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

Summary Report of the IAEA Consultants Meeting

14 – 17 December 2020
(virtual event)

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February 2022

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1. Introduction

A virtual Consultancy Meeting was held from 14 to 17 December 2020 to review existing problems in evaluations of structural materials, potential issues in the adopted experimental data, and the progress made in ongoing evaluation efforts. As the evaluation of structural materials is challenging in certain energy ranges, such as for ^{56}Fe between 1-5 MeV, an additional objective of the meeting was the discussion of evaluation methods and their possible extension. This meeting is part of a series of meetings within the framework of the International Nuclear Data Evaluation Network (INDEN) to bring together internationally recognized experts to discuss topics and issues of current relevance.

G. Nobre and V. Proniaev 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 fourteen presentations given by experts from eleven Member States and two International Organizations.

2. Presentation Summaries

2.1 New evaluations of chromium isotopes, G. Nobre

Neutron reaction data for the set of major chromium isotopes were reevaluated from the thermal energy range up to 20 MeV. In the low energy region, updates to the thermal values together with an improved R-matrix analysis of the resonance parameters characterizing the cluster of large s-wave resonances for ^{50,53}Cr isotopes were performed. In the intermediate and high energy range up to 20 MeV, the evaluation methodology used statistical nuclear reaction models implemented in the EMPIRE code within the Hauser-Feshbach framework to evaluate the reaction cross sections and angular distributions. Exceptionally, experimental data were used to evaluate relevant cross sections above the resonance region up to 5 MeV in the major ^{52}Cr isotope. Evaluations were benchmarked with Monte Carlo simulations of a small suite of critical assemblies highly sensitive to Chromium data, and with the Oktavian shielding benchmark to judge deep penetration performance with a 14-MeV D-T neutron source. A significant improvement in performance is demonstrated compared to existing evaluations.

2.2 INDEN evaluation of Fe isotopes & the ^{55}Mn update of thermal (n,γ) gammas, R. Capote, A. Trkov

A summary of the observed deficiencies in gamma emission of multiple evaluations in ENDF/B was presented. A method was shown to correct such deficiencies and improve the evaluation of emitted gammas in near-thermal neutron capture on a Mn-55 target. Results were documented in the report INDC(NDS)-0810 available online at nds.iaea.org/publications/indc/indc-nds-0810.

A comprehensive summary on modifications of the IAEA CIELO evaluation of iron isotopes was presented and discussed. Proposed changes in elastic and inelastic cross sections were reviewed. A patch aimed at fixing problems identified in neutron leakage experiments was proposed. However, a new evaluation of Fe-56 cross sections in the resonance region, at least up to 850 keV is called for. A significant improvement of evaluation regarding the leakage of fast neutrons with energies from 1 up to 6 MeV was documented.

Updated iron files are available from the INDEN webpage:

INDEN - International Nuclear Data Evaluation Network (iaea.org) (tab: Fe-isotopes).

2.3 INDEN Fe validation, A. Trkov

To view the presentation, please refer to Appendix 3 – Presentation links.

2.4 Angular distributions for neutrons with incident energy below 2 MeV scattered at ^{56}Fe, V.G. Pronyaev

Neutron induced cross sections at ^{56}Fe are well studied experimentally and the fine structure in the evaluated data files for the energy range above the usual resolved resonance range (the threshold of first inelastic scattering level at 0.85 MeV) is taken from the experimental data. The Reich-Moore evaluation by Luiz Leal up to 2 MeV for all open channels allows to predict without experimental resolution broadening the cross sections in the energy range with partially overlapping resonances.

Relative Legendre expansion coefficients for elastic and inelastic scattering angular distributions were calculated from Leal's R-M parameters in the Blatt-Biedenharn approximation for the energy range up to 2 MeV using the GRUCON code. Point-wise energy dependent coefficients were averaged with a weight of integral elastic cross sections in 299 and 28 standard energy groups. The MF4, MT2 and MT51 files were prepared for use in the calculations of benchmarks to study the influence of averaging of angular distributions on the result of calculations.

There are strong correlations between cross section and angular distributions in experimental and calculated data. These correlations can be distorted, if MF3 and MF4 files contain cross sections and angular distributions taken from different sources. Details with which the energy dependence of angular distributions should be presented in the files were studied in calculations of integral parameters (like k_{eff} in fast neutron heterogeneous systems, neutron leakage, etc.) using detailed point-wise and 299 and 28 group averaged Legendre expansion coefficients.

The following groups of related benchmarks are convenient for the study of the criticality dependence from the Fe reflector thickness:

1. PMF-022 – bare 98% ^{239}Pu sphere

   PMF-025 – 98% ^{239}Pu sphere with 1.55 cm iron reflector

   PMF-026 – 98% ^{239}Pu sphere with 11.9 cm iron reflector.

2. HMF-008 – bare 90% ^{235}U sphere

   HMF-013 - 90% ^{235}U sphere with 4 cm iron reflector

3. HMF-018 – bare 90% ^{235}U sphere at different (comparing with HMF-008) installation

   HMF-021 - 90% ^{235}U sphere with 9.7 cm Iron reflector.

The trend in the dependence of C/E for k_{eff} from the reflector thickness will show if the ^{56}Fe evaluated data file describes the properties of iron as reflecting material at different thicknesses well. Data can be presented as ratio to C/E for k_{eff} of bare sphere of a given group (double ratio). This will practically remove the biases in k_{eff} due to different data for ^{235}U and ^{239}Pu driven benchmarks in different libraries.

