https://doi.org/10.61092/iaea.zn77-f2r9

INDC(NDS)-0746
Distr. G+IN+J

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Integral Data in Nuclear Data Evaluation

Summary Report of an IAEA Consultants Meeting
IAEA Headquarters, Vienna, Austria
14 - 17 November 2017

Prepared by

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January 2018

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Printed by the IAEA in Austria

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Contents

The meeting was opened by Andrej Trkov. Patrick Griffin was elected as Chairman and Vladimir Radulović was elected as Rapporteur.

1. Summary of Presentations

1.1. Survey on the Use of Integral Data in Evaluated Libraries (M. Ishikawa, JAEA)

Outline:

- History of criticality evaluations
- Statistics of integral data evaluation by JENDL-4.0
- Effect of integral data inclusion in a library
- A primitive trial to alleviate the discrepancy (introduction of new negative correlations, in group constant form)

Discussion during the presentation:

- The physical basis for the introduction of negative correlations was discussed, particularly related to correlations between data sets from model calculations, microscopic and integral experimental data.
- Adjusted cross-sections and their covariance matrices can be obtained by a Bayesian maximum likelihood approach. The *posterior* covariance matrix is determined by the *prior* covariance matrix and an additional term which depends on the experimental uncertainty matrix and the sensitivities.
- From the above, it follows that missing correlations do not depend on the prior nominal values of nuclear data.
- By the inclusion of integral experiments, correlations are introduced, linking the parameters that affect the k_{eff}, which may not be present in the original evaluations based on microscopic data alone.
- Existing general purpose libraries can give good results on k_{eff}, but with high uncertainties because some correlations do not exist in microscopic data (for example, there is no correlation in the measured data between nu-bar and fission), but they may be strongly correlated in critical assemblies. The exercise of adding ad-hoc (missing) correlations to the *a priori* covariance matrix demonstrates that the uncertainties in the integral result can be reduced (see the contribution of M. Ishikawa in the Appendix). The introduction of such correlations is an »easy fix«, but should not be part of a general purpose library, even though it improves the performance in specific integral benchmarks.
- Evaluators must document the adjustment steps made in the evaluation procedure.
- The adjustment procedure based on criticality benchmarks is not unique. For major benchmarks, the currently available major libraries perform well. However, if for example ^{235}U data is taken from one library and inserted into another, the results are often less good due to compensating errors in the cross-sections.
- It is difficult to extract meaningful data from sodium void reactivity cases on account of the multitude of processes and nuclear reactions, which affect the integral data.
- In Japan, generally the authorities and designers do not embrace the use of adjustment procedures.
- To avoid the use of the term »hidden correlations« which appeared in documents, the terms »non expressed correlations« or »application implicit correlations« are proposed.

1.2. Integral data in Nuclear Data Evaluation (M. Košťál, Research Centre Řež)

Outline:

- Introduction to the experimental activities at the Research Centre Rež.
- Brief description of the research infrastructure:
  - LR-0 research reactor
  - Si-filtered spectra
  - LVR-15 research reactor
  - ^{252}Cf source and spheres
- Summary of selected experimental results.
- Engagement in integral experiments (such as spectrum average cross-sections in ^{252}Cf and the high-energy part of reactor spectra) that are usable in data evaluation.
- Engagement in integral experiments usable in data validation (such as well-characterized neutron spectra in various locations of complex reactor assemblies and leakage neutron spectra from spheres, containing a ^{252}Cf neutron source).

Discussion during the presentation:

- Measurements using ^{252}Cf neutron source and spheres of various materials and dimensions.
- Reactor assemblies with large uncertainties on the fuel specifications (like IRT-4M in LVR-15) are of limited use as criticality benchmarks. They can be used, however, for other kinds of integral measurements, such as transmission, reaction rates, dynamic parameters.
- The usefulness of dynamic reactivity measurements was discussed, regarding the verification and validation of kinetic parameters. Differences in the calculated results using different evaluated libraries have been observed. The source of the differences needs further investigation.
- The potential of using the LVR-15 spectra with a Silicon filter, which feature distinctive peaks, as a neutron field for the energy calibration of stilbene detectors was presented.
- Measurements of spectrum averaged cross-sections in the LR-0 reactor and the ^{252}Cf neutron fields were recognized as valuable for the validation of dosimetry reaction cross-sections.
- Complex experiments are preferable for nuclear data validation only, and not for nuclear data adjustment.
- Measurements of leakage spectra from ^{252}Cf in light and heavy water spheres and spectrum measurements in the special LR-0 core (Central cavity) are sensitive to the reactions on oxygen. Some anomalies have been observed in the spectra between 3 and 4 MeV. A similar trend was also observed in the spectrum behind concrete blocks (VVER-1000 reactor benchmark). The observations point to possible deficiencies in the oxygen evaluations.
- The presented benchmarks are useful in that they indicate problems in the differential data.
- Regions where the discrepancy between the measurements and calculations exceeds 2 sigma are worthy of more detailed investigations.

1.3. Integral data assimilation strategy (G. Noguere, CEA/DEN Cadarache)

Outline:

- Introduction
- History of integral data assimilation in Cadarache:
  - Presentation of the BARRAKA method.
  - Presentation of the ERALIB application library and its limitations (problems with inelastic scattering on ^{23}Na due to missing constraints).
- Integral data assimilation strategy in the framework of the COMAC covariance database:
  - COMAC mic: covariances based on experimental microscopic data and "clean" integral data (sensitive to one reaction channel only) → results can be included in a general purpose library.
  - COMAC mac: covariances based on macroscopic integral data from mock-up and power reactors → results are usable only for application-specific libraries.
  - CONRAD is a nuclear data analysis code, based on equations similar to D.W. Muir's.
- COMAC strategy applied to MOX fuel calculations:
  - Evaluation of ^{239}Pu (use of oscillation measurements in the MINERVE reactor).
  - Evaluation of ^{240}Pu (use of post-irradiated fuel experiment in power reactors).

General discussion:

- Propagation of ^{239}Pu results: covariances corresponding to microscopic data result in large uncertaitnies in k_{eff} (~ 1000 pcm), but good C/E values. After the assimilation of the MINERVE results, the uncertainty in k_{eff} is reduced to ~ 400 pcm.
- The large uncertainties in the general purpose libraries should not disturb the community. To reduce the uncertainties, adjustments to general purpose libraries are needed. The resulting *adjusted libraries* are specific to a given application.

1.4. Integral measurements, neutron spectrum adjustment and cross-section validation activities at the Jožef Stefan Institute (V. Radulović, Jožef Stefan Institute)

Outline:

- Integral measurements of reaction rate ratios, neutron spectrum filters, uncertainties.
- General features of the GRUPINT spectrum adjustment code.
- Neutron spectrum adjustment:
  - Fitting analytically defined spectra to M/C calculation results.
  - Fitting spectra to measured reaction rate ratios.
  - Generation of neutron spectrum covariance matrices.
- Cross-section validation.
- Collecting experimental data in a well-defined format is recommended. A template is available from the IAEA https://www-nds.iaea.org/naa/rcm2/Tasks/spcact_template.inp

General discussion:

- Measurements at the JSI TRIGA reactor indicated:
  - Inconsistencies in the IRDFF-v1-05 dosimetry library were found for the ^{58}Fe(n,g)^{59}Fe in the upper end of the resonance range, using cadmium and boron nitride covers (15-20%, x sigma, rr_unc)
  - Large discrepancies in the ENDF/B-VII.1 data for the ^{117}Sn(n,n')^{117m}Sn reaction (100%) were observed. This reaction is being suggested for inclusion in the IRDFF library because of its low threshold and suitable nuclear properties, but requires enriched monitor samples.

1.5. What is the Role of Integral Benchmark Data in Support of Nuclear Data (P. Griffin, Sandia National Laboratories)

Outline:

- Fundamental axioms on dosimetry data.
- Historical perspectives.
- Terminology.
- Challenges in a spectrum adjustment.
- Reaction / isotope / element cross-correlations.
- Path forward.

Discussion during the presentation:

- All information, to have any meaningful content, must be associated with an uncertainty statement. The uncertainty must be derived in a manner consistent with the methodology used to derive the data/information. The development of covariance matrices needs to be an integral part of the nuclear data evaluation process.
- Terminology: within the dosimetry context, distinctions were provided between an adjustment and unfolding process. Adjustment is a formal mathematical process which requires the use of a *prior*, whereas unfolding does not require an initial guess.
- The community is challenged to define a *prior* in the absence of experimental data.
- Issue: how to make recommendations to the nuclear data evaluation community while preserving all the caveats for an adjustment process.
    - The community needs to consider which integral data are used in an adjustment and which data are reserved for use in validation. These two data sets must be distinct and non-overlapping.
    - Covariances are not physical quantities intrinsic to the variable being described. Different methodologies used to evaluate cross-sections will result in different covariances. The covariances reflect the process used to derive the characterization of the variable.
    - Large uncertainties may result from nuclear data evaluation methodologies based purely on differential data. They should not be criticized because they do not include correlations which are implicit in specific integral benchmarks. They should only be criticized if they fail to clearly detail the data on which they are based and the methodology used to extract the covariance.

1.6. On the use of integral experiments in nuclear data evaluation (A. Trkov, IAEA)

Outline:

- Types of integral data were discussed, with comments on their applicability.
- Some aspects of the IAEA-CIELO evaluation strategy was presented, with examples.

Discussion during the presentation:

- Selection criteria for the choice of integral data in the evaluation process of a general purpose library were discussed and are listed in Section 2.2. “Summary of recommendations”.
- Recommendations on the applicability of specific experiment categories in the evaluation process of a general purpose library were discussed and are listed in Section 2.2. “Summary of Recommendations”.
- ^{235}U nubar evaluation: The starting point was the ENDF-VII.1 library (adopted from ENDF/B-VII.0) which was already adjusted, however, in the IAEA CIELO evaluation the »tweak« made in order to get good results for main benchmarks, has been undone. The thermal value has been increased by 0.2 % compared to the total uncertainty from Standards-2017 of 0.5 % (i.e. 0.2 % from the fit and 0.4 % from unrecognized sources of uncertainty).

General discussion:

- Standards do not change frequently. In dosimetry libraries, reactions that are Standards are updated only when Standards change.
- Dosimetry evaluations change more frequently than general purpose evaluations. However, when general purpose evaluations change, the dosimetry evaluations should be reflected in the general purpose libraries.
- General purpose libraries may not be in sync with dosimetry libraries; therefore, the latter must be used for reaction rate calculations.
- Gilles Noguere provided information that JEFF 3.3 uses Standards-2017 for ^{235}U(n,f) but not for ^{239}Pu(n,f) and ^{238}U(n,f).
- Thermal cross sections and resonance integrals can be deduced from the k_0 and Q_0 factors in the Kayzero-NAA library. This information can be used for cross-checking, but not in the evaluation process (some are taken from literature and in some cases represent averages of discrepant data).

2. Discussion

2.1. General observations emerging from the discussions:

Observations regarding the evaluation process and the use of the covariances were as follows:

- In an evaluation, the microscopic experimental data must be the basis. Integral experiments can be used as guidance in the evaluations, to discriminate between discrepant data. The generalised least squares (GLS) is blind to statistically discrepant data; using such data procedures produces mathematically correct but physically wrong results, so the evaluator often has to make choices (e.g.: increase uncertainties or discard one or more of the data sets); such choices may introduce a bias in the results and are inevitably subjective, but are unavoidable.
- The evaluator must document which data sets were considered in the evaluation and (if applicable), which corrections to the data were made. The evaluator should provide a rationale for the selection of the data sets. A rationale for deselected datasets is also desirable.
- In the IAEA-CIELO: ^{235}U and ^{238}U were evaluated simultaneously, in order to decrease the compensating errors.
- General purpose libraries, based on experimental data only, can give good results on multiplication factor k_{eff}, but with high uncertainties. In order to reduce the uncertainties in integral benchmarks the user has to introduce correlations that are specific for that benchmark. It has been demonstrated in a simple example (see Appendix, contribution by M. Ishikawa) that the addition of ad-hoc (sometimes referred to as "missing") correlations to the *a priori* covariance matrix reduces the uncertainties in the integral result. The introduction of such correlations is an "easy fix", but should not be part of general purpose library, even though it improves the performance of the library in certain integral benchmarks.
- Users should be "educated" on the IAEA-CIELO and similar evaluations that follow similar principles, where the uncertainties arise from experimental data and do not include correlation, which would arise from integral measurements. For example, the microscopic measured prompt nu-bar is uncorrelated with the fission cross section and the variance in the calculated k_{eff} of a reactor assembly using microscopic data alone is the sum of the variances of the two parameters. However, we know that in modelling reactor systems the two are strongly correlated; when such correlations are introduced, the uncertainty in the calculated k_{eff} is significantly reduced. We note however, that the correlations are case-specific and should not be placed into a general purpose library.
- Licensing authorities and reactor designers should use general purpose libraries to derive adjusted libraries based on benchmarks representative of the system they are licencing or designing.

Observations regarding covariance processing:

- The most widely used nuclear data processing code NJOY can only process the P_1 component of angular distributions in a particular variant of the ENDF format. Higher order terms and cross-correlations cannot be processed and so the scattering moments for deterministic libraries cannot be calculated correctly in some cases. This could be important for reflector materials and in deep-penetration problems.

2.2. Summary of Recommendations

2.2.1. Integral Data

The formal criteria for acceptability of integral measurements include:

- Sensitivity only to an individual reaction channel which are being measured.
- Measurement does not introduce correlations between other nuclides / reaction channels.
- High precision and accuracy in the measurement process.

A classification of integral measurements, according to the fulfilment of the above criteria is proposed. Class 1, Class 2, Class 3, and Class 4.

Recommended use of particular integral measurements for general purpose evaluations:

Class 1: integral experiments that fully fulfil the above criteria:

- Spectrum averaged cross sections in standard and secondary standard neutron fields (^{252}Cf, thermal fission in ^{235}U)
- MACS measurements in Maxwellian fields (30 keV, below the ^{7}Li(p,n) threshold, i.e. 1.8 MeV)

Class 2: integral experiments that are conditionally acceptable when no more reliable data are available and are sensitive to individual reaction channels:

- Oscillation measurements of enriched samples in reactors.
- Post-irradiation measurements on enriched samples with mass spectrometry methods.
- Spectrum averaged cross sections in neutron fields well-defined from basic Physics principles.
- Measurements in thermal Maxwellian fields (usually in reactor thermal columns).
- Resonance integrals (RI). Note that the definition of RI has to be clearly specified.

Class 3: integral experiments that are conditionally acceptable when no more reliable data are available, understanding that significant cross-correlations are introduced by using these data.

- Criticality benchmarks that can be modelled accurately and contain a minimum number of materials (ideally applicable for application-specific libraries; not applicable in general purpose evaluations).

Class 4: integral experiments that are not acceptable for inclusion in the evaluation process, but can be used for data validation.

Some examples are:

- Transmission, shielding, leakage spectrum benchmarks, etc.
- Reactivity coefficient measurements (e.g. sodium void reactivity, etc.).
- Complex criticality benchmarks.
- Neutronics parameters from power reactor experiments.

2.2.2. Evaluated Data Files

Distinguish two categories for evaluated data:

A) General purpose libraries.

B) Application libraries derived form a general purpose library with the additional classification that is used in some user-communities:

1) Mean values and covariances are preserved, only additional correlations (+/-) are added.

2) Mean values and standard deviations are preserved, correlations are added/updated.
3) Mean values are preserved, standard deviations and correlations are added/updated.
4) Both mean values and covariances are updated.

Items 1) and 3) are illustrated with results presented in the talks of Makoto Ishikawa and Gilles Noguere respectively.

A General purpose library is expected to faithfully reflect differential data and corresponding uncertainties and correlations (e.g., from cross-section ratio measurements), and is expected to be used as a *prior* to derive application libraries for specific applications.
Note that in a broad sense typical adjusted libraries correspond to application library #4.
Uncertainties propagated to integral parameters in applications from a general purpose library are expected to be much larger than those propagated from application libraries to a relevant application.
Evaluators must provide clear and comprehensive information on which integral experiments have been used, and how those experiments were used in the evaluation process. Note that only Class 1-3 type of integral experiments are acceptable for use in the evaluation process.

APPENDIX: Participants' Presentations

I. Makoto Ishikawa, JAEA

Chap. 1 History of Criticality Evaluation for Fast Reactors

In this chapter, we summarize the history of performance for the criticality evaluation of fast reactors by ENDF/B and JENDL libraries, with the use of integral criticality data in the evaluation process, according to open documents.

1.1. ENDF/B case (Ref. 1-9)

Fig. 1.1 shows the prediction performance of ENDF/B libraries for the criticality of fast reactor cores. From this figure, it is apparent that ENDF/B was adjusted from version VII.0 in 2006. The major actinide data were taken over to ENDF/B-VII.1. It is noticed that the discrepancies of C/E values from 1.0 beyond ±1% were not unusual, before the adjusted ENDF/B-VII.0.

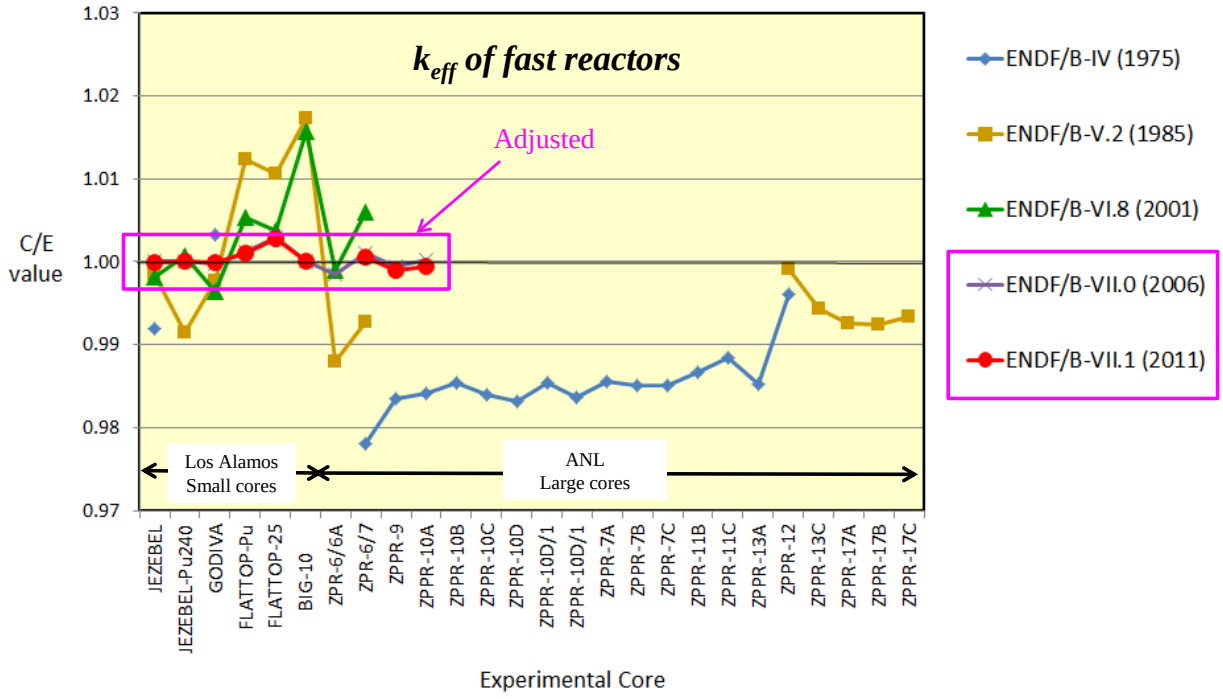

Fig. 1.1. ENDF/B history of criticality evaluation performance for fast reactors.

<Background of ENDF/B benchmarks>

ENDF/B-IV was developed and used in 1975-79. At the time, the use of deterministic 1D- or 2D-transport calculation was usual for reactor calculation. Since 3D-transport calculation was impossible due to poor computer ability at the time, the uncertainty induced from the analytical method was comparable with the uncertainty induced from nuclear data. Therefore, we guess that nuclear data evaluators did not apply the adjustment technique to improve the performance of criticality prediction.

ENDF/B-V.2 was developed and used in 1985-90. At the time, the use of deterministic 3D-transport and/or continuous-energy Monte Carlo calculations was not impossible, but very expensive. Therefore, it is supposed that nuclear data evaluators did not apply the adjustment technique to improve the performance of criticality prediction performance.

ENDF/B-VI.8 was developed and used in 2001-06. At the time, the use of massive Monte Carlo calculations was adopted for the library benchmarks based on the integral benchmarks such as ICSBEP, but nuclear data covariance and sensitivity analysis were not common yet. Therefore, it is considered that nuclear data evaluators did not apply the adjustment technique to improve the performance of criticality prediction performance.

ENDF/B-VII.0 was developed and used from 2006. At the time, the use of massive Monte Carlo calculations was adopted for the library benchmarks. In the development paper of ENDF/B-VII.0, the authors clearly mention that they applied the adjustment procedure in the evaluation procedure, that is, "..... In the case of ^{233}U and the major actinides ^{235}U and ^{239}Pu, the final step in the evaluations was to make minor adjustments in prompt ν (generally within experimental data uncertainties) to enhance agreement with simple fast critical benchmark measurements .... (Ref. 10)".

1.2. JENDL case (Ref. 11-14)

Fig. 1.2 shows the prediction performance of JENDL libraries for the criticality of fast reactor cores. Since JENDL was originally developed to apply the fast reactor analysis and design, the evaluators were keen to improve the prediction performance of criticality for fast reactors. This is the reason the performance of JENDL-2 or -3.2 was not so poor compared with the same generation of ENDF/B libraries, though the discrepancies of C/E values from 1.0 close to ±1% were not surprising, before the adjusted JENDL/Actinoid file 2008. It is clearly reported that JENDL/AC-2008 was completely adjusted with the mathematical maximum likelihood methodology (Ref. 15), and the results can be seen in Fig.1.2.

<Background of ENDF/B benchmarks>

JENDL-2 was developed and used in 1982-89. Practically, JENDL-2 was the first version of JENDL which was used to analyse reactor parameters. For the application to large fast reactors, there were two significant problems, that is, 1) the large space-dependency of C/E values for control rod worths and reaction rate distributions, and 2) the extreme overestimation of sodium void reactivity.

JENDL-3.2 was developed and used in 1994-2002. The above deficiency of JENDL-2 was almost solved. " ..... The revision work of JENDL-3 has been made by considering feedback information of various benchmark tests. (Ref. 16)", but it seems no systematic adjustments were performed.

