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

Summary Report of the IAEA Consultants' Meeting
IAEA Headquarters, Vienna, Austria
29 October to 1 November 2018

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EC-JRC Geel, Belgium

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March 2019

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1. Introduction

A Consultancy Meeting was held at IAEA Headquarters in Vienna, Austria, from 29 October to 1 November 2018, to address current problems in the evaluation of nuclear data and structural materials. This work was carried out in the framework of the International Nuclear Data Evaluation Network (INDEN) with experts from eight Member States and one International Organization attending the meeting.

2. Presentations Summaries

1.1. Overview of the structural evaluation challenges: "There is never inelastic without elastic", R. Capote Noy

Within this INDEN working group on structural materials the status and problems of the evaluations for mid-mass nuclei in the vicinity of closed shells are going to be addressed. All the nuclei addressed have rather low level densities, therefore the evaluations will have to cope with similar problems which are essentially different from the problems encountered in other mass regions. One of the main problems for the mid-mass region is that the models usually applied in evaluations reach the end of their applicability, e.g. in the energy range between 1 and 5 MeV the cross sections still exhibit strong fluctuations, fluctuations that can no longer be addressed by R-matrix analysis (or treatment by methods of URR), but the energies are also too low and the fluctuations are too large for optical model calculations. This, in turn, means that the methodology for evaluation at higher masses can no longer be applied and, so far, no consistent methodology has been developed and applied. Therefore, one of the main goals of this working group should be to develop a more structured approach for future evaluations, and create evaluations applying such new methodology. Another point of concern is that for many of these isotopes direct capture might be of importance, and a consistent approach how direct capture could/should be included in evaluated data files would be desirable. Many of the elements addressed have a number of stable isotopes, and although the evaluations are done per isotope, the performance for a combined natural composition is most important for application. Finally, such new evaluations should address shortcomings of presently available evaluated data files.

Observed deficiencies in iron evaluations:
The observed leakage through iron shields seems to be overestimated around the cross-section minima of Fe-56. and in the energy range between 1 and 4 MeV (see also presentation by S. Simakov, p 13). At the moment a number of possible pathways to address the problem can be considered, including a significant component of direct capture of Fe-56. However, this approach does not seem to solve the problem fully, due to constraints in the observed total cross sections of Fe-54. Another reason could be lying in the total cross section of Fe-54 itself. For inelastic scattering below 800 keV, only the contribution of Fe-57 is important, even if the natural abundance is only 2%. For the ENDF evaluations, it is observed that the average for experimental data is lower than model calculations, presently the origin of this discrepancy is still unclear, but should be investigated.

A recent measurement of the thermal capture reported by R. Firestone came approximately 10% lower than the previously recommended value, far outside the uncertainties of the measurements. From analysis of integral experiments no clear indication for either of the values can be obtained.

For Cr deficiencies between 2-10 kev have been observed, most likely caused by ether Cr-50 or Cr-53, and overall the natural capture seems not to be reproduced by the sum of the isotopes.

1.2. ORNL Nuclear Data Evaluations, V. Sobes

Prior to the release of ENDF/B-VIII seemingly a wrong file for Cr-53 resonance parameters has been transmitted.

ORNL has been working on the resonance region of Fe-54, and from this work it is clear that the problems observed in integral experiments with natural iron cannot be solved by further adjusting the Fe-54 contributions, as otherwise the consistency with total cross section of Fe-54 would no longer be maintained.

ORNL is planning some more work on the copper evaluations, especially as quite some effort has been devoted to Cu-63 and Cu-65 prior to the latest ENDF release, efforts that are unfortunately not reflected in the presently available ENDF/B-VIII files, e.g. capture measurements have been performed and analysed up to 300 keV, but the file only contains average capture widths, and the fast region starts at 100 keV. Similarly, it has been shown that the Cu angular contributions are very important for transport/reflection properties, but the full information has not been included in the present files. The covariance matrix prepared in the original work at ORNL is included in the final version of the ENDF file, but the resonance parameters are not.

For the silicon isotopes (mostly Si-28) tests to identify the most suitable model for deriving the direct capture component have been performed. Originally the TEDCA code has been employed, but this seems to lead to unphysical cross sections at higher energies (above approx. 10 keV). Using the CUPIDO code seems to strongly improve the consistency of the results. This will be included in a new evaluation of the resolved resonance region of silicon isotopes.

Vanadium measurements have been performed and it seems that files describe the data satisfactorily below 200 keV, whereas at energies above 300 keV some deficiencies can be observed.

Finally, at ORNL work addressing the methodologies is performed., e.g. sensitivity analysis of integral benchmarks to resonance parameters is developed. This is done within the TSUNAMI/SCALE package.

1.3. Evaluation of n + ^{56}Fe Reaction Data (+ covariances) and Experimental Validation, D. Bernard

At CEA Cadarache efforts are underway to make a new evaluation for Fe-56. The goal is to extend the resolved resonance region above the 850 keV presently included in the file. This will build on the work of L. Leal who has included elastic and inelastic scattering in a R-matrix analysis using SAMMY. Overall the code CONRAD will be used, for the description/adjustment of experimental data and a full covariance matrix will be included in the new file.

