

## **INDC International Nuclear Data Committee**

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

Summary Report of the IAEA Consultants Meeting

13 – 16 December 2021  
(virtual event)

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November 2022

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## 1. Introduction

A virtual Consultancy Meeting was held from 13 to 16 December 2021 with the objective of bringing together the collaborators of the INDEN network to discuss the progress made and the issues identified regarding the evaluation of structural materials. The International Nuclear Data Evaluation Network (INDEN), managed by the IAEA, has been initiated in 2018 as a platform with regular meetings of internationally recognized experts to 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. A close interaction with national and international evaluation projects is held.

The focus of discussions at this meeting leaned towards the evaluation and validation of Fe isotopes, but significant progress of evaluation work was also presented for copper isotopes including new integral experiment for validation. Moreover, benchmark studies for zirconium, copper and lead complemented the presentations on evaluations and provided further indications for data issues and possible improvements. Regarding evaluation methodology, the utility of evaluations based on Monte Carlo sampling and Bayesian statistics has been presented and discussed.

Maria Diakaki, Stefan Kopecky and Andrej Trkov agreed to serve as Rapporteurs of the meeting. R. Capote agreed to take on the role of Chairperson to lead through the meeting program consisting of twelve presentations given by experts from seven Member States and the IAEA.

## 2. Presentation Summaries

### 2.1 Benchmarking of the evaluations in the $^{56}\text{Fe}$ Resolved Resonance Range, V. Pronyaev

The presentation shows the fit of the experimental data for narrow neutron beam transmission measurements for 37 neutron energy groups between 4 keV and 2 MeV. The Monte Carlo code using real geometry and accounting neutron multiple scattering was used in the calculations with the data files evaluated by L. Leal in the resolved resonance range using the R-matrix limited format between  $10^{-5}$  eV and 2 MeV. The angular distributions for elastic and inelastic scattering cross section and angular distributions with excitation of the first level were calculated from resonance parameters using the GRUCON code. Resonance parameters evaluated by L. Leal in 2014 and revised in 2021, and resonance parameters from ENDF/B-VIII.0 were used in the calculations for comparisons. The resonance range in the ENDF/B-VIII.0 file is limited by 850 keV and point-wise cross sections above this energy contain the structures of high-resolution experimental data.

It was shown that the extension of the resolved resonance range up to 2 MeV and the use of angular distributions calculated from the resonance parameters generally improve the fit of neutron transmission for large thicknesses. There are few energy groups where the fit of transmissions should be improved by further adjustment of resonance parameters. The evident loss of narrow neutron resonances with the increase of energy up to 2 MeV can be corrected by introducing pseudo-resonances, or some background addition. This can be important for inelastic scattering and especially for capture cross sections.

Although  $^{56}\text{Fe}$  is a major isotope in natural iron, and many results of transmission measurements are available, the use of the results of super high resolution TOF measurements for natural iron in the resonance parameters search can improve the evaluated values of  $^{56}\text{Fe}$  resonance parameters.

## 2.2 Analysis of the post-CIELO <sup>56</sup>Fe evaluation, A. Trkov

The problems with the CIELO Fe-56 evaluation are well-known. They were identified prior to the release of the ENDF/B-VIII.0 library (which adopted the CIELO evaluation), but there was no time to fix it before the release of the library. Since then, considerable effort has been devoted to identifying and fixing the problems. The most significant change was the reduction of the inelastic cross section and compensating the difference with the elastic such that unitarity with the total cross section was preserved. An option to fix the overprediction of the neutron flux in the resonance windows in deep penetration experiments was to increase the elastic cross section in the resonance minima of Fe-56. However, a thick 90 mm transmission measurement at the nELBE facility showed that the patch to the elastic cross section minima in Fe-56 was not appropriate. Shortly before the meeting it was discovered that Fe-57 only had resonances up to 190 keV and that there was significant structure in the total cross section above this energy as measured by Pandey. Preliminary analysis showed that introducing the fluctuations in the Fe-57 total cross section solves the flux overestimation problem and brings simulations in agreement with the thick transmission measurements at nELBE.

