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Methods and Approaches to Provide Feedback from Nuclear and Covariance Data Adjustment for Improvement of Nuclear Data Files

Intermediate Report

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The mission of the NEA is:

– to assist its member countries in maintaining and further developing, through international co-operation, the scientific, technological and legal bases required for a safe, environmentally sound and economical use of nuclear energy for peaceful purposes;

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Foreword

The Working Party on International Nuclear Data Evaluation Co-operation (WPEC) has been established under the aegis of the Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation and related topics. Its aim is also to provide a framework for co-operative activities between the members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The WPEC determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

This project is organised by the Nuclear Energy Agency in close co-operation with several parties such as BROND (Russian Federation), ENDF (United States), JENDL (Japan), JEFF (other NEA Data Bank member countries) and also CENDL (China) through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

This report gives an overview of the first activities undertaken by WPEC/Subgroup 39. The first chapter focuses on the adjustment methodologies and the definition of the criteria to assess the reliability and robustness of an adjustment. This chapter also presents guidance on assuring the quantitative validity of the covariance data and enlarging the experimental database in order to avoid as much compensations as possible and to meet needs that were identified by the cross-section adjustment. The second chapter reviews the current covariance data files associated with the latest versions of the JENDL and ENDF evaluated data files.

Acknowledgements

The NEA Data Bank would like to gratefully acknowledge the contribution of all the scientists involved in the WPEC/SG39. In particular, the NEA Data Bank wishes to express its gratitude to all the researchers and experts from the different institutions who participated in WPEC/SG39 meetings. The list of participants is found in Appendix A.

List of abbreviations and acronyms

ANL	Argonne National Laboratory
BNL	Brookhaven National Laboratory
BROND	Russian Evaluated Neutron Data Library
CEA	Commissariat à l'énergie atomique et aux énergies alternatives
CENDL	China Evaluated Nuclear Data Library
ENDF	Evaluated Nuclear Data File
FCA	Fast Critical Assembly
JENDL	Japanese Evaluated Nuclear Data Library
JEFF	Joint Evaluated Fission and Fusion File
IAEA	International Atomic Energy Agency
JAEA	Japan Atomic Energy Agency
LANL	Los Alamos National Laboratory
MC	Monte Carlo
NRG	Nuclear Research and consultancy Group
NSC	Nuclear Science Committee
ORNL	Oak Ridge National Laboratory
STD	Standard deviation
WPEC	Working Party on International Nuclear Data Evaluation Co-operation

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1. Summary of methodology

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In the summary report of the Subgroup 33, it was indicated that future development should focus on a research activity to provide criteria and practical approaches for the effective use of the results of sensitivity analyses and cross-section adjustments in order to provide feedback to evaluators.

It was pointed out that this goal requires addressing and solving a new series of issues. In particular, the definition of criteria to assess the reliability and robustness of an adjustment, criteria to assure the quantitative validity of the covariance data and to suggest guidelines to enlarge the experimental database in order to avoid compensations as much as possible and to meet needs that were identified by the cross-section adjustment.

The present report provides an analysis and an extension of the adjustment methodologies, both in terms of criteria to avoid compensations as much as possible in terms of practical indicators to be used and in terms of criteria in the selection or planning new meaningful experiments.

1. Introduction

To provide useful and physical feedback to nuclear data evaluators from cross-section adjustment results, it is necessary to assess the reliability of the adjustment results. For instance, the adjustment results may include the so-called "compensation effects", which cause fictitious alterations of adjusted cross-sections by the cancellation of two or more reactions of cross-sections. Typical compensation effects have been observed for the following reactions:

- ^{239}Pu fission spectrum and inelastic in general;
  - equivalent effect through neutron spectrum changes;
- capture and (n,2n) for irradiation experiments;
  - same impact of disappearing the associated isotope;
- capture and fission for spectral indices;
  - e.g. ^{238}U capture (C28) and ^{239}Pu fission (F49) for C28/F49;
  - compensation between numerator and denominator;
- many reactions for criticalities;
  - capture, fission, ν, χ, inelastic, elastic, etc.

In addition, useless and unphysical systematic effects may occur in the cross-section adjustments. In order to avoid the compensation effects and to point out systematic effects, several criteria with associated parameters/indices are recommended to be used. This document summarises the methodology with the definitions of the parameters/indices. Although a lot of parameters/indices are reported in the intermediate report of Subgroup 33 [1], many institutions use their own different nomenclature to describe the parameters/indices about the cross-section adjustment. Therefore, Subgroup 39 proposes a common nomenclature for convenience.

2. Preparation and review

2.1. Common nomenclature

The following nomenclature is proposed and consistently used here.

- $\mathrm{N_E}$: number of experimental values used in cross-section adjustment;
- $\mathrm{E_i}(\mathrm{i}=1,\dots,\mathrm{N_E})$: experimental value of measured integral parameter i;
- $\mathrm{C_i}(\mathrm{i}=1,\dots,\mathrm{N_E})$: "a priori" calculated value of integral parameter i;
- $\mathrm{C_i'}(\mathrm{i}=1,\dots,\mathrm{N_E})$: "a posteriori" calculated value of integral parameter i;
- $\sigma_\mathrm{i}(\mathrm{i}=1,\dots,\mathrm{N_E})$: "a priori" cross-section;
- $\sigma_\mathrm{i}'(\mathrm{i}=1,\dots,\mathrm{N_E})$: "a posteriori" cross-sections;
- $\mathrm{S_{ij}}(=\mathrm{S_{\sigma,ij}})$: sensitivity coefficient for integral parameter i and cross-section j;
- $\mathrm{M_{EC}}(\equiv \mathrm{M_E}+\mathrm{M_C})$: integral parameter covariance matrix;
- $\mathrm{M_E}$: integral parameter covariance matrix due to experiment covariance;
- $\mathrm{M_C}$: integral parameter covariance matrix due to calculation covariance;
- $\mathrm{M_\sigma}$: "a priori" cross-section covariance matrix;
- $\mathrm{M_\sigma'}$: "a posteriori" cross-section covariance matrix;
- $\chi^2(\tilde{\sigma})$: chi-square as a function of cross-section $\tilde{\sigma}$ to be minimised in the adjustment;
- χ^2_{min}: minimised chi-square value;
- $\mathrm{G}(\equiv \mathrm{M_{EC}}+\mathrm{SM_\sigma S^T})$: total integral-parameter covariance matrix (to be inverted in adjustment formulas);
- Matrix indexing:

$$\mathrm{A_{ij}} = (\mathrm{A})_{\mathrm{ij}} = \mathrm{a_{ij}} \tag{2.1}$$

$$A_{i\cdot} = (A)_{i\bullet} = (a_{i1} \quad a_{i2} \quad \cdots \quad a_{in}) \tag{2.2}$$

$$\mathrm{A_{\cdot j}} = (\mathrm{A})_{\ \mathrm{j}} = \begin{pmatrix} \mathrm{a_{1j}} \\ \mathrm{a_{2j}} \\ \vdots \\ \mathrm{a_{mj}} \end{pmatrix} \tag{2.3}$$

where:

$$\mathrm{A} = \begin{pmatrix} \mathrm{a_{11}} & \mathrm{a_{12}} & \cdots & \mathrm{a_{1n}} \\ \mathrm{a_{21}} & \mathrm{a_{22}} & \cdots & \mathrm{a_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{a_{m1}} & \mathrm{a_{m2}} & \cdots & \mathrm{a_{mn}} \end{pmatrix}. \tag{2.4}$$

2.2. Adjustment formulas

In this section, the formulation of the cross-section adjustment is reviewed with the common nomenclature. The "a posteriori" cross-section σ' is calculated as:

$$\sigma' = \sigma + M_\sigma S^T G^{-1}(E - C). \tag{2.5}$$

The associated "a posteriori" cross-section covariance matrix M'_σ is denoted as:

$$M'_\sigma = M_\sigma - M_\sigma S^T G^{-1} S M_\sigma. \tag{2.6}$$

In the cross-section adjustment, the chi-square function $\chi^2(\tilde{\sigma})$ to be minimised is described as:

$$\chi^2(\tilde{\sigma}) = (\sigma - \tilde{\sigma})^T M_\sigma^{-1}(\sigma - \tilde{\sigma}) + \left(E - C(\tilde{\sigma})\right)^T M_{EC}^{-1}(E - C(\tilde{\sigma})). \tag{2.7}$$

The minimised chi-square value χ^2_{min} can be represented as below:

$$\begin{aligned} \chi^2_{min} &= (E - C)^T G^{-1}(E - C) \\ &= (\sigma - \sigma')^T M_\sigma^{-1}(\sigma - \sigma') + (E - C')^T M_{EC}^{-1}(E - C'). \end{aligned} \tag{2.8}$$

In contrast with the minimised chi-square value, one can define the initial chi-square value χ^2_{init} as:

$$\begin{aligned} \chi^2_{init} &= \left. (\sigma - \tilde{\sigma})^T M_\sigma^{-1}(\sigma - \tilde{\sigma}) + \left(E - C(\tilde{\sigma})\right)^T M_{EC}^{-1}\left(E - C(\tilde{\sigma})\right) \right|_{\tilde{\sigma}=\sigma} \\ &= (E - C)^T M_{EC}^{-1}(E - C). \end{aligned} \tag{2.9}$$

3. Premises of valid adjustment

We should consider that the following premises are required for a valid cross-section adjustment:

- no missing/underestimation of uncertainty;
- reliable nuclear data covariance: M_σ;
- reliable experiment covariance: M_E;
- reliable calculation covariance: M_C;
- consistency of C/E values and covariance matrices (=chi-square test), i.e. the following equation should be satisfied:

$$\chi^2_{min}/N_E \approx 1. \tag{3.1}$$

In addition, we should note the following points in the adjustment:

- If there are missing isotopes and reactions in nuclear data covariance (i.e. extreme underestimation), variations of some other cross-sections could be unreliable due to compensations. In addition, we should note that the correlations with the missing isotopes and reactions are also neglected. For example, if an important reaction is missing, other reactions that have similar sensitivity will compensate the adjustment.
- Underestimation of experiment and/or calculation uncertainty could give unreliable results as well.
- Overestimation of experiment and/or calculation uncertainty results does not contribute to the adjustment because it is equivalent to eliminating the related experiment.

4. Assessment of adjustment

It is possible to classify assessment techniques into two major categories of (1) assessment before adjustment that can be performed “a priori”, and (2) assessment after adjustment, therefore “a posteriori” using the adjustment results. In fact, these assessments are often applied repeatedly by changing the set of experiments. These repeated assessment procedures can be used for understanding the adjustment results.

4.1. Assessment before adjustment

The assessment before adjustment is useful for selecting the integral experiments.

(1) Experiment correlation factor

Correlation factor between two experiments, i and $\mathrm{i'}$is defined as:

$$f_{ii'} \equiv \frac{(S_{i'}M_\sigma S_i^T)}{\left[(S_{i'}M_\sigma S_{i'}^T)(S_iM_\sigma S_i^T)\right]^{1/2}}. \tag{4.1}$$

The correlation factor corresponds to the representativity factor when one of the experiments is replaced by a target reactor. The complementarity of the experiments can be established by examining the correlation factor $f_{ii'}$ among the selected experiments.