Another modification will be the inclusion of the data of IAEA/EGAF into the file, as it has been shown that with these data a satisfactory description of the photon heating could be obtained.

For determining the fluence in the RPV and a correct description of the dpa and their respective uncertainties, the importance of including the correct angular dependence of the elastic scattering cannot be stressed enough, especially the inclusion of higher Legendre polynoms is essential.

An experimental validation of neutron transmission in stainless steel has been performed. This was done in the EOLE core, for which the penetration into the stainless steel reflector has been determined. The performance of the JEFF-3.3 file in this case is satisfactory.
The deep penetration experiments will be most sensitive to the inelastic cross section, as already pointed out in a publication by Bethe and co-workers in 1956, therefore such experiments could be very useful in achieving the target uncertainty for the ratio elastic/inelastic cross section around 2%, as requested by users.
Finally, a new set of experiments at PETALE an PSI in a collaboration between PSI, EPFL and CEA will measure the deep penetration at the crocus reactor for Fe, Cr and Ni.

1.4. Recent ND developments and plans at UU, G. Schnabel

Within the process of data evaluation, problems with similar mathematical properties can be encountered at various steps, i.e. steps in which "models" have to describe "observations". In many cases a situation is encountered when not enough model parameters are available to be adjusted to describe the observations (" model defect") or the almost opposite case, when too many parameters could be adjusted ("overfittig" as would be encountered when adjusting evaluations to integral benchmark). Although these cases seem to be fundamentally different, the same mathematical process – a Gaussian process – could be employed to improve results and obtain uncertainties (and covariance matrices) consistent with the available data.

In this presentation a number of examples for which the Gaussian process can be applied are given.
The method can be successfully applied for determining energy dependent model parameters and create a consistent description of data and a respective consistent covariance matrix. The description of model defects has been extended with the introduction of an energy dependent scaling function and an energy dependent length scale. Such an energy dependent scaling function could be applied e.g. when using optical model calculation down to the resolved resonance region. With this approach the application region for a model will be reflected in the defect function, which in essence will prevent the adjustment process to use data outside the region in which the model can be deemed to be adequate/good. This, in turn, will lead to better model predictions and in addition to more reliable estimates of the uncertainties.

Finally, the Gaussian process can be used for experiment selection in a large database. Depending on the chosen prior/constraints to all the observation, a "defects functions" can be fitted. This implies that observation strongly deviant from the best value will be assigned a larger uncertainty and will, therefore, have a lower weight in the fitting procedure. It has to be emphasized that depending on the choice of constraints, the values assigned can vary strongly, emphasizing the importance of the choice of prior done by the evaluator.

1.5. Status of nuclear data of structural materials in JENDL-4,0, N. Iwamoto

Most of the evaluation that will be included in the future release of JENDl-5.0 for structural materials (Cr, Cu, Ni) will employ the same program package. This package consists of CCONE in the fast range, coupled to KALMAN-CCONE to determine the uncertainties/ covariance matrix. In general the resolved resonance parameters will be taken from a previous evaluation, in some case the R-matrix code AMUR would be used in the process as well.

Cr-isotopes:
Fast region done with CCONE system, resonance parameters either from JENDL-3.3 (Cr-50, Cr-54) or an analysis of L. Leal (Cr-52, Cr-53)

Cu
Copper isotopes will be redone for the JENDL-5 evaluation. CCONE in the fast region, with parameters taken from the RIPL library.
This new evaluation has been compared to a Cu(n,a) benchmark performed employing a graphite cylinder in the field of a D-T neutron source. A large improvement compared to the previous JENDL release (an increased cross section by a factor of 10) has been observed.

Ni
Problems at neutron energies of approximate 5 MeV in the present JENDL file have triggered efforts for new evaluation of the nickel isotopes to be prepared for the JENDL-5.0 release.

Additionally, Co, Mn will be new files in the next release.

1.6. The status of evaluation for structural materials at CNDC, Y. Chen

The evaluations at CNDC are done using the same framework. In fact, the resolved resonance parameters are adopted from previous evaluations, the focus of the work lies in improving the files in the fast energy region. For this work the code UNF is employed. UNF uses a spherical optical model to determine the total, the shape-elastic cross section and the angular distribution. Additionally, a unified Hartree-Fock model plus an exiton model can be used. This code package can also be used for obtaining a covariance matrix.

So far Ni-58 and Ni-61 have been updated. Overall an improvement in the description of the double differential cross section has been achieved.

A new file for Fe-56 was created within the framework of the CIELO project. Using the UNF package in this case also a covariance file has been provided.
An improvement in the (n,a) angular dependence and better agreement of the double differential cross section with experimental data has been achieved.

An additional new file presently under development will be included in the next release of the CENDL library (within the next 2-3 years).

A new experimental setup has been developed at CNSN. A proton beam hitting a spallation target provide for the neutron beam, that is characterized by a rather high intensity but a limited time resolution. The experiments presently performed are "leakage" and "back scattering" experiments.