## 2.3 Comments on fast region evaluations, R. Capote

A review of the current status of INDEN evaluations in the fast region on iron and copper isotopes was given in two separate presentations.

### Iron isotopes:

A good performance of existing INDEN files in the fast region (above 1 MeV) was confirmed in new neutron leakage experiments (50 cm stainless steel cube), undertaken at CV Rez, Czech Republic (still unpublished) that include direct neutron measurements as well as In-115(n,n') and Ni-58(n,p) dosimetry foil measurements.

- Lower inelastic data by 10-15% are needed, compared to Negret et al measurements, especially above 2 MeV. Further measurements are needed to clarify the situation.
- Problems in the optical model description below 4 MeV were emphasized related to near-magicity and low-level density of iron isotopes. Such problems raise questions about the use of theoretical calculations below 4 MeV. It is pointed out that an  $l$ -dependent optical model potential derived by Kawano et al [1] is the only one that may solve these issues.
- The need to include background in the capture channel in the resolved resonance region was emphasized: the  $1/v$  background below the 28 keV resonance dramatically improves the performance of the ZPR9/34 benchmark (the iron uranium benchmark) which is highly sensitive to iron data. The background above 600 keV is needed to reproduce the measured RPI capture yield in Fe-56. Both capture backgrounds may be explained by direct capture contributions (see Section 2.4).
- It is stressed that the capture in the IAEA CIELO file was fitted to measured RPI data above 850 keV up to 1.3 MeV, evaluations are expected to be very close in the fast neutron energy range.
- Recently measured elastic angular distributions of Fe-56 by Pirovano et al [2] are in very good agreement with the IAEA CIELO evaluation (adopted by ENDF/B-VIII.0) from 2 to 6 MeV. There are problems to deconvolute the inelastic cross sections and angular distributions, it is suggested to compare the sum of elastic+inelastic data vs the evaluations as the sum features much lower uncertainty than the elastic and inelastic data separately.
- A fix for the thermal capture gammas in the evaluated file is needed.
- For Fe-57, it is emphasized that a better evaluation in the resolved resonance region of the inelastic scattering is needed. Data derived by Negret et al [3] may help to define the inelastic cross section in the whole energy range.

## Copper isotopes:

The status of copper evaluations was reviewed and results of new Copper neutron leakage benchmark (50 cm copper cube) from CV Rez discussed [4]. It was noted that the JEFF-3.3 evaluation performed poorly in the whole energy range, the ENDF/B-VIII.0 evaluation underestimates the data above 4 MeV, while the JENDL-4 evaluation overestimates the data below 4 MeV. Combining these results and a good criticality performance of the ENDF/B-VIII.0 evaluation, a new INDEN Cu-63,65 evaluation was assembled by using the ENDF/B-VIII.0 evaluation below 4 MeV and the JENDL-4 evaluation above 4 MeV. Newly assembled INDEN files show good criticality performance and good neutron leakage performance in the Rez experiment as well as better agreement with differential experimental scattering data. However, a new evaluation of Cu isotopes in the fast range is very desirable.

The following requirements should be met:

- preserve/improve the achieved criticality performance of ENDF/B-VIII.0 (check JENDL-4 performance) and the shielding performance of the newly assembled INDEN files;
- achieve good fusion performance (JENDL-4/TENDL-2019 were good there).

JENDL-4 gives the best total cross section vs data above 1 MeV (see slides 5 and 6 of the Cu presentation). The ENDF/B-VIII.0 evaluation slightly underestimates data below 2 MeV.

The Finlay and Guenther total cross section data on natural copper show good agreement with JENDL-4 above 1 MeV. It looks like JENDL-4 total and elastic cross sections should be preferred in this energy region.

- ENDF/B-V gives the best agreement with measured angular distributions on natural copper at least up to 5 MeV and should be preferred there. The ENDF/B-V angular distributions are expected to improve the agreement with RPI quasi-differential data above 0.5 MeV, especially at angles near 90 and backward angles.

