lower the entrance barrier for new evaluators to engage in evaluation work.

Validation

- MAESTRO validation results are available for Fe, Ni, Cr, and various stainless-steel types.
- MAESTRO results can be used to validate the assessment of thermal capture cross section by Firestone using pile oscillation measurements.
- It is recommended to review the thermal capture cross sections of ENDFB8.1, JEFF4, JENDL5, CENDL and compare them with C/E for JEFF-3.2 for all materials involved in the MAESTRO project.
- It is recommended to consider recent results of ALANINE-5 for validating cross sections in current libraries, e.g., ^{117}Sn(n,n'), ^{64,67}Zn(n,p), ^{64,68}Zn(n,γ).
- POSEIDON results (within the APRENDE projects) will become available sometime between 2024 and 2028.
- There is an ongoing experimental programme led by Rez on producing benchmarks to validate mostly prompt thermal capture gammas ($MnSO_4$, $FeSO_4$, NaCl).
- The IMF21 benchmark uses the same machine and fuel in the core as IMF20 and IMF22, but with a natural uranium reflector instead of Cu. Therefore, it can be used to estimate potential criticality bias due to U evaluations and IMF20,21,22 benchmark specifications. For existing U evaluations, the bias is estimated to be around +250 pcm.
- A list of benchmarks for Cu and Fe will be pertinent for a more streamlined validation in the future. It will also be helpful to indicate the relevance of each benchmark for different energy ranges (i.e. fast, intermediate, and thermal) and parameters (e.g. k_{eff} and leakage). The list of benchmarks defined by PSI, NRG, IRSN, and UPM for JEFF may be a good starting point:

https://git.oecd-nea.org/databank/nds/jeff/jeff-validation/benchmarks/-/blob/main/Experiments_in_common_PSI_NRG_IRSN_UMP.xlsx Also the benchmarks performed and documented in the recently published FENDL reference paper should be considered for this list.

- In general, it is recommended to perform a sensitivity analysis when using integral data to provide feedback for isotopic nuclear data. One essential prerequisite for this analysis is the careful verification of the integral benchmark specification.
- It is recommended to further explore and develop methodologies to incorporate integral feedback into the evaluation process, also considering possibly under-reported benchmark uncertainties.

Use of angular distributions

- The use of angular distributions reconstructed from resonance parameters instead of optical model results should be encouraged.
- Missing resonances have a weak impact on average elastic scattering cross sections, hence angular distributions are expected to be weakly affected by missing resonances at the upper range of the RRR.
- Related to the previous point, the proper spin assignment to resonance is a challenge and requires transmission, capture and scattering data. Moreover, the spin assignment becomes increasingly difficult at higher energies due to overlapping resonances.
- Reconstructed angular distributions are at 0K. Doppler broadening to room temperature needs to be considered before including them into the file.
- Comparison of angular distributions reconstructed from RP vs measured angular distribution data is recommended to be undertaken for Cu and Fe isotopes. For instance, Popov measured the angular distribution for Cu and Kinney data can be used for Fe. Essential features of the experimental setups need to be considered for the comparison, such as the detector resolution, Doppler broadening, and the spread in incident energy.

Appendix 1

IAEA Consultancy Meeting of the International Nuclear Data Evaluation Network (INDEN) on the Evaluated Data of the Structural Materials

18 – 21 December 2023
IAEA, Vienna

ADOPTED AGENDA

Monday, 18 December

10:00 – 16:30	**Opening of the meeting,** A. Koning / NDS Section Head	
	Welcome and introduction, Georg Schnabel **Election of Chair and Rapporteur(s), adoption of Agenda**	
	Participants' presentations	
	G. Nobre	The ENDF/B-VIII.1 release and future plans on structural materials
	E. Alhassan	Accounting for model uncertainty in Bayesian evaluation of nuclear data
	A. Göök	The nuclear data evaluation pipeline of Uppsala University (NEPU) - addressing model defects and data inconsistencies
	G. Schnabel	Lowering the ENDF-6 entrance barrier for evaluators
	M. Kostal	New integral experiments in Rez - focus on PFGS of ^{252}Cf(s.f) and ^{235}U(n_{th},f)

Tuesday, 19 December

10:00 - 16:00	**Participants' presentations** cont'd	
	D. Foligno	JEFF-4T3 status and NEA pipeline developments
	V. Pronyaev	Neutron inelastic cross section derived from gamma-production cross section (n,n'γ) reactions and Pygmy dipole resonance
	M. Diakaki	Updates on the study of the Fe isotopes
	Y. Danon	Measurements and Evaluation of structural materials at RPI
	A. Trkov	Some issues with the INDEN structural material evaluations

Wednesday, 20 December

13:00 - 15:30	**Participants' presentations** cont'd	
	D. Bernard (P. Leconte)	Nuclear data feedback on structural, moderating and absorbing materials through MAESTRO experimental programme in MINERVE
	E.A. Sunden	Half way Monte Carlo for integral adjustment
	R. Capote	Overview of selected INDEN evaluations ^{56,57}Fe, ^{63,65}Cu, and ^{19}F

Thursday, 21 December

10:00 – 15:00	**Technical Discussions & drafting of the meeting summary report**
	Closing of the meeting

Appendix 2

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