Another model benchmark was proposed by V. Sinitsa. It is based on calculations of the k_{eff} dependence for Godiva with a ^{235}U sphere radius reduced to 8 cm and variable thickness of a ^{56}Fe reflector. Three different sets of MF4, MT2 files were prepared: with detailed energy dependence of Legendre expansion coefficients for elastic and inelastic scattering (few tens of thousands angular distributions), with 299 standard energy groups and 28 standard energy groups for angular distributions in the energy range below 2 MeV. The influence of details of angular distributions presentation from energy can be seen comparing the calculated criticality coefficient in dependence from the reflector thickness.

Comparing the results of V. Fillipov's narrow neutron beam transmission measurements through natural iron with the transmissions calculated using different iron evaluations may indicate a problem in the evaluations. Transmissions are sensitive to the averaged total cross sections as well to the cross sections at the minima between resonances. For the large thicknesses the influence of the cross sections at the minima is dominating.

This leads to the following conclusions:

1. The angular distributions of scattered neutrons in the resolved resonance range should be calculated from the evaluated resonance parameters.
2. The resolved resonance range can be extended up to the threshold of the second excited state, where it is possible.
3. Remote resonances (even fictitious) at the upper boundary of the resonance range should be added to the fit.
4. The cross sections most sensitive to the missed (narrow) resonances (e.g., capture cross section), can be corrected through the inclusion of the background component.
5. The contribution of direct processes in the inelastic scattering cross section with excitation of the first level in the resolved resonance range can be accounted as the background.
6. The use of angular distributions averaged on 299 energy groups in the benchmark calculations allows to obtain results that are very close to the results based on the detailed energy dependence for angular distributions.

It is expected that these changes in the files will allow to get a better description of benchmarks with reflector from a given material and experiments with deep penetration of neutrons in the materials.

2.5 Status of the evaluation of n+^{56}Fe reaction data – Focus on (n,inl), M. Diakaki

A new evaluation of the ^{56}Fe isotope neutron induced reaction cross sections is ongoing at CEA Cadarache, with the goal to cover the whole energy range, from the Resolved Resonances Region (RRR) to the continuum, with consistent uncertainties treatment. The motivation was the CIELO project that showed that it is very difficult to extend the RRR to higher energies than the initial 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 JEFF 3.1.1 was used as a basis and, on the whole, nicely reproduced the cross-section data, apart from certain issues (need for increase of the total cross section minima, small changes in the Resolved Resonance Parameters -RRP).

Above 850 keV, in an effort to extend the RRR to the highest energy limit, the initial RRP from the CIELO project (ORNL4 by Luiz Leal, available at www-nds.iaea.org/CIELO) has been used as a basis. Many resonances have been added to this file in order to better reproduce the following (n,inl) data available at EXFOR: Negret (2013-GELINA, JRC-Geel) and Perey (1971-ORNL). The data of Dupont (1998) had normalization issues and have only been used to find the position of the peaks to be added, thanks to the very high neutron energy resolution. New preliminary RRP have occurred until 2 MeV. It was observed that the higher the energy the more difficult it gets to reproduce the inelastic by adding resonances without spoiling the reproduction of the transmission datasets. This could mean that the data of the inelastic reaction cross section are too high or that there is the need to change the elastic cross section, still under investigation.

The older PERLE experiment at the EOLE reactor (CEA Cadarache) was used for the validation of the new resonance file and especially the region 850 keV-2 MeV. The experiment was interpreted with the Monte Carlo code TRIPOLI-4. The new 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).

Throughout this new evaluation effort, it has been noticed that high accuracy microscopic data are needed in order to be able to properly extend the RRR well above the current limit (850keV). To this purpose a new experimental campaign with a set of microscopic measurements on ^{56}Fe starts soon at JRC-Geel, and a PhD student from CEA Cadarache will be working on the subject.

2.6 MCNP simulation of Fe transmission measurements, S. Kopecky

This contribution investigates if measurements by Harvey et al (1975 EXFOR 13765), transmission measurements of thick iron samples, would be sensitive enough for testing the cross-section minima in the energy range from 100keV to 1 MeV. These investigations try to reproduce the experimental data by MCNP simulations, with the goal to understand the experimentally observed transmission spectra, in particular estimate the contribution of multiple scattering and forward scattering events.

Using MCNP, the trajectories of the neutrons emitted from the ORELA source through the sample until they reach the detector are simulated and the timing of the detected neutron is registered. For all simulations the start time of all neutron is set to zero. The resolution of the target assembly is accounted for by modifying the spatial distribution of the emitted neutrons.

The source distributions were derived using simulation of the ORELA target, the geometry and dimension of the target have been taken from a report by S. N. Cramer and F. Perey. The accuracy of the ORELA resolution function was validated by simulating transmission measurements through thick U-238 samples.

From the documentation of the EXFOR 13765 entry the dimension of the neutron detector is not entirely clear. However, it could be established that most likely a 2 cm thick Ne-110 detector was employed for the measurements. As first approach to derive the detector resolution function, the neutron flux multiplied with the elastic cross section of hydrogen was used. The cut-off energy for neutrons was 20 keV, and the time information of these events was recorded. This timing resolution was compared to more detailed and time-consuming models, and while the detection efficiency was differing, the time resolution for these detectors was similar. As the same detectors are used for sample-in and sample out, detailed simulations for detection efficiencies are for the presently desired accuracies not needed. No background effects, such as room returns, etc., are considered in the simulation and therefore the simple model is more than adequate.