## References:

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## 2.4 First Results on the DRC calculations for the $^{56}\text{Fe}$ isotope

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In the context of this work, the calculations of the neutron Direct Radiative Capture (DRC) process for the  $^{56}\text{Fe}(n,\gamma)$  were performed with a dedicated code, developed by A. Mengoni, which has given successful results in the past on light nuclei [1,2]. The first results were presented and discussed.

The motivation behind this work was that issues occurred with the  $^{56}\text{Fe}(n,\gamma)$  reaction within the CIELO project [3], leading to important implementations in the evaluation of the  $^{56}\text{Fe}(n,\gamma)$  reaction in the latest ENDF/B-VIII.0 library. More specifically, an artificial background was added in the energy region 10 eV - 100 keV, which seems to be validated by integral measurements [3-4]. Furthermore, the results

above 860 keV based on experimental data from the RPI [5] showed an increase of  $(n, \gamma)$  at  $\sim 850$  keV, where the  $(n, \text{inl})$  channel opens. The previously mentioned issues need physical interpretation, and this was attempted via the Direct Radiative Capture mechanism. Finally, from transmission measurements, it was shown that some valleys between resonances are not well described in the Resolved Resonance Region [4,5], pointing to a need of increasing the total cross section below the opening of the  $(n, \text{inl})$  channel, which could be mainly attributed to the elastic channel contribution of  $^{56}\text{Fe}$  or minor isotopes and potentially some small contribution of the direct capture mechanism.

The DRC calculation in the codes of A. Mengoni is performed in two steps: firstly, the calculation of the bound state wave functions based on available experimental information of bound states takes place and secondly the calculation of the DRC cross section for a given Optical Model Potential (OMP) is performed. The different partial waves were calculated independently in order to study their effect at the different neutron energy ranges.

For the bound state configuration, we used all the levels available at the ENSDF file (evaluation 1998), which were obtained from  $^{56}\text{Fe}(d, p)$ ,  $^{57}\text{Fe}(p, p')$ ,  $^{59}\text{Co}(d, \alpha)$  reactions, but also other bound state configurations were tried (e.g. grouping of fragmented single particle bound states, following [7]). It turned out that the bound state configuration did not play an important role, as expected.

A typical DRC calculation is shown in Fig. 1. This result should only be qualitatively considered, since the proper normalization to the thermal point will be performed after the compound capture reaction is added to the calculation. Nevertheless, some first interesting features can already be observed: i) the s-wave DRC is able to reproduce the  $1/v$  behavior that was needed in the energy region 10 eV - 100 keV and was artificially added for the latest ENDF/B-VIII.0 file and ii) the increase at the capture cross section observed at the RPI data, at approximately 850 keV could be attributed to the d-wave DRC. However, there are some shape resonances above 2 MeV, attributed to higher l-wave DRC which are not physically likely, since above  $\sim 2$  MeV collective effects should also be considered and Direct-Semidirect models [9] should be used instead of a simple Direct Capture model.

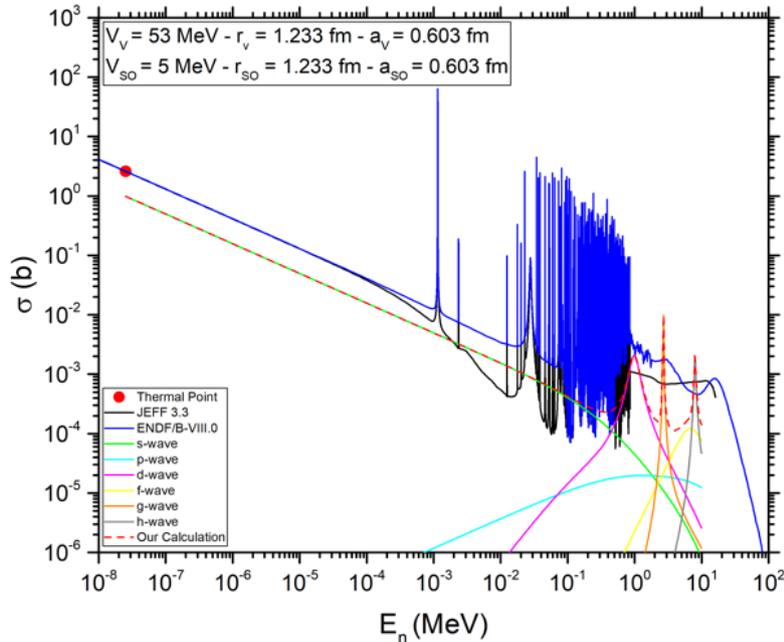


FIG. 1. First results of the DRC calculation of the  $^{56}\text{Fe}(n, \gamma)$  reaction. The different partial wave DRC components are shown.