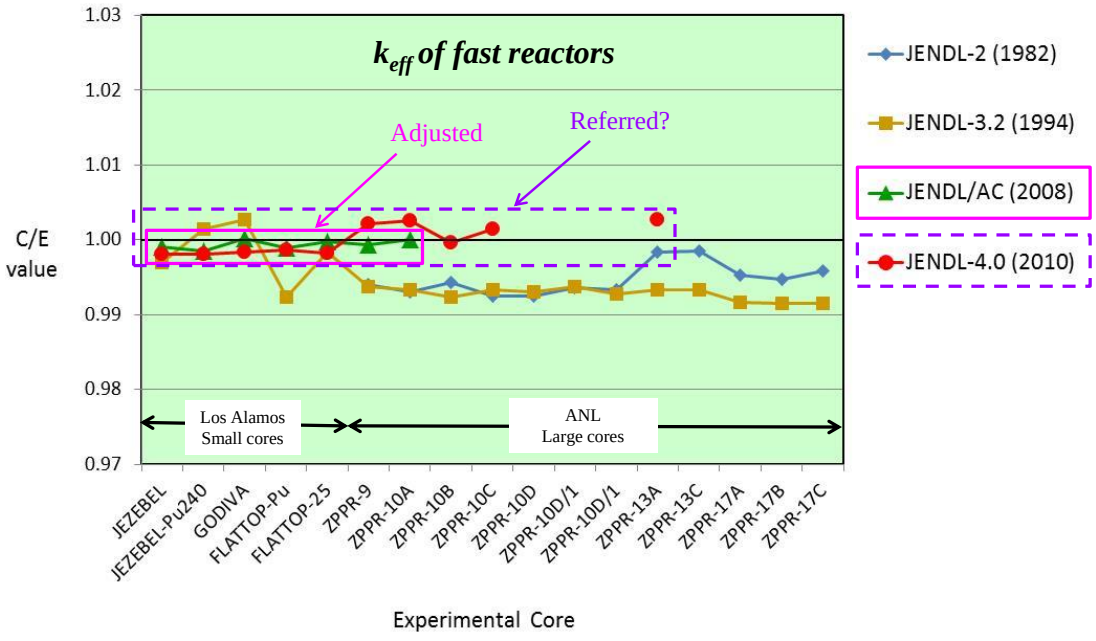

Fig. 1.2. JENDL history of criticality evaluation performance for fast reactors

JENDL/Actinoid file 2008 was developed as a special purpose file in 2008. In the development paper of JEND/AC-2008, the authors clearly mention that they applied the adjustment procedure in the evaluation procedure, that is, "..... The evaluated data for $^{233, 235, 238}$U, $^{239, 240, 241}$Pu, and ^{237}Np explained above were slightly corrected by taking account of the integral data of fast reactors since the evaluated results underestimate the criticality values of some small systems beyond the range of their uncertainties uniformly ..... (Ref. 15)".

JENDL-4.0 was developed and used since 2010. The adjustment of major actinides was not officially adopted unlike JENDL/AC-2008, but it seems to have "reflected" the results of some integral benchmarks, judging from the excellent performance of criticality prediction.

Chap. 2 Statistics of Integral Data Evaluation by JENDL-4.0

JENDL-4.0 was validated with a fast reactor benchmark dataset which contains more than 400 data including various reactor core characteristics such as criticality, reaction rate and reactivity. In this chapter, the prediction performance (C/E-1) and covariance-based uncertainty (GMG[1]) by JENDL-4.0 are statistically compared for the three categories of core characteristics and discussed regarding their consistency.

2.1. Integral Database used for the Study of Statistical Consistency

Table 2.1 summarizes the fast reactor database which was used to make the statistical consideration. This database and the analytical results by JENDL-4.0 are openly reported in Ref. 17.

TABLE 2.1(1/2) INTEGRAL EXPERIMENTAL DATA FOR JENDL-4.0 STATISTICS

Facility (Institute, Country)	Name of Experimental Core (Total Number)	Core Features	Core parameters*1) collected in database	Open to Public
ZPPR <JUPITER Program> (ANL-W, USA)	**ZPPR-9, 10A -10C** (4)	600-800 MWe-class, two-region homogeneous MOX cores.	keff, RR, CRW, SVR, and DR(sample).	**Yes.** (**IRPhE**)
	ZPPR-13A (1)	650 MWe-class, Radially-heterogeneous MOX cores.	keff, RR, CRW, SVR, and DR(sample).	
	ZPPR-18A, 18C, 19B (3)	1,000 MWe-class, two-region homogeneous MOX cores with enriched-uranium regions.	keff, RR, CRW, and SVR.	
ZEBRA <MOZART Program> (Winfrith, UK)	**MZA** (1)	550 liter-sized one-region MOX core as a clean benchmark.	keff and SVR	**Yes.** (**IRPhE**)
	MZB, MZC (2)	2,300 liter-sized two-region homogeneous MOX cores to simulate the prototype fast reactor MONJU.	keff, CRW, and SVR	
JOYO (JAEA, Japan)	**JOYO Mk-I** (1)	300 liter-sized fast power reactor core with mixed Pu and enriched-uranium fuel with blanket.	keff, CRW, SVR, ZMRR, Isothermal temperature reactivity, and Burnup reactivity.	**Yes.** (**IRPhE**)
	~~**JOYO Mk-II** (1)~~	~~240 liter-sized fast power reactor core with mixed Pu and enriched-uranium fuel with reflector.~~	~~MA post-irradiation test.~~	~~No.~~

*1) keff: Criticality, RR: Reaction rate, CRW: Control rod worth, SVR: Sodium void reactivity, SSW: Small sample worth, DR: Doppler reactivity, ZMRR: Zone material replacement reactivity

Table 2.1(2/2) Cont'd

Facility (Institute, Country)	Name of Experimental Core (Total Number)	Core Features	Core parameters*1) collected in database	Open to Public
MONJU (JAEA, Japan)	**MONJU Start-up Tests** (2)	280 MWe prototype fast breeder reactor with two-region homogeneous MOX core.	keff, CRW, and Isothermal temperature reactivity.	No.
BFS (IPPE, Russia)	**BFS-62-1 -62-5, 66-1** (6)	3,400 liter-sized three or four-region enriched-uranium and/or MOX fuel cores with or without radial blankets.	keff, RR, CRW, and SVR.	No. (**Yes. BFS-62-3A**) (**IRPhE**)
	BFS-67, 69, 66 (3)	10 kg of NpO_2 loading cores in central MOX region with weapon-grade Pu, high enriched Pu, and degraded Pu.	keff, RR, CRW, and SVR.	
MASURCA (CEA, France)	**ZONA-2B** (1)	380 liter-sized core in the CIRANO experiment series, which aimed at the study of plutonium burner cores	SVR and ZMRR.	No.
SEFOR (General Electric, USA)	**SEFOR CORE-I, II** (2)	20MWt fast power reactor core fueled with mixed PuO_2-UO_2 and cooled with sodium.	DR(whole core).	**Yes.** (**PHYSOR 2004**)
Los Alamos (LANL, USA)	**FLATTOP-Pu, FLATTOP-25, JEZEBEL, JEZEBEL-Pu240, GODIVA** (5)	sphere-shaped cores of approx. ten centimeter in diameter with metallic fuel consisted of Pu-239, or degraded Pu, or U-235.	keff.	**Yes.** (**IRPhE**)

The size of experimental cores ranges from ultra-small ones (LANL experiments) to 1,000 MWe-class large cores (ZPPR experiments), the fuels of the cores are not only Pu, but Uranium (BFS experiments), and the features of the experiments include not only critical experiments, but also power reactors such as JOYO and MONJU. The number of data and the variety of experiments are considered sufficient to make the statistical study.

2.2. Summary of JENDL-4.0 Performance

We classified the whole reactor core characteristics (447 data) into three categories, that is, (1) Criticality (total number of data is 31). (2) Reaction rate (218 data, both distribution data and ratio data are included), and (3) Reactivity (198 data, control rod worth and sodium void reactivity are included). Table 2.2 summarizes the statistics of JENDL-4.0 performance. The first column of the table shows the category of reactor core parameters, the second one is the averaged values of C/E-1 which are defined as the square root of average value of $(C/E-1)^2$ to compare them with the total uncertainty values evaluated by summing up the covariance-based uncertainty and the integral parameter uncertainty. Figures 2.1 - 2.5 show the C/E values and the total uncertainties of typical characteristics by JENDL-4.0, that is, Criticality, ^{235}U fission-rate ratio, ^{238}U fission-rate ratio, Control rod worth and Na void reactivity, respectively. We can find the following facts from Table 2.2 and these figures:

For the criticality, there are large discrepancies between the averaged C/E-1 value (0.18%) and the total uncertainty based on nuclear data covariance (0.88%). Since the major contribution to the total uncertainty is nuclear-data-induced uncertainty (GMG^t: 0.82%), we can judge that the prediction performance of criticality by JENDL-4.0 is unreasonably good compared with the covariance-based uncertainty (a factor of 5)[1].

On the other hand, the statistics of Reaction rate and Reactivity do not show such unreasonable inconsistency between the averaged C/E-1 values and the covariance-based uncertainty.

[1] G. Palmiotti gave us the same statistics by ENDF/B-VII. The average of C/E-1 values for criticality is 0.16%, and the covariance-based uncertainty is 0.65%. The ENDF/B-VII has also large discrepancy for these two values (a factor of 4).

In detail, Fig. 2.2 shows that the total uncertainty of ^{235}U fission-rate ratio (2.3%) seems a little larger than the averaged C/E-1 values (1.1%), but the reason for this difference can be considered the estimation of experimental uncertainty assigned to this reaction-rate ratio (approx. 2%), not caused by the covariance-based uncertainty.

Fig. 2.5 shows that the total uncertainty of Na void reactivity (19.6%) seems a little larger than the averaged C/E-1 values (11.7%), but considering that the results by the Monte Carlo calculation in Fig.2.5 show reasonable agreement between the averaged C/E-1 values and the total uncertainty, the cause of above discrepancy may be the overestimation of analytical modeling uncertainty (Vm) for the deterministic calculation. The evaluation of the analytical modeling uncertainty is based on the recommendation of the NEA/WPEC/SG33 final report (Ref.18).

As discussed in Chap.1, this large discrepancy between the averaged C/E-1 value and the covariance-based uncertainty for criticality by JENDL-4.0 (and ENDF/B-VII) is considered the result of the integral data inclusion in the library evaluation without its reflection to the covariance data.

TABLE 2.2. SUMMARY OF JENDL-4.0 PERFORMANCE

Core Parameter **(number of data)**	**Square root of Average value of $(C/E-1)^2$**	**Average value of Total uncertainty of C/E values** $\sqrt{Ve+Vm+GMG^t}$*1	**Average value of Nuclear-data-induced uncertainty** $\sqrt{GMG^t}$
Criticality (31)	0.18 %	0.88 %	0.82 %
Reaction rate (distribution, ratio) (218)	2.2 %	3.3 %	2.4%
Reactivity (control rod worth, sodium void reactivity, etc) (198)	7.3 %	11.4 %	7.4 %

Compare

Contribution

*1 *Ve*: Experimental uncertainty (1 sigma)
Vm: Analytical modeling uncertainty (1 sigma)
G: Sensitivity coefficients
M: Covariance data of JENDL-4.0 (1 sigma)

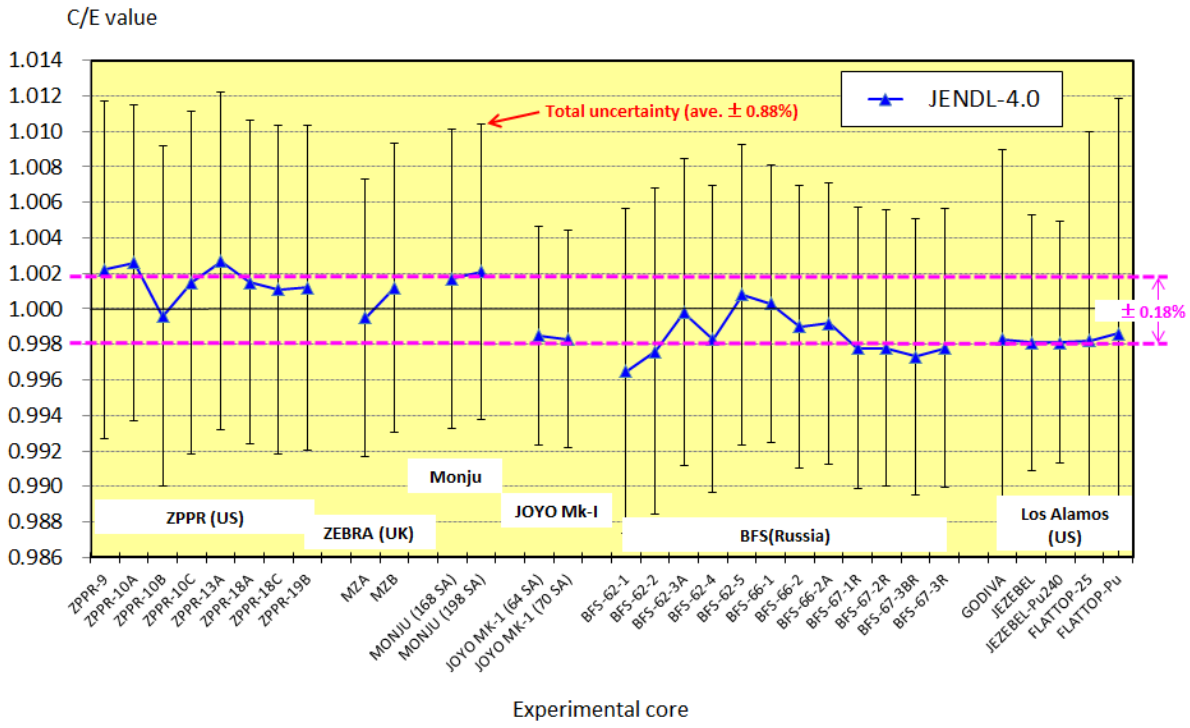

Fig. 2.1. C/E value and Total uncertainty for Criticality by JENDL-4.0

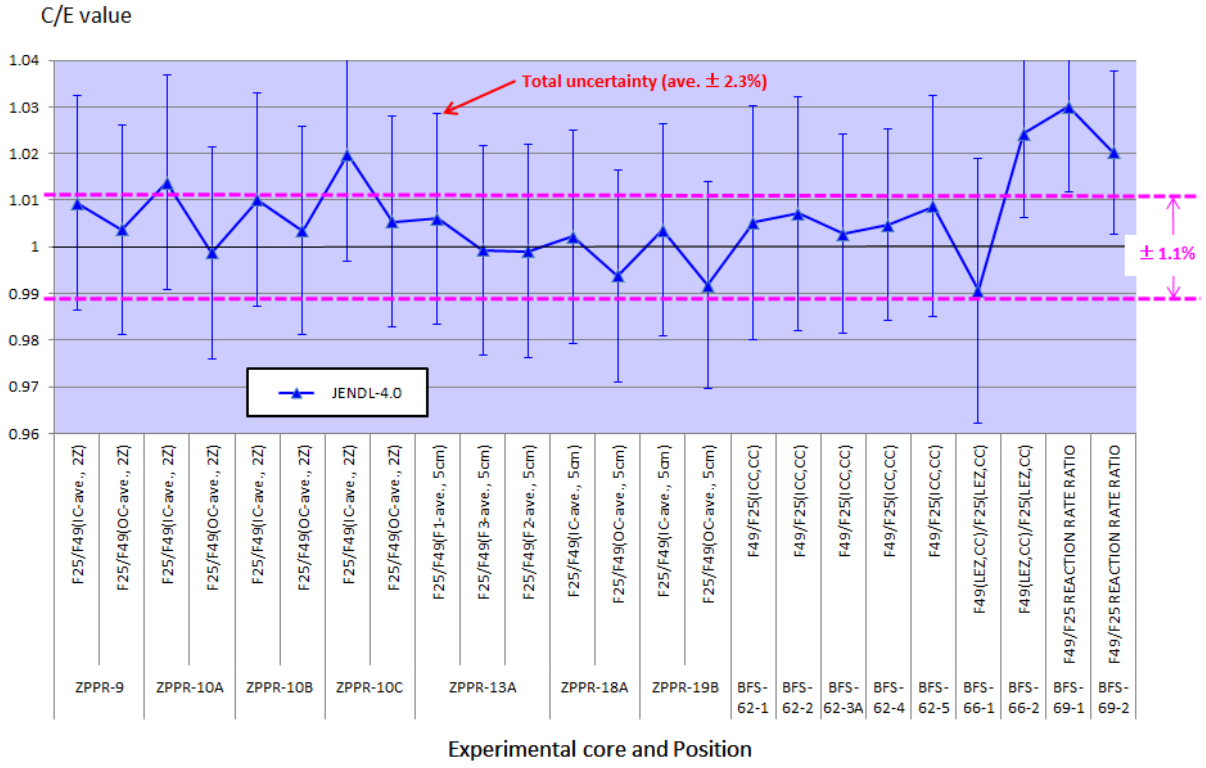

Fig. 2.2. C/E value and Total uncertainty for ^{235}U Fission-rate ratio by JENDL-4.0

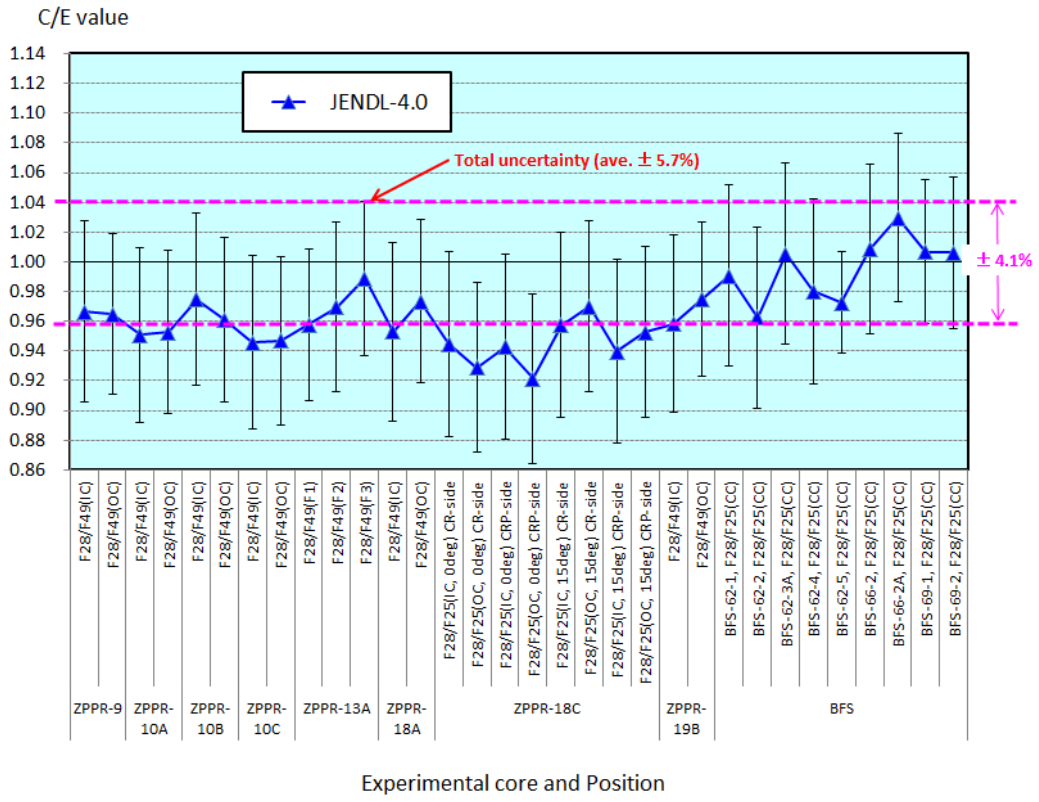

Fig. 2.3. C/E value and Total uncertainty for U238 Fission-rate ratio by JENDL-4.0

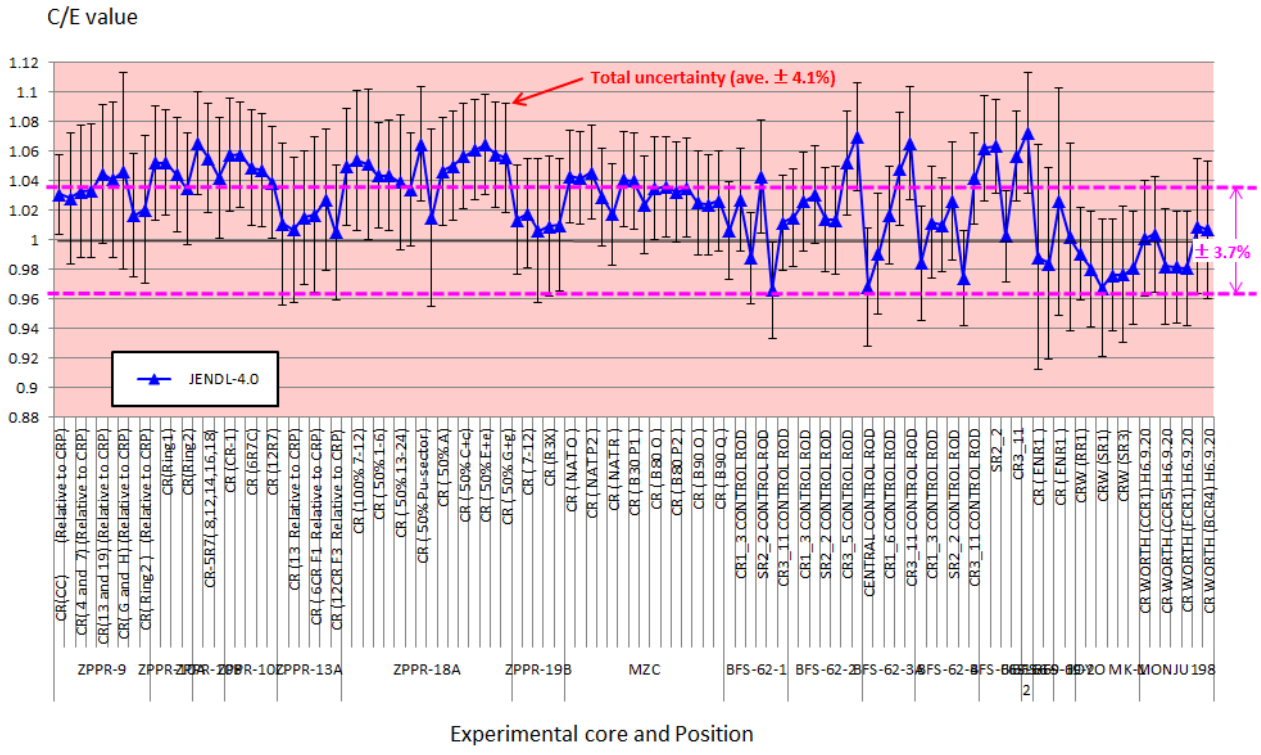

Fig. 2.4. C/E value and Total uncertainty for Control rod worth by JENDL-4.0

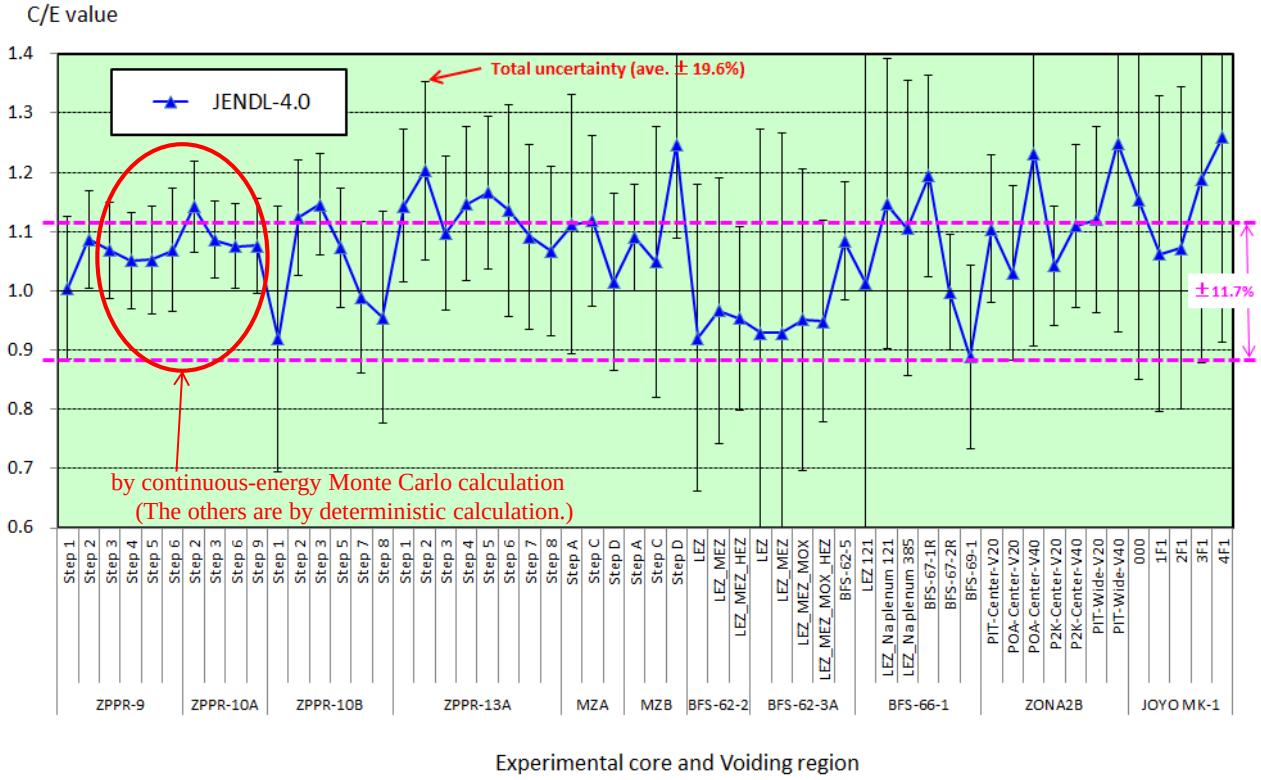

Fig. 2.5. C/E value and Total uncertainty for Na void reactivity by JENDL-4.0

Chap. 3 A Primitive Trial to Alleviate the Discrepancy

As seen in Chap.2, the adjusted libraries, JENDL-4.0 and ENDF/B-VII, show a large discrepancy between the averaged C/E-1 value and the covariance-based uncertainty for criticality evaluation by a factor of 4 – 5. This discrepancy may be caused by the fact that the evaluators adjusted (or calibrated) the nuclear data to meet the integral critical experiments, but they did not make the covariance data consistent with the adjusted libraries. This may cause a serious problem, if the library and associated covariance data are used in the licensing evidence of an atomic power reactor, from the viewpoint of recent V&V trends and accountability requirements by the authorities. In this chapter, we demonstrate the effect of negative correlations between reactions or isotopes which is inevitably generated if library evaluators use some integral experimental data to determine the final values of nuclear data.

