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

Summary Report of the IAEA Consultants Meeting

IAEA Headquarters, Vienna, Austria
2 – 5 December 2019

Andrej Trkov
Institut Jozef Stefan, Ljubljana, Slovenia

Stefan Kopecky
EC-JRC Geel, Belgium

Roberto Capote Noy
IAEA, Vienna, Austria

December 2020

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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International Atomic Energy Agency
Vienna International Centre
PO Box 100
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Austria

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1 Introduction

A Consultancy meeting was held at IAEA Headquarters in Vienna, Austria, from 2 to 5 December 2019, to address current problems in the evaluation of nuclear data and structural materials and discuss both the evaluation methodology, evaluation issues and existing data problems. Dimitri Rochman was elected Chairman, and Stefan Kopecky agreed to serve as Rapporteur of the meeting. This work was carried out in the framework of the International Nuclear Data Evaluation Network (INDEN) with experts from six Member States and one International Organization attending the meeting.

2 Presentation Summaries

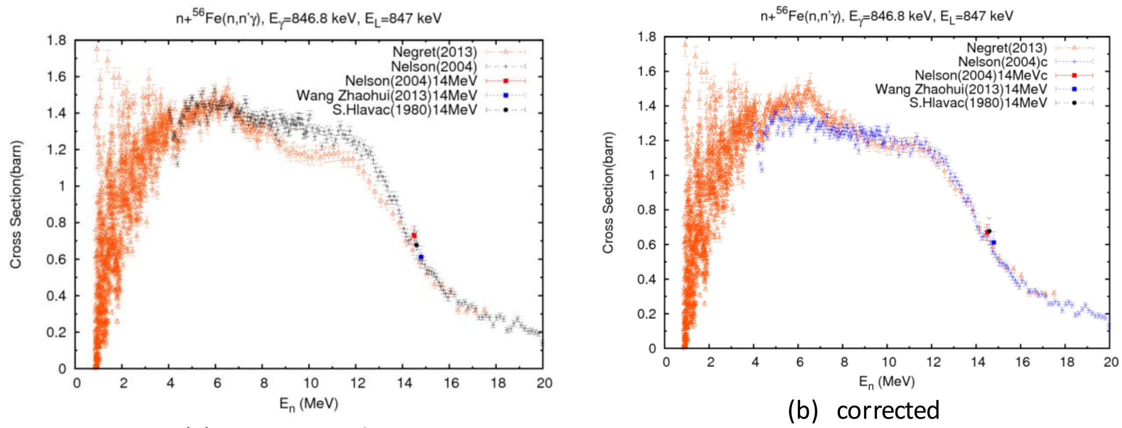
2.1 Re-evaluation of Fe-56 data based on CENDL-3.2b1, H. Wu

To solve the problem of serious under predictions of the neutron leakage caused by the Fe-56 evaluations, such as CENDL-3.2b1(C32b1) and ENDF/B-VIII.beta4 (B8b4), in deep penetration shielding calculation, an improved revision (C32b5) had been evaluated based on C32b1 in 2018.

2.1.1 Experimental data of ^{56}Fe(n,n'γ) were re-evaluated and recommended.

Gamma production data of ^{56}Fe(n,inl) reaction since 1970 have been reviewed. Corrections of partial cross sections for gamma-ray anisotropy have been applied as recommended by D.L. Smith [1].

Above 4 MeV, Nelson (2004) data with a normalization factor 91.754% applied was recommended. The correction factor was obtained based on the analysis of (n, inl) cross sections measured with D-T neutron source, including Hlavac (1980), Nelson (2004) and Wang Zhaohui (2013). Good agreements with the Negret (2013) data above 8 MeV are shown in Fig. 1(b). At the same time, Negret (2013)'s data between 4-8 MeV were rejected because an unreasonable bump around 6 MeV was found.



(a) Uncorrected

(b) corrected

Fig. 1 Comparison of gamma production cross sections for 847 keV gamma-ray of Fe-56 measured by Negret (2003) and Nelson (2004).

Below 4 MeV, cross-section integrals of 5 data sets were compared and are shown in TABLE 1. The data below 4 MeV measured by Voss (1971), Savin (1976) and Dickens (1991) show better agreement than the other two, and were recommended for the further evaluation.

TABLE 1: COMPARISON OF CROSS SECTION INTEGRAL BELOW 4 MeV

Data Sets	XS. integral <4MeV (Barn*MeV)	Residual
Voss (1971)	2.53	-5%
Savin (1976)	2.69	1%
Dickens (1991)	2.71	2%
Nelson (2002)	2.31	-13%
Negret (2013)	3.02	14%
Average	2.65	
Relative Uncertainty	10%	

2.1.2 A new version of Fe-56 evaluation, C32b5, was evaluated based on the recommended data and C32b1.

4 sets of gamma production cross section for 847 keV gamma-ray recommended above were converted to ^{56}Fe(n,inl) cross sections and evaluated with Korzh (1994) and Perey (1971) data together (Fig. 2). Korzh (1994) was rejected because of not enough background reduction. Perey (1971) was rejected because cross section integral below 2 MeV is about 14% higher than that of Voss (1971). Finally, C32b5 was evaluated based on recommended experimental data by editing (n,inl) and (n,el) cross sections of C32b1. The cross sections for discrete levels were re-accommodated to fit the (n,inl) cross section. The comparison of the evaluated (n,inl) cross sections with the recommended experimental data is shown in Fig. 3.

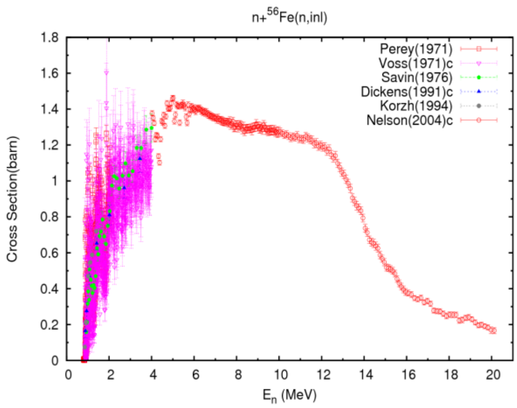


Fig. 2 Comparison of experimental ^{56}Fe(n,inl) cross sections

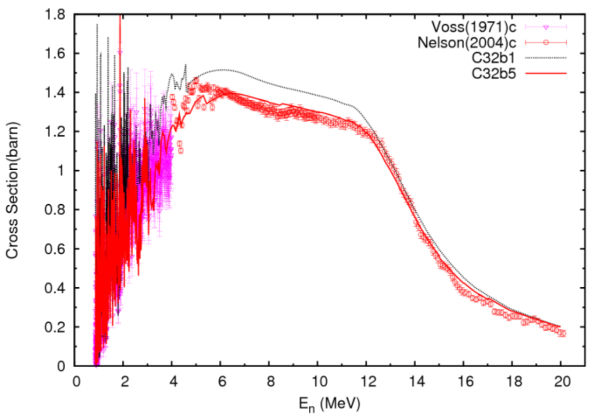


Fig. 3 Comparison of ^{56}Fe(n,inl) cross sections for C32b1 and C32b5

2.1.3 Benchmarking performance

The new and previous evaluations were tested with the IPPE iron sphere benchmarks. The results for 70 cm dia. sphere are shown in Fig. 4. The prediction of neutron leakage spectra for shielding calculation is now significantly improved with the C32b5 revision. The data were also tested with the criticality benchmarks sensitive to Fe-56. The prediction of k_{eff} values for fast and intermediate spectra benchmarks sensitive to Fe-56 are also improved.

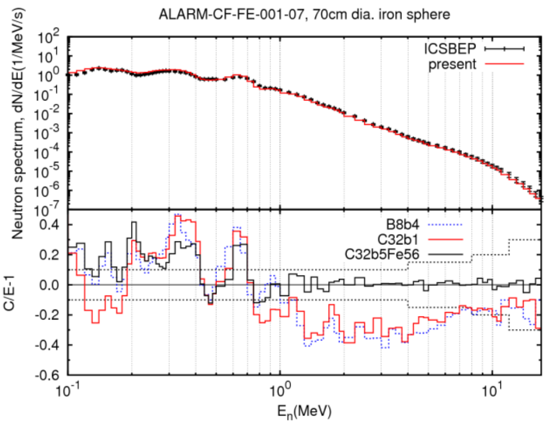


Fig. 4 The comparison of the calculated and experimental neutron leakage spectra from the IPPE iron sphere in 70 cm dia..