Some of the data are not published yet, neither is a full simulation model of the facility. Nevertheless, the experimental data could already be used for the validation of libraries. More experiments with structural materials would be very valuable for validation.

1.7. Nuclear data evaluations of structural materials in BNL, G. Nobre

After the iron files have been updated — although there are still unsolved issues related to iron — the chromium isotopes will be one of the next priorities at BNL. Overall a few problems with the chromium files can be observed:
The strong fluctuation at higher energies might have an impact on the flux in critical assemblies. Leakage through stainless steel may require rescaling of the inelastic scattering data set of Nelson (Fe-56). There is also a more general problem in the analysis of the transmission data.
Overall the resolved resonance region is based on an ORNL evaluation from 2010, whereas the fast region dates basically back to ENDF/B-VI (1989).
The "recent" inelastic data of Mihailescu are not included in the ENDF file. And finally, for testing of the files, a few of benchmark experiments very sensitive to Cr have been identified.

Resolved Resonance Region
Firstly, the correct data file for capture has to be identified (related to the inclusion of under-corrected preliminary Cr-50 capture data reported by Guber in 2010).
The measurements for transmission performed at the 200m flight station at ORELA have been using a Cr^2O^3 (samples enriched in Cr-52 and Cr-53). The data available in EXFOR have not been corrected for the oxygen content in the sample. An increased difficulty to correctly determine the oxygen content comes from the fact that the powder is hygroscopic and the amount of water stored in the sample is not known accurately. A procedure to subtract the correct oxygen contribution from the reported cross section values has yet to be established.

Fast region:
Overall the challenge will be to include the fluctuation in the cross sections up to energies of approximately 10 MeV.
At the moment it seems most likely that a dispersive optical model with soft rotor coupling as reported by Li et al. will be employed, which needs to be extended for all Cr isotopes. With the presently used OMP, the angular distribution of elastic scattering is quite well reproduced, the average inelastic cross section derived by the model is discrepant with the latest measurements. Overall it is observed that the status of the inelastic data is not fully satisfactory, i.e. disagreement between theory and experiment and some not fully understood features in the measured inelastic cross section.

For the file it is envisaged that the smooth cross section will be derived with the EMPIRE code, and the fluctuation of the experimental data will be overlaid on top of the theory.

1.8. TENDL and BMC evaluations: advantages and limits, D. Rochman

The TENDL system, including TALYS, TARES, has been developed over the last years and reached a status in which a fully automated system can create a full evaluated data library, e.g. the TALYS model parameter can be taken from default values, adjusted to experimental data or normalized. For the resolved resonance region the parameters could come from experiments/existing evaluations or using the HFR approach.

Combining TENDL with BMC/BFMC could quite easily allow for incorporating integral measurements into the evaluation procedure. Presently adjustments of evaluated files to integral benchmarks are already performed at the evaluation stage. This helps to make the files "cleaner", and allows to reduce the uncertainties in the files by benchmark experiments as well as to derive covariance matrices including cross-isotope correlations. A scheme of how such an integration of the integral experiments can be achieved is presented. One of the critical/most important points is how to correctly assign weights to experiments, especially when the C/E is deviating strongly from unity. A first scheme for such weighing has been developed.

To sample model defects, different models (from TALYS and EMPIRE) have been tested, in an attempt to sample the full model space, and not to be restricted by a prior choice. This is the logical extension of the BMC/BFMC approach in that sense that not only model parameters but also models themselves are sampled.

1.9. TENDL approach for Ni isotopes, A. Koning

The TENDL approach has been successfully applied over the full mass range, and by doing so it has been observed that global/local adjustment can reduce uncertainties and predict cross section for isotopes for which data are sparse.
The predictive power of such global analysis can be shown eg. for (n,2n) peak cross sections. The hope/assumption would be that if the TENDL system can be adjusted for a few rather well known isotopes, this could lead to a significant improvement over a much wider mass range. It was therefore considered interesting to apply TENDL to the Ni isotopes.

The choice of the goodness-of-fit estimator is discussed since a number of estimators is already considered in the analysis such as chi-squared, root-mean-square asymmetry, etc.

Some challenges are specific to the TENDL approach, such as how to access experimental data automatically and maintain corrections/adjustments of the data done by previous evaluators, a format already exists within the EXFOR library, but so far entries have only been made for dosimetry reactions.
Other challenges are more general, and rather depend on the choice of nuclei, e.g. how to correctly/consistently include fluctuations of cross section when models are smooth, the available experimental data have different resolution, and how to ensure that the sum of the partials equals the total.

1.10. Integral experiments with structural materials in Research Center Rez, M. Kostal

At the RC Rez two reactors are operated that can be used for nuclear data experiments.

The reactor LVR15, which is a high power reactor that uses IRT type fuel. In its tangential channel HK-1, that has a neutron spectrum dominated by the U-235 fission spectrum, a 1m silicon filter is installed. One experiment at this position is to determine the transport through this Si filter with the activation filter placed in front and behind the filter. More experiments are planned to use the Si windows to measure transport through Fe, oxygen and nitrogen at these quasi mono-energetic neutrons.