3.1. Assumption to Estimate the "Missing Correlations" in JENDL-4.0

Since there is no information how the evaluators of JENDL-4.0 included the integral information during the evaluation process, we make very simple assumptions to estimate the “Missing Correlation” as below:

(1) The nominal values and the associated standard deviations (i.e., diagonal terms of the covariance matrix) possess the firm technical basis from the viewpoint of the differential evaluation for nuclear data.
--> We give NO changes to the nominal values and the standard deviations, that is, we modify only the correlation factors.

(2) The evaluators only cared for, and tried to improve the criticality benchmark results, but NOT more complicated core characteristics such as Na void reactivity, which have large ambiguities from the integral viewpoint.
--> We should improve the covariance-based uncertainty ONLY for the criticality.

(3) The "missing correlations" are given only between different reactions of a nuclide, that is, NOT between the reactions of the different nuclides.
(4) The energy dependency of nuclear data (i.e., shape) is NOT changed, since the evaluators gave their confidence to the shape which was based on the nuclear model calculation.

3.2. Correlations Given to Improve the Covariance-based Uncertainty of Criticality

We chose effective reactions to modify keff values. From the adjustment equation based on the maximum likelihood consideration, the reactions and isotopes with large sensitivity coefficients are effective to compensate the keff values. Fig. 3.1 gives typical sensitivity coefficients for ^{239}Pu and ^{238}U for the keff of a large fast reactor core, ZPPR-9.

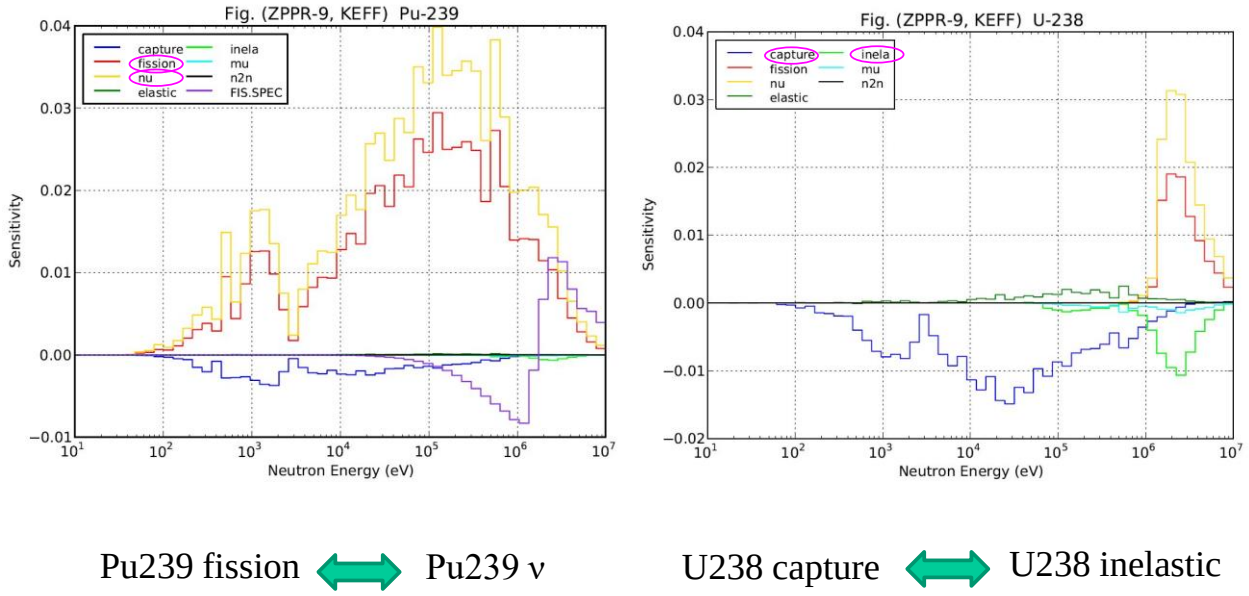

Fig. 3.1. Sensitivity coefficients for keff of a large fast reactor core ZPPR-9

Taking into account that there are uranium-fuelled fast reactor cores, i.e., BFS experiments, we finally selected Table 3.1 as the minimum reactions to improve the discrepancy between the averaged C/E-1 value and the covariance-based uncertainty for criticality evaluation. The values of correlation factors were decided with several iteration calculations, but not perfectly optimized.

TABLE 3.1 CORRELATIONS GIVEN TO IMPROVE THE COVARIANCE-BASED UNCERTAINTY OF CRITICALITY

Nuclide	Reactions	Correlation Coefficients (among all energy groups)
Pu239	fission vs. ν	-0.7
U235	fission vs. ν	-0.6
U238	capture vs. inelastic	-0.3

By adding the new negative correlations of Table 3.1 to the original 70-group covariance based on JENDL-4.0, we obtained the revised values of the total uncertainty for the statistic table of 447 data as shown in Table 3.2 and Fig.3.2. As can be seen, the covariance-based uncertainty of criticality was

greatly reduced and becomes close to the averaged C/E-1 value, while there are no changes about those of reaction rate and reactivity.

TABLE 3.2 REVISED SUMMARY OF JENDL-4.0 PERFORMANCE BY ADDING CORRELATIONS

Core Parameter (number of data)	**Covariance**	**Square root of Average value of $(C/E-1)^2$**	**Average value of Total uncertainty of C/E values** $\sqrt{Ve+Vm+GMG^t}$	Average value of Nuclear-data-induced uncertainty $\sqrt{GMG^t}$
Criticality (31)	**JENDL-4.0**	0.18 %	**0.88 %**	0.82 %
	Additional Correlations		**0.58 %**	0.49 %
Reaction rate (218)	**JENDL-4.0**	2.2 %	**3.3 %**	2.4%
	Additional Correlations		**3.2 %**	2.3 %
Reactivity (198)	**JENDL-4.0**	7.3 %	**11.4 %**	7.4 %
	Additional Correlations		**11.4 %**	7.5 %

Compare

Contribution

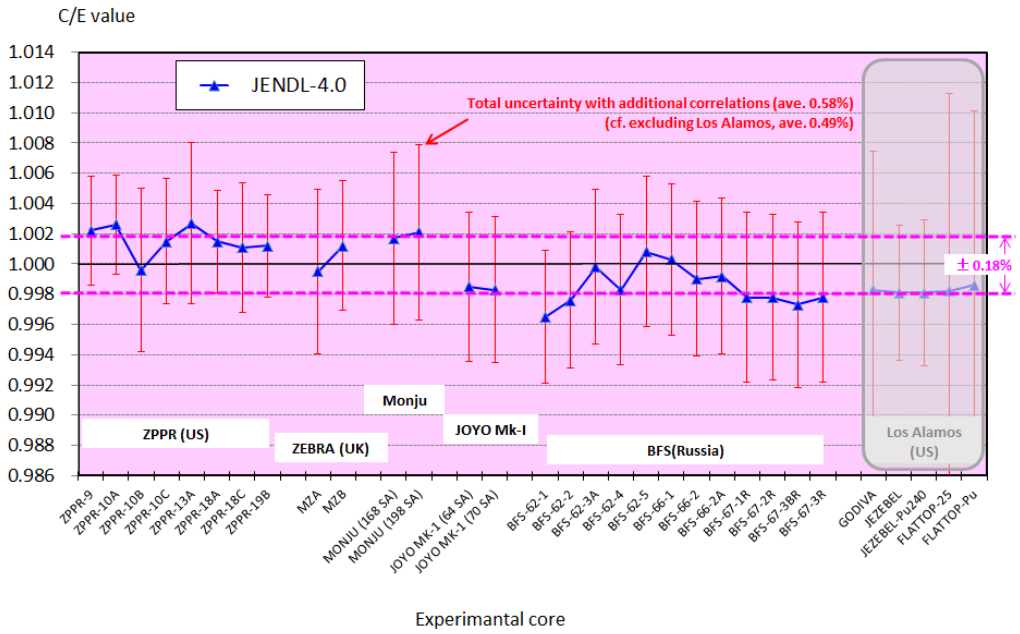

Fig. 3.2. C/E value and Total Uncertainty

(Criticality with Additional Correlations to JENDL-4.0)

In detail, the isotope- and reaction-wise contributions of the covariance-based uncertainty are shown in Fig. 3.3, without and with the addition of new correlations for the criticality of three typical experiments, ZPPR-9 (a large Pu core), BFS-62-1 (a large uranium core), and GODIVA (an ultra-small uranium

core). The three negative correlations assumed in Table 3.1 worked very well for ZPPR-9 and BFS-62-1, since the assumed correlations are very effective for the major uncertainty components. However, the improvement of GODIVA is not so large, the reason of which is clear: GODIVA has other uncertainty components such as ^{235}U elastic, inelastic, and mu-bar, which were not assigned new correlations here.

ZPPR-9 (Pu large core)

(ZPPR-9, KEFF)		JENDL-4.0	With Additional Correlations
U238	Capture	0.46	0.46
	Inelastic	0.50	0.50
Pu239	Capture	0.22	0.22
	Fission	0.30	0.30
	ν	0.14	0.14
	χ	0.42	0.42
Fe56	Inelastic	0.18	0.18
Sum of Diagonal		0.94	0.94
Sum of Non-diagonal		0.12	−0.87
Total Uncertainty (GMG^t)		0.94	0.34

BFS-62-1 (U large core)

(BFS-62-1, KEFF)		JENDL-4.0	With Additional Correlations
U235	Capture	0.24	0.24
	Fission	0.44	0.44
	ν	0.17	0.17
	χ	0.33	0.33
U238	Capture	0.45	0.45
	Elastic	0.11	0.11
	Inelastic	0.26	0.26
Fe56	Capture	0.10	0.10
	Inelastic	0.11	0.11
Sum of Diagonal		0.86	0.86
Sum of Non-diagonal		0.12	−0.80
Total Uncertainty (GMG^t)		0.86	0.31

GODIVA (U small core)

(GODIVA, KEFF)		JENDL-4.0	With Additional Correlations
U235	Capture	0.19	0.19
	Fission	0.33	0.33
	ν	0.28	0.28
	Elastic	0.42	0.42
	Inelastic	0.74	0.74
	μ	0.38	0.38
	χ	0.15	0.15
Sum of Diagonal		1.05	1.05
Sum of Non-diagonal		0.05	−0.54
Total Uncertainty (GMG^t)		1.06	0.91

※ ▭ shows the reactions which were given the additional correlations.

Fig. 3.3. Isotope- and Reaction-wise Contributions of the Covariance-based Uncertainty for ZPPR-9, BFS-62, and GODIVA

As a conclusion, we demonstrated that even very few negative correlations could improve the agreement between the C/E-1 value and the covariance-based uncertainty, as well as the fact that they would not work efficiently if other isotopes or reactions provide dominant contributions to the uncertainty. This kind of remedy is not appropriate for generous purpose libraries, but should be added to application-dependent libraries.

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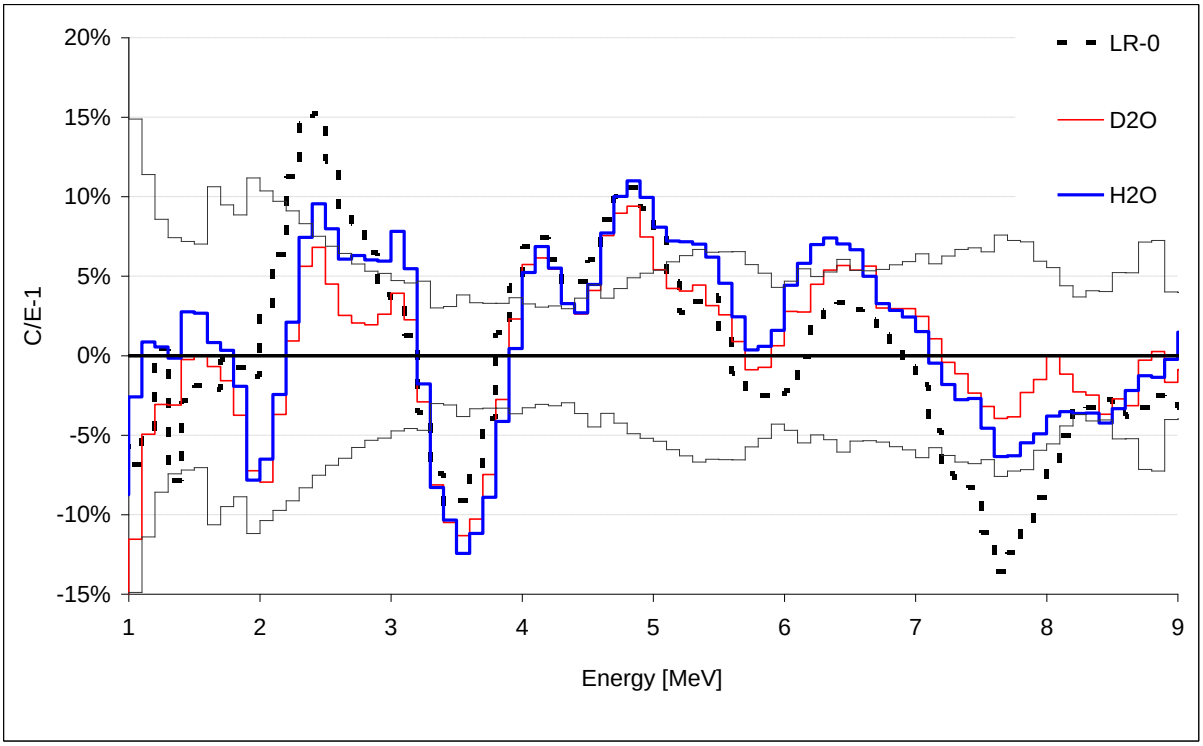
II. Michal Košťál, Research Centre Řež

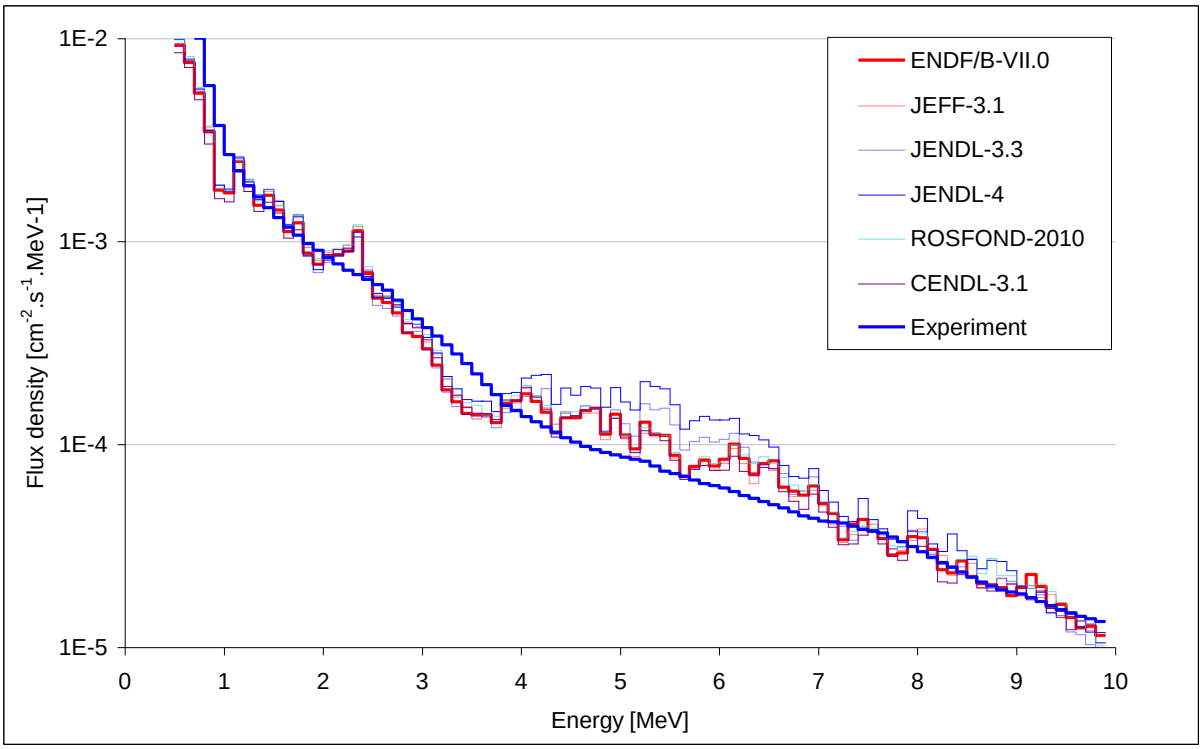
The physical quantities in integral experiments can usually be measured much more accurately than differential nuclear data, if well performed. Integral data imply spectrum-averaged cross sections or cross section ratios, kinetic parameters, leakage spectra, scattered-neutron yields, multiplication factor, etc. The major disadvantage during their possible use for data tuning, is, that they integrate many parameters, where many of them have compensating effect. Based on this fact, only integral data integrating reference spectra with cross section (spectral averaged cross sections) can be used during data adjustments.

The other data – criticality, leakage spectra, scattered-neutron yields, multiplication factor, and data from complex reactor benchmarks (criticality, reactivity, reactivity effects, reactivity coefficients, fission/power profile, distribution of neutron flux, distribution of reaction rates, neutron spectra or spectral parameters in various locations, buckling parameters, kinetic parameters are recommended to be used for validation of evaluated nuclear data libraries. Also, the results from integral experiments are an essential and important tool in the finding of deflections in data evaluations.

The results presented by M. Kostal might serve as an expample. In the Research Center Rez, a set of measurements of neutron leakage spectra from H2O and D20 spheres with ^{252}Cf in the center was realized. It shows notable discrepancies in some regions. Based on various oxygen accompanying element (hydrogen or deutrerium) it can be assumed, that the discrepancy is connected with oxygen. This is fully consistent with the integral measurement of neutron spectra in the center of LR-0 core (LR(0)-VVER-RESR-003: CRIT-SPEC). Moreover, the same manner can be observed for integral measurements of neutron spectra in biological shielding (Neutron deep penetration through reactor pressure vessel and biological concrete shield of VVER-1000 Mock-Up in LR-0 reactor, Annals of Nuclear Energy, Vol. 94, (2016), pp 672-683).



C/E comparison of neutron leakage spectra from H2O/D2O sphere, D=30cm, calculation realized with ENDF/B-VII.1



Neutron flux density in biological shielding simulator (Point 8), (Kostal et al, Annals of Nuclear Energy, Vol. 94, (2016), pp 672-683)

SACS in ^{252}Cf

A large set of cross sections measured. Many of them were published in: M. Schulc et al., Validation of differential cross sections by means of ^{252}Cf spectral averaged cross sections, Appl. Rad. and Isot., 132 (2018) 29–37. Significant discprepancies were observed in case of:

^{54}Fe(n,α)^{51}Cr; ^{54}Fe(n,p)^{54}Mn; ^{55}Mn(n,2n)^{54}Mn

Reaction	CVR SACS [mb]	Unc. [%]	IRDFF SACS [mb]	Unc. [%]	Difference
^{23}Na(n,2n) ^{22}Na	8.84E-03	3.6	8.77E-03	7.03	-0.79%
^{90}Zr(n,2n) ^{89}Zr	0.2162	3.5	0.2181	5.08	0.88%
^{89}Y(n,2n) ^{88}Y	0.3409	3.6	0.3461	4.37	1.51%
^{19}F(n,2n) ^{18F}	0.01561	3.8	0.01634	5.26	4.68%
^{54}Fe(n,α)^{51}Cr	1.003	4.3	1.112	3.88	10.90%
^{27}Al(n, α)^{24}Na	0.9851	3.5	1.017	1.77	3.23%
^{27}Al(n,p)^{27}Mg	4.976	3.5	4.747	2.35	-4.60%
^{54}Fe(n,p)^{54}Mn	78.72	3.9	86.51	3.16	9.89%
^{127}I(n,2n)^{126}I	2.044	3.6	2.104	3.82	2.94%
^{197}Au(n,2n)^{196}Au	5.446	3.5	5.5232	2.75	1.42%
^{55}Mn(n,2n)^{54}Mn	0.4821	4.1	0.4162	3.72	-13.66%
^{169}Tm(n,2n)^{168}Tm	6.358	3.9	6.259	3.14	-1.56%
^{59}Co(n,2n)^{58}Co	0.41985	3.6	0.4079	3.6	-2.84%
^{59}Co(n,p)^{59}Fe	1.79514	3.6	1.714	3.65	-4.52%
^{93}Nb(n,2n)^{92}Nb*	0.8188	3.7	0.79014	2.38	-3.50%

SACS in ^{235}U

The previously measured set: ^{23}Na(n,2n), ^{75}As(n,2n), ^{90}Zr(n,2n), ^{89}Y(n,2n) are benchmarked now.