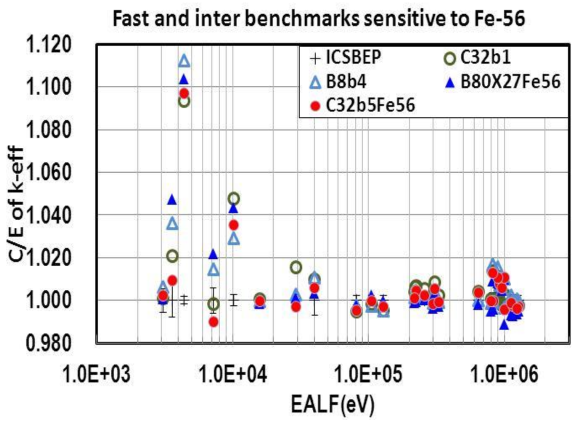


Fig. 5 Comparison of the C/E values of k_{eff} for the fast and intermediate spectra benchmarks sensitive to Fe-56.

References:

[1] D.L. Smith, Fast-Neutron Gamma-Ray Production From Element Iron: En ≤ 2MeV, Argonne National Laboratory, 1976.

2.2 Status of Cr Evaluations, G. Nobre

We presented the most recent developments in the evaluations of the stable chromium isotopes (^{52}Cr, ^{53}Cr, ^{50}Cr, ^{54}Cr) by the BNL/INDEN collaboration.

Performance-wise, one of the main challenges for new chromium evaluations resides in the proper description of the cluster of resonances seen in ^{53}Cr capture cross section between 2 and 10 keV neutron incident energy, centered at around 6 keV. The other impactful issue is the description of the wide resonance observed in the ^{50}Cr capture, centered also at around 6 keV. In this case there seems to be an energy shift relative to data (Stieglietz, 1971). Despite the low abundance ratios of both isotopes, these resonances dominate capture in natural chromium in this important energy range.

On ^{53}Cr(n,g), the only two important measurements in this region are from Stieglitz et al. (1971) and the more recent by Guber et al. (2011). However, those two data sets are inconsistent with each other. Integral benchmarks suggest that capture should be higher than Guber, much closer to Stieglitz values. Even though those two datasets have nearly the same shape, their normalization differs significantly due to different approximations needed and applied in each case to convert measured capture yield to cross sections (multiple scattering corrections may be as high as 80%). Because of this, we cannot simply renormalize Guber data to Stieglietz's. There is an entry in the High Priority Request List (HPRL) for a new measurement in this region. Also, RPI is planning to perform an experiment to address this. However, no new data are available and it is not clear whether new experiments will be capable to solve the issue as very thin and expensive targets are needed. Therefore, in the meantime, the solution found was to fit transmission data of Guber on natural chromium between 1 and 10 keV. In this energy window only ^{53}Cr and ^{50}Cr are relevant. With the set of resonance parameters fitting the magnitude of the natural data, normalized Guber (0.48 to theoretical) and Stieglitz (0.8 to theoretical) data and, with these normalized data refined the fit also using the transmission data. This is the best solution that can be implemented without explicitly sorting out the issues with ^{53}Cr capture data. This approach leads to significant improvement in benchmark performance, supported by differential data.

Regarding fast region, we have begun calculations using newly developed chromium-specific soft-rotor dispersive optical model potential (OMP), identified in RIPL as #616. This has led to improvements in threshold reactions. The OMP fitted natCr transmission data from Abfalterer. The total cross-section data from Foster Jr., natural and isotopic, seem to be compatible with Abfalterer, albeit slightly different. To confirm compatibility, we will construct covariances for Abfalterer measurement. It would be helpful to be able to use data from Foster Jr. (it extends to lower energy and has fluctuations).

For the inelastic channel, we performed spline fits (without considering covariances yet) to smooth out inelastic data for partial levels and total. When comparing our calculations of total inelastic with experimental data from EXFOR we found that data from Mihailescu and Tagesen labeled as MT=4 (total neutron inelastic cross section) actually correspond to inelastic gamma cross sections for the transition from the first excited level to the ground state. We will report these findings of mislabeled data to EXFOR community. We will also derive the total neutron inelastic cross section from the original gamma cross section measurements from Mihailescu and also send it to EXFOR.

We believe to have identified solutions to the main issues, and we hope to produce a complete beta file in the next few months.

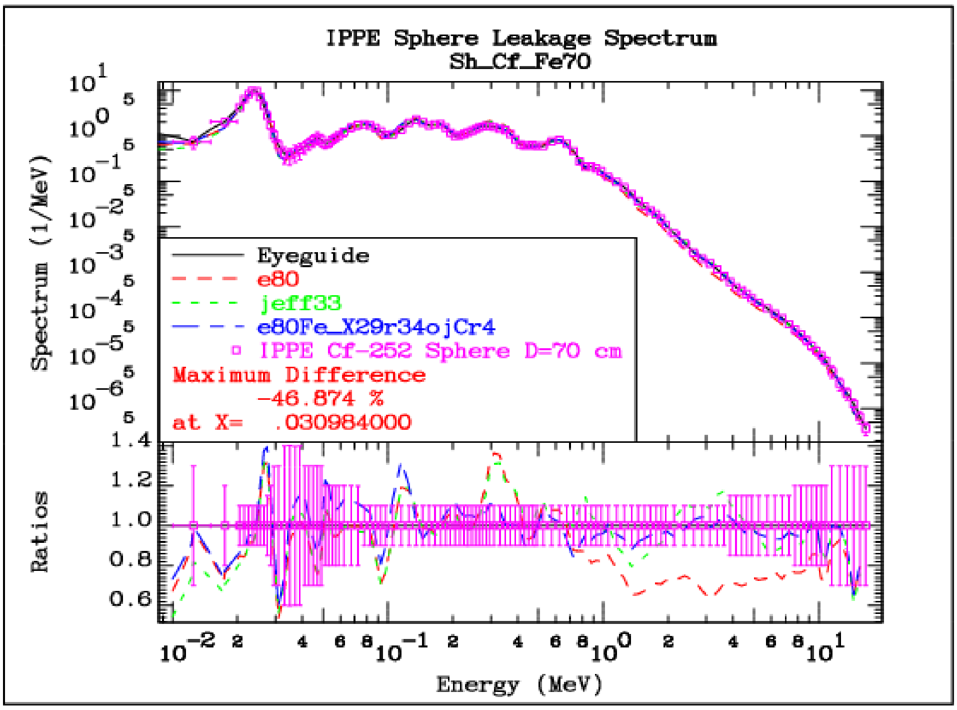
2.3 TENDL-2019 and the Ni isotopes: what to expect, D. Rochman

In this presentation, the global method to produce the TENDL library was presented, with an emphasis on the modifications for the latest release, TENDL-2019. A new version of TALYS was used, with improved gamma strength functions and specific adjustments for important cross sections (such as activation cross sections from IRDFF-II). In the resonance range, a new version of the TARES code was used, with resonance parameters coming from the latest library releases (JEFF-3.3, ENDF/B-VIII.0 and JENDL-4.0), as well as from the latest version of the Atlas of Neutron Resonances. The TENDL-2019 version is planned to be released before the end of December 2019. Within this context, specific efforts for the Ni isotopes were done. Selections of resonance parameters were based on the Atlas and the JENDL library. The resonance uncertainties were adjusted to reproduce the values provided in the Atlas, for isotopic components, as well as for the natural Ni. In the fast neutron range, a specific (new) method was applied. In TALYS (or T6), a random parameter search, combined with a Bayesian search was used for the first time. Parameters are changed so that cross sections become in agreement with ENDF/B-VIII.0. This method is planned to be combined with an in-depth evaluation based on EXFOR selection. This is under development and improved results are expected to be obtained soon. Additionally, no benchmark validation was performed yet, and no assessment for the unresolved resonance range was performed. These are the next steps for coming efforts. The future improvements are planned to be included in the next TENDL version for 2021.