The LR0 reactor has a very flexible core, and is, in general, used as a VVER1000 mock-up for reactor dosimetry experiments. In support of the reactor dosimetry program a recent experiment tested if a local increase in power density could by seen be activation foils outside the reactor vessel. For this experiments, activation foils of Au, Ni were placed behind the RPV, and the core was modified to increase the power density close to the foil position. In the experiment the local increase of power was clearly registered by the foils outside the vessel, confirming observation of the reactor dosimetry community.

A wide range of validation experiments were performed in the Cf-252 field. Two laboratories are available, both with their respective strengths and weaknesses in respect to observed background. The rather new source is Cf-252 dispersed in a Pd matrix. In the leakage spectra measurements, a stilbene detector was used, calibration for the neutron energy was done indirectly, using the Compton edge of various photon sources.
This setup source is/was used for measurements of the leakage spectra of Fe spheres (30,50,100 cm diameter), Ni spheres (50 cm) water (light and heavy water 30 and 50 cm diameter.
Further, experiments tested the leakage spectra through cubes of graphite, steel (including 18 % Cr) and Cu.

For the Fe measurements the prediction of the 50cm was quite good. For the 100 cm sphere a quite significant difference (up to order 50 %) was observed.

For the 50 cm Ni sphere the discrepancies were larger than for the Fe sphere of the same diameter.

A test compared the leakage spectra through a graphite sphere and a cube with similar effective thickness, the observed differences between the two experiments were of the order of 5%, and can be explained by the "edge" effects of the cube.

Furthermore, experiments tested the possible use of a AmBe source for leakage spectrum measurements. For this measurement the AmBE and Cf fields for water spheres were compared. The C/E agreement for the AmBe source was slightly worse than for the Cf source, the precise reason for this effect is presently not fully understood.

1.11. Iron sphere benchmarks with Cf source, S. Simakov

This presentation focuses on the analysis of neutron and gamma leakage spectra of iron spheres in the neutron field of a Cf source. Measurements from KFK, NIST and IPPE were compared.

For the modeling the latest MCNP version was used, the data libraries were converted to ACE files using Njoy (the latest version and NJOY-2016). The TENDL-2017 library and the TEND/BMC was used to create random files for propagating the data uncertainties to the observed leakage spectra.

For the neutron leakage spectra three measurements from KFK 1985, NIST 2000 were compared to the measurements performed at IPPE in 1985.

For the KFK75 experiment the documentation contains flaws, e.g. typos in the publication for the bare spectra, make a comparison between measured and calculated bare spectra more cumbersome than necessary.

What maybe is more worrying is that only a 15 cm shadow bare was used in the experiment, which proves too thin for ideal experimental conditions. For spheres of comparable dimension differences up to 40% in the C/E values are observed in comparison to the results of the IPPE measurement. Nuclear data uncertainties were propagated, using the TENDL/BMC system, to the leakage spectra. The calculated uncertainties were of same order as the experimentally observed ones.

For the NIST 50 cm diameter sphere the C/E values were compared to the IPPE sphere of comparable diameter. In this case, the agreement between the two measurements above 0.1 MeV — the NIST publication states clearly this as lower limit for the use of data — and below 1.5 MeV is quite good.
At higher energies the observed differences between the experiments get larger, especially with increasing sample thickness.

Overall it has to be concluded, that the KFK75 experiment should not be used for the validation of iron data.

The gamma leakage through an iron sphere has been measured in the KFK77 at the IPPE85 experiment.
The simulation of the gamma strength/ gamma spectra of the bare source was simulated. Even if some design details of the KFK source might not be known, overall the contribution of the capsule does not exceed a few percent at its maximum. The main problem lies in the fact that the gamma multiplicity of the Cf-252 source seems to be overestimated by a factor of 2-3. This is also the case for the IPPE85 bare spectrum. A study of gamma production clearly shows that the prompt gamma multiplicities as measured in "thin" sources agree rather well with theoretical predictions. On the other hand, the ABBN-93 values and measurements with larger/thicker Cf sources give multiplicities by a factor of 2-3 larger than the thin sources. The reason for this discrepancy is presently not understood.

For the KFK measurements the geometry is not ideal, as the detector is put on the surface of the sphere.
When using the data of evaluated libraries, the C/E for the KFK experiment is too low by approximately a factor of 2 for gamma energies 0.5 -2 MeV. This is consistent with the results of the IPPE experiment.

This origin of the discrepant results by a factor 2-3 is not understood. In fact, after shielding by 15cm of iron the original gamma spectrum of the Cf source is hardly seen; most of the observed gamma are the result of photon production reactions in the Fe sample.