Experimentally measured spectral averaged cross sections in ^{235}U PFNS

		^{75}As(n,2n)	^{90}Zr(n,2n)	^{23}Na(n,2n)	^{89}Y(n,2n)
Cross section in ^{235}U	[mb]	0.3205	0.1071	0.00384	0.1708
E 50%	[MeV]	12.6656	14.24	15.2269	13.698
Total combined uncertainty	[%]	4.3	3.6	4.8	3.1

A new set of measurements was realized in LR-0 as well. ^{89}Y(n,2n) (Measurement of various monitors reaction rate in a special core at LR-0 reactor; Annals of Nuclear Energy 112 (2018) 759–768), ^{55}Mn(n,2n); ^{127}I(n,2n), ^{48}Ti(n,p); ^{24}Mg(n,p) (will be published).

Validation of cross section was realized for ^{54}Fe(n,p), ^{54}Fe(n,α), ^{181}Ta(n,g) (Measurement of various monitors reaction rate in a special core at LR-0 reactor; Annals of Nuclear Energy 112 (2018) 759–768). It was observed that the new measurement is in very good agreement with previous measurement with bigger sample. But they do not correspond with exfor value 0.150, which is most probably the result of discrepant data (Measurement of ^{89}Y(n,2n) spectral averaged cross section in LR-0 special core reactor spectrum, Radiation Physics and Chemistry 141 (2017) 22–28).

Significant discrepancies between experiment and calculation using IRDFF were observed in case of: ^{54}Fe(n,α); ^{54}Fe(n,p)^{54}Mn; ^{55}Mn(n,2n). This result corresponds with ^{252}Cf measurements, thus it might be an indication on deflections in mentioned reaction cross sections.

Comparison with previous measurements

	^{235}U SACS	Unc	E/REF-1		
^{89}Y(n,2n)	0.169	4.6%	12.7%	0.150	Too many outlying values (Kostal et al, RPC, 141 (2017), 22-28
			-1.2%	0.171	IRPhEP benchmark, LR(0)- RESR 004
^{55}Mn(n,2n)	0.239	4.6%	1.3%	0.236	Manhart 2008
^{127}I(n,2n)	1.209	4.8%	-5.5%	1.279	Manhart 2008
			1.0%	1.197	K.Zolotarev, INDC(NDS)-0526
^{48}Ti(n,p)	0.311	10%	3.8%	0.300	W. Mannhart 2008
^{24}Mg(n,p)	1.476	10%	1.7%	1.451	W. Mannhart 2008
			-0.9%	1.490	K.Zolotarev, INDC(NDS)-0526

Comparison of various EXFOR data of ^{235}U SACS of ^{89}Y(n,2n) reaction

Cross section in ^{235}U PFNS [mb]	Unc.	Source
0.172	0.006	This work
0.179	0.018	Boytsov el al (1992)
0.165	0.01	
0.140	0.01	Brodskaya et al. (1977)
0.220	0.051	Braun et al. (1968)
0.144	0.02	Qaim et al. (1971)
0.200	0.01	Rau et al. (1968)
0.134	0.005	Steinnes (1970)

There was realized a new measurement of ^{90}Zr(n,2n) cross section. In this experiment yttrium was used as flux monitor. The evaluation aimed to minimize all possible discrepant effects. Reaction rates were derived from nearly the same efficiency peaks - for 909 keV peak (^{89}Zr) (1.435E-3) and 898 keV peak (1.423E-3). Due to homogenization – flux in Y is the same as in Zr – no flux recalculations. Spectral shifts are very low (0.988 in Y, 0.999 in Zr) (if used). The new result is in good agreement with the previous one, the average value is about by 4% lower than the previous value.

	Value	Unc.
Reaction rate ratio	0.6224	1.8%
Spectral shift correction	1.011	1.0%
89Y(n,2n) monitor	0.1699	3.0%
90Zr(n,2n)	0.1069	3.6%
Kostal et al 2017	0.1071	4.5%
Mannhart et al 2008	0.1027	2.7%

III. Gilles Noguere, CEA/DEN Cadarache

Gilles Noguere, Pascal Archier, David Bernard, Pierre Leconte, Cyrille De Saint Jean

Integral Data Assimilation methods for using integral data in the evaluation procedure were developed since the early years of the evaluation works. Such approaches are useful for identifying inconsistent nuclear data stored in the "general purpose libraries". However, incorporating integral trends for improving evaluated nuclear data files may change a "general purpose library" in an "application library" that restricts its use and validity to specific nuclear applications. At the CEA of Cadarache, we are trying to apply an Integral Data Assimilation strategy in the frame of the covariance database COMAC that clearly defines how far we can go with the use of integral parameters in the evaluation process so that the evaluated library is still a "general purpose library".

Origins of the Integral Data Assimilation procedure at CEA of Cadarche

One of the first results obtained from the assimilation of a given set of integral data was reported in 1968 by Barre, L'Heriteau and Ribon [bar68]. The method, namely BARRAKA, successfully provides trends on the capture-to-fission ratio of ^{239}Pu and clearly indicates major problems in the existing ^{239}Pu evaluated nuclear data (fast energy range).

Later, in the 90s, the adjusted nuclear data library ERALIB-1 were produced with a Bayesian least-squares method to fulfil Fast Reactors requirements [for96]. However, a deep inspection of the multi-group cross sections of ^{23}Na contains in ERALIB-1 reveals that the method fails to decouple neutron cross section effects [arc12]. Fig. 1 shows that the ^{23}Na(n,n') resulting from the adjustment of integral data (≡ JEFF-3.1.1) is two times smaller than all the evaluations. By using a set of integral data measured in the fast mock-up facility MASURCA of CEA Cadarache, we were able to nearly reproduce the "mistakes" found in the ERALIB-1 library. Fig. 2 shows that the underestimation of the inelastic scattering cross sections mainly comes from a lack of constraints on the total cross section. In other words, even if the cross correlations between partial cross sections, emerging from the nuclear models used in the evaluation procedure, are correctly calculated, they are not sufficient to prevent possible "compensations" between elastic and inelastic scattering cross sections.

Thanks to the valuable lessons from our past mistakes, we are trying to apply an Integral Data Assimilation strategy in the frame of the covariance data base COMAC that aims to draw a clear separation between "general purpose libraries" and "applications libraries".

Integral Data Assimilation strategy in the framework of COMAC

The COMAC library is developed at the CEA of Cadarche. It contains evaluated nuclear data files and associated covariances. Different file formats are available, such as ENDF-6 and COVFIL formats. Covariance matrices are also stored in specific multi-group structures using formatting rules similar to those used in the ERALIB-1 library.

We are trying to structure the COMAC library [arc14] in two parts. As shown in Fig. 3, the first part is labelled COMAC(mic) and it contains evaluated nuclear data with covariances compatible with the "general purpose library" rules. The second part is called COMAC(mac) and it also contains evaluated nuclear data and covariances but associated to a given "applications library". It is not always easy to apply this strategy and to respect such an ideal separation between « general purpose library » and « application library ». The fuzzy limit between them is determined by the "clean" integral data introduced during the evaluation procedure for improving at least the central values, and sometime the uncertainties. A strict definition of a "clean" integral experiment does not exist. Usually, integral experiments can be viewed as "clean" if they are sensitive to a given nuclear data for a given isotope. The selection of the integral data is routinely made by using sensitivity studies.

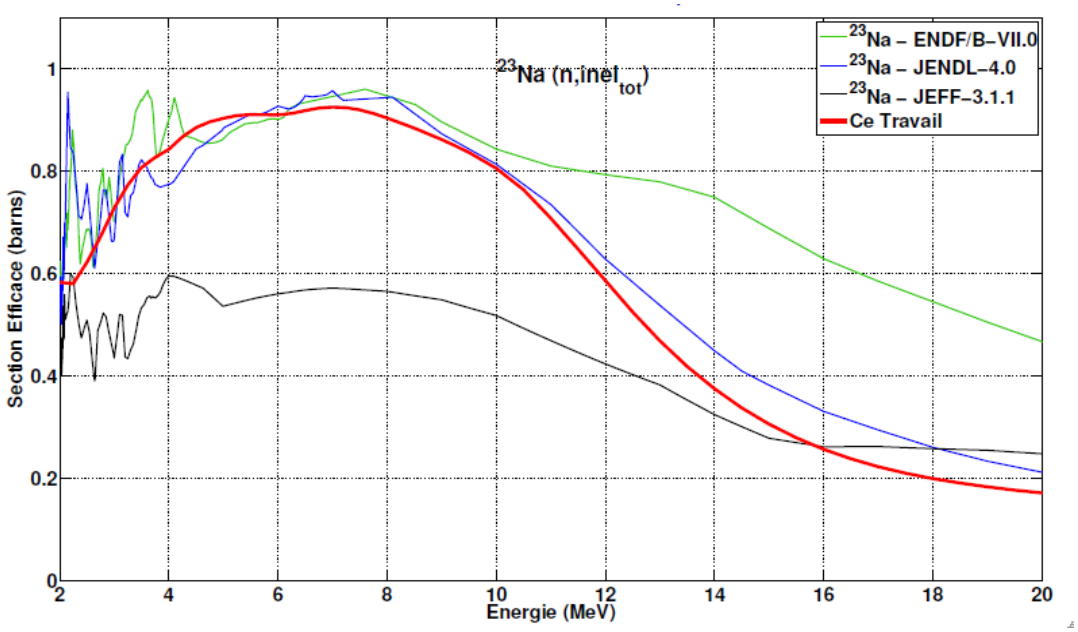


Fig. 1. ^{23}Na(n,n') cross sections available in different library. The cross section in JEFF-3.1.1 comes from integral data adjustment performed in the frame of the ERALIB libraries. The red curve is equivalent to JEFF-3.2.

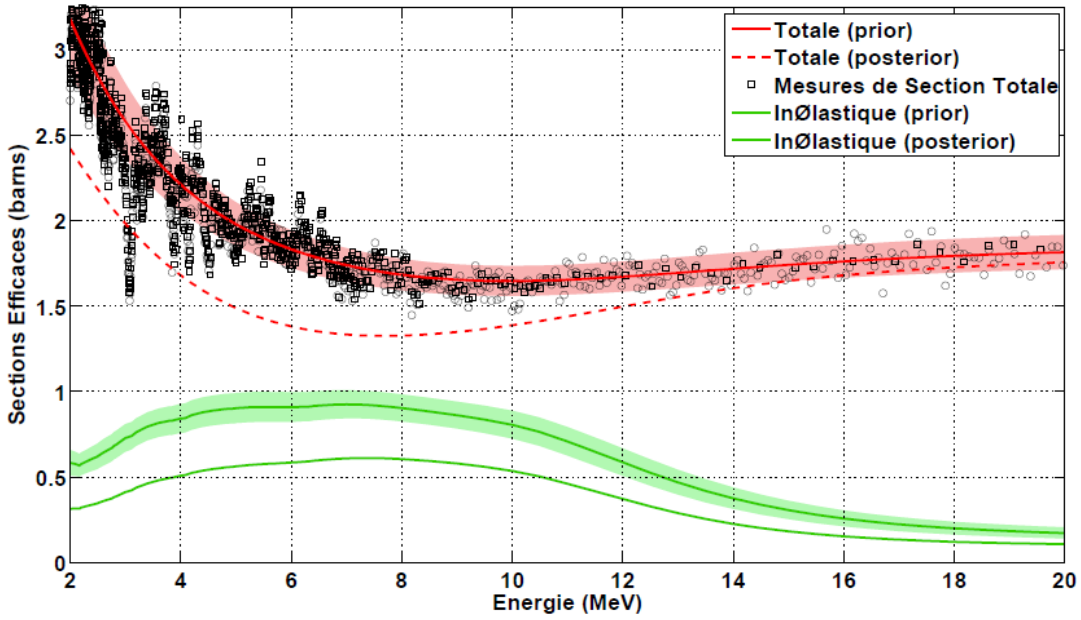


Fig. 2. Adjustment of the ^{23}Na cross sections with integral experiments performed in the fast reactor MASURCA of CEA Cadarache.

A large variety of integral benchmarks exists. The ICSBEP data base is widely used in nuclear data evaluation. Only few ICSBEP benchmarks (such as the famous GODIVA, JEZEBEL, BIGTEN, FLATTOP…) can be used with care as a "decision-making support tool". Indeed, ICSBEP are sensitive to various nuclear data (neutron multiplicities, partial cross sections, fission spectra, thermal scattering laws …). Complementary microscopic and integral trends are needed to avoid "compensation" effects between nuclear data of different isotopes; otherwise evaluated files only obtained from ICSBEP benchmarks are no longer compatible with the "general purpose library" rules.

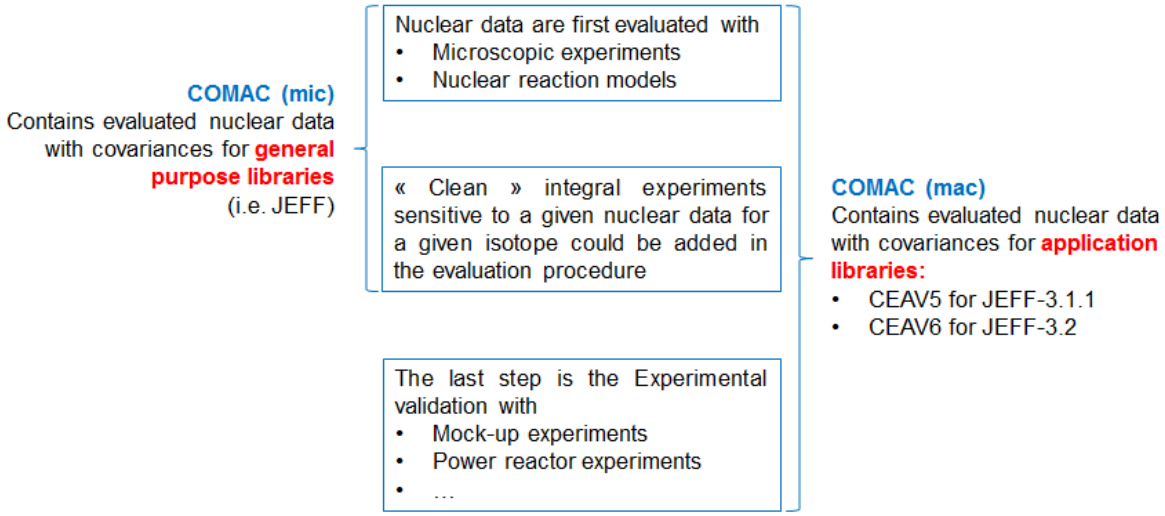


Fig. 3. Principle of the two-stage COMAC structure

Several experimental programs were performed in the CEA and European facilities (MINERVE, EOLE, MELUSINE, RAPSODIE, MASURCA, CALIBAN, GELINA) and French Power Reactors (PHENIX, PWR) for improving reactor parameter calculations and nuclear data. Among them, "clean" integral trends could be provided by oscillation measurements performed in the MINERVE facility (CEA Cadarache) and Post-Irradiated Experiments of separate isotopes performed in thermal and fast systems.

For using integral data in the evaluation procedure, an improved mathematical framework was elaborated and implemented in the nuclear data tool CONRAD [arc13]. It relies on the "variance penalty" [mui11] and Marginalization [dsj09] procedures. They provide an original way to account uncorrelated and correlated sources of uncertainties in the evaluation procedure.

Application to MOX fuel configurations

The strategy shortly described above was applied on MOX fuel calculations. The aim was to explain the increasing difference with the Pu aging observed on EOLE benchmarks between the Calculated (C) and Experimental (E) values. Three new evaluations were produced: ^{241}Am, ^{239}Pu and ^{240}Pu.

About ^{239}Pu, the resonance parameters and the corresponding covariances were re-evaluated by using microscopic data available in EXFOR. Results were included in the latest "general purpose library" JEFF library (JEFF-3.2). However, the propagation of the obtained resonance parameter uncertainties on EOLE benchmarks lead to large uncertainties on keff values, reaching ±1000pcm (top plots of Fig. 4). This large uncertainty is not satisfactory for MOX fuel applications in thermal systems, given that the prediction of the keff with the JEFF library lies below 600 pcm.

In practice, it is not possible to reduce such large uncertainties by only using microscopic data. For reducing the obtained uncertainty, we have used oscillation measurements performed in the DIMPLE and MINERVE reactors. Sensitivity analysis have shown that experimental results are sensitive to the product $\nu\Sigma f$ or to the equivalent $K1=\nu\Sigma f-\Sigma a$. As a result, the Integral Data Assimilation of many MOX configurations has suggested a decrease of the uncertainty of the ^{239}Pu(n,γ) reaction in the low energy range down to ±2%. The propagation of this lower uncertainty on EOLE benchmarks reduces the keff uncertainty to ±400 pcm (bottom plots of Fig. 4).

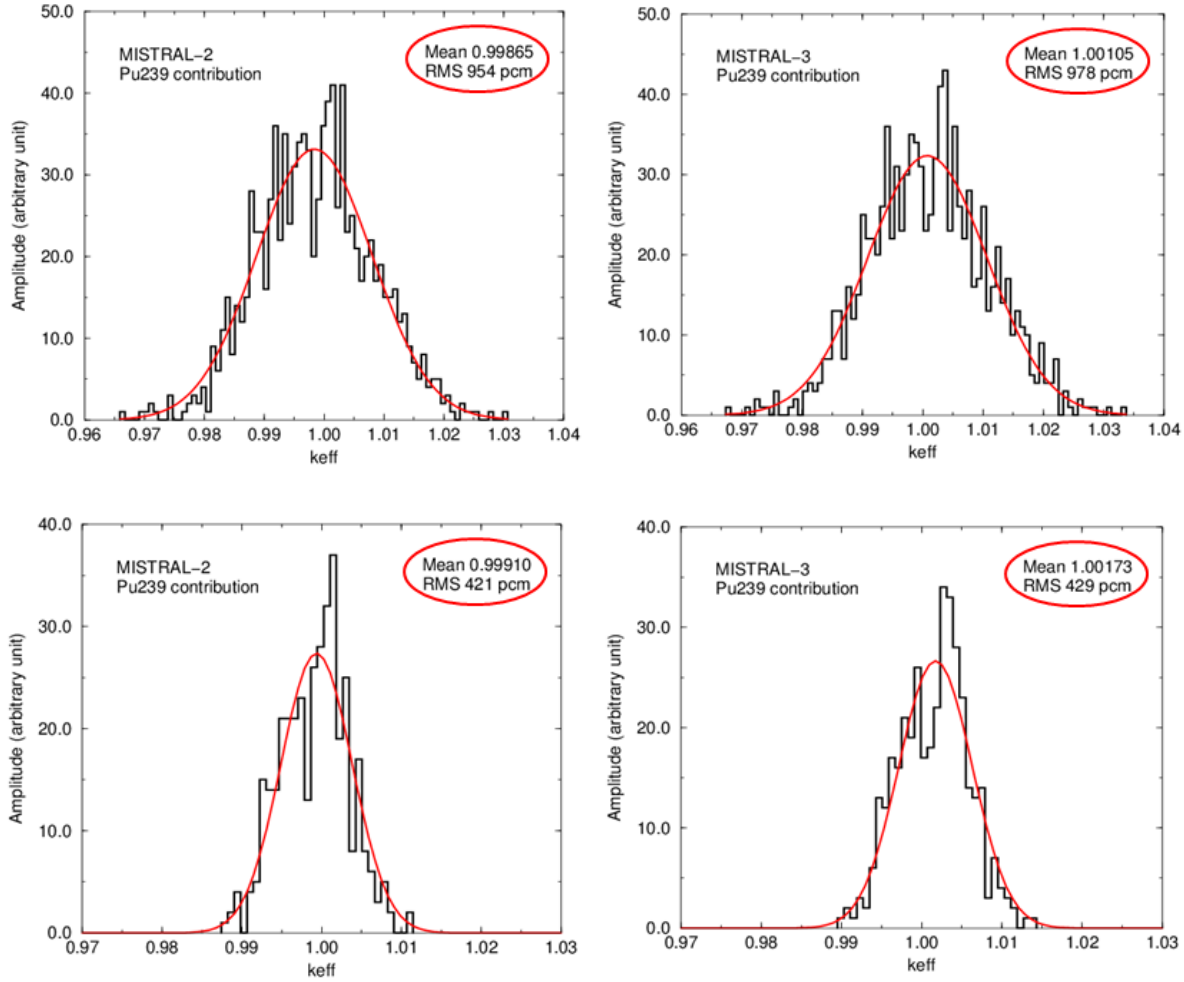


Fig. 4. Monte-Carlo propagation of the Resonance Parameter Covariance Matrix (RPCM) of ^{239}Pu on calculated keff for two MOX configurations carried out in the EOLE facility (CEA Cadarache). The top plots were obtained with RPCM coming from microscopic data only. The bottom plots are obtained after assimilation of MINERVE experiments.

Conclusions

The Integral Data Assimilation strategy developed in the frame of the COMAC library shows that large uncertainty on neutronic parameters obtained from "general purpose libraries" should not disturbed the users as long as a good agreement is obtained between the calculated (C) and experimental (E) values. Sizeable reduction of the uncertainties can be reached by using "application libraries", adequately calibrated for given nuclear applications.

The main difficulty in the strategy applied to develop the COMAC library is link to the definition and the use of "clean" integral experiments in the evaluation procedure. "Clean" integral experiments, which are sensitive to a single isotope and reaction, are not always available. Therefore, a clear separation between COMAC(mic) and COMAC(mac) is rather difficult to define.

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IV. Vladimir Radulovic, Jožef Stefan Institute

Neutron spectrum adjustment and cross-section validation activities at the Jožef Stefan Institute

Vladimir Radulović, Andrej Trkov, Luka Snoj

1. Introduction

Accurate knowledge on the neutron spectrum inside irradiation channels in nuclear reactors and irradiation facilities based on neutron sources is necessary for integral nuclear cross-section measurements and validation, support of experimental campaigns (primarily in research reactors and neutron sources) and neutron fluence determination (primarily in nuclear power plants). Moreover, it allows for the verification and validation of computational methods, in particular Monte Carlo particle transport codes (e.g. MCNP [1], TRIPOLI [2], etc.), which are extensively used for the determination of the experimental conditions in irradiation facilities. Therefore, considerable effort has been dedicated to the development of codes which adjust neutron spectra based on *a priori* information, to sets of measurements - reaction rates or Bonner sphere signals. There are numerous adjustment (unfolding) codes in existence, mostly based on Least Squares algorithms [3-5], in the last decade adjustment codes based on neural networks have gained considerable popularity [6-9]. To our knowledge there are only two unfolding codes based on the parametrization of the neutron spectrum with an analytical function. FRUIT [10] is a code designed to unfold the neutron spectrum from measurements with Bonner spheres, GRUPINT from classical dosimetry measurements.

An overview of the GRUPINT neutron spectrum adjustment code, developed at the Jožef Stefan Institute (JSI) in Ljubljana, Slovenia is given. GRUPINT is a complex code package, which was primarily developed for the calculation of constants relevant to Neutron Activation Analysis (NAA) from neutron spectra and cross sections in standard SAND-II 640-energy group structure. Over time the original code has been extensively upgraded and numerous features have been added. The neutron spectrum in GRUPINT is parametrized by an analytical function based on physical models, described by a maximum of 19 parameters. The parameters of the analytic function can be fitted by GRUPINT, firstly to reproduce input spectra from Monte Carlo calculations and secondly, to adjust the neutron spectra, on the basis of sets of measured reaction rate ratios or ratios of the same reaction rate, bare and under cover (e.g. Cd-ratios). Another important feature of the GRUPINT code is the possibility of generation of the neutron spectrum covariance matrix through a Monte Carlo algorithm, in which selected parameters of the analytic function are sampled uniformly and the covariances are computed by definition. The covariance matrix thus generated is one of the inputs for a final adjustment step using the ZOTT99 code [11], implemented into GRUPINT, which yields physical uncertainties and correlations in the neutron spectrum.