Precise information on the flight path geometry was not available in the EXFOR. Therefore, some assumptions on location and size of the collimators had to be made. These assumptions were guided by information available for other experiments performed at that flight path in the same time period.

With all these ingredients simulation for the "open beam" and the "sample" were performed, and the transmission calculated. After converting the recorded time-of-flight into energy – using the parameters given for the ORELA experiments – comparisons between measured and simulated transmission spectra could be made.

It could be observed that the simulations using ENDF/B-VIII and JEFF3.3 libraries show a tendency to slightly overestimate the transmission through the transmission maxima below 800 keV. For the tested IAEA file, the picture is more mixed, as some transmission maxima are underestimated while others are overestimated. It might be too early to draw any strong conclusion, as the full impact of the uncertainties in the measurement geometry is hard to quantify. However, the simulations clearly show the value of such thick transmission measurements and for the case of Fe new measurements with well-documented geometries might proof very valuable.

2.7 Inelastic measurements on Fe isotopes at GELINA - Results and future plans, A. Negret

C. Borcea, M. Boromiza, Ph. Dessagne, Gr. Henning, M. Kerveno, N. Nankov, M. Nyman, A. Olacel, A.J.M. Plompen, C. Rouki

The presentation summarizes the experimental details of the neutron inelastic cross section measurements performed by our group at the neutron source GELINA of JRC-Geel. The results on ^{56}Fe, ^{57}Fe and ^{54}Fe were published in 2014, 2017 and 2018, respectively. All experiments applied the time-of-flight method combined with gamma spectroscopy techniques using HPGe detectors to build gamma production cross sections as primary experimental results. In case of ^{57}Fe the determination of the 14-keV gamma production cross section implied a combination of the experimental investigation with a detailed theoretical description of the reaction.

In view of the renewed interest in the inelastic cross sections on ^{56}Fe within the INDEN project we present our plans for a future new measurement of the inelastic cross section of this isotope.

2.8 Evaluation of ^{59}Co for the JENDL Library, N. Iwamoto

New evaluations of structural materials progress for the development of JENDL-5. The presentation at this meeting was focused on the evaluation of Cobalt-59, which is only stable isotope of Cobalt. Cobalt is one of the structural materials in nuclear and accelerator facilities. It is contained in carbon steel and concrete as well as SUS304. The nuclear data of ^{59}Co are considered to be important specifically for radioactivity estimation of $^{58,60}Co$ related to decommissioning of the facilities. JENDL-4.0 [1] includes the nuclear data of ^{59}Co, based on the evaluation performed in 1988. A major revision was carried out for the JENDL-3.3 evaluation in 2001. After the release of JENDL-3.3, many measured data for capture, (n,2n), (n,p), and (n,α) reactions have been published. Therefore, the reconsideration of nuclear data is required for JENDL-5.

The present evaluation of ^{59}Co was divided into three regions: resolved resonance region, unresolved resonance region and fast neutron energy region. In the resolved resonance region, the resonance parameters and scattering radius were taken from de Saussure et al. [2], who derived the resonance parameters up to 100 keV. The comparisons of the present data with JENDL-4.0 were made for total and capture cross sections. For capture cross section there are many resonances missed in transmission measurements. Those resonances will be taken into account after doing a detailed evaluation. The thermal capture cross section was evaluated, based on many experimental data. In this evaluation the absorption cross sections of natural boron and capture cross section of gold, which were frequently used as monitor cross sections, were corrected with those of the IAEA Neutron Data Standards [3]. The uncertainty estimation was made by the method in the report [4]. In the unresolved resonance region of 0.1 to 5 MeV, the total cross section of de Saussure et al. was adopted, though the data contain experimental effects, which should be removed from evaluated data. In the fast neutron energy region up to 20 MeV, the evaluation was performed by the nuclear reaction calculation code CCONE [5]. The evaluated data were presented with measured ones for the total cross section, elastic scattering angular distribution, capture, (n,p) and (n,α) reaction cross sections, and neutron emission double differential cross section, which were compared with the data of ENDF/B-VIII.0 and JEFF-3.3.

The direct capture contribution is considered to be important to the capture cross sections of structural materials, which have small cross sections. The calculations of direct capture cross section were carried out for 55Mn and 56Fe by a formulation [6]. The enhancement of capture cross section was seen for 56Fe in the energy region above 1 keV. This effect may have an important role in a benchmark test.

[1] K. Shibata et al., J Nucl. Sci. Technol. **48** (2011) 1.

[2] G. de Saussure et al., Ann. Nucl. Energy **19** (1992) 393.

[3] A.D. Carlson, et al., Nucl. Data Sheets **148** (2018) 143.
[4] Report OECD/NEA/WPEC/SG41, Volume 41 (2020).
[5] O. Iwamoto et al., Nucl. Data Sheets **131** (2016) 259.
[6] F. Minato and T. Fukui, EPJ Web Conf. **163** (2017) 00037.