Furthermore, different OM parameters were tried in an effort to study the effect on the final cross section shape. As a starting point the parameters of [8] were used, but various tests were made, for example by changing the depth, the radius and diffuseness of the volume part of the potential  $V_0$  and of the spin-orbit term of the potential  $V_{SO}$ . The different parameters affected in a different way the various partial waves of the direct capture reaction.

As a conclusion, the first DRC calculations of the  $^{56}\text{Fe}(n, \gamma)$  reaction showed that the Direct Capture process could explain the  $1/v$  behavior in the energy region 10 eV - 100 keV and potentially the increase of the capture cross section at ~850 keV observed at the RPI data (although this needs further investigation, both experimentally and theoretically). Further work is needed in order to perform a complete calculation, considering the resonant and direct capture component, as well as the interference term, compare with the DRC calculation implemented in the TALYS code, try other Optical Models etc. All these calculations will help us find a reasonable set of OM parameters to reproduce the basic features of the shape of the capture cross section and are planned for the near future.

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## 2.5 Update on Bayesian network developments with some $^{56}\text{Fe}$ examples, G. Schnabel

Bayesian networks are a flexible framework to model the deterministic and stochastic relationships between variables and are therefore a pertinent tool for the evaluation of nuclear data.

In the first part of the presentation, the Bayesian update formula was reviewed along with several approaches to solve it, namely Monte Carlo integration, optimization, and the GLS method. As the GLS method depends on the linearization of non-linear relationships, it may fail in practice in the presence of strong non-linearities. The Monte Carlo method provides accurate solutions and can take into account non-linearities but is computationally more expensive than the optimization-based approach. Therefore, the developments presented relied on the optimization-based approach for inference in Bayesian networks.

In the second part, basic building blocks were introduced that can be used to build Bayesian networks in a bottom-up manner. In particular, basic building blocks for nuclear data evaluation are linear interpolation to map from computational energy meshes to experimental energies, convolution to account for the finite-energy resolution of experiments, and an exponential and truncation mapping to incorporate the assumption that cross-sections must be non-negative.

In the third part, an example evaluation of neutron-induced reactions of Fe-56 between 1 and 2 MeV was presented, which relied on Gaussian processes that were interlinked within a Bayesian network to preserve the sum rules among the elastic, inelastic and total cross section channel. Another more complex example was also shown to demonstrate an evaluation with a nuclear model code (TALYS) and also accounting for model defects represented by Gaussian processes.

In the final part of the presentation, different types of users were identified, such as statisticians, nuclear data evaluators and large-scale evaluators, which have different needs and viewpoints on data and the evaluation process. It was argued that nuclear data evaluators and large scale-evaluators may not want to build a Bayesian network by hand but prefer an automated procedure. As a proof-of-concept, it was

shown how Bayesian networks can be constructed automatically for the purpose of a nuclear data evaluation by leveraging the output of a nuclear model code, such as TALYS in this demonstration.

## 2.6 Patch to INDEN on <sup>56,57</sup>Fe, A. Trkov

Refer to Section 2.2.

## 2.7 Preparing for evaluating zirconium isotopes, G. Nobre

Structural materials are present in many, if not virtually all, nuclear applications. Therefore, it is of paramount importance to describe their nuclear interactions accurately. Inspired by the success of recent evaluations of iron and more recently chromium isotopes, which leveraged the collaboration among BNL, IAEA, ORNL, JSI evaluators, we are planning to work on evaluations for zirconium isotopes. Besides cladding and in alloys (Zircaloy, Zr-Nb), Zirconium can also be found in fuel rods cladding due to its corrosion resistance and low thermal neutron absorption cross section. It is also considered in advanced reactor design studies as a moderator (in the form of zirconium hydride) and as inert matrix fuel material. The ENDF/B-VI.8 files evaluated in the 1970s relied heavily on experimental data and lacked quantities such as double-differential cross sections and gamma production.