Section 2 presents the general features of the code, in particular the implemented function used to parametrize the neutron spectrum and the code fitting abilities. The process of fitting a typical input neutron spectrum is presented for the spectrum in the Central Channel (CC) of the JSI TRIGA reactor. Section 3 focuses on the characterization of the spectra in three irradiation channels of the JSI TRIGA reactor with different spectral characteristics, based on measured reaction rate ratios for nuclear reactions with well-known cross-sections. Subsequently the validation of the nuclear data for a selection of nuclear reactions is presented. Section 4 presents the possibility of measurements of capture reactions in the epithermal range using boron nitride and boron carbide neutron filters. A proposition is made in Section 5 on an activation data collection format, which enables future reevaluations of the measured activities, in case changes in the physical data (half-lives, gamma emission probabilities) are required.

2. The GRUPINT code

GRUPINT is a complex code package, its primary purpose is the calculation of constants relevant to Neutron Activation Analysis (NAA) from input neutron spectra and cross-section libraries in 640-energy group structure. The constants are as follows: σ_0 (cross section value at 0.0253 eV), I (resonance integral), F_{Cd} (cadmium transmission factor), g (generalized Westcott g-factor), σ_{th} (thermal spectrum averaged cross section) and σ_f (fission spectrum averaged cross section).

These capabilities of the GRUPINT code have been exploited in the past in the context of NAA [12] for the assessment of capture cross-sections from evaluated nuclear data files [13] and for the experimental determination of the Q_0 factor of the $^{27}\mathrm{Al}(n,\gamma)$ reaction [14], taking into account the fission spectrum contribution to the reaction rate.

The first version of the code dates to April 2000. Over time the code has been developed extensively and has become a versatile package which, in addition to its primary purpose, allows the user to parametrize the neutron spectrum with an analytic function, fit the analytic function parameters to general input neutron spectra (e.g. obtained by Monte Carlo calculations) by the Least-Squares method, adjust the neutron spectrum parameters in order to best reproduce a set of measured reaction rate ratios (or cadmium ratios), by the Least-Squares method and to generate neutron spectrum covariance matrices by the Monte Carlo method.

2.1. Neutron spectrum parametrization

The neutron spectrum is parametrized by an analytic function, defined by a 19 possible parameters. It consists of three terms: the thermal (Ψ_t), epithermal (Ψ_e) and fast term (Ψ_f). The thermal term Ψ_t is defined as:

$$\Psi_t = C_t E^l \left[e^{-\frac{E}{kT}} + C_{t1} e^{-\frac{E}{kT_1}} + C_{t2} e^{-\frac{E}{kT_2}} \right], \tag{1}$$

where C_t is a normalization constant, which ensures continuity and k is the Boltzmann constant. The term is a superposition of three Maxwellian distributions, the main Maxwellian around temperature T and two distributions around temperatures T_1 and T_2, usually of far lesser magnitude (controlled by the constants C_{t1} and C_{t1}) which allow for an adequate representation of possible distortions in the upper thermal region. The superposition is multiplied by an E^l term, where l is the thermal slowing-down parameter.

The epithermal term Ψ_e is defined by three slope parameters, as:

$$\Psi_e = E^{-[1+\alpha_0+\alpha_1 \log(E)+\alpha_2(\log(E))^2]}, \tag{2}$$

where α_0 gives the general deviation of the spectrum from pure $1/E$ behaviour, the higher order terms α_1 and α_2, multiplied by $\log(E)$ and $(\log(E))^2$, account for distortions in the epithermal part of the spectrum.

The fast part can be modelled either by a Watt distribution (with parameters W_a and W_b), multiplied by a slowing-down term or a Maxwellian distribution around energy E_f, again multiplied by a slowing-down term:

$$\Psi_f = \begin{cases} C_f e^{-E/W_a} \sinh\left(\sqrt{E W_b}\right) \frac{1}{E^{m_0+m_1 E}} \\ C_f \sqrt{E} e^{-E/E_f} \frac{1}{E^{m_0+m_1 E}}, \end{cases} \tag{3}$$

where C_f is a normalization constant which ensures continuity. The complete spectrum is a weighted sum of the three terms:

$$\Phi = \mathrm{K}_t \Psi_t + K_e \Psi_e + K_f \Psi_f, \tag{4}$$

where the parameters K_t, K_e and K_e defined as follows:

$$K_e = \begin{cases} 1 & \text{for } E_t < \mathrm{E} < \mathrm{E}_f \\ 0 & \text{otherwise} \end{cases}$$
$$K_t = 1 + O_t - K_e$$
$$K_f = 1 + O_f - K_e \tag{5}$$

The parameters E_t and E_f are the thermal and fast region energy breakpoints, O_t and O_f are the thermal and the fast overlap parameters, which determine the fractions of the thermal and fast contributions above E_t and below E_f, respectively.

The fitting algorithm in the GRUPINT code is based on a direct search for a minimum of a functional by a systematic variation of parameters, one at a time, one after another. The parameters which can be fitted in the GRUPINT code are: $E_t, E_f, \alpha_0, \alpha_1, \alpha_2, O_t,\ O_f, W_a, W_b, l, m_0, m_1, T, C_{t1}, T_1, C_{t2}, T_2$. The normalization constants C_t and C_f, which ensure continuity between the different energy regions of the spectrum are computed automatically.

2.2. Fitting of the spectrum parameters – input spectrum

This section serves as an illustration of the meaning of the parameters of the analytical function used to parametrize the neutron spectrum and to demonstrate the fitting capabilities of GRUPINT. The starting point is an input neutron spectrum, typically obtained by Monte Carlo calculations (e.g. with the MCNP code). In the present case, the neutron spectrum in the Central irradiation channel (CC) of the JSI TRIGA reactor is considered. Fig. 1 displays the input neutron spectrum and four analytically defined neutron spectra. The spectra in Fig. 1 and all the following figures are displayed in lethargy representation. The spectra in Fig. 1 labelled "User defined" consist of a thermal Maxwellian at temperature T = 352 K, a pure $1/E$ epithermal component and a fast Maxwellian at mean energy W_a = 2.2 MeV, the thermal and fast energy breakpoints being E_t = 0.05 eV and E_f = 2 MeV. The spectra are defined with different values of the thermal and fast overlap parameters O_t and O_f; all other parameter values are default. The O_t and O_f parameters determine the relative magnitudes of the thermal and fast component.

Typically the fitting procedure is started with the thermal component parameters E_t, O_t, T and l. The spectrum in Fig. 1 labelled "Fit-1" was obtained by fitting these three parameters simultaneously, while leaving all others default. The fitted spectrum describes very well only the thermal part.

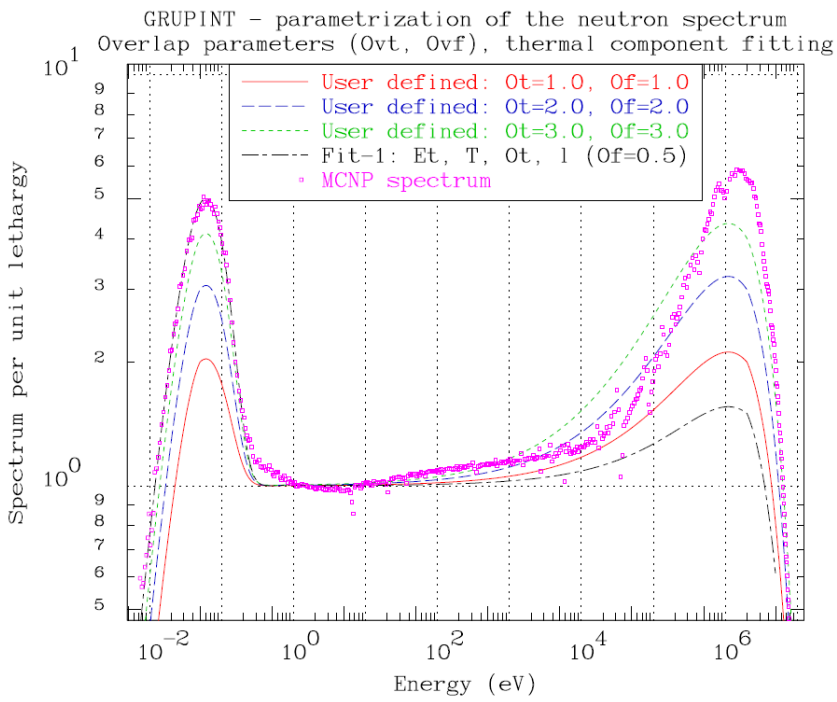

Fig. 1. Fitting the parameters of the thermal part to an input spectrum.

Fig. 2 displays the fitting of the epithermal slope parameters. The two spectra labelled "User defined" have α parameter values of -0.03 and 0.03 respectively, the remaining parameters are the same as in the spectrum labelled "Fit-1", also shown in Fig. 2.

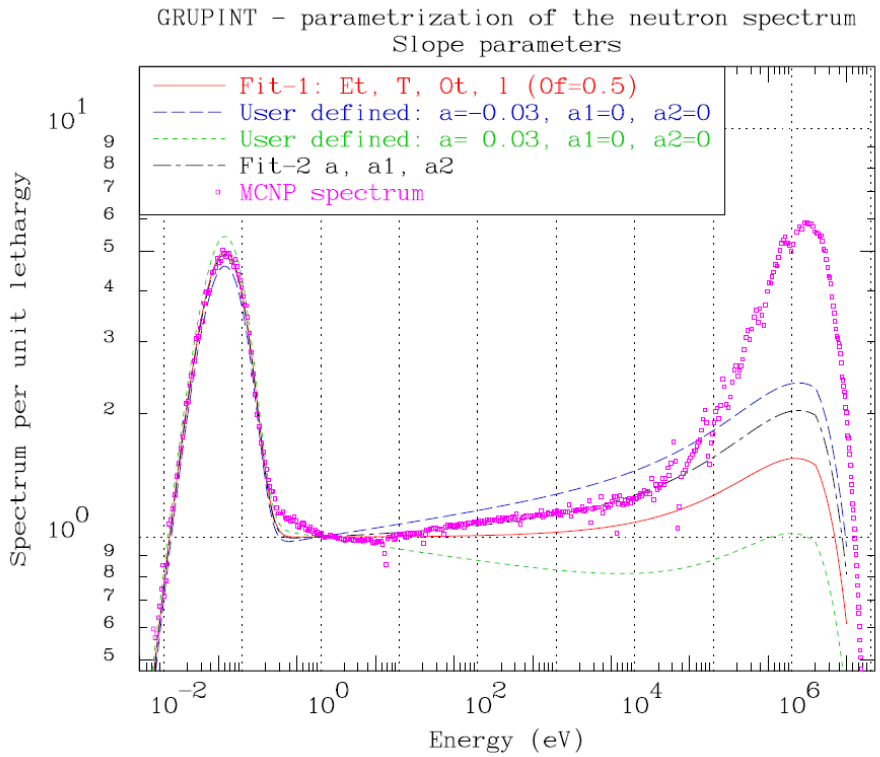

Fig. 2. Fitting the epithermal slope parameters to an input spectrum.

The spectrum in Fig. 2 labelled "Fit-2" was obtained by fitting the α and α_1 parameters simultaneously. Overall this spectrum describes well the thermal part and the epithermal slope. The α_1 and α_2 parameters are meant for fine-tuning the slope in the epithermal region and in most cases are not required (i.e. they are left default).

Fig. 3 displays the final steps in the GRUPINT fitting sequence. As seen previously in Figures 1 and 2 and indicated in Fig. 3, there is a distortion in the spectrum between the thermal and epithermal regions (from around 0.1 eV to around 1 eV), which is common. The spectrum labelled "Fit-3" was obtained by fitting the parameters O_t, C_{t1} and C_{t2}; the latter two govern the strengths of two additional Maxwellian distributions in the spectrum, at pre-set temperatures of 700 K and 1000 K. These temperatures can be fitted automatically by GRUPINT, however as a general rule, if too many parameters (> 3-4) are allowed to vary simultaneously, the fitting algorithm may fail.

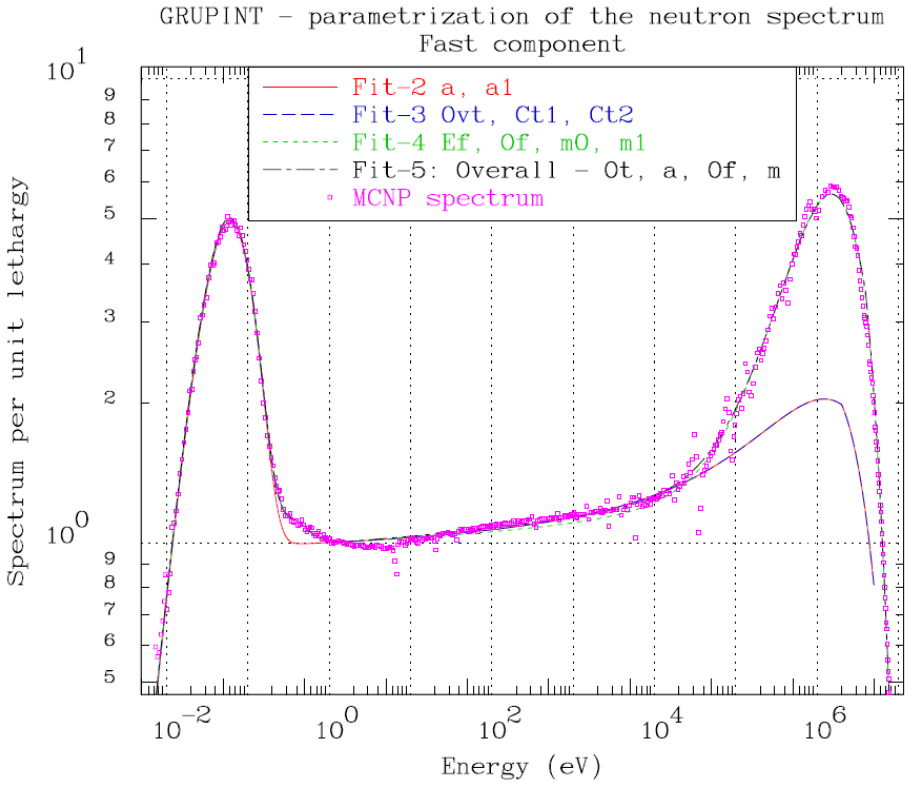

Fig. 3. Fitting the parameters of the fast part to an input spectrum, overall fit.

In the next step (spectrum labelled "Fit-4") the parameters of the fast spectrum component E_f, O_f, m_0 and m_1 were fitted. The spectrum thus obtained describes the input spectrum from the Monte Carlo calculation well, however a small deviation in the epithermal region is introduced. To refine the fit, another step is made in which the main spectrum parameters O_t, α and O_f and additionally the fast slowing-down parameter m is fitted. The final result of the analytic function fitting labelled "Fit-5".

2.3. Fitting of the spectrum parameters - measurements

After the input spectrum has been sufficiently well reproduced, a similar fitting sequence is performed, where the parameters of the neutron spectrum are fitted to measured reaction rate ratios, either ratios of one nuclear reaction to another or the same nuclear reaction, measured with and without cover – e.g. Cd ratios. It is possible for the latter ratios to be determined with a lower uncertainty than the absolute reaction rate values.

2.4. Neutron spectrum covariance matrix generation

An important feature of GRUPINT is the ability to generate the covariance matrix of the reaction rate ratios, spectrum parameters and the neutron spectrum by a Monte Carlo algorithm. A user-defined subset of the analytic neutron spectrum parameters is sampled uniformly within ranges around the initial parameter values (obtained from the previous fitting procedures). The covariances are computed by definition:

$$cov(x_i, x_j) = \frac{1}{n}\sum_{l=1}^{n}(x_i^0 - x_i^l)(x_j^0 - x_j^l)$$

where x is a vector composed of the reaction rate ratios R, the 19 parameters of the neutron spectrum and the neutron spectrum in 640 energy group structure. The covariance matrix thus generated defines the correlations between the energy groups of the neutron spectrum. It is used in the final step, in which the neutron spectrum is adjusted using the ZOTT99 code, implemented into GRUPINT.

3. Characterization of the spectra in the JSI TRIGA reactor

Here we present the results of the characterization of the neutron spectra for three routinely used irradiation channels in the JSI TRIGA reactor, namely the Central Channel (CC), located in the centre of the reactor core, the Pneumatic Tube (PT), located in the outer ring of fuel element positions and the IC40 irradiation position, part of the carousel. For the characterization the following measured reaction rate ratios have been used: $^{197}\mathrm{Au}(\mathrm{n},\gamma)\ \mathrm{R_{Cd}}$, $^{238}\mathrm{U}(\mathrm{n},\gamma)\ \mathrm{R_{Cd}}$, $^{27}\mathrm{Al}(\mathrm{n},\mathrm{p})$ vs. $^{197}\mathrm{Au}(\mathrm{n},\gamma)$, $^{27}\mathrm{Al}(\mathrm{n},\alpha)$ vs. $^{197}\mathrm{Au}(\mathrm{n},\gamma)$. Nuclear data from the IRDFF-v1-02 library [15] was used.

Figures 4, 5 and 6 display the input neutron spectra obtained from Monte Carlo calculations, the fitted analytic functions, and the final spectra obtained by fitting the spectrum parameters to the measured reaction rate ratios and Cd-ratios, and additionally, the Cd-filtered spectra. In order to visualize the differences in the spectra (which are often quite small), in the bottom parts of the figures the ratios of the spectra vs. the initial fitted analytic functions are displayed.

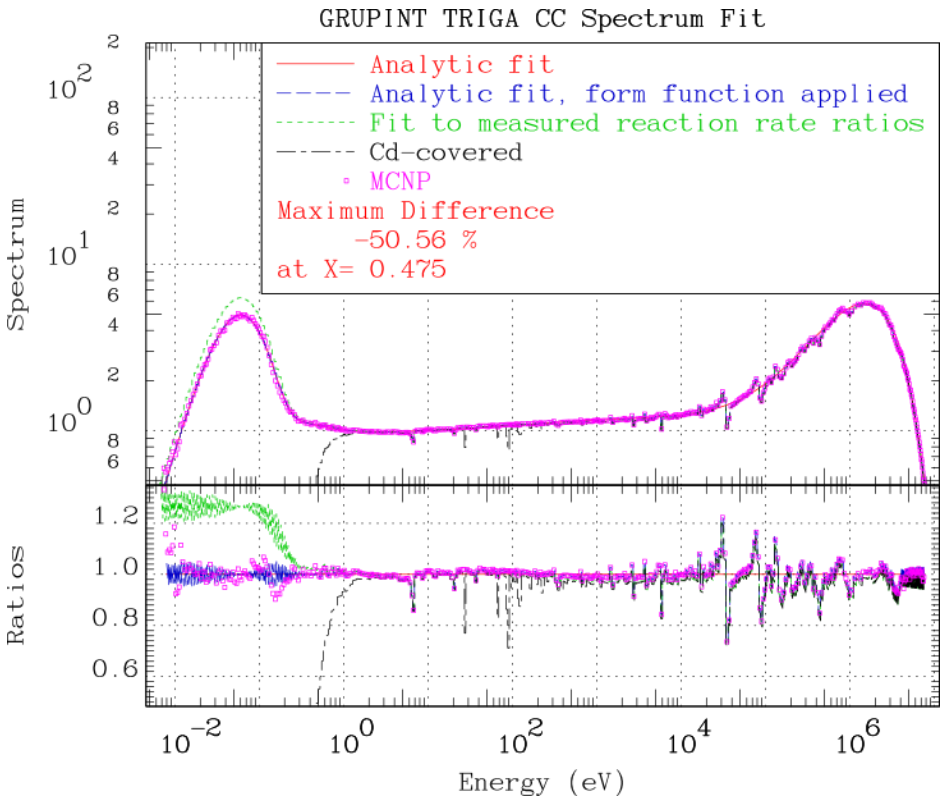

Fig. 4. JSI TRIGA Central Channel spectrum fitting.

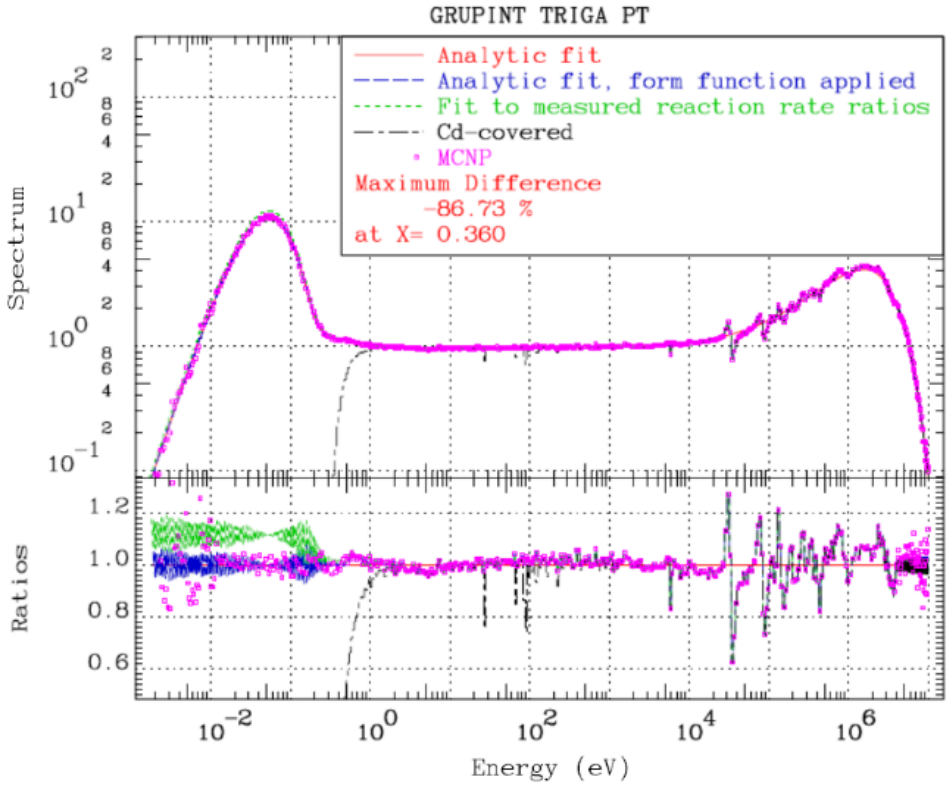

Fig. 5. JSI TRIGA Pneumatic Tube (PT) spectrum fitting.