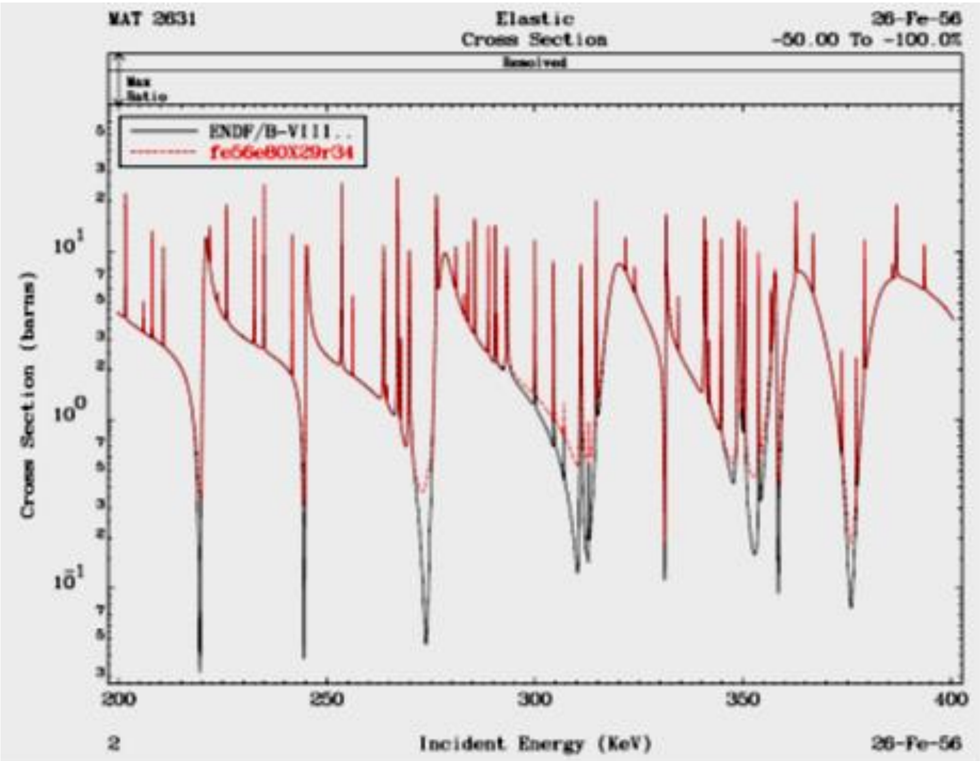
2.4 Current status of the Post-CIELO Fe-56 evaluation, A. Trkov / R. Capote

A new re-evaluation of the ^{56}Fe isotope neutron induced reaction cross sections was undertaken at the IAEA to address identified deficiencies in the Fe-56 CIELO evaluation adopted by ENDF/B-VIII.0. Detailed benchmarking revealed degraded performance in modelling neutron leakage spectra through thick iron shields with ^{252}Cf and D-T sources in the energy range from about 1 up to 10 MeV.

Additionally, a 30% overestimation of the neutron leakage has been identified in the region close to 300 keV by Rez collaborators and also found in modelling IPPE shielding spehres benchmarks as shown in the figure below for the neutron leakage in the 70cm diameter sphere measured with a Cf source. This deficiency was associated to too low total (and elastic) cross section in the minima that could be seen only in neutron leakage experiments with spherical shells above 50 cm diameter.



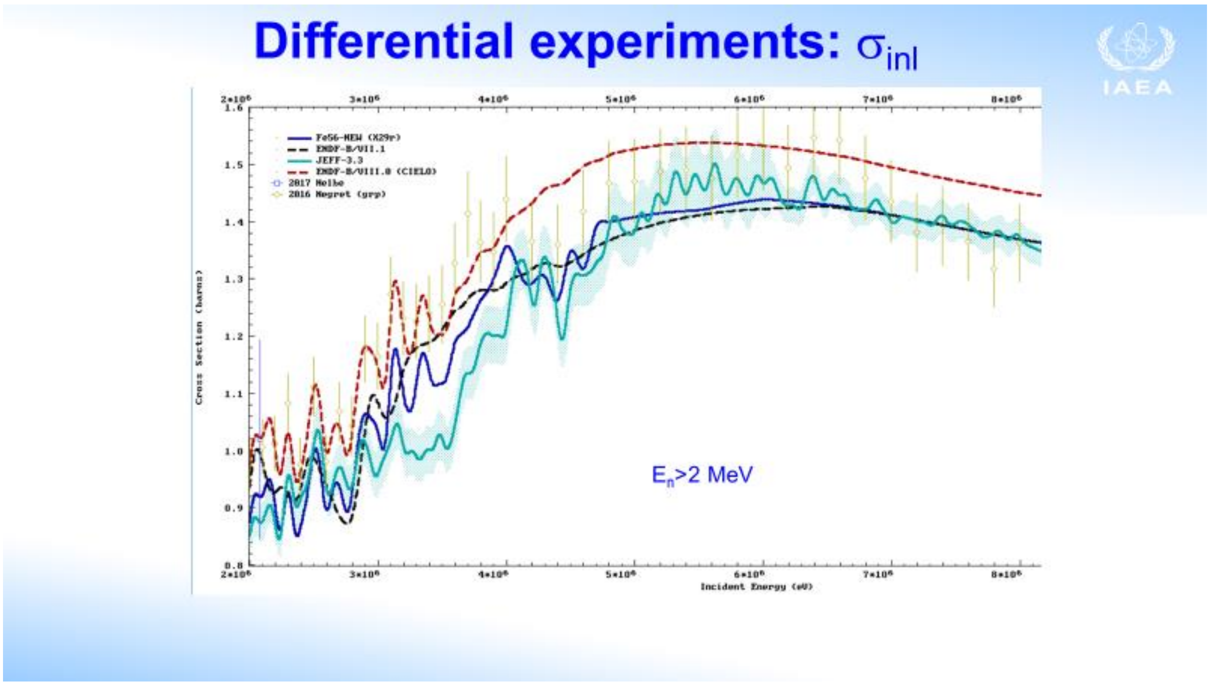
The increase in the minima of elastic peaks is shown in the figure below.



A global increase of the elastic cross section in the resonance region has a negative impact on the performance of the evaluation in criticality benchmarks. The selective increase of the elastic cross section in the minima was implemented as background cross section in MF3 of ENDF. Physically, it may be associated with a direct capture contribution or simply with the unconstrained R-matrix fit of measured yield data. Adding to the fit transmission data through very thick targets (of more than 5 cm) may help in the improvement of the RP fit and increase the elastic cross section in the minima. Traditionally, evaluators avoid using such thick targets as the thin layer approximation does not hold, and a different normalization should be used (not a simple division of the yield by the target thickness).

The problem in fast neutron leakage of the CIELO evaluation was traced to inelastic cross section being fitted to recent Negret data from 1 MeV up to around 7-8 MeV. The high inelastic cross section led to an underestimation of the elastic cross section, which directly led to an underestimated neutron leakage. Note that total cross section is well known and fixed in the whole energy range, therefore only the sum of elastic+inelastic is well constrained.