2.9 Validating nuclear data for lead with shielding benchmarks, H. Wu

Lead is a coolant material in fast reactors. However, criticality benchmark testing results of CENDL-3.2 show that Pb was one of top 10 materials whose data contributed most to the total criticality χ^2. To validate the reaction data for lead, the evaluated data from the latest major libraries were tested with the JAERI/FNS and the ALARM-Cf-Pb experiments. The sensitivity of neutron leakage flux to total cross section or mean flight path was roughly given and used to understand the results of the shielding validation. The validation results of the JAERI/FNS slabs and the ALARM-Cf-Pb experiments were analysed against the thickness of the sample. Between 1.2 to 8.4 MeV, an underestimation of neutron leakage fluxes was found, which was probably caused by the overestimation of (n, inl) scattering cross sections. Below 1 MeV, the overestimation of neutron fluxes was partially caused by the overestimation of (n, inl) cross sections.

2.10 Estimation of the elastic scattering anisotropy effect by simulation of a critical assembly with monoisotopic reflector, V.V. Sinitsa

For the overwhelming majority of isotopes presented in the modern evaluated data libraries, assessing the quality of elastic neutron scattering angular distributions is hampered by the absence of critical experiments that are sensitive to these data. As a consequence, a large scatter in these data, due to both the difference in the models used in the evaluations and the smoothing of resonance structure of angular parameters, is often detected. The approach that allows to reveal cases of inadequate representation of elastic scattering angular distribution data by its integral testing is proposed, based on using a critical assembly model with an isotope under test, used as the reflector. In this case, the bare Godiva assembly with the radius reduced from 8.7407 cm to 8 cm has been used as the core. With such a radius, the K_{eff} is equal to ~0.9280 and the sub-criticality can be compensated by the reflector. The reflector thickness $D_{C,}$ at which the assembly reaches the critical state, has been used as an integral characteristic of the elastic scattering anisotropy. In order to assess the adequacy of the anisotropy parameters representation, the file values of parameters were compared with the values retrieved from the resonance parameters using the Blatt-Biedenharn formula by the GRUCON processing code.

The MF4MT2 sections for Cr-52, Fe-56, Ni-62, Ni-64 and Pb-208 isotopes from the ENDF/B-VIII.0, JEFF-3.3, JENDL-4, ROSFOND-2010 and BROND-3.1 data libraries were prepared and included in the ACE files for computing the dependency of K_{eff} on the thickness of the reflector, from which the corresponding D_C values have been determined. Comparison of the obtained D_C values led to the following conclusions:

- the scatter of D_C values obtained for original angular distributions and reconstructed from resonance parameters, relative to the averaged over libraries values, range from -10% to +15%; a trend of decreasing of scatter for angular distributions computed from resonance parameters has been observed;
- among the considered isotopes, nickel shows the best reflection properties. In the particular case of the bare Godiva core with radius 8 cm, criticality can be achieved with a reflector thickness of about 1.3 cm, reducing the amount of fissile material by ~23%.

2.11 On evaluated angular distributions for Cr and Resonance Parameters, R. Capote

R. Capote stressed that angular distributions in natural chromium are driven by Cr-52 data.

An improvement in the description of low-resolution (in energy) angular distributions has been achieved by averaging over the appropriated energy resolution of the experiment, which depends on the incident energy. This is especially important when angular distributions are reconstructed from resonance parameters (RPs) as the assumed ideal resolution is never attained in real experiments. Without a proper averaging the comparison of derived angular distributions with measurements becomes meaningless.

It is shown that the new INDEN chromium evaluation improves angular distributions in the ENDF/B-VIII.0 evaluation and, taken together with the new iron evaluation, reproduces the observed criticality trend in stainless-steel reflected assemblies as a function of the reflector thickness.

2.12 New integral experiments in Fe / Cu validation in CVR, M. Kostal

The Research Center Rez has a wide experimental infrastructure for performing integral experiments. There are two research reactors, a strong ^{252}Cf source with well-defined emission, material blocks for validation of neutron transport in shielding arrangements – many of them are being benchmarked. In the special core in the LR-0 reactor, a new neutron reference field was identified. It is one of the neutron reference fields in the IRDFF-II database and was used in the past for the validation of the IRDFF-II neutron dosimetry library. This core is now being extensively used, not only for measurement of dosimetrical cross sections, but also for validation of neutronic parameters of many important materials – Fe, SiO_2, graphite, ^{7}LiF-BeF_2.

Iron

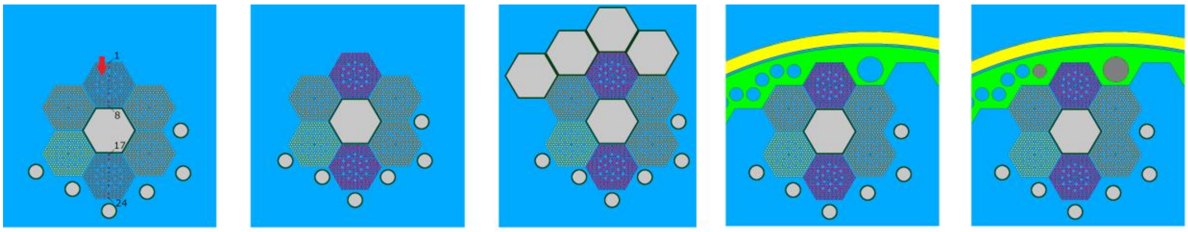
Shielding experiments have been performed in the past – transport from 1m iron sphere and 50cm sphere with Cf in diameter. The new experiments focus on the effect of stainless steel on criticality. A well-defined core was used (in its center a IRDFF-II neutron reference field was identified) which adjoins a well-defined VVER-1000 baffle simulator. For comparison, various arrangements with a reference core were studied – just water reflector, a partly non reflected core and a core adjoining to baffle were studied. It is worth noting the agreement in case when core adjoins baffle gets worse. Notable underprediction is reported.