- If the correlation factor $f_{ii'} \ll 1$,
  - there is a strong complementarity between experiments i and $\mathrm{i'}$. That is, the two experiments are useful for the adjustment.

(2) Individual chi-value measured in sigmas

Individual chi-value measured in sigmas is defined as:

$$\begin{aligned}\chi_{\mathrm{ind,i}} &\equiv \frac{|E_i - C_i|}{\sqrt{S_iM_\sigma S_i^T + (M_{EC})_{ii}}} \\ &= \sqrt{(E_i - C_i)^2 (G_{ii})^{-1}}.\end{aligned} \tag{4.2}$$

This value corresponds to the ratio of $|C/E - 1|$ to the total uncertainty.

- If the individual chi-value measured in sigmas $\chi_{\mathrm{ind,i}} \gg 1$,
  - inconsistency may exist between $|C - E|$ and covariance matrices, $SM_\sigma S$, M_E and M_C.

(3) Diagonal chi-value measured in sigmas

Diagonal chi-value measured in sigmas is defined as:

$$\begin{aligned}\chi_{\mathrm{diag,i}} &\equiv \sqrt{(E_i - C_i)^2 (G^{-1})_{ii}} \\ &= \frac{|E_i - C_i|}{\sqrt{((SM_\sigma S + M_{EC})^{-1})_{ii}}} \neq \chi_{\mathrm{ind,i}}\,.\end{aligned} \tag{4.3}$$

This value is similar to the individual chi-value $\chi_{\mathrm{ind,i}}$ but it takes into account the correlations (both among integral parameters and among cross-sections).

- If the diagonal chi-value measured in sigmas $\chi_{\mathrm{diag,i}} \gg 1$,
  - inconsistency may exist between $|C - E|$ and covariance matrices, $SM_\sigma S$, M_E and M_C.

(4) Contribution to chi-square value [2]

Contribution to chi-square value is defined as:

$$\chi^2_{con,i} \equiv \frac{(E-C)^T(G^{-1})_i\ (E_i - C_i)}{N_E}. \tag{4.4}$$

This value characterises the contribution of the experiment to the “a posteriori” chi-square value.

- If the contribution to chi-square value $\chi^2_{con,i} < 0$,
  - the corresponding integral experiment i is very effective in the adjustment.

(5) Ishikawa factor

Ishikawa factor for the integral experiment i is defined as:

$$IS_i \equiv \frac{S_i M_\sigma S_i^T}{(M_{EC})_{ii}}. \tag{4.5}$$

This factor can be used to determine whether the experiment i is useful to reduce the cross-section uncertainty. In addition, it is useful to point out the possibility of inconsistency between the cross-section covariance matrix M_σ and the integral parameter covariance matrix M_{EC}.

- if the Ishikawa factor $IS_i \gg 1$,
  - $S_i M'_\sigma S_i^T \approx (M_{EC})_{ii}$;
  - i.e. the experiment i is very useful, and the “a posteriori” cross-section covariance will be reduced to the same level as the integral parameter covariance;
  - the integral parameter covariance M_{EC} could be wrongly underestimated.
- if the Ishikawa factor $IS_i \ll 1$,
  - $\sigma' \approx \sigma$ and $S_i M'_\sigma S_i^T \approx S_i M_\sigma S_i^T$
  - i.e. the experiment i is not so useful, and the cross-sections are unchanged.
- if the Ishikawa factor $IS_i \approx 1$,
  - $S_i M'_\sigma S_i^T \approx \frac{1}{2} S_i M_\sigma S_i^T$;
  - i.e. the experiment i is useful, and the “a posteriori” cross-section covariance will be reduced by approximately half.

4.2. Assessment after adjustment

It is recommended to carefully assess the adjustment results to point out unreliable and/or unphysical adjustments as below:

- detection of unreliable adjustments;
  - rejection of the associated experiment is suggested when:
    - cross-section variation is larger than one sigma of the “a priori” standard deviation, and no abnormality is observed in the “a priori” cross-section covariance matrix;
    - unphysical results are obtained, this is the case when the cross-section change obtained by the adjustment produces negative cross-sections;

- investigation and caution is needed when:
  - large variations of the cross-sections are observed in energy ranges, isotopes or reactions that are not the main target of the adjustment;
  - large variations of the cross-sections are produced but the "a posteriori" associated standard deviation reductions are small, this happens when large standard deviations are present for the corresponding cross-sections in the covariance matrix, but the associated integral experiment sensitivity coefficients are small.
- recommended checks:
  - comparison of adjusted results with existing validated nuclear data files and/or reliable differential measurements;

- After adjustment if chi-square value is not satisfactory (> 1), experiments can be removed (chi-filtering) based either on diagonal chi-square value or chi-square contribution.
- In particular, the "a posteriori" (= minimum) chi-square contribution allows a classification of the integral experiments in a hierarchical way. Large positive values (especially those that make the total χ'2 larger than one) signal a reconsideration of the corresponding integral experiment. The reasons for large positive values can be of different nature, but the most likely is a change in the corresponding adjusted values that is larger than the starting standard deviation in the initial covariance matrix. Another possible reason is an existing correlation among experiments and/or cross-sections that is a too strong constraint in the adjustment. It has to be noted that an experiment can give a negative contribution, which means that the corresponding integral experiment is very effective in the adjustment.
- An alternative technique consists in computing the change in the Cook's distance defined by the following formula [3] due to discarding an experiment, and observing the associated impact.

$$\mathrm{CD} = (\sigma' - \sigma)^{\mathrm{T}}(\mathrm{M}'_{\sigma})^{-1}(\sigma' - \sigma). \tag{4.6}$$

4.3. Interpretation of adjustment mechanism

In some cases, it is useful to understand the adjustment mechanism for validating a specific cross-section adjustment result. One can detect the compensation effects by analysing the adjustment mechanism. For this purpose, three indices are recently proposed [4].

(1) Mobility in adjustment

Square root of mobility for the reaction j is defined as:

$$\sqrt{\mathrm{D_j}} = \mathrm{sgn}\left(\mathrm{M}_{\sigma,\mathrm{j}}\mathrm{J}\right)\sqrt{\left|\mathrm{M}_{\sigma,\mathrm{j}}\mathrm{J}\right|}, \tag{4.7}$$

where $\mathrm{sgn}(x) = x/|x|$ for $x \neq 0$, $\mathrm{sgn}(x) = 0$ for $x = 0$, and

$$\mathrm{J} = (1 \quad 1 \quad \cdots \quad 1)^{\mathrm{T}}. \tag{4.8}$$

This index is considered as a pseudo standard deviation, which includes correlation factors. If all non-diagonal elements are zero, it is equivalent to the standard deviation. The standard deviation is often used for analysing the adjustment results because it is approximately proportional to the cross-section change. However, this is not always true. In that case, it is recommended to use the square root of the mobility. For instance, a numerical experiment shows that cross-section adjustment results sometimes drastically change when the mobility is reduced by setting the correlation factors to zero, i.e. even if the standard deviation is unchanged [4].

(2) Adjustment motive force

Adjustment motive force of the experiment i for the nuclear reaction j is defined as:

$$F_{i,j} = \frac{\left\| \left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} \right\|}{\|J\|} \cos\theta. \tag{4.9}$$

where $\|\cdot\|$ is the Euclidean norm:

$$\left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} = M_{\sigma,j} S_{i,j}^{T} G_{i,j}^{-1} \left(J - \frac{C_i}{E_i}\right), \tag{4.10}$$

and:

$$\cos\theta = \frac{\left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} \cdot J}{\left\| \left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} \right\| \cdot \|J\|}. \tag{4.11}$$

Here, $(\Delta\sigma/\sigma)_{i,j}$ is a special adjustment result, in which only one nuclear reaction j is adjusted by using only one integral experiment i. The adjustment motive force is considered as an average value of the cross-section changes over all energy groups. By using the adjustment motive force, one can arrange the experiments in a unique order, and identify the experiment that has the largest impact on the change of the specific cross-section. It should be also noted that the discussion with the motive force (and the adjustment potential described later), is limited to the correlations in the energy of a specific reaction and of a specific isotope because of their definition. In other words, cross-correlation among reactions and among isotopes cannot be discussed together with the adjustment force.

(3) Adjustment potential

The adjustment potential is calculated as well as the adjustment motive force by replacing the C_i/E_i with averaged $\overline{C_I}/\overline{E_I}$ over a set of integral parameters I, which is related to the integral parameter i. For instance, one can define I as a set of specific integral parameters measured in a series of experiments, which is the same as the integral parameter i.

By using the adjustment motive force and the adjustment potential, one can discuss the mechanism of adjustment with the following assumptions:

- If only one integral experiment has a large adjustment motive force for a reaction, the cross-section of the reaction is freely adjustable.
- If more than two integral experiments with large adjustment potentials have quite different values of motive forces, it is regarded as a conflict. The cause of this conflict could be associated either with inconsistent sensitivity coefficients (e.g. opposite sign in the two experiments) or inconsistent C/E. In this case, the cross-section of the reaction is not significantly adjusted. Then, the other freely-adjustable cross-sections are altered.

For example, by iterating the adjustment calculations with increasing the number of integral experiments, it is possible to investigate the mechanism of the adjustment as follows: when you use only one integral experiment, all of the cross-sections are freely adjustable. As the number of integral experiments increases, conflict arises. Then, it can be seen how the adjustment result is changed by the conflict. Moreover, investigating the reason of the conflict, one can discuss whether the adjustment result is acceptable or not.

If the conflict is reasonable, e.g. all of the integral experiments used in the adjustment are reliable and no other inconsistency is found; the adjustment result may be accepted. In contrast, if the conflict is caused by other inconsistency, the set of the integral experiments used for the adjustment should be reconsidered.

Unfortunately, it is difficult to apply the above procedure to a large case where a lot of integral experiments are used. However, for a small case, e.g. when a specific small set of integral experiments which gives an interesting adjustment result are known in advance, this procedure can be used to investigate the mechanism of the adjustment.

5. Avoiding compensation effects

In order to avoid the compensation effects, Subgroup 39 proposes two major classes of methods, static method and dynamic method, shown below.

5.1. Static method

- Use of specific experiments:

An approach can be envisaged that expands as much as possible the use in the adjustment procedure of selected integral experiments that provide information on "elementary" phenomena or on separated individual physics effects related to specific isotopes [5]. In this respect, criticality measurements could be considered as providing a global check on selective adjustments focused on individual isotope cross-sections [6].

- The classical example is the irradiation from time "0" to time "t" of pure separate isotopes samples in variable neutron spectra within a power reactor [7,8]. That measurement gives access to the integral absorption rate of the father isotopes as well as to that of their daughter isotopes:

$$N_{A+1}(t) = N_A(0)\bar{\sigma}_A^c\Gamma$$

$$N_{A+2}(t) = \frac{1}{2}N_A(0)\bar{\sigma}_A^c\bar{\sigma}_{A+1}^c\Gamma^2$$

where the measured quantities are the NA+1 – NA+2 – NA+3 and the fluence Γ.