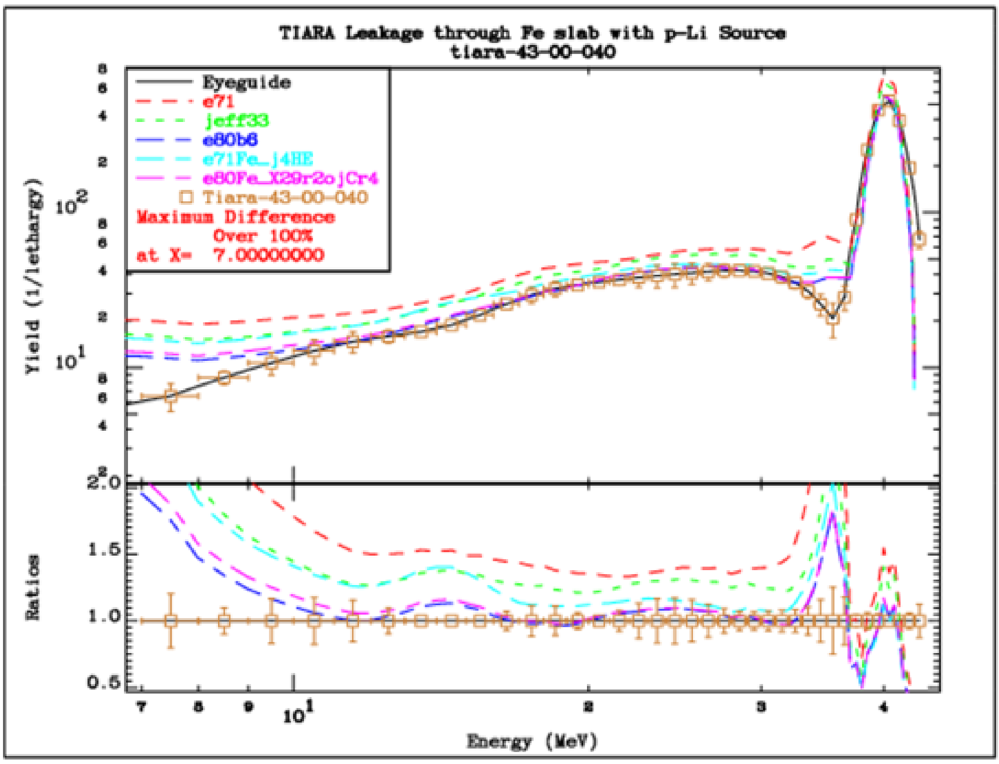
A reduction of the evaluated inelastic cross section was clearly needed, It was observed that ENDF/B-VII.1 evaluated cross sections was generally good above 4 MeV. The proposed changes are shown in the figure below (labeled Fe56-NEW).

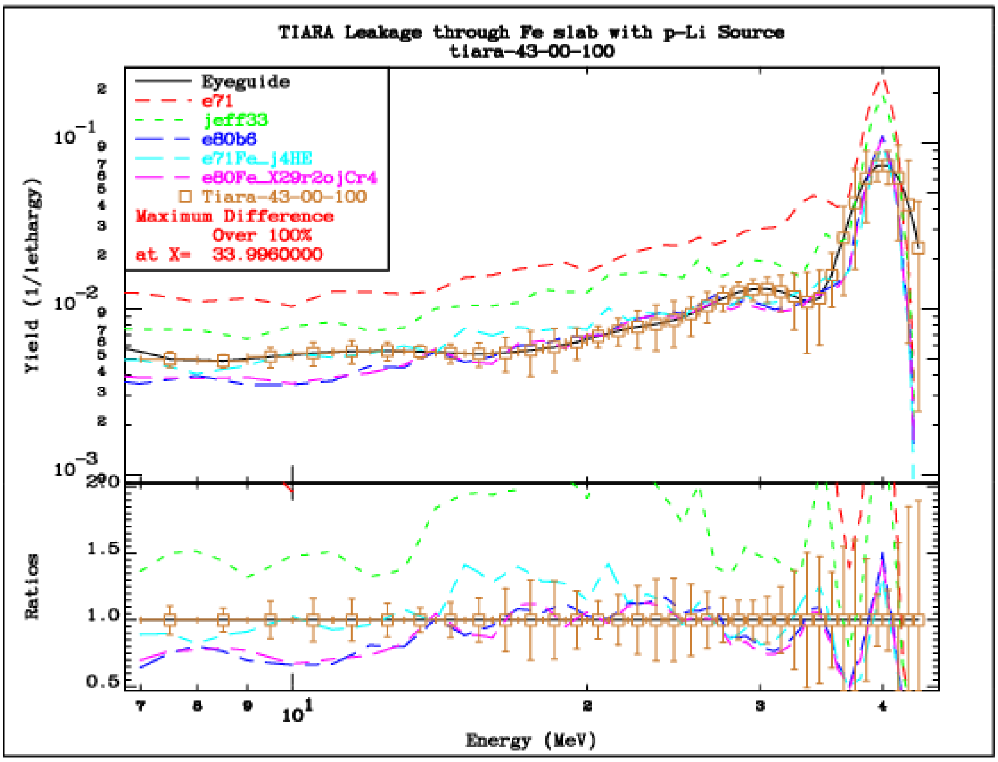


Finally, measurements reported by Firestone et al. (Phys. Rev. **C95**, 014328 (2017)) performed using PGAA suggest a lower thermal capture cross section by about 10%. Only a few stainless-steel clad thermal assemblies are affected.

Higher neutron incident energies

Very few benchmarks are available above 20 MeV of neutron incident energy. TIARA 43 and 65 MeV benchmarks are available in SINBAD. The reevaluated file shows good performance for the 43 MeV benchmark compared to the CIELO file as shown at two distances in the figures below.





Inelastic cross sections of Fe-57

Inelastic cross section of ^{57}Fe has a very low threshold of 14 keV. The cross-section shape was reconstructed from resonance parameters in the ENDF/B-VIII.0 evaluation but the resulted average cross section decreased significantly. There is a recent measurement combined with model calculation that defines higher total inelastic average cross section - A. Negret et al, Phys. Rev. **C96**, 024620 (2017). The predicted/measured total inelastic cross sections is estimated to be around 1.5b at 2 MeV with a maximum of 1.75b at 4 MeV as shown in the figure taken from the abovementioned paper below:

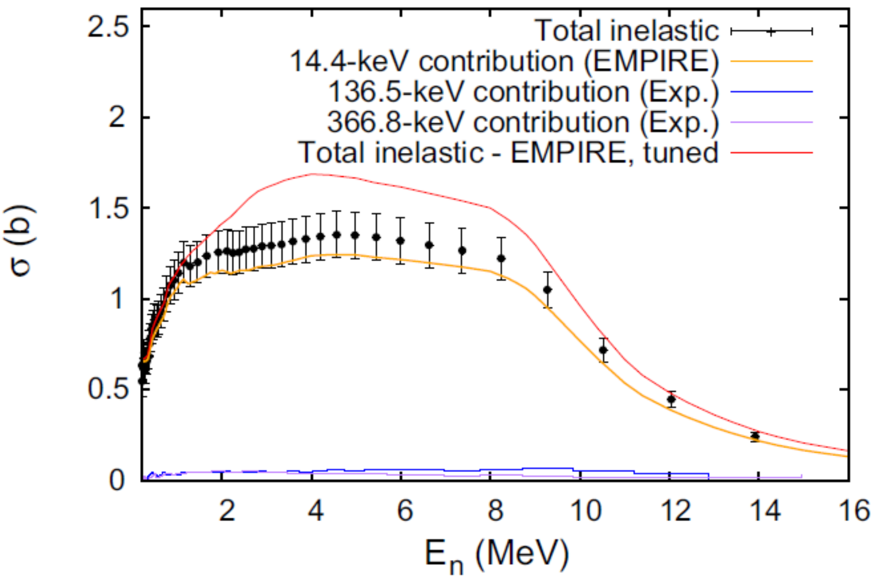
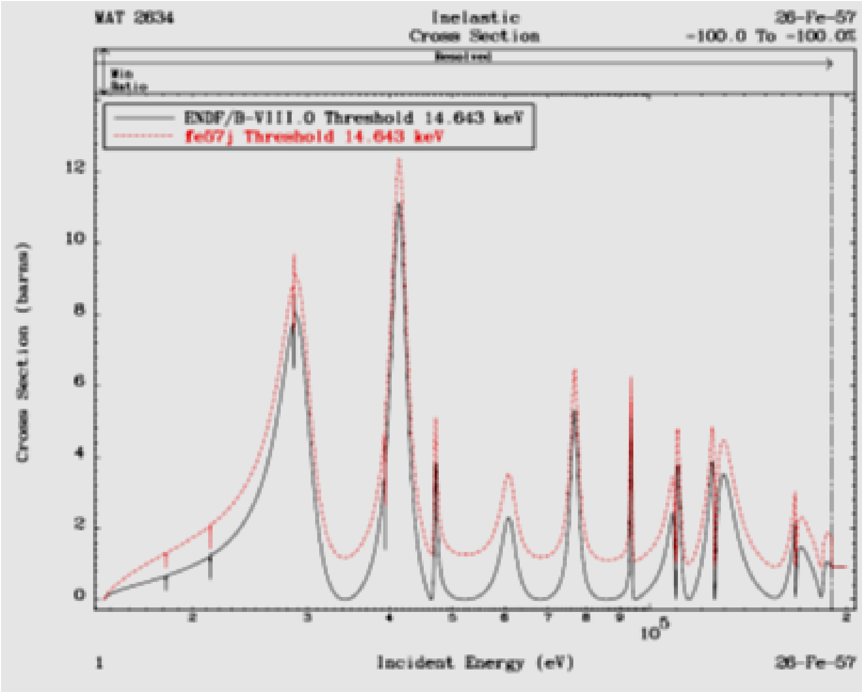
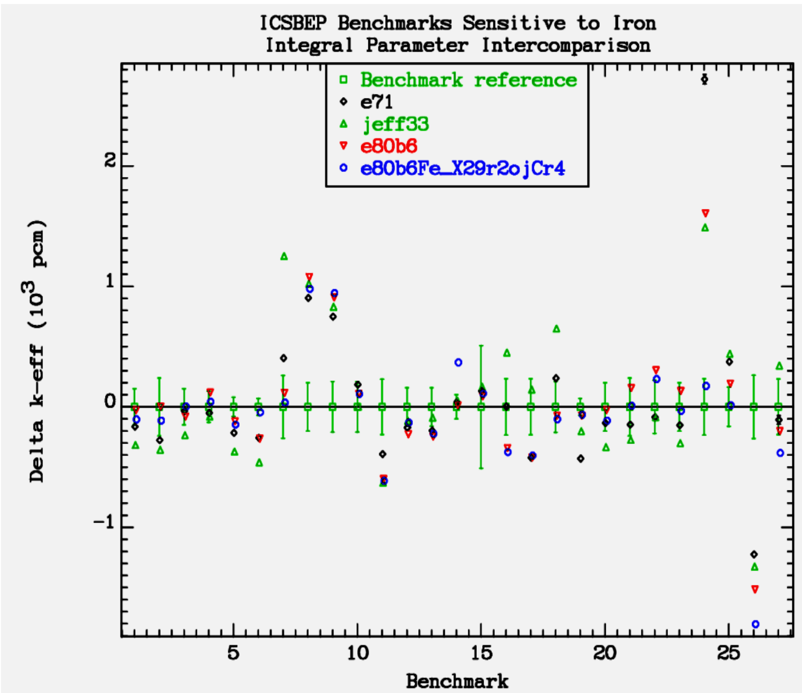


FIG. 11. Total inelastic cross section for the $^{57}Fe(n,n')$ reaction (black points), calculated based on the theoretically determined contribution of the 14.4-keV γ-production cross section (orange line), and the experimental results for the 136.5- (blue line), 366.8- (violet line), 692.0-, and 898.4-keV γ-production cross sections. The red line shows the total inelastic cross section calculated by EMPIRE using the tuned parameters.

Note that the abundance of ^{57}Fe is low, but this is the only inelastic cross section with a large slowing-down power below 0.845 MeV and a cross section below 1 MeV larager than 1 barn. The patch to the Fe-57 evaluation involves superposition of the resonance and the nuclear model contribution as shown below:



The validation of the new iron valuations in criticality benchmarks show that criticality performance was maintained for iron. The benchmarks sensitive to the thermal capture cross section on Fe-56 are numbers 5,6,7, and 14. The first two clearly improved with the new evaluation, but the last one got worse with the 10% reduction of the thermal capture.



1	hmf013	VNIITF-CTF-SS-13
2	hmf021	VNIITF-CTF-SS-21
3	hmf024	VNIITF-CTF-SS-24
4	hmf087	VNIITF-CTF-Fe
5	hmf088-001	FKBN-2/SS-PE-1
6	hmf088-002	FKBN-2/SS-PE-2
7	hmi001	ZPR-9/34
8	hmt013-002	Planet_Fe-PE-2
9	hmt015	Planet_HEU/Fe/PE
10	imf005	VNIIEF-CTF-5
11	imf006	VNIIEF-CTF-6/Al
12	lct042-001	PNL_1.68p-1
13	lct042-002	PNL_1.68p-2
14	lct043-002	IPEN/MB-01
15	lmt015-001	RB-Vinca-01
16	mcf001	ZPR-6/7(s)
17	mcf005s	ZPR-9/31(s)
18	mcf006s	ZPPR-2
19	pmf015	BR-1-3
20	pmf025	VNIIEF Pu/SS 1.55
21	pmf026	VNIIEF Pu/SS-11.9
22	pmf028	VNIIEF Pu/SS 19.6
23	pmf032	VNIIEF Pu(88%)/SS
24	pmi002	ZPR-6/10
25	pmi003-001s	ZPR-3/58(U)
26	pmi004-001s	ZPR-3/59(Pb)
27	ici005	ZPR-6/6A

2.5 Status of the evaluation of n + ^{56}Fe reaction data and experimental validation, M. Diakaki

A new evaluation of the ^{56}Fe isotope neutron induced reaction cross sections is ongoing at the CEA Cadarache, with the goal to cover the whole energy range, from the Resolved Resonances Region (RRR) to the continuum, with consistent uncertainty treatment. The motivation was the CIELO project that showed that it is very difficult to extend the RRR to higher energies (above the first inelastic level) than the original Froehner evaluation (1977). The CONRAD code is used, which is an object-oriented evaluation platform developed at CEA Cadarache.

For the energy range up to 850 keV the following has been examined up to now:

- JEFF 3.1.1 was used as a basis and overall nicely reproduced the cross section data, apart from certain minor fixes.
- The reproduction of Fe-nat total cross section minima with JEFF 3.1.1 at the different datasets has been investigated. For this, some measurements of Harvey (1975) with a thick target (6cm) available in EXFOR have been used. There is an indication of a **need of increase of the total cross section at the minima.** The origin of this discrepancy needs to be clarified.

Above 850 keV an effort is ongoing to extend the RRR, based on the initial Resolved Resonance Parameters from the CIELO project (*ORNL4* by Luiz Leal, available at https://www-nds.iaea.org/CIELO). For the moment the data of Negret (2013) and Perey (1971) have only been considered for the (n,inl) channel in order to improve the file ORNL4 and the high resolution Dupont data will be considered in the following. This is an ongoing work and for now the reproduction of these datasets (along with the transmission dataset of Pandey (1975) has been improved up to 1 MeV.

For the calculations in the continuum (> 4 MeV), the Morillon Romain optical model has been used for now, and reproduces fairly-well the average experimental data and latest evaluations above 4 MeV, but the region below (from 2 MeV up to 4 MeV) has to be revisited.

A couple of integral experiments that are/will be used to validate the evaluation have been shown:

1. the older *PERLE* experiment at the EOLE reactor (CEA Cadarache), for the validation of the Fe data and
2. the new *PETALE* experiment at the CROCUS reactor at EPFL, Switzerland (2020), for the validation of Fe, Cr and Ni data (collaboration between EPFL, PSI and CEA).

Some tests have been performed at the integral measurement PERLE (CEA Cadarache), which is interpreted with the Monte Carlo code TRIPOLI-4:

- Concerning the ^{56}Fe(n,g) cross section, the 1/v background proposed in the CIELO project has been tested and shown to improve the ^{55}Mn(n,g) dosimeter C/E results.
- Concerning the high energy region > 850 keV, the new (incomplete and preliminary) evaluation seems to improve the ^{237}Np(n,f) fission chamber C/E results (this is the most sensitive dosimeter in the region 0.6-2 MeV).