Historically, Zr evaluations date back to Drake et al. (1976) in VI.8 and then EMPIRE-based updates in VII.0 and VII.1 (done by H.I. Kim). There are many critical benchmarks sensitive to Zircalloy and Zirconium-Niobium Alloy in DICE. This shows sensitivities to Zr isotopes, major and minor ones, not only in the resonance region but also in fast range. The plan for resonances would be a collaboration with Oak Ridge/RPI and IAEA/JSI, making use of new measurements, while BNL would work on fast-region evaluations and file assemblies. For fast region, there is a good starting point from previous EMPIRE input files, but they are not perfect. The definition of NLD parameters have changed since 2011 so they will have to be refitted, which I already began to do. There are new data available since then and we need to assess which measurements to consider from older data sets. The Optical Model Potential from the Kim evaluation is good, but we need to check if previous fine tuning was appropriate. There is also somewhat “recent” inelastic gamma data available. We showed preliminary fits of level density and preliminary plots of cross sections for main reactions.

## 2.8 Need for accurate Zirconium inelastic cross sections for LWR applications, D. Bernard

This presentation was devoted to the need of an accurate evaluation of neutron induced cross sections of zirconium for LWR calculations.

As was shown, the sensitivity of radial power map (center to peripheral assemblies) of a water moderated core to the JEFF-3.1.1/<sup>90</sup>Zr(n,n') total inelastic cross section is about -0.024(4)%/% where uncertainty corresponds to neutron transport Monte Carlo convergence. Sensitivity profiles show that 80% is located in the 2.2-6.1 MeV incident energy zone for JEFF-3.1.1.

Because this sensitivity is mainly to the continuum part of the (n,n'), one has to be cautious regarding the energy cut off from discrete to continuum description because, for instance, a lower number of discrete levels will increase the cross section to the continuum by orders of magnitudes. Thus, one should aim to include as many discrete levels as possible. For JEFF-3.3, the number of levels was increased to 20 compared to 7 levels in JEFF-3.1.1. For ENDF/B8 8 discrete levels are proposed.

A second parallel topic was to ask if the following relationship at the boundary between the 2 modes (discrete and continuum) is accounted for in nuclear reaction codes at each incident energy:

$$\frac{\partial^2 \sigma_{(n,n'_i)}(E)}{\partial E' \partial \vec{\Omega}} = \frac{\partial^2 \sigma_{(n,n'_{cont})}(E)}{\partial E' \partial \vec{\Omega}}$$

However, this was affirmatively answered during the meeting.

## 2.9 Nuclear data validation for Cu and Pb, H. Wu

$k_{\text{eff}}$  trends related to Cu and Pb HMF benchmarks that contain a reflector were found in the validation of the CENDL-3.2 library. Similar trends were also found in the validation of other major libraries. To answer the question whether the data for Cu need to be improved, and to identify the nuclides and specific reaction data that might be responsible for the  $k_{\text{eff}}$  bias in the Pb reflected HMF benchmarks, a trend analysis based on nuclear data sensitivity was performed with the Cu and Pb reflected HMF benchmarks.

This trend analysis was done with the Cu reflected HMF and PMF benchmarks. Firstly, the C/E trend of  $k_{\text{eff}}$  against nuclear data sensitivity was analyzed with the HMF72 and HMF073 benchmarks. For CENDL-3.1 and CENDL-3.2 libraries, linear  $k_{\text{eff}}$  trends related to Cu and Fe were found separately, but a nonlinear trend was found for  $^{235}\text{U}$ . Secondly, the trend analysis was done with Cu reflected PMF013 and PMF040 benchmarks. Cu bias was also confirmed. Therefore, Cu data still need to be improved. When total sensitivities were broken down to reactions and energy bins, the energy region from 0.1 to 3 MeV was thought to be the most sensitive region to  $^{63,65}\text{Cu}(n, \text{tot})$  cross section.