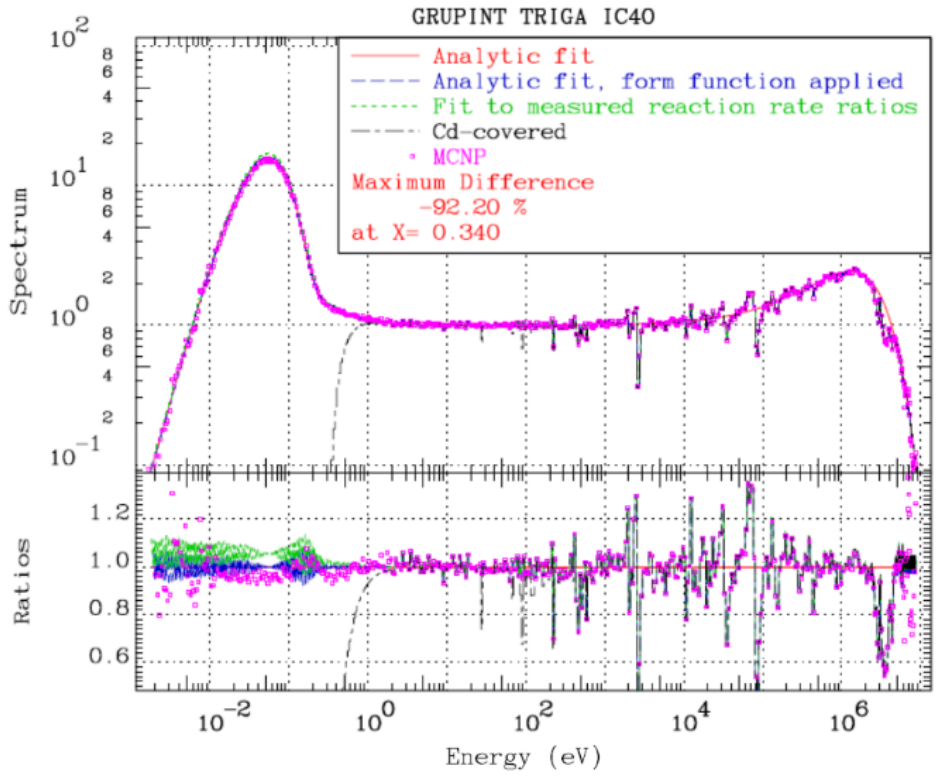

Fig. 6. JSI TRIGA IC40 channel spectrum fitting.

A positive correction in the thermal region is observed in all the fitted spectra. The magnitude of the thermal peak is increased by around 20 % in the CC, 10 % in the PT and 5 % in the IC40. The spectral shapes in the epithermal and fast energy regions remain practically unaltered. The goodness-of-fit can be judged on the basis of the relative differences between the measured and calculated reaction rate ratios. For the fitted spectra, the agreement is generally within the experimental uncertainties, i.e. within 5 % for the R_{Cd} values for the $^{197}Au(n,\gamma)$ and $^{238}U(n,\gamma)$ reactions and generally within 10 % for the reaction rate ratios $^{27}Al(n,p)$ vs. $^{197}Au(n,\gamma)$, $^{27}Al(n,\alpha)$ vs. $^{197}Au(n,\gamma)$. Figures 7, 8 and 9 display the relative differences between the measured and calculated R_{Cd} values for the $^{197}Au(n,\gamma)$ and $^{238}U(n,\gamma)$ reactions and the reaction rates ratios $^{27}Al(n,p)$ vs. $^{197}Au(n,\gamma)$, $^{27}Al(n,\alpha)$ vs. $^{197}Au(n,\gamma)$, with the final fitted spectra.

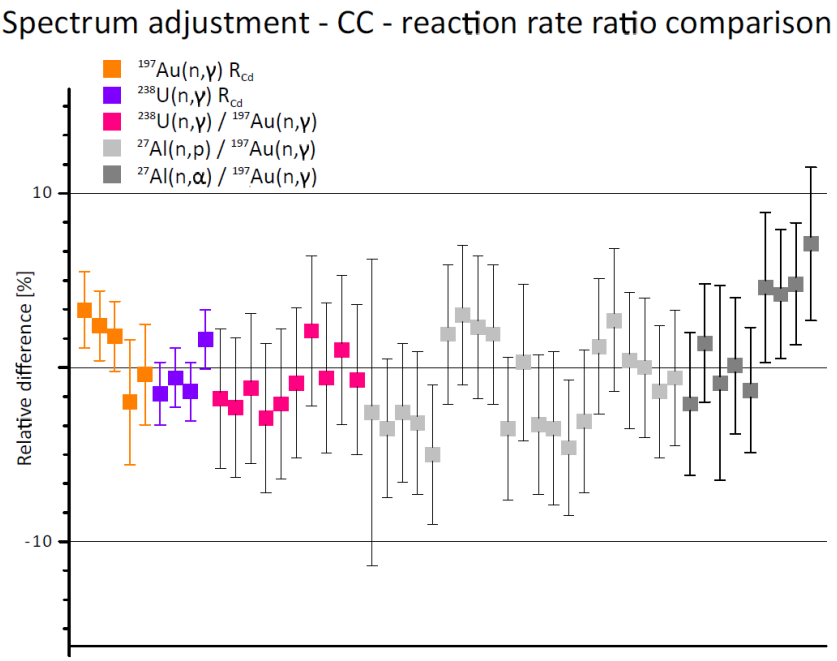

Fig. 7. JSI TRIGA Central Channel – relative differences between measured and calculated reaction rate ratios for nuclear reactions used to characterize the neutron spectrum.

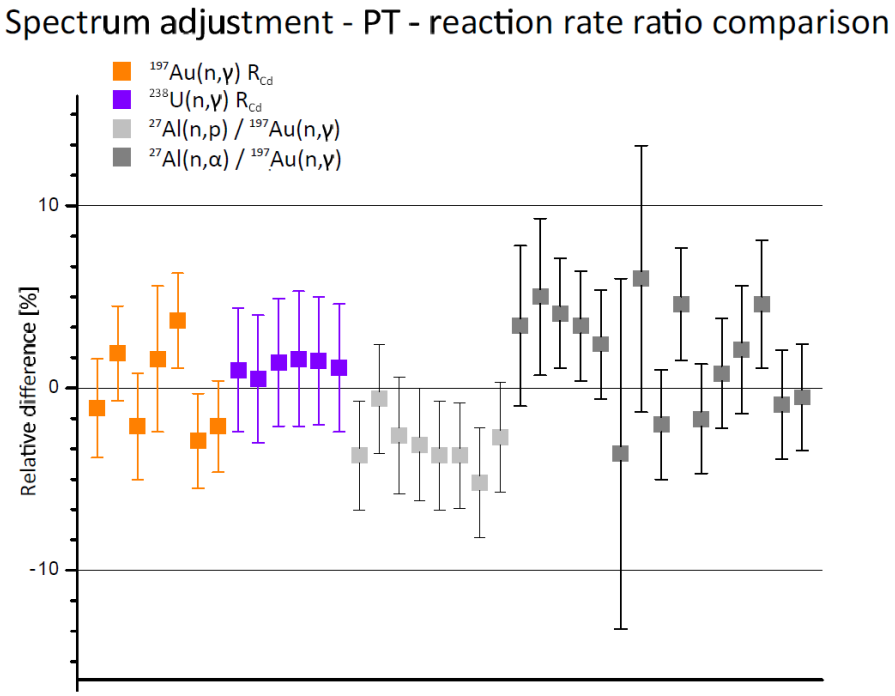

Fig. 8. JSI TRIGA Pneumatic Tube (PT) – relative differences between measured and calculated reaction rate ratios for nuclear reactions used to characterize the neutron spectrum.

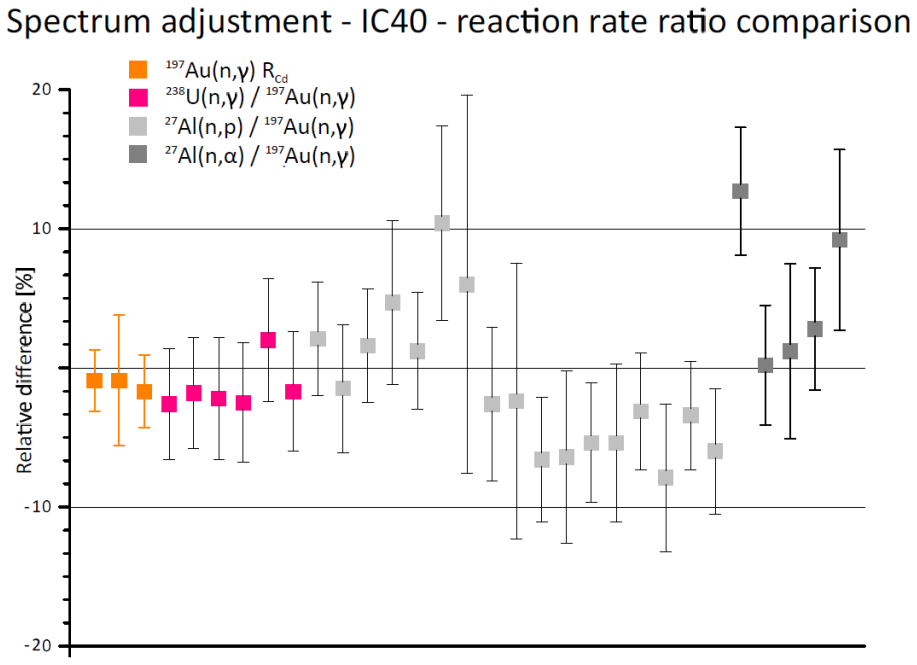

Fig. 9. JSI TRIGA IC40 channel – relative differences between measured and calculated reaction rate ratios for nuclear reactions used to characterize the neutron spectrum.

3.1. JSI TRIGA PT channel - Cross section validation

In the experimental campaign in the PT channel of the JSI TRIGA reactor measurements were performed for a selection of nuclear reactions in order to obtain experimental indications of the quality of the nuclear data. Table 1 lists the sample materials and the measured nuclear reactions. Measured R_{Cd} and reaction rate ratio values were compared to calculated values using the final fitted spectrum and the IRDFF-v1-02 cross section library, except for the $^{117}Sn(n,n')$ reaction, in which case data from the ENDF/B-VII.1 library was used.

Table 1: Sample materials and measured nuclear reactions

Sample material	**Nuclear reaction**
Al-1%Th	$^{232}Th(n,\gamma)$
Al-1%Mn	$^{55}Mn(n,\gamma)$
Al-0.1%Co	$^{59}Co(n,\gamma)$
Al-2%Sc	$^{45}Sc(n,\gamma)$
Fe	$^{58}Fe(n,\gamma)$
Sn enriched in Sn-117	$^{117}Sn(n,n')$

Fig. 10 displays the relative differences between the measured and calculated reaction rate ratios.

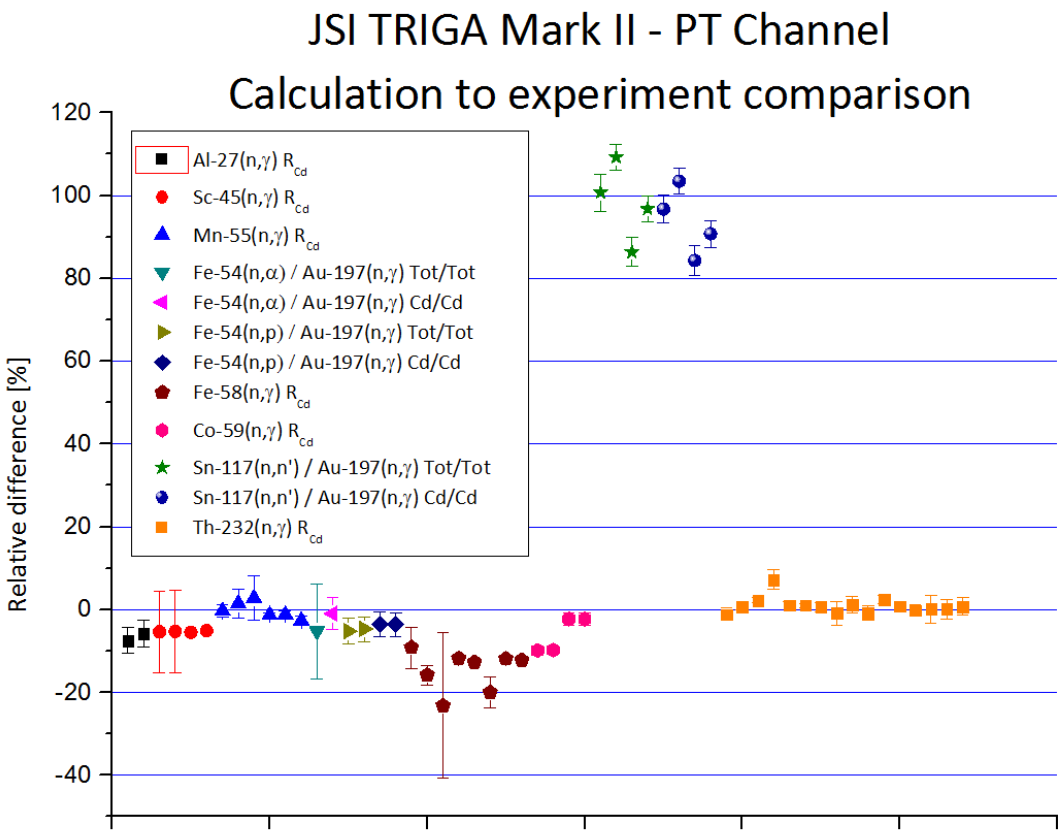

Fig. 10. Relative difference in the measured and calculated R_{Cd} values and reaction rate ratios

- The results of the measurement campaign in terms of the nuclear data quality can be summarized as follows:
- Good agreement was observed for the ^{232}Th(n,γ) and the ^{55}Mn(n,γ) reactions, which confirms the quality of the nuclear data and the usability of the reactions for neutron spectrum characterization.
- Disagreement was observed for the ^{58}Fe(n,γ) reaction, consistent with results from previous experimental campaigns, which indicates the need for improvements in the nuclear data.
- Strong consistent disagreement was observed for the ^{117}Sn(n,n') reaction, which is unfortunate, since this reaction is of particular interest for the characterization of the epithermal spectrum component, on account of its low threshold.
- The results for the ^{59}Co(n, γ) and ^{45}Sc(n, γ) reactions are inconclusive on account of the very low induced activities.

4. Spectrum characterization and cross-section validation in the epithermal range

Activation measurements have been performed in the experimental campaign in the PT channel of the JSI TRIGA reactor using boron nitride filters. The motivation behind the measurements was to shift the sensitivity of capture reaction measurements to the epithermal range, with the objectives of spectrum characterization and cross-section validation. Boron nitride filters with a wall thickness of 4 mm were used. The filter transmission functions were determined through Monte Carlo calculations. GRUPINT incorporates an exponential parametrization of the filter transmission function $t(E)$ given as:

$$t(E) = \exp\left(-nd_{eff}(\sigma_a(E) + \xi\sigma_s(E))\right), \quad (6)$$

where n is the atom density of the material, d_{eff} is an effective filter thickness, $\sigma_a(E)$ is the material absorption cross-section, ξ is a scattering fraction and $\sigma_s(E)$ is the material scattering cross-section. Material cross-sections for boron nitride were generated and the transmission function parameters d_{eff} and ξ were fitted, firstly to the Monte Carlo transmission function and subsequently to the measured ^{197}Au(n, γ) and ^{238}U(n, γ) boron nitride ratios. Fig. 11 displays a boron nitride filter used in the experimental campaign and the filter transmission function.

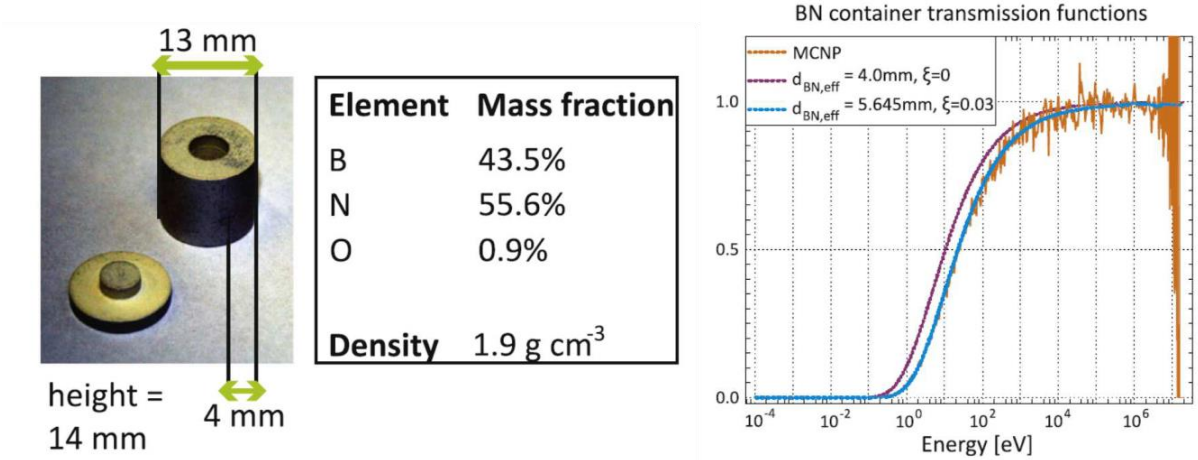

Fig. 11: Boron nitride filter used in the experiments and its transmission function.

Measured boron nitride ratios for other nuclear reactions were compared to calculated ones, using the characterized neutron spectrum and boron nitride transmission function. Fig. 12 displays the relative differences and uncertainties in the boron nitride ratios.

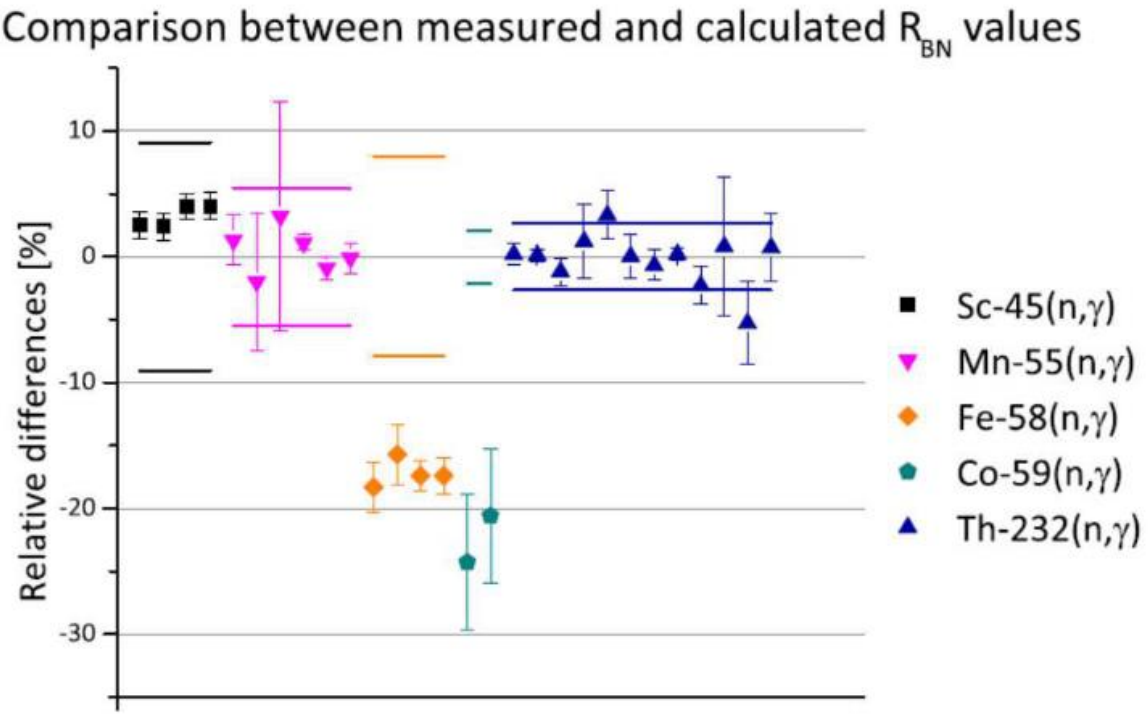

Fig. 12. comparison between the measured and calculated boron nitride ratios

Consistency was observed between the comparison for the measurements using boron nitride and cadmium filters.

A table of capture reactions from the ENDF/B-VII.1 library was made, sorted by the $E_{50\%}$ value (energy where the cumulative reaction rate reaches 50% of the total), in the JSI TRIGA PT spectrum, filtered by available boron nitride filters. The table includes comments and a final verdict on the suitability of the reactions for activation measurements [16]. As the available boron nitride filters have an effective cutoff energy at around 10-20 eV, the applicability of boron nitride, boron carbide and ^{10}B enriched boron carbide was studied with the objective to increase the effective cut-off energy and shift the sensitivity of capture reaction measurements to higher energies.

5. Data format

We hereby propose a format for the collection of activation measurement data. The aim is the collection of all the required experimental data for the computation of specific activities. The availability of complete data sets will enable future reevaluations of the activities, in case there are changes in the physical constants, e.g. the half-lives or the gamma emission probabilities.

The proposed format is based on the input format for the SPCACT code, written by Andrej Trkov. The code calculates the specific saturation activities for the measured nuclear reactions from the following data: the sample masses and mass fractions of the target isotopes, the irradiation, cooling and measurement times, the measured peak areas for specific gamma lines, the detection efficiencies at the specific gamma-ray energies, the coincidence correction fac10tors. The SPCACT code computes the uncertainties in the specific saturation activities from the uncertainties in the input data, by sequentially perturbing the values of the input data by their respective uncertainties and taking the square root of the sum of the squares (RSS) of the differences between the values computed with the perturbed and the unperturbed input data. The uncertainties in the calculated activities are combined from the uncertainties in the following input quantities: the peak areas, the irradiation, cooling and measurement times, the sample masses and the detection efficiency. The predominant source of uncertainty in the measurements is typically the uncertainty in the detection efficiency. The basic premise in the format is that any line in the data corresponds to one measurement of one reaction rate at one gamma-ray energy. The format instructions are given in the following list.

Columns 1-4, symbol “ID”: Measurement index (one line in the data corresponds to one particular gamma line in the measured gamma-ray spectra).

Columns 6-7, symbol “CV”: Identification of cover material, e.g. “Cd” for cadmium or “BN” for boron nitride.

Columns 9-11, symbol “IZ”: Target isotope atomic number.

Columns 13-14, symbol “CH”: Target isotope chemical symbol (left-justified).

Columns 16-18, symbol “IA”: Target isotope mass number.

Column 19, symbol “MM”: Target isotope state designator: “g” for ground state, “m” for first metastable state and “n” for second metastable state.

Columns 21-23, symbol “IZ”: Product isotope atomic number.

Columns 25-26, symbol “CH”: Reaction product isotope chemical symbol (left-justified).

Columns 28-30, symbol “IA”: Reaction product isotope mass number.

Column 31, symbol “MM”: Reaction product isotope state designator: blank for excited state, “m“ for first metastable state, “n” for second metastable state.

Columns 33-35, symbol “IZ”: Decaying isotope atomic number.

Columns 37-38, symbol “CH”: Decaying isotope chemical symbol (left-justified).

Columns 40-42, symbol “IA”: Decaying isotope mass number.

Columns 43-43, symbol “MM”: Decaying isotope state designator: blank for excited state, “m” for first metastable state, “n” for second metastable state.

Columns 45-52, symbol “WGT”: Total sample mass [mg].

Columns 53-56, symbol “DWG”: Uncertainty in the mass (or density) [%].

Columns 57-64, symbol “WPC”: Mass fraction of the target isotope in the sample.

Columns 65-72, symbol “Gth”: Thermal flux depression (self-shielding) factor.

Columns 73-80, symbol “SSF”: Epithermal (resonance) self-shielding factor.

Columns 81-88, symbol “TIR”: Irradiation time [s].

Columns 89-92, symbol “DTI”: Uncertainty in irradiation time [s].

Columns 93-100, symbol “TCO”: Cooling time [s].

Columns 101-104, symbol “DTC”: Uncertainty in cooling time [s].

Columns 105-112, symbol “TME”: Measurement time [s].

Columns 113-116, symbol “DTE”: Uncertainty in measurement time [s].

Columns 117-124, symbol “EGM”: Gamma-ray energy [keV].

Columns 125-132, symbol “PKA”: Measured activity (peak area) [counts].