Discrepancies on the measured quantities (e.g. in the hypothesis of negligible uncertainties on the measured fluence) can be interpreted in terms of absorption (and possibly n, xn) cross-section uncertainties.

- Spectrum indexes can help separate individual effects and oscillation experiments can produce the reactivity of single isotope samples [9,10].

Oscillation experiments are not the only experiment type that can help to separate individual isotope reactivity. Accurate experiments can be obtained in zero-power critical facilities, as it is shortly illustrated below.

- In fact, the reactivity variation per cycle can be expressed, for illustration purposes, in a simple one-group fundamental mode approximation as the sum of individual isotope i contributions (n being the core region n index):

$$\Delta\rho(\text{cycle}) = \sum\nolimits_n \sum\nolimits_i \frac{\Delta N_i(\nu\sigma_f - \sigma_a)_i}{\sum_{i,n} \nu\Sigma_{fi,n}} - \frac{\Delta N_{FP}\sigma_{FP}}{\sum_{i,n} \nu\Sigma_{fi,n}}$$

The fission product component is represented by a standard “lumped fission product” description. One can rewrite that expression as:

$$\Delta\rho(\text{cycle}) = \sum_{K} \Delta n^{K} \rho_{K}$$

where we have assumed that n=1 and that the K index includes both the “i” heavy isotopes and the lumped fission product and:

$$\Delta n^{K} = n_{F}^{K} - n_{0}^{K}$$

(F index indicates the end and the 0 index the beginning of irradiation, respectively).

In this case, measurements of the reactivity of individual heavy isotopes and of fission products should be used e.g. by means of, besides sample reactivity measurements, experiments performed in several representative neutron spectrum configurations, as should use of the C/E values in an adjustment procedure that will privilege the capture cross, fission and scattering crass sections of individual isotopes.

However, J different Pu plus minor actinide (^{241}Am) isotopic compositions can also be envisaged to be loaded successively in a predefined central region of a critical experimental configuration. Starting from the one closer to criticality, J-1 sub-critical reactivity Rj is measured [11]:

$$R^{j} = \sum_{i} (N_{i}^{Ref} - N_{i}^{j}) \times \rho_{i}$$

where: ρi is the reactivity/atom of isotope i and $N_{i}^{Ref} - N_{i}^{j}$ are the (known) atom density variations of isotopes i going from the reference to configuration j.

The calculation-experiment values can then be interpreted in terms of reactivity of each isotope:

$$R_{exp}^{j} - R_{calc}^{j} = \sum_{i} \left(N_{i}^{Ref} - N_{i}^{j}\right) x(\delta\rho_{i}) \pm \varepsilon_{Rj}$$

where j=1, (J-1) and ϵRj are the experimental uncertainties. Using the same one-group formulation for illustration purposes as above, one can use the following expressions in the nuclear data adjustment procedure:

$$R_{exp}^{j} - R_{cac}^{j} = \sum_{i}(N_{i}^{Ref} - N_{i}^{j}) \times (\delta\nu\sigma_{f} - \delta\sigma_{a}) \pm \varepsilon_{Rj} \quad (j=1, (J-1))$$

In a standard multi-group formulation, scattering effects will also be present, which account for the different importance of neutrons at different energies as given by the adjoint flux energy shape.

- In this context, if one would use integral experiments with the adjoint flux energy shapes tailored in such a way to have “flat” or steep energy shapes [12], one could separate scattering effects from capture (absorption) effects in the adjustment procedure.
- Finally, neutron leakage experiments from single material (^{238}U, Fe etc.) spheres, fed by well characterised neutron sources, have been traditionally a source of information for the evaluation or a posteriori validation of elastic and inelastic cross-sections and their angular distributions [13]. The use of the measured values (total number of neutrons, energy spectrum (e.g. by energy bands) of leaking neutrons) can lead to an adjustment procedure, which is a strong, complementary indication on some specific scattering cross-sections.
- Similar information can be obtained by neutron propagation experiments in single material blocks, fed by well characterised neutron sources [14].

5.2. Dynamic method

- physical interpretation of adjustments;
  - to understand the mechanism of adjustments;
  - if the compensation effect is reasonable and physical, we may rely on the adjustment results;
  - one possible way is to use the adjustment motive force and adjustment potential;
  - it works for limited cases, for example, a small case which uses a few of experiments;
  - more sophisticated method is needed to settle this issue.

6. Remarks on the "a posteriori" covariance matrix

Once we achieve a reliable cross-section adjustment result without compensation effects, we may provide the corresponding feedback to the nuclear data evaluation. However, it should be noted that the "a posteriori" covariance matrix has been fully correlated by the cross-section adjustment procedure. This issue has been pointed out in Subgroup 33 [5].

The global "a priori" correlation matrix M_y has the form:

$$M_y = \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix}. \tag{7.1}$$

The global "a posteriori" correlation matrix is denoted as:

$$M'_y = \left(I - M_y S_y^T G^{-1} S_y\right) M_y. \tag{7.2}$$

S_y is the global sensitivity matrix with dimension $(N_\sigma + N_E) \times N_E$ where N_σ is the total number of cross-sections and N_E is the total number of integral experiments:

$$S_y = \begin{pmatrix} S_{1,1} & S_{1,2} & \cdots & S_{1,(N_s+N_E)} \\ S_{2,1} & S_{2,2} & \cdots & S_{2,(N_s+N_E)} \\ \vdots & \vdots & \ddots & \vdots \\ S_{N_E,1} & S_{N_E,2} & \cdots & S_{N_E,(N_s+N_E)} \end{pmatrix} \tag{7.3}$$

The matrix S_y can be rewritten as a vector with two components, each being a matrix:

$$S_y = (S_\sigma \quad S_{EC}) = (S_\sigma \quad I) \tag{7.4}$$

where S_σ (dimension $N_\sigma \times N_E$) is the sensitivity matrix of the integral experiments with respect to the cross-sections and S_{EC} is a square identity matrix (dimension $N_E \times N_E$).

Finally:

$$\begin{aligned} G &= S_y M_y S_y^T \\ &= (S_\sigma \quad I) \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix} \begin{pmatrix} S_\sigma^T \\ I \end{pmatrix} \\ &= (S_\sigma M_\sigma \quad M_{EC}) \begin{pmatrix} S_\sigma^T \\ I \end{pmatrix} \\ &= S_\sigma M_\sigma S_\sigma^T + M_{EC} \end{aligned} \tag{7.5}$$

with dimension $N_E \times N_E$:

$$G^{-1} = (S_\sigma M_\sigma S_\sigma^T + M_{EC})^{-1} \tag{7.6}$$

The global "a posteriori" covariance matrix:

$$\mathrm{M}'_{\mathrm{y}} = \begin{pmatrix} \mathrm{M}'_{\sigma} & \mathrm{M}'_{\sigma,\mathrm{EC}} \\ \mathrm{M}'_{\mathrm{EC},\sigma} & \mathrm{M}'_{\mathrm{EC}} \end{pmatrix} \tag{7.7}$$

On the other hand, the global "a posteriori" covariance matrix M'_{y} is rewritten from Eq. (7.2):

$$\begin{aligned}
\mathrm{M}'_{\mathrm{y}} &= \left(\mathrm{I} - \mathrm{M}_{\mathrm{y}}\mathrm{S}_{\mathrm{y}}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{S}_{\mathrm{y}}\right)\mathrm{M}_{\mathrm{y}} \\
&= \left(\mathrm{I} - \begin{pmatrix} \mathrm{M}_{\sigma} & 0 \\ 0 & \mathrm{M}_{\mathrm{EC}} \end{pmatrix}\begin{pmatrix} \mathrm{S}_{\sigma}^{\mathrm{T}} \\ \mathrm{I} \end{pmatrix}\mathrm{G}^{-1}(\mathrm{S}_{\sigma} \quad \mathrm{I})\right)\begin{pmatrix} \mathrm{M}_{\sigma} & 0 \\ 0 & \mathrm{M}_{\mathrm{EC}} \end{pmatrix} \\
&= \left(\mathrm{I} - \begin{pmatrix} \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}} \\ \mathrm{M}_{\mathrm{EC}} \end{pmatrix}\mathrm{G}^{-1}(\mathrm{S}_{\sigma} \quad \mathrm{I})\right)\begin{pmatrix} \mathrm{M}_{\sigma} & 0 \\ 0 & \mathrm{M}_{\mathrm{EC}} \end{pmatrix} \\
&= \left(\mathrm{I} - \begin{pmatrix} \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{S}_{\sigma} & \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1} \\ \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{S}_{\sigma} & \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1} \end{pmatrix}\right)\begin{pmatrix} \mathrm{M}_{\sigma} & 0 \\ 0 & \mathrm{M}_{\mathrm{EC}} \end{pmatrix} \\
&= \begin{pmatrix} \mathrm{I} - \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{S}_{\sigma} & \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1} \\ \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{S}_{\sigma} & \mathrm{I} - \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1} \end{pmatrix}\begin{pmatrix} \mathrm{M}_{\sigma} & 0 \\ 0 & \mathrm{M}_{\mathrm{EC}} \end{pmatrix} \\
&= \begin{pmatrix} \mathrm{M}_{\sigma} - \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{S}_{\sigma}\mathrm{M}_{\sigma} & \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{M}_{\mathrm{EC}} \\ \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{S}_{\sigma}\mathrm{M}_{\sigma} & \mathrm{M}_{\mathrm{EC}} - \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{M}_{\mathrm{EC}} \end{pmatrix}
\end{aligned} \tag{7.2'}$$

By comparing Equation (7.7) with Equation (7.2), one can derive the following equations:

The "a posteriori" cross-section covariance matrix:

$$\mathrm{M}'_{\sigma} = \mathrm{M}_{\sigma} - \mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{S}_{\sigma}\mathrm{M}_{\sigma} \tag{7.8}$$

The "a posteriori" integral parameter covariance matrix:

$$\mathrm{M}'_{\mathrm{EC}} = \mathrm{M}_{\mathrm{EC}} - \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{M}_{\mathrm{EC}} \tag{7.9}$$

The "a posteriori" integral parameter/cross-section correlation matrix:

$$\begin{aligned}
\mathrm{M}'_{\mathrm{EC},\sigma} &= \left(\mathrm{M}'_{\sigma,\mathrm{EC}}\right)^{\mathrm{T}} \\
&= \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{S}_{\sigma}\mathrm{M}_{\sigma}
\end{aligned} \tag{7.10}$$

In addition, Equation (7.10) can be written more precisely:

$$\begin{aligned}
\mathrm{M}'_{\mathrm{EC},\sigma} &= \mathrm{M}'^{\mathrm{T}}_{\sigma,\mathrm{EC}} \\
&= (\mathrm{M}_{\sigma}\mathrm{S}_{\sigma}^{\mathrm{T}}\mathrm{G}^{-1}\mathrm{M}_{\mathrm{EC}})^{\mathrm{T}} \\
&= \mathrm{M}_{\mathrm{EC}}^{\mathrm{T}}(\mathrm{G}^{-1})^{\mathrm{T}}(\mathrm{S}_{\sigma}^{\mathrm{T}})^{\mathrm{T}}\mathrm{M}_{\sigma}^{\mathrm{T}} \\
&= \mathrm{M}_{\mathrm{EC}}\mathrm{G}^{-1}\mathrm{S}_{\sigma}\mathrm{M}_{\sigma}
\end{aligned} \tag{7.10'}$$

The above derivation clearly articulates that the global "a posteriori" correlation matrix is fully correlated not only for the "a posteriori" cross-sections but also for the "a posteriori" integral parameter. In addition, correlations are found between the cross-section and the integral parameters.