1.12. IAEA INDEN ^{56}Fe valuation and benchmarking, A. Trkov

In the Fe-56 CIELO evaluation some deficiencies were revealed just before release of the new libraries, coming too late to make modifications to the file before the release. The main problems detected were:
The poor performance of the evaluated files in describing the neutron leakage spectra of iron spheres of D-T and Cf-252 sources. Various benchmarks indicated that the non-elastic cross

sections in the iron files were overestimated. This assumption is corroborated by the elastic cross section measurements performed at JRC Geel. With the slightly higher elastic contribution, the strict constraint that the sum of the partial cross section is equal to the total cross section would require a further reduction of the inelastic cross section.
Another observation, mostly coming from deep penetration measurements, would indicate that the cross section minima in the total cross section of Fe-56 are underestimated in the files. In order to resolve these problems, either the total cross section of Fe-54 or the capture cross section in Fe-56 would have to be increased by a rather small absolute amount (of course in the minima the relative increase is quite substantial). New measurements of the thermal capture cross section of Fe-56 would suggest that this value should be reduced by approximately 10 % in the file.

It was therefore decided to try some ad hoc adjustments of the file. The inelastic cross section of Fe-56 was reduced since, overall, it seemed to be a bit high in the files compared to the available experimental data. After the adjustment, the values in the file were consistent with the lower edge of the uncertainty band of the experiments. Overall the elastic cross section of the files seems still a bit lower than the experimental data, but an adjustment cannot be done without either changing the total cross section or reducing the inelastic cross section further; the evaluated files and the available data would no longer be agreeing within their uncertainty band. Without any other clear evidence — or a new, full evaluation - such a change is presently not justified.

The angular distributions are very important for the correct description of reflectors of stainless steel in critical benchmarks. Presently, a rather detailed distribution for neutron energies below 2,4 MeV is included in the file, a verification of the data and/or extension of the range might be of valuable. After the described adjustments, the performance of the files for describing the leakage spectra in the neutron fields of a Cf-252 source has seemingly improved as has the ICSBEP broomstick experiment.

The following benchmark experiments proved very useful for the validation of the Fe files:

Fe sphere in Cf-252 field (IPPE)
APSIS deep penetration
Fe sphere in D-T source
OKTVIAN
FNS thick slab experiment
TIARA Fe
IPPE broomstick

Additional, potentially useful validation experiments:
KFK Fe sphere (should maybe no longer be considered according to the presentation of Simakov)
NRI & Soda leakage spectra
ORNL broomstick
NSE170 207(2012) details not available
RPI quasi differential cross section measurements

Overall the performance of the modified files has improved for a significant number of the above mentioned benchmarks.

In particular the description of the IPPE Fe sphere leakage spectra experiments has improved.

For the ASPIS experiments some improvement, the main reason for the originally observed problems are the nonelastic cross sections.

For the leakage spectra of Fe spheres in a D-T source the underprediction of the original file in the 2-5 MeV region has been reduced, unfortunately the description at higher energies has slightly deteriorated.

For the LLN sphere the overall agreement is satisfactory, although some gradient over the C/E as a function of the neutron energy is observed.

The description of the OKTAVIAN experiment is still problematic.

The TIARA benchmarks at 40 and 65 MeV are the only benchmarks for high neutron energies. Of the overall set the experiment performed with a 7 cm fe slab seems questionable due to oscillations which seem to be unphysical. For the other sets the modified file has improved the C/E ratio, but it cannot match the performance of the JENDL file for this benchmark.

The IPPE FE broomstick, an experiment measuring the transmission of quasi monoenergetic neutrons from p-T source through iron cylinders, can be better described for the minima in the total cross section. For energies above 1,2 MeV systematic differences are observed. It has been suggested that experimental effects such as e.g room return or modeling of the neutron source might be at the root of these problems.

For the Illinois sphere the source of the observed differences between the original and modified file are not understood.

For critical benchmark the modification of the thermal capture cross section is of some relevance. Unfortunately, no clear trend can be observed, while the description of some experiments benefited from the change other results show deterioration.

The problems observed in the CIELO Fe file have been addressed and, to a large extent, solved, as the overall performance in validation experiments has improved.
However, the file itself has been derived by patching and it would be desirable if a file could be created with a more consistent approach.

3. Discussion

3.1. Status of files/planned work of participants

Some reactions (Ni, Fe) are in the dosimetry file. We have to make sure that these data are reflected in new evaluations, making sure that the sum of isotopic contributions matches the measurements for natural elements.

3.1.1. Cr isotopes

Problems: capture Cr-50, Cr-53 in the energy region from 2-10 keV
Measurements: capture?

Action:

- Geel, ORNL check on available data which have not yet been considered;
- Leakage spectrum measurement of stainless steel cube at Rez (18 % Cr);

Evaluation: BNL, ORNL , IAEA
Validation: IAEA, CEA (Minerve, reactivity worth)

3.1.2. Si

Problems: thermal capture EGAF included, can value be checked with different method?
Evaluation:

- new evaluations of ORNL/IAEA have been finished (new MF 2) for all isotopes and can be made available;
- CNDC new evaluations;

Validation:

- 14 MeV leakage spectrum measurement in SiC at CNDC (IAEA will send files, CNDC will do calculations);
- KBR benchmarks (IAEA);
- CEA Minerve C/E 30% (capture compensating with elastic);
- REZ 1 m Si filter, various activation foils in front and behind of Si;

3.1.3. Fe

Problems:

- there are new files by the IAEA (patched) with improved performance in the benchmarks;
- minima of Fe-56 cross section, presently ad-hoc adjusted, can that be checked?
- reduction of inelastic cross section to the lower end of the uncertainty band, but consistent with elastic+total CS;

Evaluation:

- BNL planning modification above 5 MeV;
- JAEA new evaluation of all isotopes planned (for JENDL-5, fast range);
- CNDC new evaluation of all isotopes planned;
- UU new evaluation Fe-56 to be started within the fusion project (provide methodology for region from 850 keV up to 5 MeV)

Validation: IAEA,REZ,KIT

- CEA validation of the thermal point
- 14 MeV leakage spectrum measurement at CNDC
- validation of the dosimetry file

3.1.4. Ni

Problems: many new data since the latest evaluation done for ENDF,

Evaluation:

- BNL planning new evaluations
- TENDL to apply methodology on Ni isotopes
- JAEA new evaluations for JENDL-5.0

Validation

- validation of the dosimetry file
- leakage spectra for 50 cm Ni sphere from REZ (model?)

3.1.5. Cu

Problems:

- not all information from a resonance analysis has been included in the latest ENDF evaluation (average capture widths, limitation in resolved resonance range, angular dependence of elastic scattering, covariance matrix)
- fast range doesn't perform well in benchmarks, OKTAVIAN perfomance for ENDF is rather poor, swedish criticality benchmarks overpredict reactivity

Evaluation:

- BNL/ORNL resolved -fast region
- JAEA almost finished (new in fast region)
- CNDC in preparation (whole file)

Validation

- CEA Minerve two samples (thermal energies)
- IAEA (ZEUS,
- validation of dosimetry reaction
- FNG benchmark should be looked at
- REZ leakage spectrum from copper cube (planned)
- LANL just finished SCRAP ball (copper reflected) from high energy down to URR

3.1.6. Ti

Problems:

- are all of ORNL capture and transmission data in the recent evaluation? not aware of any severe problems of the files
- difference in thermal capture cross section between the different libraries

.Evaluation:
None are in progress.

Validation:

- KIT validation

3.1.7. Mn

Problems: (n,2n) (n,a) no high resolution capture data above RR, LSDS confirm at low energies, discrepancies around 10 keV, activation rate in fast systems and deep penetration problems with 14 MeV source are strongly overpredicted

- check if data exist that are not included yet in evaluation?

Evaluation:

- new evaluation of Mn-55 (JAEA)

Validation:

- REZ validation of dosimetry reactions
- MINERVE (oscillation technique,)

3.1.8. V

Measurements have been done, ORNL plan evaluation of RRR - BNL will address fast region

Evaluation: ORNL/BNL

Validation:
- V spheres in SINBAD, (KIT)

3.1.9. Co

Problems: similar to Cu in 14 MeV OKTAVIAN, dosimetry reaction (n,a)(n,p),(n,2n)

Evaluation:
- JAEA
- BNL/IAEA evaluation for fast region

Validation:
- MINERVE
- data on (n,p) (n,a) in Cf -field from Rez

3.1.10. Zr

Problems: neutron activation analysis for spectrum characterisation, potential dosimetry reaction (capture)

Measurements: ORNL is planning new measurements, depending on availability of samples

Evaluation:
- ORNL new evaluation in RR as soon as measurements are getting ready
- BNL new evaluation ongoing

3.2. Methodology for evaluation

3.2.1. BNL

Review of differential data (in the resonance region no fits are done at BNL, just checking of available data and agreement, in case of a problem contact ORNL, fast region, gaps in evaluations, strength weaknesses of previous evaluations, EMPIRE calculation, KALMAN for fitting, validation MCNP, but no input decks. Need to identify suitable validation experiments, collaboration (IAEA) for input decks)
The goal is to provide full evaluation files to be included in a future release of ENDF library. Covariance matrix in the fast region using KALMAN, for the resonance region not fully identified, most likely with collaboration from ORNL. Covariance file in MF-33 or MF-32 still has to be decided. The used version of EMPIRE (developing version) is clearly linked in the repository.

IRDFF cross sections are fitted as close as possible, the direct inclusion of the dosimetry is technically challenging (ensure consistency of channels etc)
Benchmark selection and input files for validation will most likely be provided by IAEA.

3.2.2. CEA

The evaluation of Fe-56 (interested in all components of stainless steel). R-matrix limited format up to approximately 1 MeV, so at the moment the methodology for the energy range between 1 and 4 MeV is not decided.
The resolved resonance region will come from IRNS (based on SAMMY). For the fast region it will be CONRAD, including covariance matrix.
Interest in Cr, Ni, not certain whether new evaluations will be done, but it is planned to perform new validation experiments (collaboration with PSI, EPFL).
Presently a wider range of experiments performed at the MINERVE facility and results are available (reactivity worth, thermal capture)
CEA could test libraries on these experiments (done with TRIPOLI)

3.2.3. CNDC

Evaluations using UNF for the fast region. The covariance file (MF-33) can be provided for the fast region, based on experimental data or on model approach (GLLS approach).
Validation for some benchmarks, some of the input files have been received from the IAEA.
Experiments for validation can be performed for leakage spectra (2.5 MeV and 14 MeV). Some measurements might be performed, especially for neutron capture in the white spallation source. As this is a new facility a clear time-scale for the measurements cannot be given.