Columns 133-140, symbol “DPK”: Measured peak area uncertainty [counts].

Columns 141-150, symbol “EPS”: Detector efficiency at gamma ray energy [fraction].

Columns 151-154, symbol “DEP”: Uncertainty in detector efficiency [%].

Columns 155-162, symbol “COI”: Coincidence correction factor [fraction].

Columns 159 and beyond are used to identify the sample.

An example dataset is reported in Figure 1.

ID	CV	Target	Product	Decaying	WGT mg	WGT %	DWG %	WFC %	Gth -	SSF -	TIR s	DTI s	TCO s	DTC s	TME s	DTE s	EGM keV	PKA counts	DPK counts	EPS -	DEP %	COI -	SAMPLE NUMBER & DESCRIPTION
1		13-Al-027	11-Na-024	11-Na-024	8.06	0.2		99.8	0.9972	0.9886	300	1	434859	1	87100.0	1	1368.6	430	25	3.99-3	2	1	V023 Al-0.2%-U (bare)
2		13-Al-027	11-Na-024	11-Na-024	8.06	0.2		99.8	0.9972	0.9886	300	1	434859	1	87100.0	1	2754.0	227	17	2.32-3	2	1	V023 Al-0.2%-U (bare)
3		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	103.7	82279	310	1.72-2	2	1	V023 Al-0.2%-U (bare)
4		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	106.1	104683	334	1.76-2	2	1	V023 Al-0.2%-U (bare)
5		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	209.8	11223	120	1.61-2	2	1	V023 Al-0.2%-U (bare)
6		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	226.4	812	53	1.49-2	2	1	V023 Al-0.2%-U (bare)
7		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	228.2	34834	196	1.27-2	2	1	V023 Al-0.2%-U (bare)
8		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	277.6	38563	217	1.25-2	2	1	V023 Al-0.2%-U (bare)
9		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	285.8	2022	60	1.16-2	2	1	V023 Al-0.2%-U (bare)
10		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	315.9	3764	77	1.11-2	2	1	V023 Al-0.2%-U (bare)
11		92- U-238	92- U-239	93-Np-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	334.2	4880	79	1.11-2	2	1	V023 Al-0.2%-U (bare)
12	Cd	13-Al-027	11-Na-024	11-Na-024	8.67	0.2		99.8	0.9971	0.9879	600	1	186903	1	172800	1	1368.6	29976	178	3.99-3	2	1	V024 Al-0.2%-U (Cd)
13	Cd	13-Al-027	11-Na-024	11-Na-024	8.67	0.2		99.8	0.9971	0.9879	600	1	186903	1	172800	1	2754.0	16848	132	2.32-3	2	1	V024 Al-0.2%-U (Cd)
14	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	103.7	591304	884	1.72-2	2	1	V024 Al-0.2%-U (Cd)
15	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	106.1	755803	984	1.76-2	2	1	V024 Al-0.2%-U (Cd)
16	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	209.8	81621	369	1.61-2	2	1	V024 Al-0.2%-U (Cd)
17	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	226.4	5862	255	1.49-2	2	1	V024 Al-0.2%-U (Cd)
18	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	228.2	250249	596	1.27-2	2	1	V024 Al-0.2%-U (Cd)
19	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	277.6	279432	555	1.25-2	2	1	V024 Al-0.2%-U (Cd)
20	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	285.8	14749	139	1.16-2	2	1	V024 Al-0.2%-U (Cd)
21	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	315.9	28383	179	1.11-2	2	1	V024 Al-0.2%-U (Cd)
22	Cd	92- U-238	92- U-239	93-Np-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	334.2	35482	200	1.11-2	2	1	V024 Al-0.2%-U (Cd)
23	B	13-Al-027	11-Na-024	11-Na-024	7.96	0.3		99.8	0.9973	0.9887	600	1	532219	1	90000.0	1	1368.6	258	20	3.99-3	2	1	V025 Al-0.2%-U (B)
24	B	13-Al-027	11-Na-024	11-Na-024	7.96	0.3		99.8	0.9973	0.9887	600	1	532219	1	90000.0	1	2754.0	148	14	2.32-3	2	1	V025 Al-0.2%-U (B)
25	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	103.7	46341	269	1.72-2	2	1	V025 Al-0.2%-U (B)
26	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	106.1	59220	364	1.76-2	2	1	V025 Al-0.2%-U (B)
27	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	209.8	6313	97	1.61-2	2	1	V025 Al-0.2%-U (B)
28	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	226.4	602	49	1.49-2	2	1	V025 Al-0.2%-U (B)
29	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	228.2	19200	149	1.27-2	2	1	V025 Al-0.2%-U (B)
30	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	277.6	21643	157	1.25-2	2	1	V025 Al-0.2%-U (B)
31	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	285.8	1211	54	1.16-2	2	1	V025 Al-0.2%-U (B)
32	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	315.9	2141	60	1.11-2	2	1	V025 Al-0.2%-U (B)
33	B	92- U-238	92- U-239	93-Np-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	334.2	2582	65	1.11-2	2	1	V025 Al-0.2%-U (B)
34		13-Al-027	11-Na-024	11-Na-024	5.87	0.3		99.9	0.9986	0.9945	300	1	33252	1	36000.0	1	1368.6	29524	174	3.96-3	2	1	V029 Al-0.1%-Au (Mn bare)
35		13-Al-027	11-Na-024	11-Na-024	5.87	0.3		99.9	0.9986	0.9945	300	1	33252	1	36000.0	1	2754.0	16488	130	2.32-3	2	1	V029 Al-0.1%-Au (Mn bare)
36		79-Au-197	79-Au-198	79-Au-198	5.87	0.3		0.1	0.9986	0.9944	300	1	33252	1	36000.0	1	411.8	2109306	1536	9.48-3	2	1	V029 Al-0.1%-Au (Mn bare)
37		79-Au-197	79-Au-198	79-Au-198	5.87	0.3		0.1	0.9986	0.9944	300	1	33252	1	36000.0	1	675.9	12101	113	6.60-3	2	1	V029 Al-0.1%-Au (Mn bare)
38	Cd	13-Al-027	11-Na-024	11-Na-024	5.91	0.3		99.9	0.9986	0.9945	600	1	23626	1	6000.00	1	1368.6	13822	119	3.96-3	2	1	V030 Al-0.1%-Au (Mn Cd)
39	Cd	13-Al-027	11-Na-024	11-Na-024	5.91	0.3		99.9	0.9986	0.9945	600	1	23626	1	6000.00	1	2754.0	7891	90	2.32-3	2	1	V030 Al-0.1%-Au (Mn Cd)
40	Cd	79-Au-197	79-Au-198	79-Au-198	5.91	0.3		0.1	0.9986	0.9944	600	1	23626	1	6000.00	1	411.8	330892	578	9.48-3	2	1	V030 Al-0.1%-Au (Mn Cd)
41	Cd	79-Au-197	79-Au-198	79-Au-198	5.91	0.3		0.1	0.9986	0.9944	600	1	23626	1	6000.00	1	675.9	1827	45	6.60-3	2	1	V030 Al-0.1%-Au (Mn Cd)
42	B	13-Al-027	11-Na-024	11-Na-024	2.83	0.7		99.9	0.9986	0.9945	600	1	114955	1	43200.0	1	1368.6	11084	106	3.96-3	2	1	V035 Al-0.1%-Au (Mn B)
43	B	13-Al-027	11-Na-024	11-Na-024	2.83	0.7		99.9	0.9986	0.9945	600	1	114955	1	43200.0	1	2754.0	6224	80	2.32-3	2	1	V035 Al-0.1%-Au (Mn B)
44	B	79-Au-197	79-Au-198	79-Au-198	2.83	0.7		0.1	0.9986	0.9984	600	1	114955	1	43200.0	1	411.8	204327	458	9.48-3	2	1	V035 Al-0.1%-Au (Mn B)
45	B	79-Au-197	79-Au-198	79-Au-198	2.83	0.7		0.1	0.9986	0.9984	600	1	114955	1	43200.0	1	675.9	1157	40	6.60-3	2	1	V035 Al-0.1%-Au (Mn B)
46		92- U-238	92- U-239	92- U-239	8.06	0.2		0.2	0.9972	0.9980	300	1	434859	1	87100.0	1	74.7	4211	109	1.21-2	2	1	V023 Al-0.2%-U (bare)
47	Cd	92- U-238	92- U-239	92- U-239	8.67	0.2		0.2	0.9971	0.9978	600	1	186903	1	172800	1	74.7	30201	768	1.21-2	2	1	V024 Al-0.2%-U (Cd)
48	B	92- U-238	92- U-239	92- U-239	7.96	0.3		0.2	0.9973	0.9980	600	1	532219	1	90000.0	1	74.7	2604	129	1.21-2	2	1	V025 Al-0.2%-U (B)

Figure 1: example dataset in the prescribed format

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R&A: 727735
SAND2017-13663 O

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What is the Role of Integral Benchmark Data in Support of Nuclear Data

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Abstract. This report summarizes the discussion and contributions made by Sandia National Laboratories in support of the International Atomic Energy Agency (IAEA) Nuclear Data Section (NDS) Consultants' Meeting on Integral Data in Nuclear Data Evaluations. This work focused on the need for all nuclear data to have an associated uncertainty and on the importance of the consistency between the methodology used to derive the nuclear data and the expression of its uncertainty.

1 Introduction

This is the report from Sandia National Laboratories (SNL) on the view from the dosimetry and radiation damage communities on the proper use of integral data in nuclear data evaluations. It is a fundamental axiom of the dosimetry community that, for any item to be considered "information/data", that item needs to have an associated uncertainty statement. There is no information transmitted in the absence of an uncertainty statement. The determination of the uncertainty can have a subjective component, i.e. a Bayesian approach to a *prior*, but the uncertainty statement needs to be consistent with the method used to derive the information/data. This means that the development of the uncertainty needs to be an integral part of the nuclear data evaluation process.

The expression of the uncertainty for nuclear data that has an energy dependence, such as a differential reaction cross section, should always be in the form of an energy-dependent covariance matrix. The visualization of this energy-dependent uncertainty is best accomplished by presenting an energy-dependent standard deviation for the data along with a two-dimensional correlation matrix.

2 Historical Perspective from Dosimetry Community

While the baseline requirement for an uncertainty expression and the consistency of the data and the associated uncertainty applies to members of both the dosimetry and the radiation damage communities, the dosimetry community, because of their emphasis on the accuracy and precision of data, has historically taken a very aggressive stance on this issue [1,2].

In 1991 the Dosimetry Integral Test Working Group of the Japanese Nuclear Data Committee, in response to a continuing dosimetry user community stated need, compiled and released the first JENDL Dosimetry Library (JENDL/D-91) [3]. This library applied the IRDF-85 [4] covariance matrices to the existing JENDL-3 cross sections. Although this was called a "dosimetry library", this library was rejected for use by the general international dosimetry community because the covariance data bore no relationship to the selected cross sections. The nuclear data evaluators are generally given a significant latitude in the data evaluation process. It is part of their job to "evaluate" the available experimental data sets and they can define a set of criteria that they will use for accepting or rejecting various sets of measurements. Aided by calculations and physics principles, they make informed judgements about how to interpolate or extrapolate between available measurement data. The only general constraint applied to the nuclear data evaluator is that they have a responsibility to be consistent in their approach and to carefully document their rationale and the resulting recommended nuclear data. It was not felt to be acceptable for other parties to retroactively

assign uncertainties to the products resulting from the nuclear data evaluation. The data evaluators themselves have to endorse and embrace any associated covariance data that is to be assigned to their product. The "tacking on" of a set of even a "reasonable covariance data" to an existing data set was not seen as satisfying the needs of the dosimetry community. The Working Group later re-evaluated the dosimetry cross sections and associated covariances, resulting in the JENDL Dosimetry File 99 (JENDL/D-99) [5]. This library was accepted and widely used by the dosimetry community [6].

At the 2008 Cross Section Evaluation Working Group (CSEWG) supported Workshop on Neutron Cross Section Covariances held in Port Jefferson [1], a similar point was made in some of the presentations and documented in the papers published in Nuclear Data Sheets [2]. During this period, the nuclear data community was taking what they called "low fidelity" covariance data computed using nuclear models and retroactively attaching this covariance data into existing cross section evaluations. The motivation was good, to support customer needs for uncertainty estimates of the criticality of shipping containers used for spent nuclear fuel, but the implementation was fatally flawed in the eyes of the dosimetry community. This approach violated the tenet that the uncertainty estimate be consistent with the derivation of the underlying nuclear data. In general, the calculated standard deviations for the cross sections (derived from the square root of the diagonal of the covariance matrix) were not out of line with expectations, but there were some exceptions. An examination of some of the details of the calculated cross sections that had consistent covariance data, and were for cross sections of reaction channels used by the dosimetry community and where good experimental data existed, demonstrated that the calculated standard deviations, as reported at that time, could be several times smaller than those associated with an experimentally-driven nuclear data evaluation and that the cross sections derived through an experiment-based nuclear data process could have mean values that differed from those obtained by the baseline calculation by over 10 standard deviations. This clearly indicated that some unaccounted for "model defect" in the calculation was being encountered and the dosimetry community viewed the situation as unacceptable. ASTM standards, such as E1018 Standard Guide for Application of ASTM Evaluated Cross Section Data File that is used to support the interpretation of surveillance data in light water pressure vessels, were modified to explicitly require a consideration of the available experimental data in nuclear data used to support dosimetry applications and to explicitly require that the covariance data be related to the underlying cross section and not merely appended from a different evaluation. The discussion at the time also highlighted the need for calculated covariance estimates to go beyond just uncertainties derived through aparametric variation of the underlying nuclear model parameters and to consider the uncertainty in the underlying physics-based models, i.e. to take into account what has been called the "model defect".

Recent dialog has taken place in conjunction with the upcoming release of the ENDF/B-VIII cross sections where the statement has been made that "I am not in favor of generating adjusted cross section data – only adjusted covariances". This position can run counter to the requirement that the uncertainties reflect the methodology used to determine the mean value of the nuclear data. The general view from the dosimetry community is that, while integral data can be used in the nuclear data evaluation process, the mean value for the energy-dependent cross section and the associated covariance data must reflect the evaluation process. In general, when integral data is considered, the resulting standard deviations will be reduced but the mean values for the energy-dependent cross sections will <u>also</u> be changed. It is a general observation, but <u>not</u> a requirement, that the use of integral data will change the mean values. There are valid evaluation/adjustment methodologies where the inclusion of integral experimental data may not change the mean energy-dependent cross sections, nor even the associated energy-dependent standard deviations, from those associated with the "*prior*" evaluation process but, in these cases, the adjustment methodology typically introduces significant cross-reaction and cross-elemental/isotopic correlations that were not addressed in the development of the "*prior*" data. These adjustment methodologies involve the use of what

has been termed "application-specific hidden correlations" that are introduced by the inclusion of the integral experimental data. The dosimetry community cares about more than just the mean value and standard deviation that come out of an evaluation process, we care about the preservation of the completer covariance matrix associated with the evaluation. However, there is no intrinsic objection to the inclusion of integral data with these "*prior*" evaluations in such a manner that the single reaction channel mean value and associated reaction-specific covariance matrix is not changed, as long as it is noted that cross-reaction correlations will result and that these cross-correlations are characterized and reported as part of the nuclear data evaluation documentation process.

3 Terminology

Before a consideration is given to any of the requirements that should be associated with the inclusion of integral data in the evaluation process, it is important that some terminology be clarified – at least in so far as it is used in this document. The following sections address some terms that will be used in the subsequent discussion.

a) Validation

A validation is the assessment of the accuracy of a model by comparison with experimental data that is independent from that used to derive the model. A validation process must always report on the uncertainty of the experimental measurement and on the uncertainty in the model prediction. As stated in Reference [7], "Validation involves the identification and quantification of the error and uncertainty in the conceptual and computational models, quantification of the numerical error in the computation solution, estimation of the experimental uncertainty, and finally, comparison between the computational results and the experimental data." A validation does not address the inference of the model accuracy for cases different from the validation comparison, thus it is important that a range of validation cases be considered and that this range encompasses the complete phase space for the intended application.

Note that a validation requires a comparison to a physical measurement. Validation should not be confused with verification. Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and of the solution to the model. A model can be verified and may bear no resemblance to what may occur in a real-world simulation – even from the perspective of the intended uses of the model.

A good software quality engineering approach generally requires an application-specific Phenomenon Identification and Ranking (PIRT) process to identify and prioritize the relevant physics models, a verification process to ensure that the models are correctly implemented, and a validation process to ensure that the models fit the real world application [8].

b) Adjustment

An adjustment, as in the adjustment of a neutron spectrum, is a formal process of using *a priori* information along with a set of integral data/measurements and applying a mathematically well-defined optimization algorithm so as to derive *a posteriori* information that better fits the constraints provided by the integral measurements as determined by the optimization algorithm. The key elements here is that there is a *prior* and the application of a well-defined optimization metric. In most applications, there is the additional constraint that the adjustment process report on an uncertainty for the resulting *posterior* information. The uncertainty in the *posterior* should consider the uncertainty in the *prior* information and in the integral

measurements along with the degree to which the optimization process was capable of enabling the model/calculated result to match the measurement integral data.

An example of a typical adjustment process is the application of a least squares optimization. The least square optimization can be in a linear space or in a logarithmic space. The least squares can be used in a logarithmic space, e.g. the LSL-M2 least squares code used for neutron spectrum adjustment [9], in order to enforce a non-negativity constraint in a physical parameter. While the least squares approach represents the use of a deterministic algorithm, this is not required for an adjustment. A Monte Carlo-based adjustment, such as is provided through the use of genetic algorithms, can also be termed to be an adjustment – as long as the "fitness" metric is well-defined and there is a *prior* and an uncertainty that is sampled in defining the sample population [10].

Some key elements of an adjustment are that it needs to be performed with a methodology that is consistently implemented and that the posterior covariance must be consistent with the mathematics of the implementation of the adjustment process.

c) Statistical Bias

Statistical bias is defined as the systematic error that contributes to the difference between the mean of a large number of test results and an accepted reference value.

Bias in a result is typically treated as the complement to the precision in a measurement. The precision in a measurement is typically reported in terms of:

- Repeatability – which addresses variability between independent test results gathered from/within a single laboratory intra-laboratory testing)
- Reproducibility – which addresses variability among single test results gathered from different laboratories (interlaboratory testing)

A bias can only be determined when there exists an accepted reference value. High fidelity integral benchmark data, such as the ICSBEP criticality benchmarks [11], can often be used to establish this reference value and support the determination of a bias in a model – when used to make the same kind of determination as is represented by the reference data.

The statistical term "bias" as addressed above, is to be differentiated from the "subjective" usage of bias in common language to refer to a "prejudice in favour or against one thing, person, or group compared with another." Both forms of the term bias may play a role in nuclear data evaluation process. An evaluator may infer a "statistical bias" to data coming out of one specific laboratory in light of tends in reported data. An evaluator might also use a "subjective bias", e.g. when they decide which datasets to consider in an evaluation, in what criteria to use to reject discrepant data, or how to interpolate/extrapolate between available data.

d) Integral Benchmark Data

There are many libraries of documented integral benchmark data that can be used to support model validation of nuclear data. These libraries include:

- International Criticality Safety Benchmark Evaluation Project (ICSBEP), see URL: http://icsbep.inel.gov/
  International Handbook of Evaluated Criticality Safety Benchmark Experiments, Nuclear Energy Agency, NEA/NSC/DOC(95)03 (2011).

- Shielding Integral Benchmark Archives and Database (SINBAD), see URL: https://www.oecd-nea.org/science/wprs/shielding/
- Reactor Physics Benchmarks, see URL: https://www.oecd-nea.org/science/projects/benchmarks.html
- International Reactor Physics Experiment Evaluation (IRPhE) Project, see URL: https://www.oecd-nea.org/science/wprs/irphe/
- International Fuel Performance Experiments (IFPE) Database, see URL: https://www.oecd-nea.org/science/wprs/fuel/ifpelst.html
- A. Yamamoto, T. Ikehara, T. Ito, E. Saji, Benchmark Problem Suite for Reactor Physics Study of LWR Next Generation Fuels, Journal of Nuclear Science and technology, Vol 39(8), pp. 900-912, August 2002.
- ASTM E2006-2017, Standard Guide for Benchmark Testing of Light Water Reactor Calculations, Annual Book of ASTM Standards, 2017.

To be acceptable for most applications, the integral benchmark experiments need to be well document and provide uncertainties for both the experiment design/set-up and for the measurements. Benchmarks are often divided into categories, e.g. standard, reference, or controlled, based on the fidelity and reproducibility of the experiment [12,13].

4 Challenges in the Use of Adjusted Nuclear Data Evaluations

When integral benchmark data is used as part of an adjustment process, challenges can arise. These challenges give rise to requirements that need to be applied to the process if it is to be used as part of the nuclear data evaluation process. The following bullets capture some of the difficulties and the associated requirements that may need to be imposed on the process.

- It can be difficult to come up with the uncertainty (including correlations) for the *prior* information input to the adjustment process.
  This is an outstanding issue for the dosimetry and neutron spectrum characterization community and one that needs to be carefully considered by the wider nuclear data community. Some subjectivity, augmented by a parameterized fitting of physics constraints, has been used by the dosimetry community to address the covariance matrix for a calculated *prior* used in neutron spectrum adjustment [14, 15]. For nuclear data evaluations, code systems such as TALYS [16] enable the nuclear data evaluator to sample, statistically, the relevant nuclear data model parameters and, after deciding upon:
    a) the allowed parameter range for parameter variation;
    b) a consideration of correlations between the model parameter; and
    c) any intrinsic "model defect" in the underlying nuclear models,
  to establish a *prior* covariance matrix that can then be considered for inclusion with integral benchmark data in further refining the nuclear data evaluations.

- "Model defect" must be considered in determining the uncertainty in model-based calculated results.
  This point was touched upon in the previous bullet. Model defect can cause some of the sample-based approaches that vary underlying nuclear model parameters to predict too small of a standard deviation. The evaluator will need to consider other factors, such as the spread in experimental data or knowledge of the limitations in the physics models, to use their judgement in increasing the strictly model-based standard deviations.

- Cross-reaction, cross-isotope, and cross-element correlations may be introduced by the inclusion of integral benchmark data.
  By their nature, integral benchmarks involve consideration of experimental measurements that may be sensitive to a variety of parameters. This dependence will introduce cross correlations between the various nuclear data components. The cross-correlations can be between the nuclear data characterization for different isotopes, or even different elements. This cross-correlation must be clearly characterized in order to ensure that the users of the nuclear data, in their application, do not violate the underlying assumptions in the nuclear data evaluation. Examples of cases where the use of integral benchmarks in the evaluation process may affect the use include:
    - One example is that inclusion of integral benchmark data from a reactor criticality benchmark for a uranium solution reactor will probably introduce cross correlations between the nuclear data for ^{235}U and ^{16}O. This means that a user of these nuclear data evaluations (obtained through the inclusion of integral benchmark criticality data) must use a consistent set of uranium and oxygen nuclear data and is no longer free to pick and choose cross section evaluations (and associated covariance matrices) from different available libraries.
    - Work by D. Rochman reported in Reference [17] from an IAEA-sponsored CRP show how inclusion of integral benchmark data for SiO_2 introduced correlations between the underlying Si and O nuclear data evaluations.
    - A third example arises in the case where the evaluation includes consideration of spectrum-averaged cross sections for a dosimetry reaction in the ^{252}Cf(sf) standard neutron benchmark field. In this case, the resulting nuclear data evaluation will be cross-correlated with the ^{252}Cf(sf) fission neutron spectrum and could not be used in further neutron spectrum adjustments of the ^{252}Cf(sf) neutron spectrum. Furthermore, if ^{252}Cf(sf) spectrum-averaged cross sections were used as integral benchmark data for several different dosimetry reactions, the evaluation process may have introduced correlations between the different dosimetry cross sections through the common use of a representation of the ^{252}Cf(sf) neutron spectrum in the evaluation process.