7. Conclusion

The methodology to assess the cross-section adjustments has been summarised with a proposed common nomenclature. Some of the assessment parameters/indices are well-established and used in many institutions. In order to achieve a reliable cross-section adjustment result, one should make full use of the methodology. In addition, the methodology itself needs to be improved to avoid the compensation effects. The following remarks can be made on the covariance matrix:

- Both standard deviation of the "a priori" covariance matrix and the correlation significantly affect the adjustment results.
- The "a posteriori" correlation matrix is full and has a significant impact on reducing the "a posteriori" uncertainty.
- The "a posteriori" correlations are useful and physical since they come from the combination of two physical data, i.e. differential and integral experiments.
- Once the adjustment is utilised, not only the adjusted cross-sections but the "a posteriori" correlations should be propagated to the nuclear data evaluation, otherwise it might result in inconsistencies between differential and integral data.
- In practice, the definition of criteria to assess the reliability and robustness of an adjustment, criteria to assure the quantitative validity of the covariance data were indicated and guidelines were suggested to enlarge the experimental database in order to avoid as much as possible compensations and to meet needs that were identified by the cross-section adjustment. Further work in the Subgroup will provide a practical implementation of the previous suggestions/guidelines
- In summary, the present report provides an analysis and an extension of the adjustment methodologies both in terms of criteria to avoid as much as possible compensations in terms of practical indicators to be used and in terms of criteria in the selection or planning new meaningful experiments.

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2. Comments on covariance data

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In the summary report of the Subgroup 33, it was indicated that future development should focus on a research activity to provide criteria and practical approaches for the effective use of the results of sensitivity analyses and cross-section adjustments in order to provide feedback to evaluators.

It was pointed out that this goal requires addressing and solving a new series of issues. In particular, the definition of criteria to assess the reliability and robustness of an adjustment, criteria to assure the quantitative validity of the covariance data and to suggest guidelines to enlarge the experimental database in order to avoid as much as possible compensations and to meet needs that were identified by the cross-section adjustment.

In this context, the present report provides a contribution to the critical analysis of current covariance data files associated to the latest versions of the JENDL and ENDF evaluated data files.

1. Introduction

The covariance matrix[1] of a scattered data set, xi (i=1,n), which must be symmetric and positive-definite, is defined as follows [1]:

- ✓ Variance: $\mu_{ii} = \mathrm{var}(x_i) = <(x_i - m_{0i})^2> \quad for\ \ i = 1, n$ $\quad (m_{0i} = \langle x_i \rangle :\ \ mean\ value)$
  - Standard deviation: $\sigma_i = std(x_i) = \sqrt{\mathrm{var}(x_i)}$
- ✓ Covariance: $\mu_{ij} = \mathrm{cov}(x_i, x_j) = <(x_i - m_{0i})(x_j - m_{0j})> \quad for\ \ i, j = 1, n\ \ with\ i \neq j$
  - Correlation factor: $\rho_{ij} = \dfrac{\mu_{ij}}{\sqrt{\mu_{ii}\mu_{jj}}} = \dfrac{\mathrm{cov}(x_i, x_j)}{std(x_i) \times std(x_j)} \quad where,\ -1 \le \rho_{ij} \le 1$

As one of WPEC/SG39 contributions to the SG40/CIELO project, several comments or recommendations on the covariance data are described here from the viewpoint of nuclear data users. To make the comments concrete and useful for nuclear data evaluators, the covariance data of the latest evaluated nuclear data library, JENDL-4.0 (J-4.0 hereafter, [2-5]) and ENDF/B-VII.1 (E-7.1 hereafter, [6-9]) are treated here as the representative materials. The surveyed nuclides are five isotopes that are most important

1. Covariance matrix is sometimes called “variance-covariance matrix”.

for fast reactor application. The nuclides, reactions[2] and energy regions dealt with are the following:

- ^{239}Pu: fission (2.5~10keV) and capture (2.5~10 keV);
- ^{235}U: fission (500eV~10keV) and capture (500 eV~30 keV);
- ^{238}U: fission (1~10 MeV), capture (below 20 keV, 20~150 keV), inelastic (above 100 keV) and elastic (above 20 keV);
- ^{56}Fe: elastic (below 850 keV) and average scattering cosine (mu-bar hereafter) (above 10keV);
- ^{23}Na: capture (600 eV~600 keV), inelastic (above 1 MeV) and elastic (around 2 keV).

2. Methodology of covariance evaluation

The covariance data of a library should be evaluated in accordance with the methodology adopted in the library to obtain the central values of the nuclear data. In other words, two covariance data of a cross-section in two libraries could be different even if the central values of the cross-section are accidentally identical, when the evaluation methodologies or the experimental data used differ from each other. Therefore, it is very important for the nuclear data evaluators to provide as much information as possible about the methodology which they adopted. Here, typical methodologies to evaluate the covariance data are briefly reviewed according to the recently published documents.

1) Generalised least-square method

If plenty of measured data are available to evaluate cross-sections in an energy range, the generalised least-square method with the GMA code (ANL, [10]) or the ZOTT code (IAEA, [11]) could be used to obtain the best-estimated cross-section values and their covariance data at once. The very critical issue to use the experimental values for the cross-section evaluation is that the systematic and statistical uncertainties[3] of the measurements must be distinguished and known quantitatively, however, the knowledge of measurement uncertainty would generally be difficult to exactly obtain [12]. For example, in the evaluation of the J-4.0 covariance for the fission cross-section of the major actinides in the high-energy range, the standard deviation (STD) values obtained with the simultaneous least-square fitting method using the SOK code (JAEA, [13]) were multiplied by a factor of 2 in order to take into account the hidden correlations among measurements [2].

2) Resonance region

To evaluate the covariance of the resolved resonance region for the major actinides such as ^{235}U, ^{238}U, and ^{239}Pu, the results of the full-scale R-matrix solution codes using the

[2] One important parameter that is not treated here is the delayed neutron fraction (nu-d, hereafter). Nu-d is a kinetic parameter to determine the reactor dynamic response to external perturbation, and also to be used as the reactivity scale to convert the delta-k unit to the dollar unit to compare the analytical reactivity with the measured one. However, the origin of the nu-d uncertainty stems from the fission product yield and related data such as decay scheme or nuclear structure. The scientific basis of these physics seems quite different from the ordinary cross-section evaluation based on nucleus models, therefore, we need to wait for the completion of WPEC/SG37 “Improved fission product yield evaluation methodologies” where the covariance of the fission yield data has been investigated since 2013. In addition, E-7.1 does not include the nu-d covariance for major actinides unlike J-4.0, and needs to be extended.

[3] The “systematic” and “statistical” means the fully-correlated and uncorrelated, respectively.

SAMMY code [14] are available. The covariance of the resonance parameters, File 32 in the ENDF format, is usually too large to accommodate in a library. Therefore, the resonance parameter uncertainties and correlations are propagated to the cross-section covariance, i.e. File 33. As mentioned in the generalised least-square fitting case, the uncertainties of the computed cross-sections from SAMMY were found to be unrealistically underestimated, although the uncertainties of resonance energies and widths seemed realistic. Therefore, in the evaluation of E-7.1 covariance data, systematic uncertainties of background, normalisation, scattering radius and other long-range correlations have been included in the analysis bringing computed cross-section uncertainties to a more plausible level [7]. For the resonance region covariance of minor actinides, the structural isotopes or fission products, more simplified methods such as the kernel approximation (BNL, [15]), or the integral uncertainty method (LANL, [16]) are applied, where some “a priori” uncertainty estimations of the resonance parameters such as those by Mughabghab [17] are propagated to the cross-section uncertainty.

3) KALMAN-filter method

The basic idea of this method is to optimise the nuclear model parameters by the inclusion of the cross-section measurement information with the Bayesian parameter estimation. In several libraries, the Bayesian code KALMAN (Kyushu University and JAEA, [18]) is used with the theoretical nuclear model codes such as GNASH (LANL, [19]), EMPIRE (BNL, [20]), TALYS (NRG, [21]) or CCONE (JAEA, [22]). The CONRAD code (CEA, [23]) also has the capability to evaluate the cross-section covariance by combining the Bayesian technique with the nuclear theoretical model parameters. The largest advantage in the KALMAN technique is that even the uncertainty of the cross-section in the energy or reaction for which no experimental data are available, can be estimated by extrapolating the obtained uncertainties of nuclear model parameters through the theoretical model. On the other hand, the KALMAN technique has some disadvantages such as the assumption of linearity through the model parameter sensitivities, or the difficulty to take into account the deficiency of the adopted nuclear models themselves [24,25]. Since the KALMAN method utilises the experimental information, it is also unavoidable to suffer from the unrecognised correlation problems.

4) Monte Carlo-based method

The recent increase in computer speed and memory allowed for the Monte Carlo (MC) calculations to evaluate the covariance of nuclear data as well as the best-estimated values (NRG, [26,27]). One of the advantages for the MC-based method is that it does not need the sensitivity of nuclear model parameters, which makes the method free from the assumption of linearity. The MC method, however, not only requires enormous computing time to obtain sufficiently small statistical errors, but also has similar disadvantages to other deterministic Bayesian methods such as the need for prior model parameter uncertainty, shape and correlation for random sampling, the difficulty of taking into account the deficiency of the nuclear models, and the quality and quantity of the cross-section measurements.

3. Comments on covariance data of JENDL-4.0 and ENDF/B-VII.1

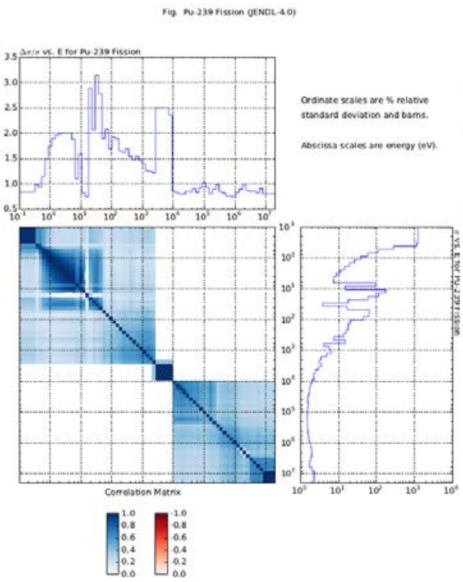
3.1. ^{239}Pu fission

The neutron energy discussed here is in the range 2.5 keV to 10 keV, which is the lower part of the unresolved resonance region, 2.5~30 keV, in both J-4.0 and E-7.1. Figure 1 shows the covariance data of ^{239}Pu fission cross-section of both libraries, the comparison of the STD values and the adjusted result based on J-4.0 (ADJ2010, [28]). In (a) and (b) of the figure, the upper part is the energy dependency of the STD values, the right part that of the cross-section values, and the central part the energy distribution of the correlation factors. In (c) of the figure, the comparison of the STD values between two libraries, and in (d) the alteration of ^{239}Pu fission cross-section by the ADJ2010 adjustment are shown, respectively.