3.2.4. IAEA

Review of experimental data is performed, with correction and renormalization where necessary and possible. The methodology to store this information is available, but not consistently used. Dosimetry reactions are directly included. Model calculation with EMPIRE after carefully tuning the model parameters. The covariance prior is generated by MC technique from random sampling and then combined with experimental data by GANDR (GLS).
IAEA has a collection of approximately 1200 benchmarks, selection for criticality is based on DICE, for shielding the number of available benchmarks is much smaller (search from SINDBAD, publications??)

3.2.5. JAEA

Evaluations in the fast region use the CCONE code, the covariance is the KALMAN-CCONE code system.
Review of experimental data for the fast energy range and for the resolved resonance region for which the AMUR code will be used, if experimental data are available.
Shielding benchmarks are used for validation, already applied for JENDL-4.0 (PHITS and MCNP can be used)

3.2.6. JRC-Geel

Selection and review of experimental data, gaps in the data base are identified and new experiments are performed, if required.

Analysis in the resolved resonance range has been done using REFIT.

3.2.7. KIT

Validation of libraries against shielding benchmarks and to propagate the library uncertainties through the integral experiments. The work is based on the latest versions of MCNP and NJOY.

3.2.8. ORNL

Review of experimental data in the resonance range. Evaluation with SAMMY, covariance with SAMMY. Collaboration with UU on covariance, collaboration with BNL on high energy evaluation.
Method development for systematic inclusion of direct capture in the evaluation.
Validation using the in-house suite, either using MCNP and SCALE (VALID benchmark suite, suite that has been internally reviewed) and validation through collaboration outside the institute.
Have the ability to run sensitivity analysis if required/requested.

3.2.9. PSI

The TENDL methodology is used, further are BMC and MD (model defect) employed.
Provide random files, will mix EMPIRE/TALYS, some benchmarking of integral data.

3.2.10. RC Rez

A variety of validation facilities and detectors are available.

3.2.11. UU

Bayesian modelling between 1 and 5 MeV consistently using optical model code (TALYS) and possible resonance files from ORNL. Collaboration with PSI/IAEA on model defects.

4. Action

1. IAEA: can provide codes (GNTOEN) for converting GENDF into ENDF, which might be useful for the wider INDEN community.
2. IAEA: There will be INDC reports of ASPIS and TIARA, including input files for Monte Carlo calculation.
3. IAEA: Send the new Fe files to CEA (David) and to KIT (Stanislav)
4. CEA: perform the validation of iron at MINERVE for checking the thermal capture.
5. IAEA: Ongoing efforts to improve GUI for GANDR which should be available early 2019, to make more user friendly.
6. KIT: analysis of Oak Ridge Broomstick experiment validation, improvement of model.
7. KIT: analysis of Cf-252 leakage sphere from the REZ experiment
8. REZ: provide data of neutron leakage spectra Ni and Fe sphere experiments
9. ORNL: check if Ni data of Guber and Ti were already considered in the latest ENDF evaluation
10. ORNL, check Cr data (Guber)
11. ORNL check with IRNS (Luiz) the Cr-53 resonance parameter file
12. PSI after testing provide the weights of experimental data

13. UU: publication and distribution of analysis code
14. IAEA: provide evaluated EXFOR "input" for e.g. U-238, Ni f
15. IAEA/KIT explore possibility to obtain models for additional benchmark experiments (Livermore pulsed sphere experiments)

5. Recommendation

5.1. Experimental data

5.1.1. Measurements

Identified gaps in the experimental data:

- Fe-56 total cross section minima up to 500 keV
- Fe-56 capture, 10-25 keV
- Cr (natural) check of capture yields in the energy range between 2-10keV
- Cr (natural) check on total cross section
- Si thermal capture
- Inelastic data (especially for Fe-56) above the second exited level data would be very useful
- High resolution angular distribution measurements (only available for Fe-56 at present)
- Semi-integral experiments (can be very useful for checking the correctness of the file)

5.1.2. EXFOR correction database

Identification and recommendation of reliable data available in the EXFOR database. A system has been developed at IAEA to mark and store the choices and corrections evaluators have applied. The system will still need some more development to allow for extracting the correction files provided by an evaluator (search by name, etc). All evaluators are strongly recommended to use and store and submit their data into this system, to allow for later reproduction of their work and results.

5.2. Evaluation

Optical models have to be improved for structural materials for energies below 5 MeV (at least total cross section should be correct on average).

How do we treat fluctuations for evaluations? (below first inelastic level, between first and second) Can the creating of artificial resonance ladders serve as a solution to this problem, below the first inelastic level).

Model defect approach might be helpful above the first inelastic level.

Systematic inclusion of the direct capture component in the evaluations (e.g. some problems in the Fe-56 capture between 10-20 keV maybe solved by direct capture. Evaluations of Ar-40, Ca-48, Sc-45 might benefit from direct capture calculations).