The calculations in SCALE imply strong sensitivity for elastic and nonelastic scatter in the stainless steel reflector. In the case of the reference core, where steel also plays a significant role in the neutron balance – the sensitivity of scattering to k_{eff} is significantly lower than sensitivity of capture.

Calculated k_{eff} in various libraries for various reflected arrangements

	ENDF/B-VIII**	ENDF/B-VIII*	ENDF/B-VIII	ENDF/B-VII.1	JEFF-3.3	JENDL-4	ROSFOND-2010	CENDL-3.1
Case 1A	1.00251	1.00111	1.00002	1.00075	1.00107	1.00035	1.00015	0.99946
Case 1	1.00223	1.00096	0.99987	1.00072	1.00092	1.00032	1.00007	0.99916
Case 2	1.00204	1.00063	0.99969	1.00032	1.00083	1.00001	0.99968	0.99894
Case 3	1.00020	0.99893	0.99774	0.99838	0.99895	0.99818	0.99769	0.99657
Case 4	1.00054	0.99920	0.99797	0.99873	0.99931	0.99843	0.99807	0.99678

** The Fe was replaced by the INDEN evaluation, O was replaced by the ENDF/B-VII.1 evaluation
* The Fe was replaced by the INDEN evaluation



Case 1A Case 1 Case 2 Case 3 Case 4

Cases where the critical parameter was determined.

Sensitivities for selected reactions in core and baffle [a]

	Case 1 (in whole core)			Case 3 (effect of baffle)		
	(n, el)	(n,inl)	(n,g)	(n, el)	(n,inl)	(n,g)
^{56}Fe	302	99	-1560	613	106	-216
^{52}Cr	64	22	-137	143	20	-20
^{58}Ni	65	7.1	-266	132	6.6	-38
^{54}Fe	22	4.2	-88	49	3.6	-13
^{60}Ni	16	3.8	-59	33	3.4	-8.9
^{57}Fe	6.2	3.5	-35	13	6.6	-5.5

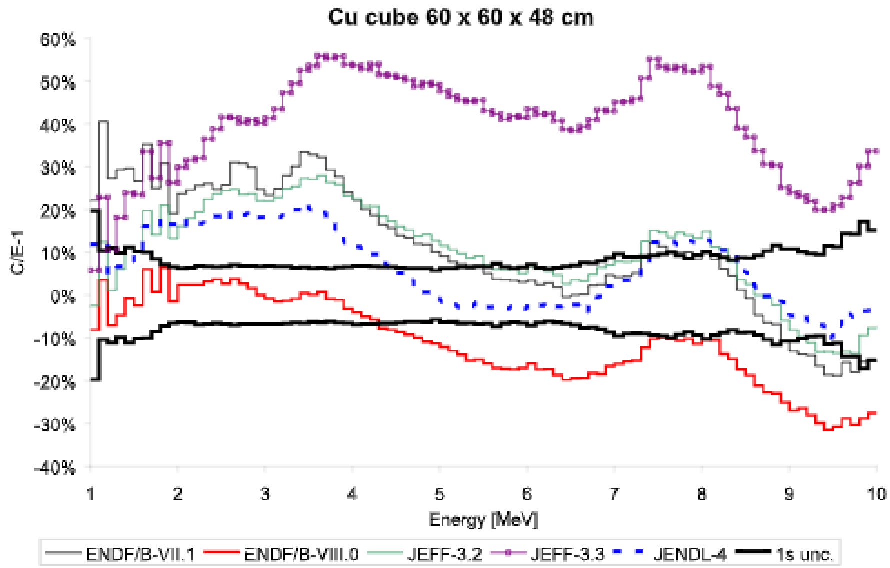
[a] Adapted from: Košťál, M., Losa, E., Czakoj, T., Schulc, M., Šimon, J., Juříček, V., Rypar, V., Ulmanová, J., Trkov, A., Capote, R., The effect of heavy reflector on neutronic parameters of core, Ann. Nucl. Energy **168** (2022) 108898.

The case of Copper

The new copper cube (Cu >= 99.95wt.%) was developed in the Research Center Rez. The neutron leakage spectra was measured and compared with calculations using various evaluations. In all evaluations there are discrepancies. In the leakage neutron spectra ENDF/B-VIII agrees below 4.5 MeV, over 4.5 MeV JENDL-4 or ENDF/B-VII.1 agree.

The leakage spectra measurement was accompanied by reaction rates measurements. It is worth noting that the agreement in the measured higher energy range shows similar discrepancies to those observed in the leakage spectra measurement. In case of ENDF/B-VIII - ^{58}Ni(n,p) is satisfactory, ^{93}Nb(n,2n) is underpredicted, in case of ENDF/B-VII.1 or JENDL-4 - ^{58}Ni(n,p) is overpredicted, ^{93}Nb(n,2n) is good (JENDL-4 similar trend).