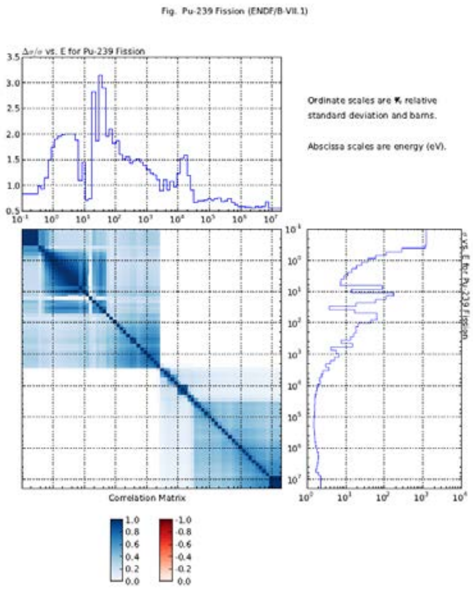
Figure 1 shows that the STD values of 2.5~10keV show an abrupt peak in J-4.0, on the contrary, no such discontinuity is seen in E-7.1.

Figure 1. JENDL-4.0 and ENDF/B-VII.1 covariance–^{239}Pu fission

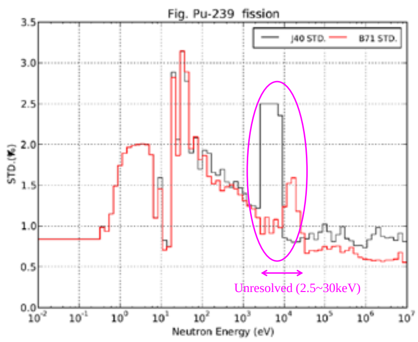
(a) JENDL-4.0



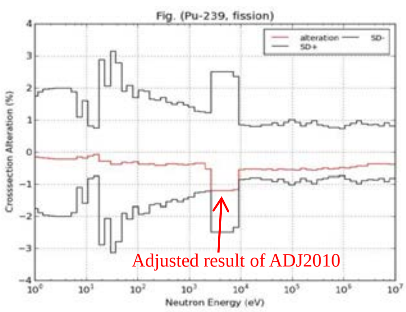
(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



(d) Alteration of Pu-239 fission cross-section by the adjustment based on JENDL-4.0



As a result, the following information has been obtained. In the former JENDL-3.3 (J-3.3 hereafter, [29]), the covariance data of the whole unresolved resonance region were evaluated from the uncertainty of resonance parameters, consequently, the STD values were generally large. Above 10 keV, J-4.0 changed to adopt the simultaneous evaluation for the center cross-section values of major fission isotopes, and the resonance parameters were only used to calculate the shielding factors. Since the simultaneous evaluation was found to evaluate the STD values too small,[4] the STD values of J-4.0 were multiplied by a factor of 2 to compensate for this defect as mentioned in the previous section, but were still small compared with the STD values of J-3.3, which were carried over to J-4.0 in 2.5~10 keV [30]. Since the evaluation method of the covariance data is consistent with that of the central value of cross-section, the discontinuity at 2.5~10 keV in J-4.0 is methodologically acceptable. However, this discontinuity was found to unnaturally affect the cross-section change by an adjustment as can be seen in Figure 1 (d).

Recommendations

It is desirable for J-4.0 to improve the covariance evaluation of the 2.5~10 keV region.

3.2. ^{239}Pu capture

The energy range is 2.5~10 keV the same as that of ^{239}Pu fission. Figure 2 shows the covariance data of ^{239}Pu capture cross-section in J-4.0 and E-7.1, the STD comparison, and the adjusted result of ADJ2010.

Figure 2 shows that the STD values of E-7.1 are notably large in 2.5~10 keV, while, those of J-4.0 are quite smooth above 2.5 keV.

It can be concluded that above 2.5 keV, J-4.0 adopted the results of the CCONE-KALMAN calculation [4], therefore, the STD values tend to be smooth in the high-energy region [30]. On the other hand, there seems to be no explanation in the E-7.1 comment file [8] to correspond to its discontinuity. In the United States, there is an option according to which the ^{239}Pu capture cross-section above 2.5 keV should be 10% larger than E-7.1 [31], but no information was obtained on this covariance trend. The adjusted result of ADJ2010 in Figure 2 (d) seems to be somewhat coincident with the expectation of ^{239}Pu capture increase, but it needs to be further confirmed.

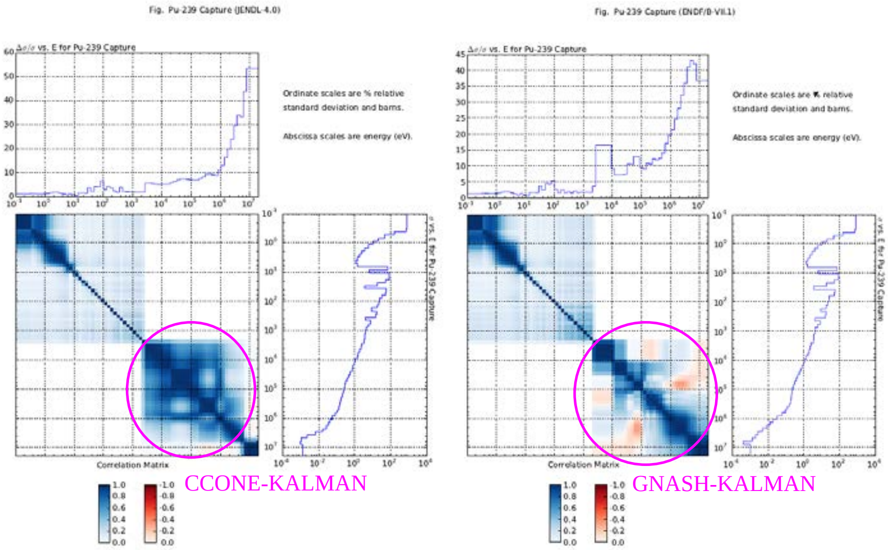
Recommendations

The ENDF evaluators may be asked if there is any physical reason for this discontinuity at 2.5 keV.

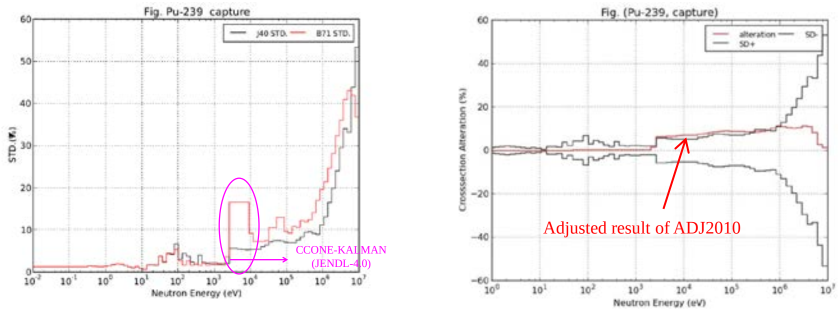
4 The underestimation of the fission variance is attributed to the fact of “so many experimental data points were considered without correlation among different data sets” ([2] p.22).

Figure 2. JENDL-4.0 and ENDF/B-VII.1 covariance–^{239}Pu capture

(a) JENDL-4.0 (b) ENDF/B-VII.1



(c) Comparison of Standard Deviation (d) Alteration of Pu-239 capture cross-section by the adjustment based on JENDL-4.0



It can be concluded that above 2.5 keV, J-4.0 adopted the results of the CCONE-KALMAN calculation [4], therefore, the STD values tend to be smooth in the high-energy region [30]. On the other hand, there seems to be no explanation in the E-7.1 comment file [8] to correspond to its discontinuity. In the US, there is an option according to which the ^{239}Pu capture cross-section above 2.5 keV should be 10% larger than E-7.1 [31], but no information was obtained on this covariance trend. The adjusted result of ADJ2010 in Figure 2 (d) seems to be somewhat coincident with the expectation of ^{239}Pu capture increase, but it needs to be further confirmed.

Recommendations

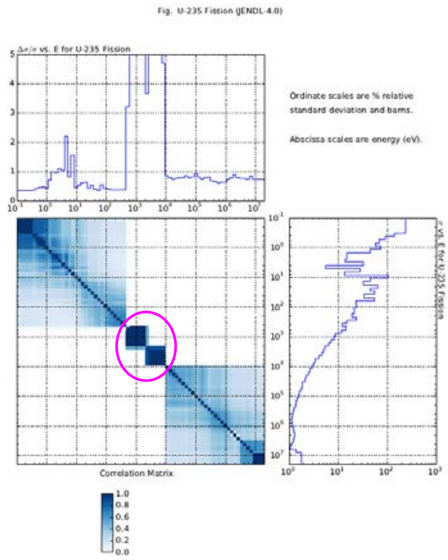
The ENDF evaluators may be asked if there is any physical reason for this discontinuity at 2.5 keV.

3.3. ^{235}U fission

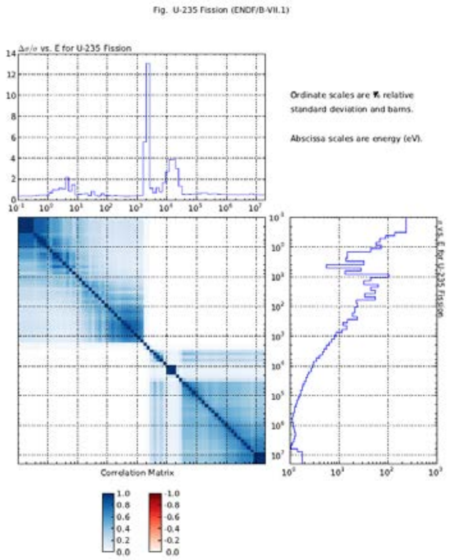
The energy range treated here is 500 eV~10 keV, which is a part of unresolved resonance region in J-4.0 and a part of resolved and unresolved resonance region in E-7.1. Figure 3 exhibits the covariance data and the STD comparison of ^{235}U fission cross-section.

Figure 3. JENDL-4.0 and ENDF/B-VII.1 covariance–^{235}U fission

(a) JENDL-4.0



(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation

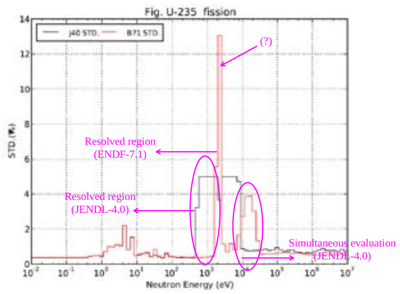


Figure 3 shows that the STD values of E-7.1 in 500 eV~2 keV are extremely low, on the other hand, J-4.0 shows the large values around 5%. Further, E-7.1 has very sharp peak near 2 keV.