- Adjustments will introduce correlations between the *a posteriori* and the *a priori* information.
  The previous bullet included examples where the adjustment process using integral benchmark data will reflect a dependence on the *prior* information used in the adjustment process. This dependence can result in correlations between different sets of nuclear data that result from a similar adjustment process. This correlation must then be properly reflected in the subsequent use of the nuclear data evaluations and any derived products.

- One cannot iterative "adjust" a set of nuclear data to reduce the resulting uncertainty or to achieve a better convergence metric.
  When an adjustment is performed, there is a correlation between the *prior* and the *posterior* products – and between resulting products when the adjustment is done on more than one isolated nuclear data component. For example, use of reactor criticality benchmark data in the evaluation process may have introduced a correlation between an angular distribution and a cross section. If a subsequent "adjustment" is performed using this nuclear data, this correlation between the two quantities must be properly reflected in the methodology used to perform the second adjustment. Capturing these correlations between all of the nuclear data is very complex. As a boundary condition on any iterative approach, it needs to be noted that any "iterative" adjustment performed without the introduction of new data must yield the exact same result if these correlations in the *prior* are correctly reflected. Thus, there is no value in an iterative adjustment process. If multiple

sets of integral benchmark data are to be considered, they should be included as *prior* data in a single integrated adjust process.

5 Conclusions

This input to the Consultants' Meeting, input which is heavily influenced from the perspective of the dosimetry community's use of nuclear data files, has observed that, while there is nothing intrinsically wrong with including the use of integral benchmark data in the nuclear data evaluation process, the inclusion of this data can greatly complicate both the development of and the use of the resulting data and will require great care to properly document the evaluation process so that subsequent use of the adjusted evaluation data does not violate assumptions that went into the evaluation process. If integral benchmark data is used, it is critical that:

- the methodology used to include this data be formally correct, i.e. the *posterior* covariance must be consistent with the adjustment process;
- detailed cross-reaction/isotope/element correlations be provided for all relevant channels in order to permit the user to properly address any correlation between the adjusted nuclear data and his application data when this nuclear data is utilized;
- detailed documentation of the adjustment methodology and optimization metrics be provided within (or referenced within) the resulting nuclear data files so that the user can ensure that his intended application is consistent with any (statistical) bias provided by the inclusion of the integral benchmark data.

It is also recommended that the resulting "adjusted" nuclear evaluation be accompanied by a consistent "unadjusted" nuclear data evaluation, i.e. the *prior* used in the adjustment process, so that users can check for the influence of unexpected cross isotope/element correlations that may not have been specifically addressed in the evaluation process.

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VI. Andrej Trkov, IAEA

On the use of integral experiments in nuclear data evaluation

A. Trkov, R. Capote

Background

Adjustment of evaluated nuclear data files through integral experiments is a long-standing issue. There are two distinct schools of thought: one that advocates absolutely no use of integral data and the other that would favour full adjustment using as much integral data as possible. The reasonable approach is somewhere in between. There are clean measurements like the spectrum averaged cross sections in well-defined neutron fields, which provide information on one reaction channel and are practically uncorrelated with other reaction channels and other materials. The other extreme are criticality benchmarks, where all materials and reactions, including differential and double-differential data are correlated.

Selection of applicable integral data

As already mentioned, there is no reason to oppose the use of clean integral measurements in well-defined neutron fields directly in the evaluation process, but not all integral measurements are suitable for such purpose.

- Spectrum-averaged cross sections in the spontaneous fission spectrum of ^{252}Cf are the cleanest because the spectrum is a standard, published with the Standards-2017. The key point is the analysis of such measurements: note that measurements of the cross sections of the high-threshold reactions are difficult because the spectrum is dropping rapidly as the energy increases. Similarly, measurements of non-threshold reactions require large corrections due to room-return and multiple scattering to lower energies, which is best dealt with by Monte Carlo simulations.
- Spectrum-averaged cross sections in the thermal-neutron induced fission spectrum of ^{235}U can be a suitable neutron field since it was included in Standards-2017 as a secondary standard, but one must be aware that in practice the measurements are usually made in a reactor environment. Purity of the spectrum must be checked by (Monte Carlo) simulations.
- Resonance integrals are less clean, since they usually involve some filter to suppress thermal neutrons from a reactor spectrum. In the epithermal energy range, the spectrum may deviate from the pure 1/*E* behaviour and the fast fission contribution needs to be accounted for. Such measurements are more suitable for data verification/validation than for the adjustment.
- Spectrum-average cross sections in other neutron fields, like fast reactor spectra, astrophysical Maxwellian spectra (MACS), etc. are likewise more suitable for data verification/validation rather than for the adjustment. Their usefulness depends on the accuracy with which the spectrum is known. Ideally it should be supplied with the full covariance matrix, or at least the uncertainties.
- Criticality benchmarks used in data evaluations introduce complex correlations between all reaction channels (including differential and double differential data) and all materials. The adjustments are not unique and represent local minima that depend on the choice of the benchmarks for adjustment. This is clearly demonstrated by the fact that different major libraries reproduce the most commonly used criticality benchmarks fairly well, but the substitution of one material from one library into another one causes differences in the results that are often bigger that the uncertainties in some reactions.

- Transmission, shielding, leakage spectrum and similar measurements may produce useful information to the evaluator to search for weaknesses in the basic data, but they are not suitable for direct use in the evaluation process.

Case: IAEA CIELO evaluations for ^{235}U and ^{238}U

There is a lot of misunderstanding regarding the IAEA-CIELO evaluation process, because it is stated that integral benchmarks "were used as guidance in the selection of the measured cross section data". The situation is best illustrated on a practical example.

Capture to fission ratio above thermal range

- PFNS of ^{235}U was evaluated for the Standards-2017 and resulted in a decrease of the average neutron energy.
- This change had a severe impact on thermal solution benchmarks, particularly on the high-leakage cases. To monitor the situation a representative selection of HEU thermal solution benchmarks listed in Table 1 was used. The "above-thermal leakage fraction" (ATLF) is used as a kind of spectral index.
- We checked the data and found that measured data by Brooks were not used in the previous resonance analysis. The data are given in the form of capture-to-fission ratios and better constrain the cross sections in the valleys between the resonances. The improvement in the fit of these data is shown in Fig. 1.

In short, the integral benchmarks helped us to identify the deficiency in the nuclear data. The results of benchmark calculations did not propagate into the uncertainties and correlations of the evaluated cross sections, which were based purely on measured cross section data.

TABLE 1: LIST OF THERMAL SOLUTION BENCHMARKS CONSIDERED IN THE EVALUATION

No.	ICSBEP name	Short name	Common name	ATLF
1	HEU-SOL-THERM-009	hst009-001	ORNL_S1	0.56252
2	HEU-SOL-THERM-009	hst009-004	ORNL_S4	0.54880
3	HEU-SOL-THERM-013	hst013-001	ORNL_T1	0.14375
4	HEU-SOL-THERM-032	hst032	ORNL_T5	0.05300
5	HEU-SOL-THERM-001	hst001-004	R04	0.44310
6	HEU-SOL-THERM-001	hst001-005	R05	0.33800
7	HEU-SOL-THERM-001	hst001-007	R07	0.33800
8	HEU-SOL-THERM-042	hst042-1	ORNL_C1	0.09900
9	HEU-SOL-THERM-042	hst042-004	ORNL_C4	0.03800
10	HEU-SOL-THERM-042	hst042-008	ORNL_C8	0.00900
11	HEU-SOL-THERM-043	hst043-003	ORNL_LS3	0.14290
12	HEU-SOL-THERM-010	hst010-001	ORNL_S10T0	0.49647
13	HEU-SOL-THERM-012	hst012	ORNL_S91	0.20665

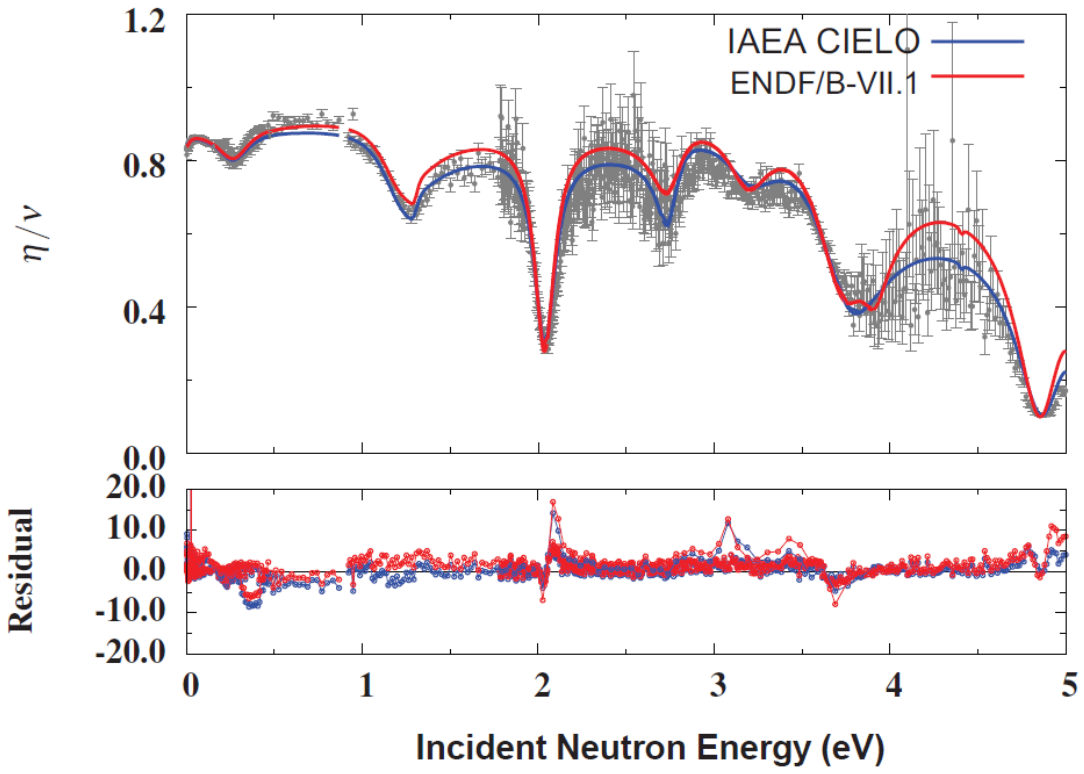

Fig. 1. Comparison of the fit to Brooks data comparing ENDF/B-VII.1 and IAEA-CIELO evaluations for ^{235}U.

Average number of prompt neutrons per fission

The second example is the average number of prompt neutrons per fission (nu-bar). The starter file was the ENDF/B-VII.1 library, including the covariances, which were based on the evaluation of experimental data. The analysis was not repeated for the IAEA-CIELO evaluation, but reasonable adjustments were made as described below.

- To compensate the overprediction of reactivity of Godiva a 0.28 % reduction of nu-bar was made in the energy range 1.2 - 2.4 MeV. After a discussion with the ENDF/B-VII.1 evaluators it was clear that this was effectively un-doing the tweak made to nu-bar in the ENDF/B-VII.1 library. The data from the original evaluation by Phil Young with the GLUCS code were provided by P. Talou from the archive at the LANL. The ratios of the IAEA-CIELO and Young's original evaluation with the GLUCS code of the prompt nu-bar of ^{235}U relative to the ENDF/B-VII.1 evaluation are shown in Figure 2. From there it is clear that smoothing was applied to the fitted curve before insertion into the ENDF/B-VII.1 evaluation. The IAEA-CIELO seems to be in better agreement with the original fit in general than the ENDF/B-VII.1 data.
- At thermal energies, the nu-bar was determined by the Standards-2017. In this particular case, the value at the thermal point was indeed increased by 0.2 % (from 2.40915 to 2.414), which is within the uncertainty of the Standards (0.2 % from the fit and 0.4 % from the unrecognized sources of uncertainty, recommended by Standards-2017). Note however, that the recommended value in the Standards-2006 was 2.41965.
- Above the thermal point the shape of nu-bar was taken from experimental data by Reed and by Simon, with uncertainties adopted from the experimentalists. Above 75 eV up to 100 keV there are no measured data, so we felt free to choose the *prior* in any way we want. Below 200 keV we preferred the shape of nu-bar from JENDL-4.0, but we extended the dip horizontally to lower energies. In this region, there are no experimental data; we were guided by integral benchmarks listed in Table 2. The ENDF/B-VII.1 and IAEA-CIELO prompt nu-bar values are compared to experimental data in Fig. 3. The IAEA-CIELO curve is the red one (adopted for ENDF/B-VIII) and is given with the uncertainty band. The data of Reed and of Simon are not plotted to avoid cluttering of the figure.
- Measured nu-bar data *are not* correlated to the fission cross section. The correlation to PFNS is very weak because the uncertainty from dedicated measurements of nu-bar is an order of magnitude smaller than what can be deduced from the PFNS measurements. For this reason, no correlations are given in the general purpose library. The shape of the nu-bar curve where no data are given is a *pragmatic choice* of the *prior* by the evaluator. A small inconsistency is acknowledged at the thermal point, where the correlations between thermal nu-bar and the thermal cross sections were evaluated with the standards. The largest correlation amounted to 0.08 % and was neglected for simplicity.

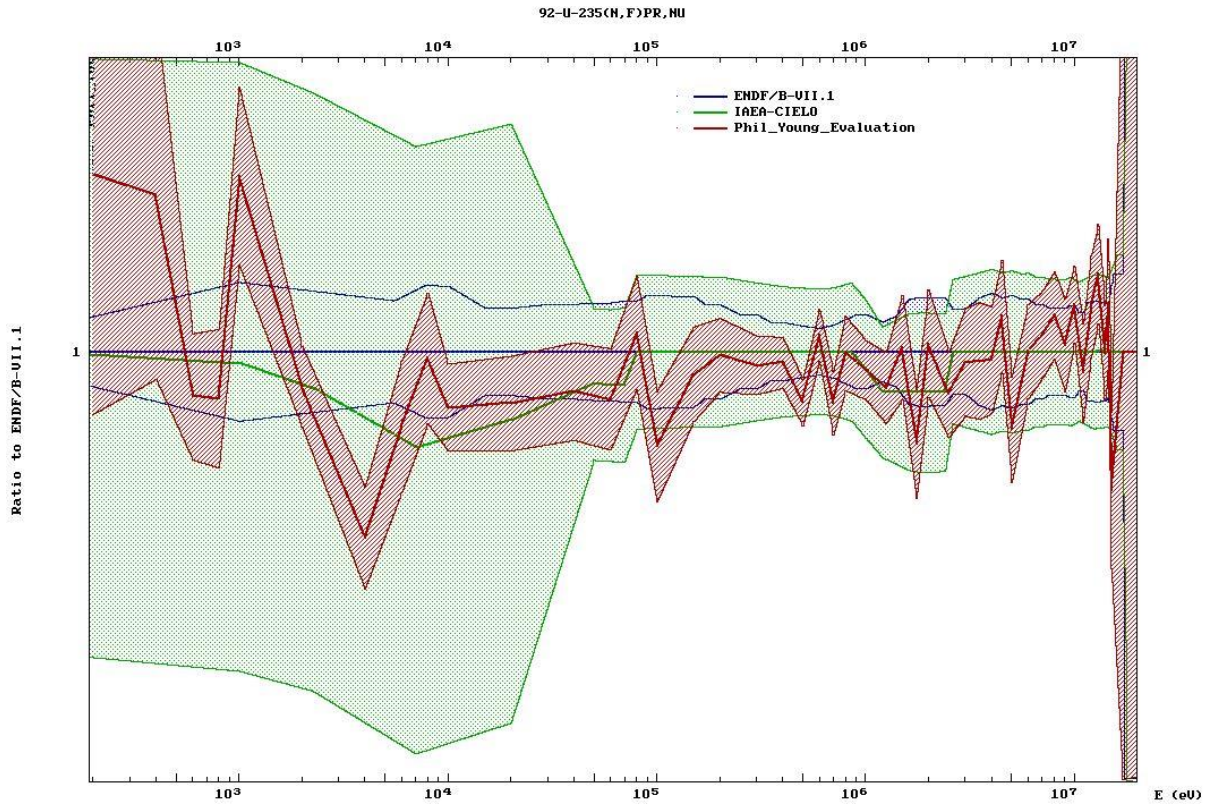

Fig. 2. Comparison of the ratios of the IAEA-CIELO and original evaluation with the GLUCS code by Phil Young of the prompt nu-bar of 235U relative to the ENDF/B-VII.1 evaluation.

Conclusions

- Different types of integral benchmarks were discussed, including the implications of their use in nuclear data evaluation.
- The limited use of criticality benchmarks in the IAEA-CIELO evaluations was described by specific examples. We strongly believe that our use of integral information does not imply usage of such benchmarks as adjustment.
- Covariances are not physical quantities. They may differ, depending on the information that is used to derive them. They are not "inconsistent" (as argued by M. Williams at CSEWG), they are simply different from some adjusted set to which the information from integral benchmarks is added.
- Regarding the release of *adjusted libraries*, we strongly believe that the *general purpose* library is the *one and only*! Any adjustment leads to an adjusted library, *derived* from the general purpose library and is user-specific. Such libraries should be treated similarly like application libraries, which may be produced by experts for a particular end-user or a specific application.

Table 2: Fast benchmarks used for guidance in choosing the *prior* for the prompt nu-bar.

No.	ICSBEP name	Short name	Common name
1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-028	hmf028	Flattop-25
3	IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
11	IEU-MET-FAST-001	imf001-001d	Jemima-1d
12	IEU-MET-FAST-001	imf001-002d	Jemima-2d
13	IEU-MET-FAST-001	imf001-003d	Jemima-3d
14	IEU-MET-FAST-001	imf001-004d	Jemima-4d

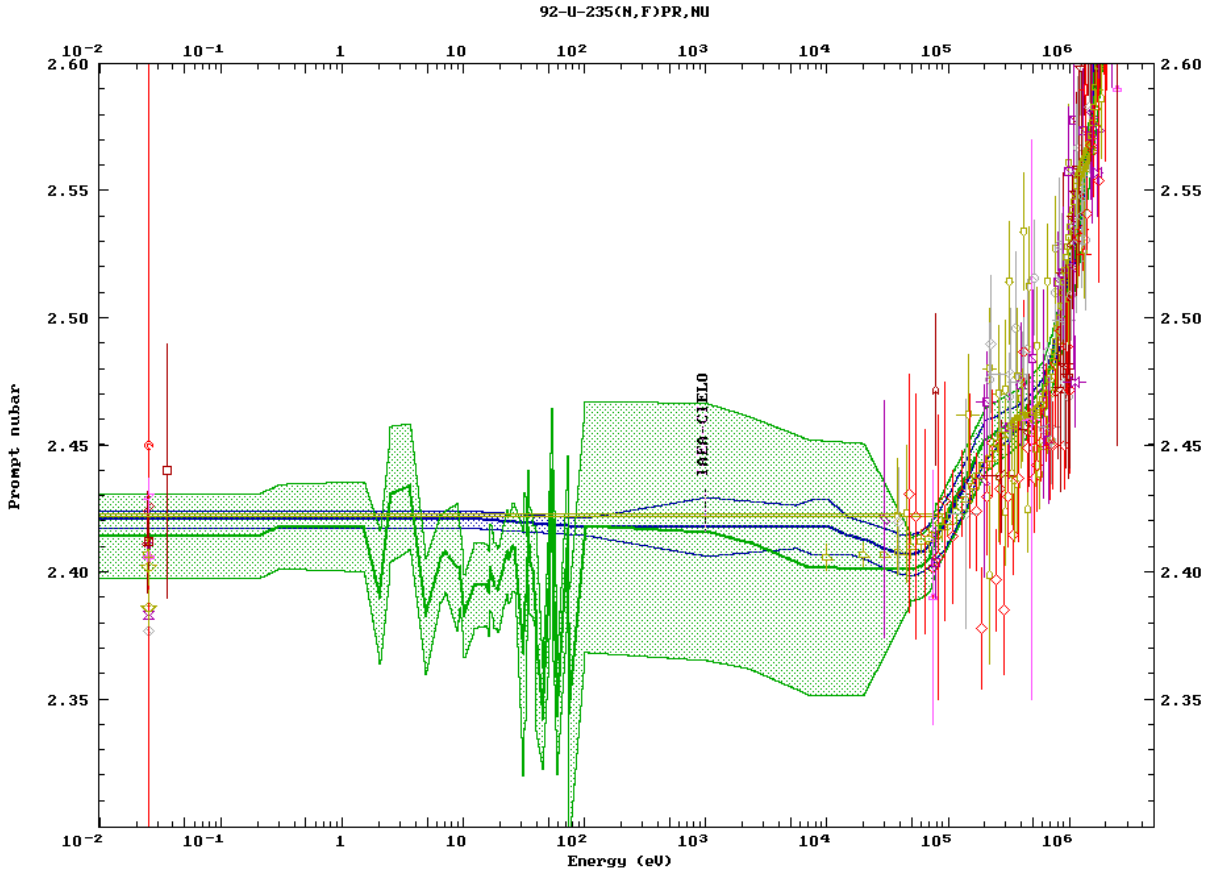

Fig 3. Comparison of prompt nu-bar from ENDF/B-VII.1 and IAEA-CIELO evaluations for ^{235}U with available experimental data.

Consultants' Meeting on

Integral Data in Nuclear Data Evaluation

IAEA Headquarters, Vienna, Austria
14-17 November 2017
Meeting Room VIC MOE75

Preliminary AGENDA

Tuesday, 14 November

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

09:30 - 10:15 **Opening Session**

Welcoming address and Introduction: Andrej Trkov *(NDS/NDDU)*
Election of Chairman and Rapporteur
Adoption of Agenda
Administrative matters

10:15 - 12:30 **Presentations by participants**

1. M. Ishikawa (Kenji Yokoyama & M. Ishikawa / JAEA, Japan)

- A "Tiny" Adjustment of Nuclear Data and Associated Correlation Factor (~ 20 min)
- Survey on Use of Integral Data in Evaluated Libraries (~ 60 min)

12:30 – 14:00 ***Lunch***

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

2. M. Kostal (Research Centre Rez, CZ)
3. G. Noguere (CEA Cadarache, FR) *Coffee breaks as needed*

Wednesday, 15 November

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

4. V. Radulovic (JSI, SL)
5. P. Griffin (Sandia National Lab., Albuquerque NM, USA)

12:30 – 14:00 ***Lunch***

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

6. A. Trkov (IAEA) *Coffee breaks as needed*

19:00 ***Dinner at a downtown Restaurant (see separate information)***

Thursday, 16 November

09:00 - 12:30 Round Table Discussion

12:30 – 14:00 Lunch

14:00 – 17:30 Round table discussion (cont'd)

- Drafting of the Summary Report and Action List

Coffee breaks as needed

Friday, 17 November

09:00 - 16:00 Drafting of the summary report

- Finalisation of the Summary Report and Action List

16:00 Closing of the meeting

Coffee and lunch break(s) in between

Consultants' Meeting on

"Integral Data in Nuclear Data Evaluation"

IAEA, Vienna, Austria
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