The lower threshold reactions are underpredicted in all studied evaluations.



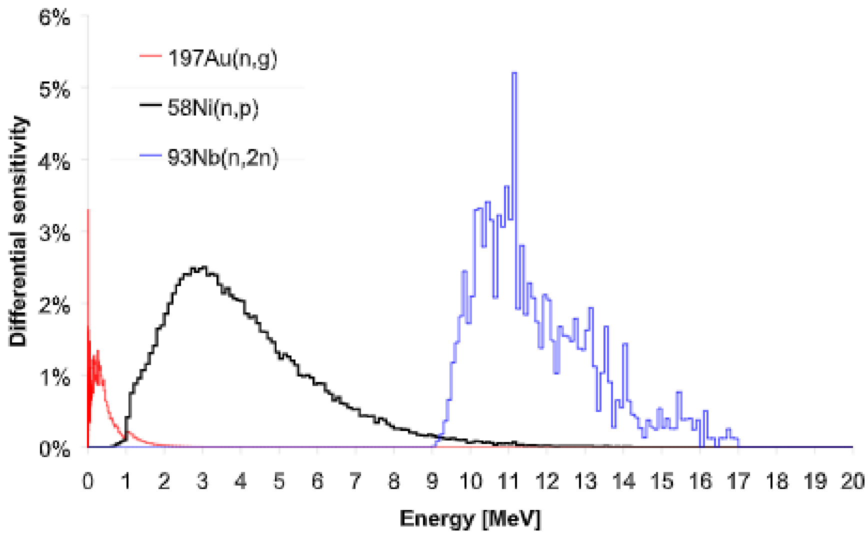
C/E-1 comparison of neutron leakage spectra after passing by 24cm of Cu

Summary of C/E – 1 comparison of reaction rates measured in Cu [b]

	^{58}Ni(n,p)	^{93}Nb(n,2n)	^{197}Au(n,γ)	^{55}Mn(n,γ)
ENDF/B-VII.1	25.3%	-2.6%	-4.3%	
ENDF/B-VIII.0	4.1%	-13.7%	-6.8%	-4.8%
JEFF-3.3	40.0%	23.4%	-5.4%	-2.7%
JEFF-3.2	24.0%	-3.1%	-4.5%	-4.0%
JENDL-4.0	17.5%	1.6%	-5.7%	-2.8%
CENDL-3.1	20.2%	-6.3%	-9.4%	-6.4%

[b] Adapted from:

Schulc, M., Košťál, M., Matěj, Z., Czakoj, T., Novák, E., Fast neutron spectra measurement in a copper using a ^{252}Cf standard neutron source, Radiat. Phys. Chem. **192** (2022) 109871.
Schulc, M., Košťál, M., Novák, E., Šimon, J., Copper neutron transport libraries validation by means of a ^{252}Cf standard neutron source, (2021) Nucl. Eng. Technol. **53**/10 (2021) 3151.



Sensitivities of selected reactions

2.13 Exploring an updated evaluation methodology at the example of iron, G. Schnabel

This presentation was divided into two parts. The first part reviewed a recently released nuclear data evaluation pipeline tailored to an evaluation of Fe-56 [1]. The pipeline is a sequence of scripts to perform the evaluation through various stages. It begins with the retrieval of experimental and preparation of data from the EXFOR library [2]: Experimental datasets are retrieved from a MongoDB database with the EXFOR data [3], then additional uncertainties are added to the experiments based on simple rules and finally additional normalization uncertainties, as determined by Marginal Likelihood Optimization (MLO), are assigned to the datasets. Afterwards, the parameters of the nuclear model code TALYS [4] are adjusted based on the experimental data using Bayesian inference. For the adjustment of energy-dependent parameters in TALYS, Gaussian processes are employed. The inference procedure also yields an evaluated covariance matrix reflecting the remaining uncertainty in the values of the adjusted parameters. Finally, a collection of model parameter sets is obtained by sampling from a multivariate normal distribution centered at the adjusted parameters and using the evaluated covariance matrix. Corresponding TALYS calculations are performed, and the resulting output files of each calculation processed by TEFAL to generate an ensemble of ENDF files. The adjusted parameters obtained by Bayesian inference are also used to create a best ENDF file with covariance information, achieved by the TASMAN code. TALYS, TEFAL and TASMAN are part of the T6 evaluation system [4], which is used to produce the TENDL library [5].

The second part of the presentation focused on the energy range between a few hundred keV and five MeV of Fe-56, which is difficult to evaluate by R-Matrix and nuclear model fits. A proof-of-concept evaluation was presented based on Gaussian processes that preserves the constraint that the sum of the partial cross sections must always yield the total cross section. It was shown how a Gaussian process can be defined by a sum of components. In the presented schematic evaluation, two components were defined in each channel to capture an average trend of the cross section and an overlaid highly fluctuating cross section. First results were presented to give an idea of how the procedure performs.

[1] G. Schnabel, H. Sjöstrand, J. Hansson, D. Rochman, A. Koning and R. Capote, Conception and software evaluation of a nuclear data evaluation pipeline, Nucl. Data Sheets **173** (2021).

[2] N. Otsuka, et al, Towards a more complete and accurate experimental nuclear reaction data library (EXFOR): International Collaboration between Nuclear Reaction Data Centres (NRDS), Nuclear Data Sheets **120** (2014).