It is important to note that J-4.0 adopted the resonance parameter values obtained from Oak Ridge National Laboratory (ORNL) below 500 eV, and re-evaluated in the range of 500 eV~2.25 keV based on those of ENDF/B-VI.5 (= J-3.3) [2]. In 2.25~9keV, the CCONE code was used, and above 10 keV, the simultaneous evaluation was adopted. J-4.0 assumed the STD values of 5% in 500 eV~9 keV [4], but the reason is unknown. The covariance data of E-7.1 in the resolved resonance region (1.0E-5 eV~2.25 keV) were adopted from ORNL-SAMMY analysis. The covariance of E-7.1 in the fast energy region was evaluated with GNASH-KALMAN [9].

Recommendations

The JENDL evaluators could be asked about the physical basis of 5% in the range of 500 eV~ 9 keV, and the ENDF evaluators may explain the reason for the sharp peak around 2 keV, which might be a problem for the processing code NJOY.

3.4. ^{235}U capture

The focused energy range is 500 eV~30 keV, which is the unresolved resonance region of J-4.0, while, the unresolved resonance region of E-7.1 is 2.25 to 25 keV. Figure 4 shows the covariance data and the STD comparison of J-4.0 and E-7.1.

Figure 4 shows that the STD values of J-4.0 in 500 eV~2.25 keV are 10% constant with perfect positive correlations, on the other hand, E-7.1 increases from a few % to 35%. In 2.25~30 keV range, E-7.1 gives the STD values of 35% with almost perfect positive correlations, while J-4.0 shows several % with weak correlations. Further, the negative correlations with high-energy region were found in E-7.1, whereas, no such trend was found in J-4.0.

It can be seen that the resonance parameters of J-4.0 have the same explanation with ^{235}U fission, but the correction was added to make the centre cross-section values close to those of JENDL-3.2 in 500 eV~2.25 keV, according to the discussion made in WPEC/SG29 [5] [2], and the uncertainty was assumed as 10% [4]. Above 2.25 keV, the covariance data were obtained with the least-square calculation with the GMA code, based on the experimental results of the alpha values [6]. The resonance parameters of E-7.1 below 2.25 keV adopted the ORNL results, but the constant STD values of 35% would reflect the recent LANL measurements. The reason for the slope from several % to 35% is unknown.

Recommendations

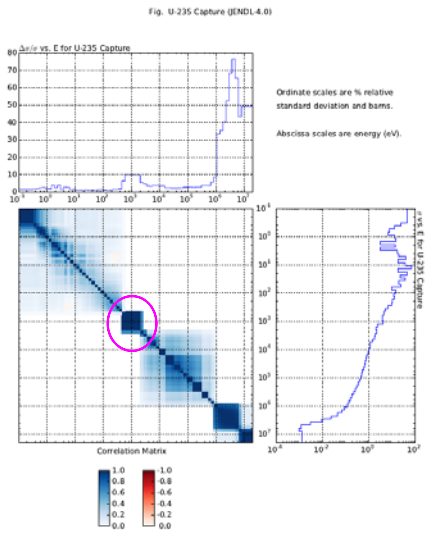
The causes of the observed facts need to be confirmed for both J-4.0 and E-7.1 evaluators.

5 The report of WPEC/SG29 concluded that "The possible overestimation of ^{235}U capture cross-section in the 0.1 to 2.5 keV range is consistent with the alpha measurement and the integral experiments of Na-void reactivity of BFS and FCA, and the criticality trends of FCA and ZEUS. The new FCA experiments were described better with JENDL-3.2 and JENDL-4.0, which have lower ^{235}U capture cross-sections around 1 keV than other libraries. The magnitude of the overestimation could be ~10% or more."

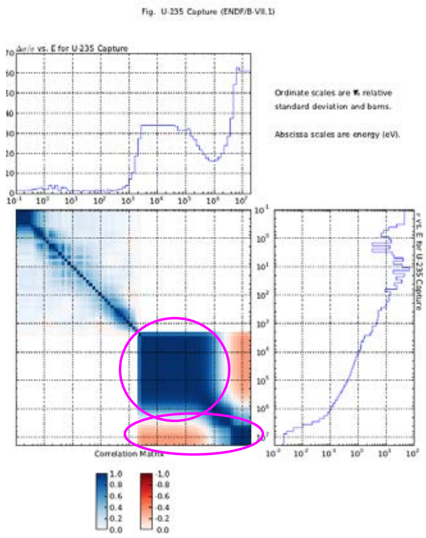
6 Alpha value is defined as the ratio of capture to fission cross-section.

Figure 4. JENDL-4.0 and ENDF/B-VII.1 covariance–^{235}U capture

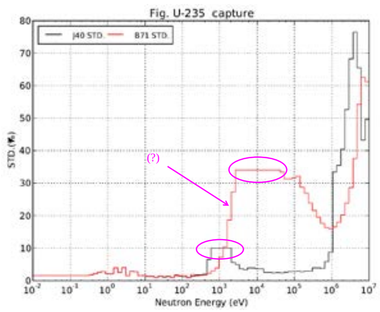
(a) JENDL-4.0



(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



3.5. ^{238}U fission

The energy range treated here is 1~10 MeV above the fission threshold energy. Figure 5 shows the covariance data and the STD comparison for J-4.0 and E-7.1.

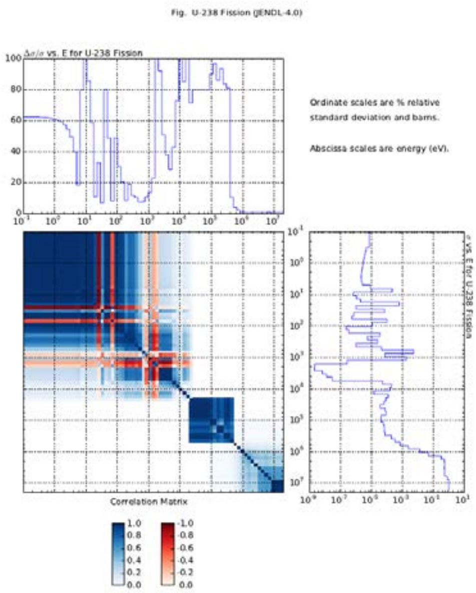
As can be seen in Figure 5, the cross-section and STD values in 1~10 MeV seem very similar between J-4.0 and E-7.1. According to the documents, J-4.0 adopted the results of the simultaneous evaluation [2], while, the covariance data of E-7.1 applied the evaluation done with GNASH-KALMAN [8]. The similar results from the different evaluation methods might come from the ample experimental data of ^{238}U fission.

Recommendations

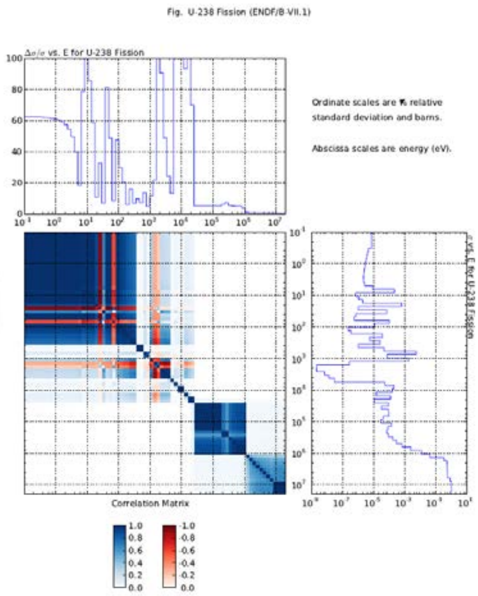
No comments were made on the covariance data of ^{238}U fission.

Figure 5. JENDL-4.0 and ENDF/B-VII.1 covariance–^{238}U fission

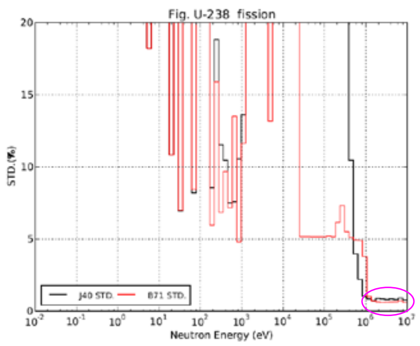
(a) JENDL-4.0



(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



3.6. *^{238}U capture*

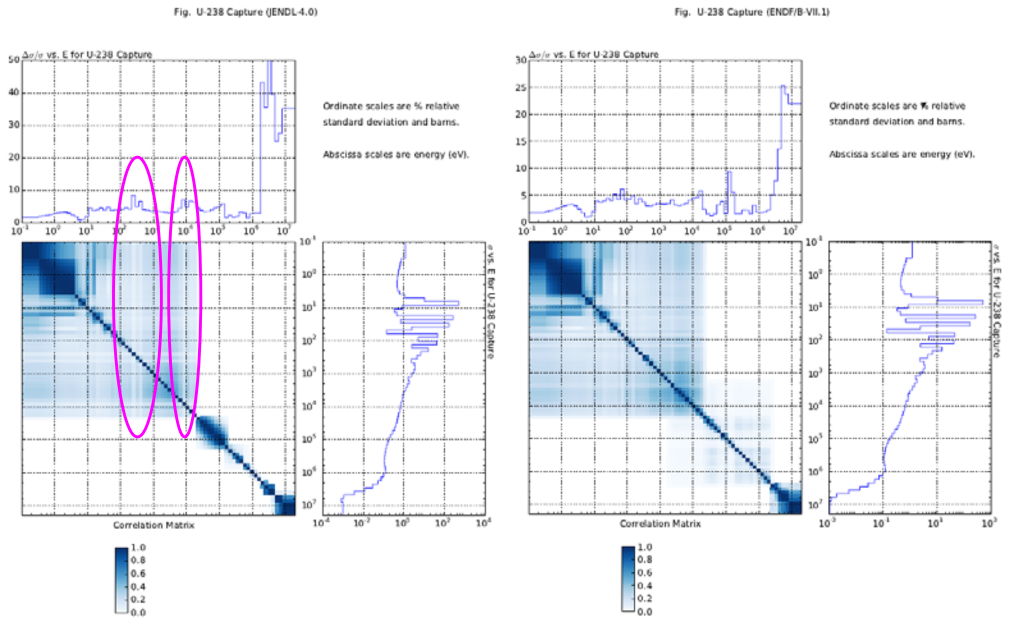
Two energy ranges discussed here are as follows: the first below 20 keV (resolved resonance region), and the second 20~150 keV (unresolved resonance region). The covariance data and the STD comparison of J-4.0 and E-7.1 are depicted in Figure 6.

The covariance data below 20 keV are almost identical between J-4.0 and E-7.1, but the spikes of the STD values appear only in J-4.0, and in the unresolved region of 20~100 keV, the STD values of J-4.0 are significantly larger than those of E-7.1, and vice versa in 100~150 keV.