How to treat the cross section minima in the resonance analysis, i.e. to make sure that the minima are maintained.

5.3. Validation

Identification and recommendation of reliable benchmarks.

Shielding benchmarks proved to be very useful for this mass range, as they are very sensitive to the minima in the cross section.

Criticality benchmarks for testing structural materials as reflectors.

Average cross section measurements (SACS) in Cf-252 spectrum and in well characterized reactor spectra are extremely useful, as well as leakage spectra measurements, when available.

It is very important to have reliable, well documented benchmark experiments (including tested Monte Carlo input files) e.g. it would be very appreciated if in the SINBAD collection more MCNP input files could be included.

IAEA
International Atomic Energy Agency
Atoms for Peace and Development

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

IAEA Headquarters, Vienna, Austria
29 October to 1 November 2018
Meeting Room MOE69

AGENDA

Monday, 29 October

08:30 – 09:00 **Registration** (IAEA Registration desk, Gate 1)

09:00 - 09:30 **Opening Session**

Welcoming address – Roberto Capote Noy / IAEA
Introduction – Andrej Trkov / IAEA
Election of Chairman and Rapporteur
Adoption of Agenda
Administrative matters

09:30 - 12:30 **Presentations by participants** (~ 30 min' each)

1. R. Capote / IAEA, *Overview of the structural materials' evaluation challenges*
2. S. Kopecky, EC-JRC-IRMM, *Known problems in structural material data and possible ways to address them*
3. V. Sobes, ORNL / USA, *ORNL Nuclear Data Evaluations*
4. D. Bernard, CEA / FR, *Evaluation OF n + ^{56}Fe reaction DATA (+Covariances) and experimental validation*
5. G. Schnabel, Univ. Uppsala, *Recent ND developments and plans at UU*

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **Presentations by participants** (cont'd)

6. N. Iwamoto, JAEA /JPN, *Status of nuclear data of structural materials in JENDL-4.0*
7. Y. Chen, CIAE / CPR, *The status of evaluation for structural materials at CNDC*
8. G. Nobre, BNL / USA, *Nuclear data evaluations of structural materials in BNL*
9. D. Rochman, PSI / SWI, *TENDL and BMC evaluations: advantages and limits*

Coffee breaks as needed

Tuesday, 30 October

09:00 - 12:30 **Presentations by participants** (cont'd)

10. M. Kostal, Research Centre Řež / CZR, *Integral experiments with structural materials in the Research Center Rez*
11. S. Simakov, KIT / GFR, *Iron sphere benchmarks with ^{252}Cf source: IPPE cf. with KFK and NIST*
12. A. Koning / IAEA, *TENDL-approach for Ni isotopes*
13. A. Trkov / IAEA, *IAEA INDEN (post-CIELO) ^{56}Fe evaluation benchmarking*

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **Round table discussions**

Discussion on the presentations

Coffee breaks as needed

19:00 ***Dinner at a restaurant (see separate information sheet)***

Wednesday, 31 October

09:00 - 12:30 **Round table discussions** (cont'd)
Discussion on the presentations

12:30 – 14:00 ***Lunch***

14:00 – 17:30 **Round table discussions** (cont'd)
Drafting of the Summary Report

Coffee breaks as needed

Thursday, 1 November

09:00 - 16:00 **Drafting of the summary report** (cont'd)
Finalisation of the Summary Report and Action List

16:00 **Closing of the meeting**

Coffee break(s) and lunch in between

ANNEX II

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

29 Oct to 1 Nov 2018
IAEA, Vienna

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Presentations

#	Author	Title	Link
1	Gustavo Nobre	Nuclear data evaluations of structural materials in BNL	PDF
2	David Bernard	Evaluation of n + 56Fe Reaction Data (+covariances) and Experimental Validation	PDF
3	Noboyuki Iwamoto	Status of nuclear data of structural materials in JENDL-4.0	PDF
4	Chen Yongjing	The status of evaluation for structural materials at CNDC	PDF
5	Vladimir Sobes	ORNL Nuclear Data Evaluations	PDF
6	Stefan Kopecky	Known problems in structural material data and possible ways to address them	PDF
7	Georg Schnabel	Recent ND developments and plans at UU	PDF
8	Stanislav Simakov	Iron sphere benchmarks with 252Cf source: IPPE cf. with KFK and NIST	PDF
9	Michal Kostal	Review of integral experiments with structural materials in Research Center Rez	PDF
10	Dimitri Rochman	TENDL and BMC evaluations: advantages and limits	PDF
11	Roberto Capote	Challenges of evaluation structural materials	PDF
12	Arjan Koning	TENDL approach applied to Ni isotopes	PDF
13	Andrej Trkov	IAEA INDEN (post-CIELO) 56Fe evaluation benchmarking	PDF
14	Andrej Trkov	IAEA INDEN (post-CIELO) 56Fe evaluation benchmarking (Long)	PDF
15	Viktor Zerkin	EXFOR data renormalization system	PDF

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