The trend analysis based on sensitivity was also performed with the lead reflected benchmarks, HMF057 and HMF063. The analysis of HMF057 benchmarks has shown that the over prediction of the  $k_{\text{eff}}$  values was not linearly correlated to the Pb or U-235 sensitivities. Some other factors may cause the nonlinear variety in the  $k_{\text{eff}}$  trend. The quality of HMF057 benchmarks is doubtful. So, the Pb bias in HMF benchmarks was not confirmed.

Finally, it was suggested that the (n, tot) cross sections between 0.1 and 3 MeV be reviewed in the Cu evaluation.

## 2.10 Latest development on Cu evaluation with benchmarking, D. Rochman

Following the work performed in 2012 and presented in NSE170(2012)265, a new analysis of the Cu isotopes was performed using the TENDL approach (production of a number of “random” ENDF-6 files based on TMC). Each Cu ENDF file was then used in validation (with differential data, criticality and shielding benchmarks). The performance of each validated file was quantified using a simple  $\chi^2$  value. Finally, the best performing files for  $^{63}\text{Cu}$  and  $^{65}\text{Cu}$  were presented as potential new Cu evaluations. This work will be complemented in the future by additional benchmarking, and combined with the Bayesian network update.

## 2.11 Updates to the n+ $^{63,65}\text{Cu}$ angular distributions, J. McDonnell

Progress in the evaluation of neutron reactions on  $^{63,65}\text{Cu}$  was presented, focusing especially on the elastic scattering angular distributions.

In the ENDF/B-VIII.0 evaluations, the Legendre coefficients for both isotopes were reconstructed from the resonance parameters up to 300 keV and subsequently smoothed on a coarse energy grid for inclusion in the ENDF-6 format. This procedure produces a discontinuity in the average cosine of the scattering angle between the resolved resonance region and the high energy regions. In this work, it was shown that a simple adjustment to the Legendre coefficients to achieve a smooth transition had a negative impact on integral benchmark performance. The plan was established to base the Legendre coefficients on measured angular distribution data.

## 2.12 Benchmarking of neutron cross sections and angular distributions of Cu and Pb in the RRR, V. Pronyaev

This presentation considers the degree of consistency between the evaluations of angular distribution of elastic scattering in the resolved resonance range (RRR) based on optical model calculations and calculated from resonance parameters using the Blatt-Biedenharn approximation. Most of the current libraries contain evaluations based on optical model calculations. However, it is well known that the

optical model often gives a poor cross section fit below 1 MeV for incident neutrons (e.g. for structural materials) and produces angular distributions of neutron elastic scattering with a smoother shape than indicated by measurements. Angular distributions calculated from resonance parameters have a strong mu-bar variation correlated with the resonance cross section.

First, the tests using simulated critical assemblies presenting sub-critical  $^{235}\text{U}$  sphere (Godiva type) with  $k_{\text{eff}}=0.92808$  surrounded by a spherical reflector from studied material with a thickness restoring the  $k_{\text{eff}}$  to 1, were considered. The calculations were done with files taken from original nuclear data libraries and with files where elastic scattering angular distributions were calculated from the resonance parameters using the GRUCON code. It was shown for Copper and Lead, often used as reflectors for compact assemblies or lead cooling reactors, that the difference in the thickness of the reflector leading to criticality may differ by few per-cents. The upper boundary of the RRR for Copper isotopes in modern libraries is 99.5 keV. In this case only a small part of the assembly spectrum covers the RRR. Because of this, the sensitivity to the mu-bar below 99.5 keV is small.