2.6 Interfacing TALYS with a Bayesian treatment of model defects and inconsistent data, G. Schnabel

Fe-56 is an important structural material but notoriously difficult to properly evaluate due to the fact that the energy range between few hundred keV and 5 MeV is difficult to represent accurately by R-matrix fits or optical models calculations. Therefore new evaluation concepts are of interest that aim to incorporate the idea of model deficiency into the evaluation procedure. Another issue affecting not only evaluations of structural materials are wrongly specified uncertainties of experimental data.

This presentation outlined an evaluation method featuring several innovations in evaluation methodology addressing the issues mentioned to alleviate their impact. The evaluation method was applied for a tentative evaluation of neutron-induced cross sections of Fe-56. Experimental data including associated uncertainties retrieved from the EXFOR library are first corrected using a rule-based approach, similar to the rules suggested in [1]. Remaining inconsistencies are removed or at least reduced by automatically introducing systematic uncertainties using marginal likelihood optimization (MLO). This approach is a special case of the method for automatic covariance matrix correction described in [2]. Model defects are addressed by imposing Gaussian processes on energy-dependent model parameters of TALYS as prior knowledge. This method to simulate a treatment of model defects was first described in [3]. After the pre-processing of experimental data and the setup of Gaussian process priors on energy-dependent model parameters, energy-dependent and independent parameters of the nuclear models code TALYS are adjusted to the experimental data by using a modified Levenberg-Marquardt (LM) algorithm, which was presented in the context of nuclear data evaluation in [4]. After the LM algorithm has located the maximum of the posterior distribution, a second-order Taylor approximation of the log-posterior distribution of the model parameters is constructed, i.e., a multivariate normal distribution. Random parameters sets are drawn from this approximated posterior distribution and the corresponding TALYS calculations performed. The calculation results are then written to ENDF files by virtue of the TEFAL code. A modified version of TASMAN enables the generation of a best ENDF files with covariance matrices. TALYS, TASMAN, and TEFAL are part of the the T6 code system employed for the generation of the TENDL library [5].

The mathematical and information technology aspects of the evaluation method outlined in the presentation are described comprehensively in a recently published preprint [6]. Even though the innovations incorporated into the evaluation procedure are significant advancements, the tentative evaluation of Fe-56 brought to light shortcomings that need to be addressed in the future. The most important one being that the treatment of model defects by using energy-dependent model parameters does not provide enough flexibility to fully match the model prediction to the experimental data, which manifests itself in very small evaluated uncertainties. The introduction of a treatment of model defects on the observable side as suggested and explored in, e.g. [7,8,9] is therefore important and should also be implemented and used in full scale evaluations in the future.

[1] Helgesson, P., Sjöstrand, H., Koning, A.J., Rydén, J., Rochman, D., Alhassan, E., Pomp, S., Combining Total Monte Carlo and Unified Monte Carlo: Bayesian nuclear data uncertainty quantification from auto-generated experimental covariances. Progress in Nuclear Energy 96 (2017) 76–96. https://doi.org/10.1016/j.pnucene.2016.11.006

[2] Schnabel, G., 2018. Fitting and Analysis Technique for Inconsistent Nuclear Data. arXiv:1803.0096. https://arxiv.org/abs/1803.00960

[3] Helgesson, P., Sjöstrand, H., Treating model defects by fitting smoothly varying model parameters: Energy dependence in nuclear data evaluation. Annals of Nuclear Energy 120 (2018), 35–47. https://doi.org/10.1016/j.anucene.2018.05.026

[4] Helgesson, P., Sjöstrand, H., Fitting a defect non-linear model with or without prior, distinguishing nuclear reaction products as an example. Review of Scientific Instruments 88 (2017) 115114. https://doi.org/10.1063/1.4993697

[5] Koning, A.J., Rochman, D., Sublet, J.-Ch., Dzysiuk, N., Fleming, M., van der Marck, S., TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology. Nuclear Data Sheets 155 (2019) 1–55. https://doi.org/10.1016/j.nds.2019.01.002

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[9] Schnabel, G., Leeb, H., Differential Cross Sections and the Impact of Model Defects in Nuclear Data Evaluation. EPJ Web of Conferences 111 (2016) 09001. https://doi.org/10.1051/epjconf/201611109001

2.7 Evaluation progress in the nuclear data of structural materials in JENDL, N. Iwamoto

New evaluations of structural materials (e.g., Cr, Mn, Fe, Co, Ni and Cu) progress for the development of JENDL-5. The presentation at this meeting was focused on the evaluation of Manganese-55, which is the only stable isotope of Mn and is used as an alloy material in a nuclear facility.

In JENDL the previous major revision of nuclear data on 55Mn was made 30 years ago [1]. Minor revisions were continuously performed for JENDL-3.2, JENDL-3.3 and JENDL-4.0. In the JENDL-4.0 resolved resonance parameters (RRPs) were replaced into those of Derrien et al. [2] who derived them with SAMMY code, and the resolved resonance region was extended from 100 keV to 125 keV. On the other hand, it is being difficult to reproduce the nuclear data in a smooth region, since some codes were involved with their calculations.

For JENDL-5 the RRPs revised from the original Derrien et al. Evaluation in JEFF-3.2 evaluation were adopted. In a smooth region the evaluation efforts were made by CCONE code which is a comprehensive nuclear reaction model code. In the presentation, newly evaluated data of ^{55}Mn (total, elastic scattering, total and partial inelastic scattering, capture, (n,2n), (n,p), and (n,a) reaction cross sections; angular distributions of elastic scattering; gamma-ray and neutron emission double differential cross sections) were shown, together with the data of JENDL-4.0, ENDF/B-VIII.0, JEFF-3.3 and measurements. The present results well reproduce the measured data, except for 126 keV-gamma-ray production cross section at inelastic scattering, in which the data of Lashuk et al.[3] are larger than the calculated ones by ~150 mb below 1 MeV. Their data will be taken into account in the evaluation. Special care was needed in the unresolved resonance region (URR). The URR was divided with three regions: (i) 125-175 keV, (ii) 175-500 keV and (iii) 500 keV-4 MeV. The region (i) has point-wise cross sections derived from the RRPs of Derrien et al. with statistical p-wave resonances. The region (ii) consists of smooth cross section calculated by coupled channels optical model. The region (iii) is expressed by the data of Cierjacks et al.[4].
It was realized that the gamma-ray production cross sections at inelastic scattering and (n,a) reaction cross sections in ENDF/B-VIII.0 and JEFF-3.3 are extremely small above incident neutron energies corresponding to upper limit of adopted discrete levels in residues, compared with the present results. This fact comes from the missing of continuum level components.

[1] K. Shibata, J. Nucl. Sci. Technol. **26**/10 (1989) 955.

[2] H. Derrien, L.C. Leal, N.M. Larson, K. Guber, D. Wiarda, G. Arbanas, Int. Conf. Phys. Reactors (PHYSOR 2008), p.124.

[3] A.I. Lashuk, A.I. Gonchar, I.P. Sadokhin, Vop. At.Nauki i Tekhn., Ser. Yadernye Konstantys, Issue 1 (1994) 26.

[4] S. Cierjacks, P. Forti, D. Kopsch, L. Kropp, J. Nebe, H. Unseld, Kernforschungszentrum Karlsruhe Reports, No.1000, Vol. (SUPP.2) (1969).

3 Discussion

3.1 General comments

For criticality applications, typically a good description of capture and inelastic cross section is required. This implies that minor isotopes can become very important. For most of the structural materials the energy region of highest importance is close to the transition between resonance and fast region, therefore carefully modelling that transition will be absolutely essential for any evaluation.

For shielding applications, a good description of the elastic (total) cross section for the major isotopes is important. Without correctly describing the interference minima in the total cross section, deep penetration problems cannot be modelled adequately.

3.2 Resolved resonance region

All of the structural material considered have a few stable isotopes, it will be therefore essential that already during the evaluation process all naturally occurring isotopes are considered. Only such an approach can ensure that the final evaluation(s) can reproduce the properties of the natural materials correctly. For all new evaluations all open channels should be considered, and a direct capture component will have to be accounted for in the evaluation process.

However, at the moment we are not aware of any publicly available code that can do the calculations of direct capture. We were informed that TALYS has in principle the possibility, but this option has not yet been broadly used, as the accuracy of the results has not been tested /validated yet. In the absence of an openly available code, a possible (temporary) solution might be to provide tabulated values of the direct capture components of the nuclei of interest.