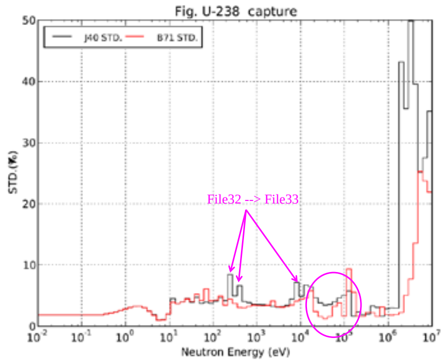
J-4.0 [4] and E-7.1 [9] adopted the same resonance parameters obtained from ORNL, and converted the parameter covariance to File 33. The process from File 32 to File 33 has some arbitrariness such as energy boundaries, therefore, some differences are possible even if the resonance parameters are identical [30]. The ^{238}U capture in the energy range of 20~150 keV greatly affects the breeding ratio and burn-up reactivity loss in the fast reactor applications, therefore, these differences are very important from the nuclear design viewpoint. The covariance data of J-4.0 unresolved resonance parameters were evaluated with ASREP-KALMAN in 1997 [5], but the details are not recorded. The cross-section covariance in this energy region of E-7.1 was evaluated with GNASH-KALMAN [9].

Figure 6. JENDL-4.0 and ENDF/B-VII.1 covariance–^{238}U capture

(a) JENDL-4.0 (b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



Recommendations

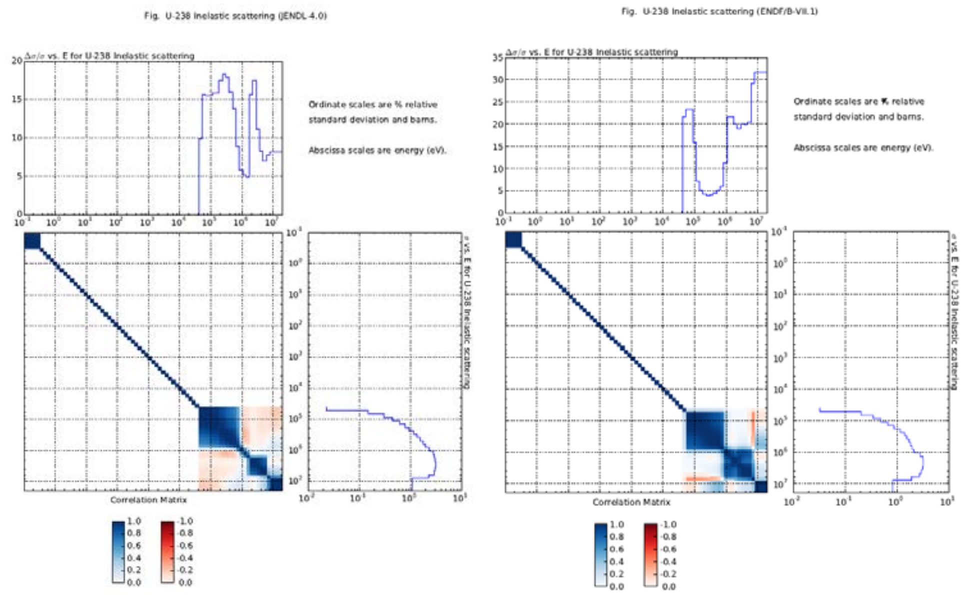
It is very important for fast reactor experts to explore the reason for the observed facts for both J-4.0 and E-7.1 evaluators.

3.7. ^{238}U inelastic

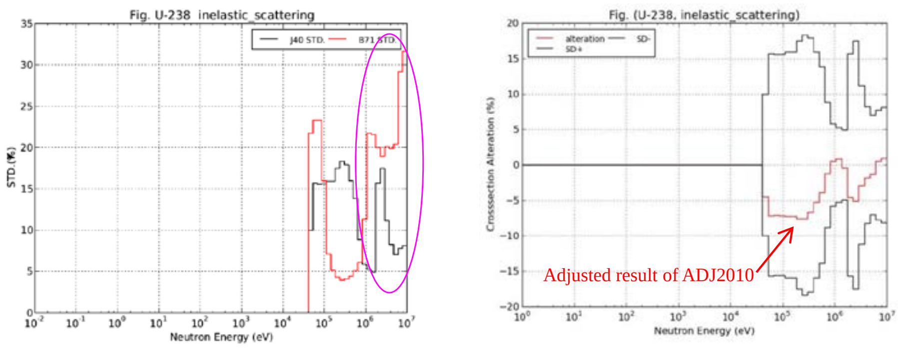
The energy range treated here is above 100 keV with meaningful inelastic cross-section values. Figure 7 shows the covariance data, the STD comparison and the adjusted result in ADJ2010.

Figure 7. JENDL-4.0 and ENDF/B-VII.1 covariance–^{238}U inelastic

(a) JENDL-4.0 (b) ENDF/B-VII.1



(c) Comparison of Standard Deviation (d) Alteration of U-238 inelastic cross-section by the adjustment based on JENDL-4.0



As can be seen in Figure 7, the total inelastic cross-section seems quite similar between J-4.0 and E-7.1, but the STD values and their energy shapes are extremely different.

The authors speculated as to whether the excitation level-wise evaluation of both libraries was different, but the total inelastic cross-section was forced to be similar because of ample measurements etc. However, the total of inelastic cross-section is simply a summation of each level-wise value, unlike the relation between the total and the elastic cross-section case, therefore, this idea was found not to be the reason of the STD differences [30]. The adjusted result of ADJ2010 in Figure 7 (d) shows a possible decrease in ^{238}U inelastic cross-section. [7]

Recommendations

It is recommended to consult both J-4.0 and E-7.1 evaluators about the reason for the STD differences.

3.8. ^{238}U elastic

The energy range discussed here is above 20 keV, which corresponds to the unresolved resonance and the continuous energy regions. The covariance data and the STD comparison are presented in Figure 8, where the STD values and energy shapes of both libraries are rather similar, but the energy regions with strong negative correlations were found in J-4.0, but not in E-7.1.

It was reported that the covariance data of J-4.0 were evaluated by CCONE-KALMAN [4], and those of E-7.1 by GNASH-KALMAN [8], while both applied the relation of "Elastic = Total - Nonelastic" to evaluate the central elastic cross-section values [4,8]. This means that there must be negative correlations between elastic and other partial cross-sections in both libraries, since the accuracy of the total cross-section measurements is generally high. As can be seen in Figure 8 (d), strong negative correlations appear between the elastic and inelastic cross-sections in E-7.1, while J-4.0 does not give such correlations at all.

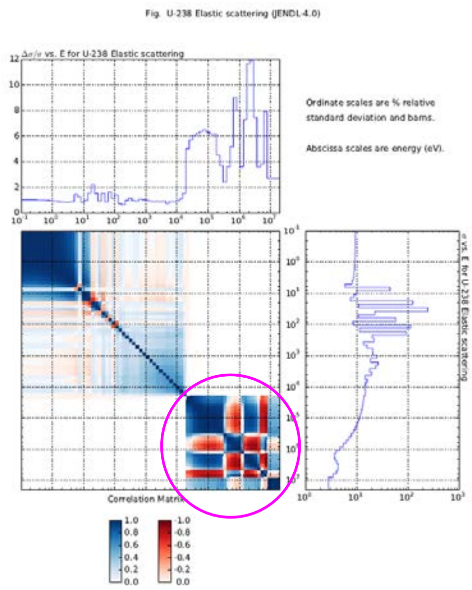
Recommendations

J-4.0 and E-7.1 evaluators should be consulted about the possible reason of the correlation differences in order to deepen the knowledge of the mechanism of the nuclear data evaluation.

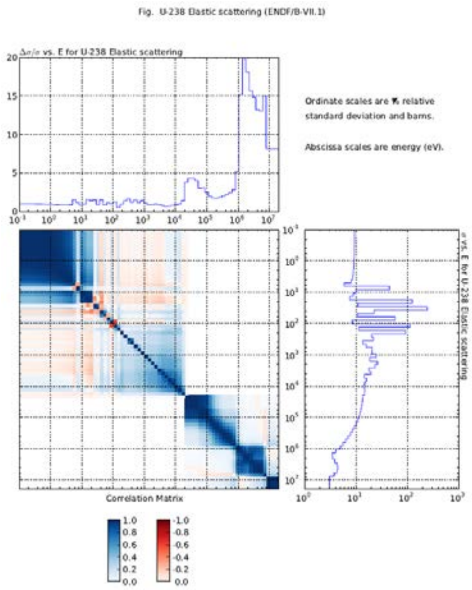
7 The reduction of ^{238}U inelastic cross-section results in the hardening of neutron spectrum. However, we have to be careful about the cross-section alteration, since the alteration of ^{239}Pu fission spectrum always compensates the effect of ^{238}U inelastic cross-section in the fast reactor cores.

Figure 8. JENDL-4.0 and ENDF/B-VII.1 covariance–^{238}U elastic

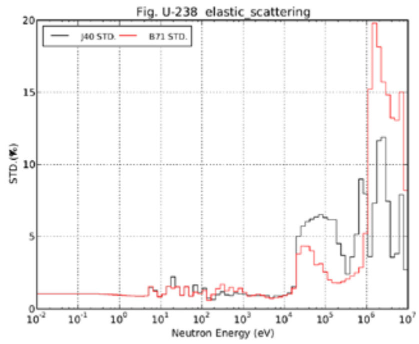
(a) JENDL-4.0



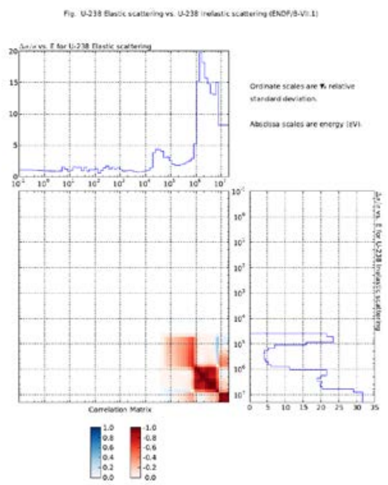
(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



(d) Covariance between U-238 elastic and inelastic cross-sections in ENDF/B-VII.1



3.9. ^{56}Fe elastic

The energy region treated here is below 850 keV, that is, the resolved resonance region. Figure 9 shows the covariance data and the STD comparison.

As can be seen in Figure 9, the covariance data of E-7.1 in the energy region of 30~300 eV and 300 eV~30 keV show the complete correlations respectively, but the the STD values of E-7.1 and J-4.0 are rather similar around 6~8%. Above 30 keV, the STD values of both libraries are utterly different. Further, a sharp peak near 10 keV appears in J-4.0, but not in E-7.1.