The RRR for  $^{63,65}\text{Cu}$  isotopes was extended to 300 keV by L. Leal. New files for  $^{63,65}\text{Cu}$  and  $^{206,208}\text{Pb}$  were prepared for the BROND library release. The capture cross section for Copper files was corrected at missed resonances above 100 keV by adding a smooth background cross section. The elastic scattering angular distributions were calculated from resonance parameters using the GRUCON code (freely available from the IAEA/NDS website). They were presented in MF4, MT2 as relative Legendre coefficients for several tens of thousands energy mesh points, or Legendre coefficients for 642, 299 or 28 energy groups averaged with a weight of elastic cross section. The benchmark experiments from ICSBEP database most sensitive to the Copper and Lead reflectors and Lead in the form of coolant were used in the standard MC calculations of  $k_{\text{eff}}$ . The main conclusions from the analysis of the results are the following:

- the  $k_{\text{eff}}$  for files with angular distribution calculated from the RRR for Copper isotopes is lower than for files with evaluated optical model angular distributions between 0.1 and 0.5%, depending on the hardness of the neutron spectrum;
- compact assemblies with Lead reflector files, where angular distributions were calculated from the RRR, reduce the  $k_{\text{eff}}$  value by about 0.2%. However, the observed negative trend with increasing reflector thickness remained. This probably indicates that the integral elastic cross section in the Lead isotopes could be a little low;
- for large assemblies with Lead in the core the  $k_{\text{eff}}$  increases at about 0.3%;
- the 642 or 299 energy groups for presentation of angular distributions in the RRR give results of MC calculations for  $k_{\text{eff}}$  that are close to the results based on a detailed point-wise energy representation of angular distributions reconstructed from resonance parameters.

This leads to the conclusion that in modern files angular distributions in the RRR should be calculated from the resolved resonance parameters and not from optical model calculations.

### 3. Summary and conclusion

This meeting on structural materials within the International Nuclear Data Evaluation Network (INDEN) managed by the IAEA brought together internationally recognized experts with expertise in nuclear data evaluation, experimental nuclear physics, benchmarking and evaluation methodology.

Several presentations on iron indicated that evaluation work has advanced significantly. A. Trkov demonstrated that a problem of overestimation of neutron flux in iron deep penetration benchmarks (e.g., around 300 keV of neutron energy) can be resolved by using available experimental Fe-57 total cross section data by Pandey et al from 190 keV up to 2 MeV, and that a 30% underestimation of neutron leakage from 1-10 MeV was related mainly to too high inelastic cross section. R. Capote's presentation provided a good overview of the current state of the INDEN iron and copper evaluations

and pointed out necessary improvements. V. Pronyaev studied the potential extension of the resolved resonance range up to 2 MeV and the use of angular distributions calculated from resonance parameters and found that reconstructed angular distributions can improve the consistency with neutron transmission experiments for large thicknesses. M. Diakaki presented significant progress in model developments to account for the Direct Resonance Capture (DRC) contribution in Fe-56, which helps to explain the  $1/v$  behavior in the energy region 10 eV - 100 keV and potentially the increase of the capture cross section at about 600 keV observed at RPI. G. Schnabel outlined a methodology based on Bayesian networks and presented results stemming from its tentative application to the evaluation of Fe-56 between one and two MeV.

Copper isotopes were also covered by several presentations. J. McDonnell presented ongoing evaluation work with a focus on the elastic scattering angular distribution. He explained the benefits of a smooth transition in the angular distribution between the resolved resonance range and the high energy range, but also pointed out the negative impact on integral benchmark performance, thereby highlighting the importance of a well evaluated elastic angular distribution. V. Pronyaev studied, for copper and lead, the consistency between elastic angular distribution obtained by an optical model and the Blatt-Biedenharn R-matrix formalism and found differences of  $k_{\text{eff}}$  in Godiva-type benchmarks ranging from 0.1% to 0.5% depending on the approach. D. Rochman presented an evaluation of the Cu isotopes using the Monte Carlo-based TENDL approach and a  $\chi^2$  ranking score. H. Wu investigated the quality of evaluations in the CENDL library by analyzing trends in HMF benchmarks containing copper or lead and concluded that there is a bias present in copper evaluations. No such statement could be made for lead due to potential issues in the benchmarks.

Two presentations dedicated to zirconium were given. G. Nobre emphasized the importance of good nuclear data for zirconium for applications, elaborated on the historical development of its evaluation and outlined the plan for a re-evaluation within a collaboration between BNL, IAEA, ORNL and JSI. The importance of zirconium was further substantiated by D. Bernard who showed the impact of zirconium data for LWR applications, in particular the strong influence of the location of the boundary between the discrete level and continuous level representation. Guided by this study, he recommended to include as many discrete levels as possible, such as done for the JEFF 3.3.