[3] G. Schnabel, A computational EXFOR database, EPJ Web Conf. **239** (2020).

[4] A. Koning and D. Rochman, Modern nuclear data evaluation with the TALYS code system, Nucl. Data Sheets **113** (2012).

[5] A. Koning, D. Rochman et al, TENDL: Complete nuclear data library for innovative nuclear science and technology, Nucl. Data Sheets **155** (2019).

2.14 NEA resources for validation, M. Fleming

To view the presentation, please refer to Appendix 3 – Presentation links.

2.15 New evaluation of ^{181}Ta, M.W. Herman

Tantalum is almost a mono-isotopic metal with ^{181}Ta being 99.988% of the natural mixture. Therefore, there is an exceptional wealth of experimental data available, including total, capture, (n,p) and (n,2n) cross sections, elastic angular distributions, as well as neutron and gamma spectra (and double-differential cross sections). There are also some fragmentary data for inelastic scattering.

^{181}Ta is a strongly deformed nucleus which requires Coupled-Channel (CC) modeling of the incident channel. There is a RIPL-3 (#610) regional CC potential that covers ^{181}Ta and extends up to 200 MeV but it was not designed specifically for tantalum and needs adjustments to optimally describe the incident energy region from 50 keV up to 20 MeV. The two very reliable and consistent measurements of total by Poenitz et al, which cover this energy range entirely and match each other around 4 MeV, were used to refine the RIPL-3 potential. The fitting has been performed using a Kalman filter and resulted in rather minor corrections to three geometry parameters and somewhat more substantial to the three deformation parameters.

The calculations were performed with the EMPIRE-3.2.3 reaction model code. In view of multiple choices available in the EMPIRE code for selecting specific models, various combinations of these models were first explored in an attempt to reproduce a vast set of available experimental data while refraining from adjusting individual model parameters. Apart of the 6 optical model parameters mentioned above, only two parameters have been adjusted to obtain the results presented in this report. The finally adopted models are:

- Coupled-Channels with dispersive Optical Model potential;
- Quantum-mechanical Multistep Direct (MSD) model for pre-equilibrium neutron emission;
- Heidelberg formulation of the Multistep Compound (MSC) model for pre-equilibrium neutron and gamma emission;
- Exciton model for pre-equilibrium proton emission;
- Exciton model with Iwamoto-Harada extension for pre-equilibrium cluster emission.

The combination of MSD and MSC models provides a very good description of the high energy tail of the neutron spectra, which is the major advantage over the classical exciton model of pre-equilibrium emission. Proper description of neutron spectra is essential for correct description of channels such as (n,2n) and (n,p). Several of the options in MSD were tested.
Also, one of the two adjusted parameters is pertinent to MSD. This parameter was tuned to improve neutron spectra and at the same time ameliorate agreement for (n,2n) and (n,p) reactions. This parameter should not be affected by potential further adjustments of other parameters.

Gilbert-Cameron level densities were chosen over EGSM and microscopic Hartree-Fock-Bogoliubov because the former produce better capture cross sections between 1-3 MeV, and slightly better gamma spectra. The effect on the neutron spectra is mixed with GC, working better at incident energies around 14 MeV while EGSM has an advantage at 20 MeV.

The overall results, obtained with very limited parameter adjustment, and without any manual or energy dependent corrections are very encouraging.

3. Conclusion

The presentations covered experimental work, updates to evaluations, ongoing evaluation work, new validations, as well as suggestions on how to improve aspects of evaluation methodology and validation. Regarding evaluation work, the structural materials ^{50,52,53,54}Cr, ^{56}Fe, ^{55}Mn, ^{59}Co and ^{181}Ta were covered. Validation results using benchmarks sensitive to Cr, Cu, Fe, Pb were also presented.

Besides the ongoing evaluation work of Cr isotopes at Brookhaven National Laboratory (BNL) (presented by G. Nobre), and the evaluation of ^{181}Ta, (presented by M. Herman) the focus of INDEN currently lies on the evaluation of ^{56}Fe, which is undertaken at CEA Cadarache (presented by M. Diakaki) and other participants in collaboration with the nuclear data section of the IAEA. In these evaluation efforts, the difficulty to evaluate the energy range above the first inelastic level at 850 keV to about 5 MeV was recognized. For the evaluation at CEA Cadarache, one objective is to extend the resolved resonance range by including more resonances starting from the CIELO evaluation performed by Luiz Leal (ORNL4). The ^{56}Fe evaluation presented by R. Capote addresses an issue in the capture cross section first identified in the context of oil-well logging and another issue, which is a significant overestimation in some leakage benchmarks. Thick target transmission measurements can help in the proper evaluation of minima in the total cross section. The analysis of the thick target transmission measurement of Harvey performed in 1975 (presented by S. Kopecky) indicates that this measurement can provide additional useful information even though the details of the geometry are not entirely certain and, by extension, that well-documented thick target transmission measurements are valuable information for evaluators. V.G. Pronyaev gave a detailed presentation of a new evaluation of ^{56}Fe in the resolved resonance range below 2 MeV with particular focus on the impact of different choices of the number of groups used to represent the angular distribution on criticality. Concerning the experimental side, A. Negret presented the results of and an outlook for the GAINS experiment at GELINA to obtain data for the neutron-induced inelastic cross section of ^{54,56,57}Fe. As a final note on the evaluation side, N. Iwamoto covered the evaluation of ^{59}Co in preparation for the release of JENDL-5, which at the time of writing is already publicly available.