As describing the interference minima of the elastic (total) cross section is a prerequisite for correctly reproducing the results of shielding benchmarks, very thick transmission measurements (thickness of few centimeters) should be included during the evaluation process (e.g., Fe-56 Harvey thick transmission with 40% transmission in the cross section minima). Special attention should be paid to existing experiments, or specially designed experiments.

Various validation methods can and should be used at the end of the evaluation, such as

- The k0 database can provide thermal capture cross section (e.g., see Ref. [1,2]).
- Validation for the resolved resonance region, data from LSDS can help to identify weaknesses in the RRR.(e.g., Grenoble LSDS [3,4]; Mn, Ni, W have been tested)
- The use of the KADONIS database [v0.3, v1.0] cannot be recommended for validation of capture as it contains a mixture between theoretical calculations and experiments. Nevertheless, it is valuable to obtain guidelines for evaluation, after the sources given in the database have been checked and experimental data recovered.

3.3 Transition RRR to URR

It is recommended to check the average capture cross section at the end of the resonance region. Deviations from the shape of calculated capture using the Hauser-Feshbach CN decay model may indicate the existence of missing levels, which need to be addressed.

When the percentage of missing levels exceeds 30-40% of the total number of resonances the description of the cross section with resolved resonance parameters is questionable.

Three possible options of addressing missing levels are available:

1) Reduction of the RR energy range.
2) If the RRR can not be reduced, then the missing strength at the upper end of the resolved resonance region due to the missing levels can be compensated by introducing fictitious resonances. This will ensure that the ensemble of resonances will pass the statistical test (e.g., see https://www-nds.iaea.org/missing-levels/ for a comprehensive review and codes).
   A comparison between the strength function calculated from the optical model to the strength function derived from the resonance parameters can be used to estimate the missing capture strength, especially for L>0 partial waves. This has the advantage of guaranteeing consistency between the fast and the resonance regions.
3) A common, but very rough way of dealing with this problem is adding background. Ideally, background should be added before undertaking the R-matrix fit, otherwise it may violate unitarity.

We would recommend adding an ENDF-6 (GND) flag in the evaluated file for the resonances that have been added based on statistical analysis, as this would allow for a clear distinction between observed and fictitious resonances.

3.4 Unresolved resonance parameters

Consistency between RRR, URR and fast range cross sections is extremely important. If no experimental data are available the OM should be used to derive the average parameters. If data are available, still the strength functions calculated from the proper optical model for L>0 may be considered (and not be taken as a fitting parameter).

When do we need URR ? If there are large non-statistical fluctuations in the measured total cross sections it is difficult to define URR (e.g., Fe-56 above 850 keV up to 4 MeV) and often these fluctuations are considered in the fast neutron range.

With these parameters the self-shielding factor can be calculated, and when this factor becomes small enough then transition between URR and fast region (smooth cross section) can take place. Such a test could be done either using MCNP to describe transmission through a thick sample – with and without Probability Table (PT) –or by calculating self shielding factors with NJOY. The use of UNRESR module is enough for this purpose. Additional tests using experimental data have been discussed (e.g., see Yaron's presentation at the INDEN meeting on resonances in actinides – available online at https://www-nds.iaea.org/index-meeting-crp/TM-INDEN-2019/docs/Danon-ResAct-INDEN.pdf ").

[1] The Kayzero database, available online at http://www.kayzero.com/k0naa/k0naaorg/Nuclear_Data_SC/Nuclear_Data_SC.html.

[2] A. Trkov and V. Radulovic, « Nuclear reactions and physical models for neutron activation analysis, », J. Radioan. Nucl. Chem. **304**, 763-–778 (2015).

[3] L. Perrot et al, « Precise validation of (n,g) cross-section database using a Lead-Slowing-Down-Spectrometer and simulation from 0.1 eV to 30keV : Methodology and data for a few elements », Nucl. Sc. & Eng. **144**, 142-156 (2003).

[4] Luc Perrot Ph.D. Thesis, 4 Dec. 2001, Institute of Nuclear Sciences, Grenoble, France.

3.5 Fast range

Medium-mass structural materials (iron region) are characterized by large fluctuations in the measured total (and correspondingly inelastic) cross sections below ~5 MeV in a region that is very important for many applications, including reactor and shielding, criticality safety, radiation damage, etc.

Additionally, many existing optical model potentials (OMP) have shown deficiencies in describing the average total cross sections below 5 MeV, in particular the very low total cross sections near 1 MeV (there are l-dependent potentials especially developed, e.g., Kawano and Froehner [1] that accurately reproduce low average cross sections near 1 MeV).

If we neglect cross section fluctuations in the fast range (i.e., OMP calculations are used) and we do not define URR then it is implicitly assumed that self-shielding is negligible in applications. This fact should be considered by evaluators to either define the URR or to consider fluctuations in the energy range if self-shielding is important for a given applications.

OMPs should be checked vs the averaged total cross section data from EXFOR. Comprehensive measurement sets by e.g., Foster Jr. *et al*, Abfalterer *et al*, Poenitz *et al*, Finlay *et al.*, should be considered for testing the consistency of the selected OMP.

Inelastic (and n,xn) data measured by gamma detection should be considered once the used decay data are updated. Experimentalists are encouraged to provide measured gamma-production data (on isolated transitions) in addition to derived inelastic data. This may allow improving the data analysis. Use of gamma detection for inelastic studies require consideration of the anisotropic gamma angular distribution for conversion to angle-integrated gamma-production cross section for incident neutron energies lower than about 2 MeV. The use of newly defined gamma-production reference cross sections on Li-6(n,n'g), B-10(n,n'g), and Ti-48(n,n'g) is recommended [2], see also (n,n'g) reference cross-section data online at https://www-nds.iaea.org/standards/.

There is a question of the impact of those fluctuations on calculated integral quantities. Intercomparison of calculated integral quantities using fluctuating vs average cross sections should be studied to define recommendations.

There have been observed inconsistencies for several targets between (differential) inelastic experiments from different labs, as well as inconsistencies between inelastic data needed to describe deep-penetration shielding experiments and results of inelastic differential measurements (e.g., Fe-56). Such discrepancies indicate the need to investigate their origin.

[1] T. Kawano and F.H. Froehner, « Partial-Wave Analysis with the Optical Model for the Resolved and Unresolved Resonance Regions of 56Fe », Nucl. Sc. Eng. **127**, 130 (1997).

[2] A.D. Carlson, V.G. Pronyaev, R. Capote et al., « Evaluation of the Neutron Data Standards, » Nucl. Data Sheets **148**, 143 (2018).

3.6 Status of files/planned work of participants

3.6.1 Fe-56

Thermal capture

Firestone et al [Phys. Rev. **C95**, 014328 (2017)] suggests a reduction of approximately 10 % of the thermal capture. Can that be supported by any other measurement? There has been a recent measurement at n_TOF, results are not available yet. (M. Diakaki to provide feedback of the thermal capture data as soon as data are available).

Capture in the 10-20 keV energy range

There is consensus that the capture in the region follows a 1/v behaviour, the dip observed in older evaluations is considered an artefact caused by the introduction of bound states. It is preferable that a direct capture component is introduced instead.

(G.Nobre will check on availability of CUPIDO, D. Rochman will check on TALYS, M. Diakaki will contact A. Mengoni, N. Iwamoto to provide tabulated data for Fe-56)

The resonance analysis should include (really) thick target (>5cm) transmission data (Harvey 75 picture), to improve the description of the interference minima in the total cross section.

At the upper end of the resonance region, additional fictitious resonances will have to be included, especially for higher partial waves. It will be attempted to increase the upper limit of the RRR. Comparisons with integral benchmark will be made. Fe-56 evaluation is in progress at CEA Cadarache. There is a new file produced by Trkov and Capote (available from the INDEN webpage – r39) which shows good integral performance, but the resonance region has beeen corrected in an adhoc manner. A proper R-matrix fit including direct capture is very desirable.

Test a MCNP model for ORELA transmission model for Fe transmission. (S. Kopecky).