Overall, the presentations and discussions highlighted the significant advances made in the knowledge of structural materials since the inception of INDEN. Knowledge sharing and collaboration are essential for improving nuclear data due to the complexities of nuclear data evaluation and its connection with experimental data and applications. The identified issues and on-going evaluation work indicate that knowledge sharing and collaboration will remain essential in the future and that INDEN is a valuable platform for this purpose.



## Appendix 1

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

13 – 16 December 2021

## ADOPTED AGENDA

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**Monday, 13 December (2:00 – 6:00 pm, open 1:45pm Vienna time)**

14:00	<b>Opening of the meeting</b>	
	<b>Election of Chair and Rapporteur(s), discussion/adoption of Agenda</b>	
14:20	<b>Participants' Presentations</b>	
	V. Pronyaev	Benchmarking of the Evaluations in $^{56}\text{Fe}$ Resolved Resonance Range (25')
	A. Trkov	Analysis of the Post-CIELO Fe-56 evaluation (25')
	R. Capote	Comments on Fe fast region evaluations (25')
	<b>Discussion</b>	

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**Tuesday, 14 December (2:00 – 6:00 pm, open 1:45pm Vienna time)**

14:00	<b>Participants' Presentations (cont')</b>	
	M. Diakaki	First results on the DRC calculations for the $^{56}\text{Fe}$ isotope (25')
	G. Schnabel	Update on Bayesian network developments with some $^{56}\text{Fe}$ examples (25')
	A. Trkov	Patch to INDEN on Fe-56,57
	G. Nobre	Preparing for evaluating zirconium isotopes (25')
	D. Bernard	Need for accurate Zirconium inelastic cross sections for LWR applications
	<b>Discussion</b>	

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**Wednesday, 15 December (2:00 – 6:00 pm, open 1:45pm Vienna time)**

14:00	<b>Participants' Presentations (cont')</b>	
	H. Wu	Nuclear data validation for Cu and Pb (25')
	D. Rochman	Latest development on Cu evaluation with benchmarking (25')
	J. McDonnell	Updates to the n+63,65Cu Angular Distributions (25')
	V. Pronyaev	Benchmarking of neutron cross sections and angular distributions of Cu and Pb in the RRR (25')
	<b>Discussion</b>	

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**Thursday, 16 December (starting 2pm, open 1:45pm Vienna time)**

14:00	<b>General discussion</b>	
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## Appendix 2

### PARTICIPANTS

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## Appendix 2

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## Appendix 3

### PRESENTATION LINKS

#	Author	Title	Link
1	V.G. Pronyaev	Benchmarking of the Evaluations in $^{56}\text{Fe}$ Resolved Resonance Range	<a href="#">pdf</a>
2	A. Trkov	Analysis of the Post-CIELO Fe-56 evaluation	<a href="#">pptx</a>
3	R. Capote	Comments on Fe fast region evaluations	<a href="#">pptx</a>
4	M. Diakaki	First results on the DRC calculations for the $^{56}\text{Fe}$ isotope	<a href="#">pdf</a>
5	G. Schnabel	Update on Bayesian network developments with some $^{56}\text{Fe}$ examples	<a href="#">pptx</a>
6	A. Trkov	Patch to INDEN on Fe-56,57	<a href="#">pptx</a>
7	G. Nobre	Preparing for evaluating zirconium isotopes	<a href="#">pdf</a>
8	D. Bernard	Need for accurate Zirconium inelastic cross sections for LWR applications	<a href="#">pdf</a>
9	H. Wu	Nuclear data validation for Cu and Pb	<a href="#">pptx</a>
10	D. Rochman	Latest development on Cu evaluation with benchmarking	<a href="#">pdf</a>
11	J. McDonnell	Updates to the $n+^{63,65}\text{Cu}$ Angular Distributions	<a href="#">pptx</a>
12	V.G. Pronyaev	Benchmarking of neutron cross sections and angular distributions of Cu and Pb in the RRR	<a href="#">pdf</a>





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