As validation is an important part of the evaluation process, the presentations on specific evaluations also covered the performance of evaluated files in integral benchmarks. Some presentations, however, were completely focused on validation.
H. Wu presented the benchmark results of the CENDL-3.2 Pb evaluation, as lead is an important coolant material in fast reactors and can also serve as shielding material. Comparisons to the other major libraries showed that the libraries exhibited similar performance, with some overestimation of the elastic and inelastic cross section, which indicates the need for an improved evaluation in the resolved resonance range.
M. Kostal gave an overview of the research infrastructure at the Research Centre Rez (CVR), including a strong ^{252}Cf source, a D-T generator, and two reactors, and its capacities to validate evaluations. Among other measurements, such as one involving a Cu cube, the effect of stainless steel on criticality was studied and the performance of various major libraries compared. In this study, evaluations of O and Fe in ENDF/B-III have been tentatively substituted by INDEN evaluation candidates to study their impact, as these isotopes have been identified to have a large impact on these integral experiments.
V.V. Sinitsa presented several benchmark results that demonstrate how the preparation of angular distributions, either taken directly from the MF4 section or reconstructed from resonance parameters in MF2 section in the evaluated ENDF file, may impact the benchmark results. In a variety of structural materials an estimate of the thickness of the reflector material to achieve criticality can be quite different (i.e., -10 to 15%) depending on the specific preparation of the angular distributions.

Nuclear data evaluation is a complex undertaking that involves differential and integral experiments, theory, statistical methods and validation. This is especially true for structural materials, as it is often difficult to model the region between the resolved resonance energy range and the range where the assumptions of statistical models fully apply. This meeting has again shown that the International Nuclear Data Evaluation Network (INDEN) is an important framework to bring together experts of those domains with the goal to obtain a comprehensive picture in order to produce high-quality evaluations and to determine data needs and beneficial future activities. With the important scientific contributions of universities and research laboratories, and the collaboration between international organizations, such as the OECD/NEA and IAEA, which disseminate nuclear data and provide software, a unified effort in this direction is made.

Appendix 1

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

14 – 17 December 2020
(virtual event)

Adopted AGENDA

Meeting starts at 14:00 CET each day

Monday 14 December	
A. Koning	Opening and Welcome
G. Schnabel	Discussion of the agenda, election of chair and rapporteur(s)
	Presentations:
G. Nobre	New evaluation of chromium isotopes
R. Capote	INDEN evaluation of Fe isotopes & the ^{55}Mn update of thermal (n,γ) gammas
A. Trkov	INDEN Fe validation
Tuesday 15 December	**Presentations cont'd:**
V.G. Pronyaev	Angular distributions for neutrons with incident energy below 2 MeV scattered at ^{56}Fe
M. Diakaki	Status of the evaluation of n + ^{56}Fe reaction data - Focus on (n,inl)
S. Kopecky	MCNP simulation of ORELA transmission measurements
A. Negret	Inelastic measurements on Fe isotopes at GELINA Results and future plans
N. Iwamoto	Evaluation of ^{59}Co for the JENDL library
Wednesday 16 December	**Presentations cont'd:**
H. Wu	Validating nuclear data for lead with shielding benchmarks
V.V. Sinitsa	Estimation of the elastic neutron scattering anisotropy effect by simulation of a critical assembly with monoisotopic reflector
R. Capote	On evaluated angular distributions for Cr and Rps
M. Kostal	New integral experiments in Fe / Cu validation in CVR
Thursday 17 December	**Presentations cont'd:**
G. Schnabel	Exploring an updated evaluation methodology at the example of iron
M. Fleming	NEA resources for validation
M.W. Herman	New Evaluation of ^{181}Ta

Appendix 2

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Appendix 3

PRESENTATION LINKS

#	Author	Title	Link
1	G. Nobre	New evaluation of chromium isotopes	pdf
2	R. Capote	INDEN evaluation of Fe isotopes & the ^{55}Mn update of thermal (n,γ) gammas	pptx
3	A. Trkov	INDEN Fe validation	pptx
4	V.G. Pronyaev	Angular distributions for neutrons with incident energy below 2 MeV scattered at ^{56}Fe	pdf
5	M. Diakaki	Status of the evaluation of n + ^{56}Fe reaction data - Focus on (n,inl)	pptx
6	S. Kopecky	MCNP simulation of ORELA transmission measurements	pptx
7	A. Negret	Inelastic measurements on Fe isotopes at GELINA Results and future plans	pdf
8	N. Iwamoto	Evaluation of Co-59 for the JENDL library	pdf
9	H. Wu	Validating nuclear data for lead with shielding benchmarks	pptx
10	V.V. Sinitsa	Estimation of the elastic neutron scattering anisotropy effect by simulation a critical assembly with monoisotopic reflector	pdf
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12	M. Kostal	New integral experiments in Fe / Cu validation in CVR	pdf
13	G. Schnabel	Exploring an updated evaluation methodology at the example of iron	pptx
14	M. Fleming	NEA resources for validation	pdf
15	M.W. Herman	New Evaluation of ^{181}Ta	pdf

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