For the inelastic cross section the available experimental data are not fully in agreement, evaluators will have to consider integral benchmark information (shielding experiments) for selection of differential data.

Fe-57 inelastic data has a low threshold, therefore it defines the total inelastic for natural iron below 800 keV (impact in critical benchmarks has been observed by Trkov validation). The status of experimental data is not satisfactory, new measurement would be desirable. However, the first inelastic level at 14 keV which defines the total inelastic is very much converted and difficult to measure with gammas.

3.6.2 Cr

Thermal capture: At low energies the capture is dominated by the cross sections of the odd isotopes. First indication of currently ongoing resonance analysis suggests to increase the thermal cross section, still to be checked. The k0 database only lists a value for Cr-51, the agreement with the values in evaluated files is within a few percent, for Cr-50 the difference is significant.

There may be problems in the resonance integral in the Atlas, some values are significantly larger than in the evaluations. The RI for natural Cr seems to be underestimated. Future evaluations will test against RI. This observation is consistent with observations of integral experiments. Activation measurements (MACS, Si filtered beam…) for Cr-50 might be helpful.

Inelastic measurements seem to have similar problems as observed for Fe-56. Some inconsistencies between EXFOR and data in publication.

The calculation using OM overestimates measured total cross section data below 4 MeV.

Natural data exist, the measurements of isotopic samples suffer from problems with the sample material, new measurements would help for resonance analysis.

3.6.3 Ni

Ni-64 is the only isotope that can be measured by activation. The thermal capture cross section values by Mughabghab and derived from the Kayzero library are in good agreement (1.63+/-1.2% and 1.622+/-0.7%, respectively.

Likewise, the resonance integrals are in similarly good agreement (1.07+/-14%, 1.09+/-0.7%, respectively).

The cross sections in the resonance range need to be validated. The Grenoble LSDS experiment can be used for this purpose.

The direct capture contribution should be checked.

Unless the fluctuations above the resolved resonance region are considered explicitly, the unresolved resonance region should be included.

The fluctuations in the inelastic cross sections of Ni-58,60,62 are available in EXFOR and should be included in the evaluations.

3.6.4 Mn

There is a new JENDL evaluation in preparation.
Current: RRR (up to ~125keV) + URR up to 1 MeV.
Mn-55(n,2n), Mn-55(n,g) is an IRDFF-II evaluation (2019).
Investigate issues in epithermal neutron dosimetry using Mn. Some differences in (n,a) formatting and gamma-production should be investigated (see 2.7).

3.6.5 Cu

ORNL is working on revising the evaluation and addressing issues in capture/angular distributions.

RRR exists up to 300 keV, but the capture decreases showing a possible impact of missing levels. Other evaluations had the RRR up to 100 keV. This problem needs to be addressed.

New measurements of angular distributions below 500 keV are needed. High sensitivity to angular distributions below 1 MeV has been shown in criticality testing.

Criticality experiments of the ZEUS assembly are highly sensitive to copper (HMI006-4 cases, HMF72-2 cases,HMF73, Swedish benchmarks …)

Fast range:

There are issues in shielding 14 MeV benchmarks (Oktavian) with ENDF/B-VIII.0 evaluation.

There is an FNG copper shielding benchmark (SINBAD), dosimetry measurements inside the copper block.

IRDFF-II Cu-63(n,g), Cu-63(n,a), Cu-63(n,2n) and Cu-65(n,2n). However, there are issues noted in validation of the Cu-63(n,2n) reaction that need to be investigated.

3.6.6 Pb

Very important as coolant (Pb/Bi), shielding and criticality safety.
Big issues in C/E for critical assemblies (especially reflectors) …
New resonance evaluation (Pb-204,206,207,208) on-going (IRSN/ORNL).
Direct capture should be considered.
Additional data needs may require new HPRL entries.
Fast range:
Possible efforts may include BNL, IAEA, JENDL (inelastic).

3.7 Issues for next meeting

- Self-shielding estimates (definition of the URR, stat reson vs explicit fluctuations)

Thick sample transmission data are needed for testing.

- Impact of fluctuations in the fast region on applications. Can we use smooth cross sections?

Appendix 1

Atoms for Peace: The First Half Century
1957–2007

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

IAEA Headquarters, Vienna, Austria

2– 5 December 2019

Meeting Room **M0E23**

Adopted AGENDA

Monday 2 December

08:30 – 09:30	**Registration** (IAEA Registration desk, Gate 1)
09:30 – 10:00	**Opening Session** Welcoming address – Arjan Koning Introductory Remarks – Roberto Capote Election of Chairman and Rapporteur Adoption of Agenda
10:00 – 13:00	**Presentations**
10:00 – 11:00	Re-evaluation of Fe-56 data based on CENDL-3.2b1, H. Wu
11:00 – 12:00	Status of Cr Evaluations, G. Nobre:
12:00 – 13:00	TENDL-2019 and the Ni isotopes: what to expect? D. Rochman

Coffee break as needed

13:00 – 14:00	*Lunch*
14:00 – 18:00	**Presentations** (cont'd)
14:00 – 15:00	Current status of the Post-CIELO Fe-56 evaluation, A. Trkov / R. Capote:
15:00 – 16:00	Status of the evaluation of n + ^{56}Fe reaction data and experimental validation, M. Diakaki
16:00 – 17:00	Interfacing TALYS with a Bayesian treatment of model defects and inconsistent data, G. Schnabel
17:00 – 18:00	Evaluation Progress in the Nuclear Data of Structural Materials in JENDL, N. Iwamoto

Coffee break as needed

Tuesday 3 December

09:00 – 13:00 **Technical discussions**

Coffee break as needed

13:00 – 14:00 *Lunch*

14:00 – 18:00 **Round Table Discussions**

Coffee break as needed

19:00 ***Social Dinner**: Restaurant Das Heinz, Rudolfsplatz 12, 1010 Wien*

Wednesday 4 December

09:00 – 13:00 **Round Table Discussions (cont'd)**
Drafting of the summary report

Coffee break as needed

13:00 – 14:00 *Lunch*

14:00 – 18:00 **Drafting of the summary report (cont'd)**

Coffee break as needed

Thursday 5 December

09:00 – 13:00 **Review of the summary report**
Discussion of the actions

Coffee break as needed

13:00 **Closing of the Meeting**

Appendix 2

IAEA
Atoms for Peace: The First Half Century
1957–2007

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

List of Participants

China	Wu HAICHENG China Nuclear Data Center China Institute of Atomic Energy P.O. Box 275 (41) Beijing Email: haicheng@ciae.ac.cn
France	Maria DIAKAKI Centre d'Etudes Nucleaires de Cadarache SAINT PAUL LEZ DURANCE 13108 Email: Maria.DIAKAKI@cea.fr
Japan	Nobuyuki IWAMOTO Japan Atomic Energy Agency (JAEA) 2-4 Shirakata, Nagka-gun 319-1195 Tokai-Mura Ibaraki Email: iwamoto.nobuyuki@jaea.go.jp
Sweden	Georg SCHNABEL Uppsala University Department of Physics and Astronomy Division of Applied Nuclear Physics 75120 Uppsala Email : georg.schnabel@physics.uu.se
Switzerland	Dimitri ROCHMAN Paul Scherrer Institut (PSI) 5232 Villigen Email: dimitri-alexandre.rochman@psi.ch
United States of America	Gustavo NOBRE Brookhaven National Laboratory National Nuclear Data Center Bldg 817 Upton, NY 11973-5000 Email: gnobre@bnl.gov
	Vladimir SOBES Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 Email : sobesv@ornl.gov

EC-JRC	Stefan KOPECKY European Commission Joint Research Centre Directorate G - Nuclear Safety & Security Retieseweg 111 2440 Geel Email: stefan.kopecky@ec.europa.eu
IAEA	Andrej TRKOV Email: a.trkov@iaea.org Roberto CAPOTE NOY Email: Roberto.CapoteNoy@iaea.org Both: International Atomic Energy Agency Nuclear Data Section Wagramer Strasse 5 P.O. Box 100 1400 Vienna Austria

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://nds.iaea.org