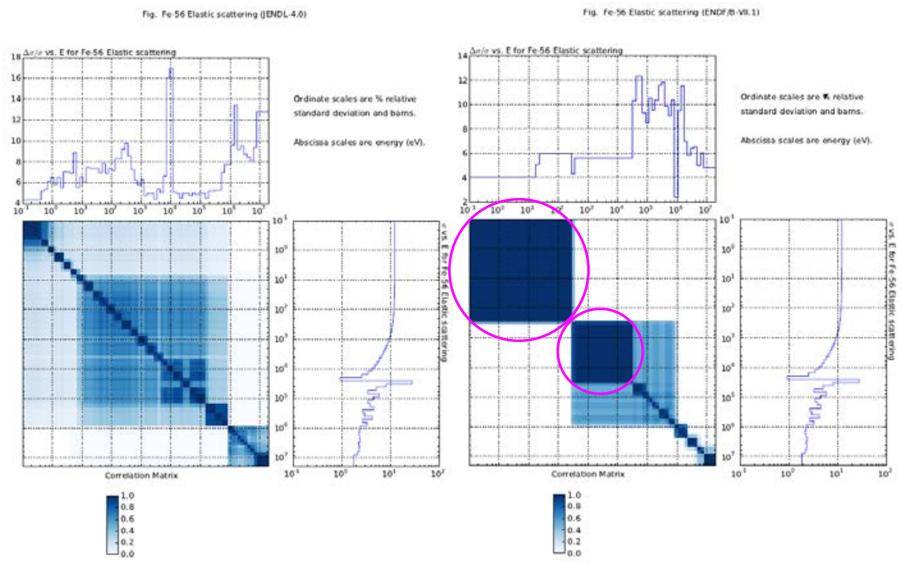
The central cross-sections are almost identical, since they are evaluated with almost the same resonance parameters based on Pereys' evaluation in 1990 [32]. The covariance data of E-7.1 were evaluated by Kernel approximation [8] [15] with the resonance parameter uncertainty of Mugahabghab [9], while those of J-4.0 adopted the least-square calculation of ^{56}Fe experimental data, and corrected the covariance data based on the difference of the least-square-based central values and J-4.0 [4].

Recommendations

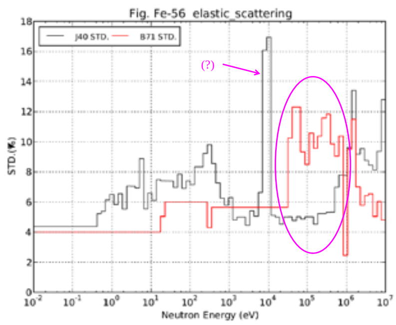
J-4.0 and E-7.1 evaluators should be consulted about the plausibility of the ^{56}Fe elastic covariance data.

Figure 9. JENDL-4.0 and ENDF/B-VII.1 covariance–^{56}Fe elastic

(a) JENDL-4.0 (b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



8 There is a description about the correlation evaluation with Kernel approximation in [15] p.32: “Difficult part of establishing correlation coefficients in our procedure consists in the fact that they are not available in Atlas. Making their plausible estimate is therefore one of the most important issues that an evaluator must resolve.”

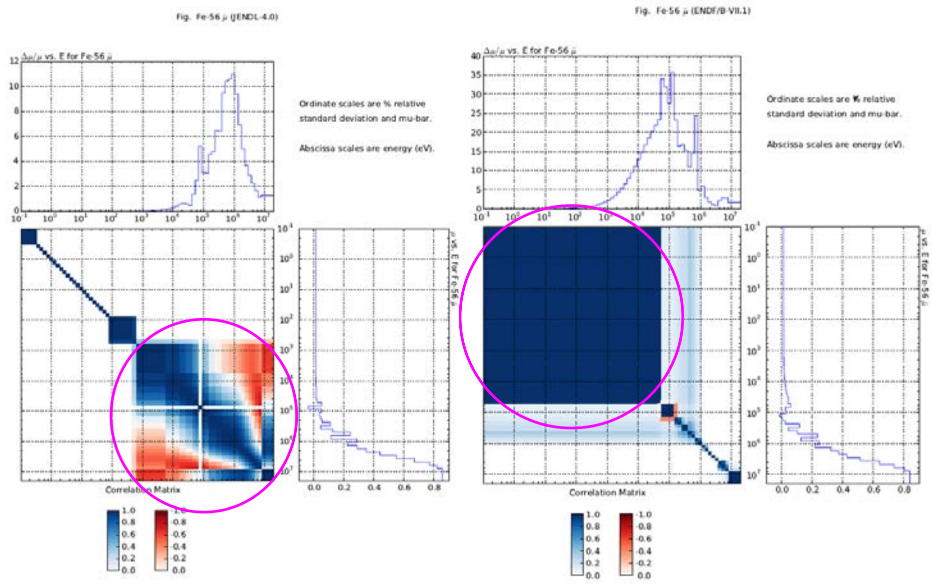
3.10. ^{56}Fe mu-bar

The energy region discussed here is above 10 keV, which has meaningful mu-bar values. Figure 10 shows the covariance data and the STD comparison.

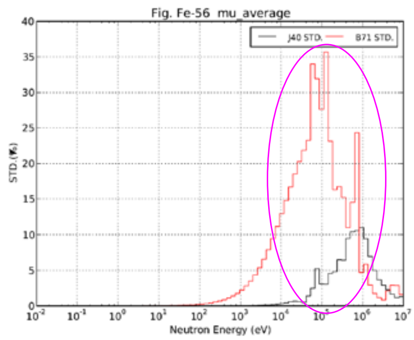
Figure 10 reveals quite a different evaluation of both libraries. In J-4.0, the maximum value of STD is 10%, on the other hand, 35% in E-7.1. The strong negative correlations appear in J-4.0, but not in E-7.1. Further, the correlation factors are a value of +1.0 below 50 keV in E-7.1, but not in J-4.0.

Figure 10. JENDL-4.0 and ENDF/B-VII.1 covariance–^{56}Fe mu-bar

(a) JENDL-4.0 (b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



According to the documentations, the covariance data of J-4.0 were evaluated with ELIESE3-KALMAN in 1997 [5]. Those of E-7.1 are supposed to be obtained with Kernel approximation as well as those of the elastic cross-section [9]. The reason for these large differences between J-4.0 and E-7.1 is unknown.

Recommendations

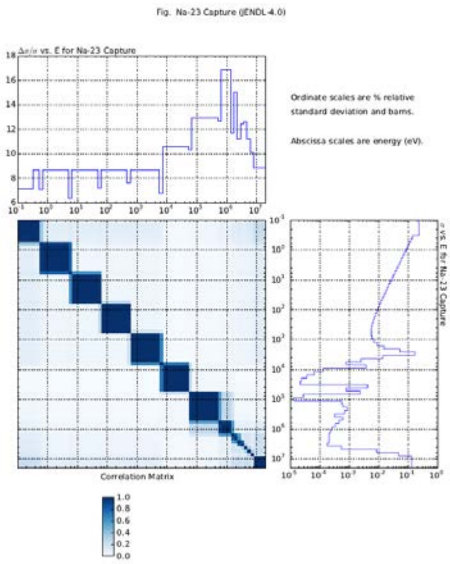
J-4.0 and E-7.1 evaluators should be advised about the reason for the large differences. In addition, E-7.1 has only the covariance data of mu-bar for ^{23}Na, ^{56}Fe and minor actinides, but those of other isotopes such as ^{238}U are also necessary for the reactor application.

3.11. ^{23}*Na capture*

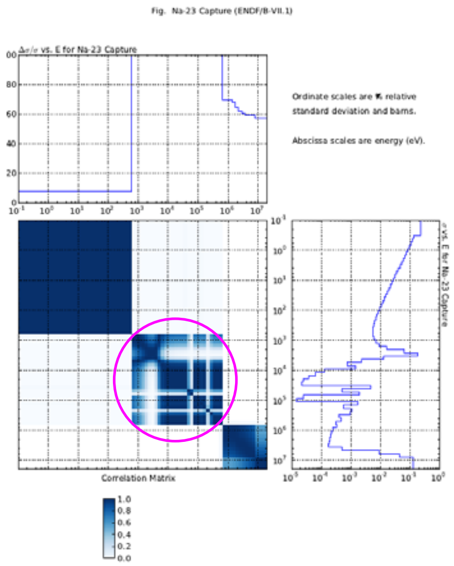
The energy region treated here is 600 eV~600 keV, which is the upper part of resolved resonance in both libraries, and a part of the continuous energy region only in J-4.0. Figure 11 shows the covariance data and the STD comparison.

Figure 11. JENDL-4.0 and ENDF/B-VII.1 covariance–^{23}Na capture

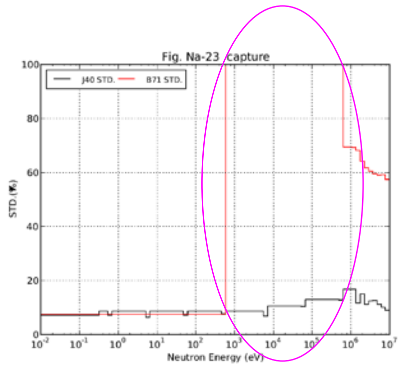
(a) JENDL-4.0



(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



In J-4.0, the STD values are around 10% in the energy range, on the other hand, 100% in E-7.1, although the cross-section values are very small, in milli-barn.

It was reported that the covariance data of J-4.0 were evaluated from the experimental values with the least-square fitting with the GMA code [5], while E-7.1 adopted the results of EMPIRE-KALMAN [9]. The 100% STD value of E-7.1 might have been an assumption which was not changed due to the large experimental uncertainty.

Recommendations

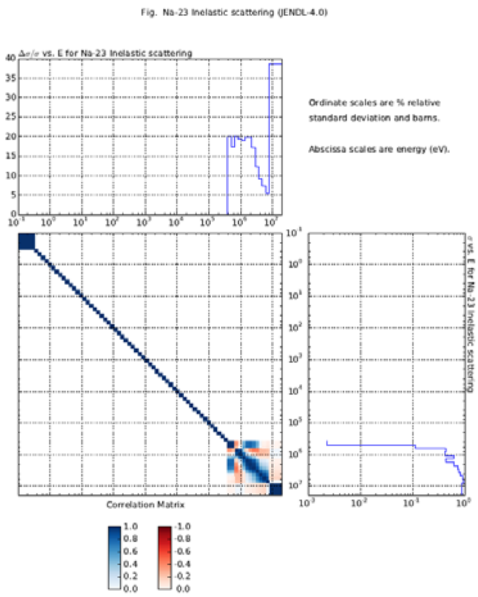
Although this reaction is not important for the reactor application, there would be some concerns from the viewpoint of the sodium activation related to plant maintenance work. J-4.0 and E-7.1 evaluators should be consulted about the reason for the STD differences between 10% and 100%.

3.12. ^{23}Na inelastic

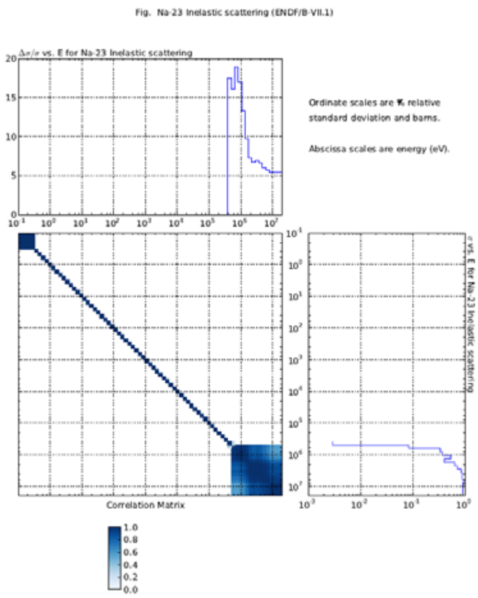
The energy region discussed here is above 1 MeV where the inelastic cross-section has meaningful values. Figure 12 shows the covariance data, STD comparison and the adjusted result of ADJ2010.

Figure 12. JENDL-4.0 and ENDF/B-VII.1 covariance–^{23}Na inelastic

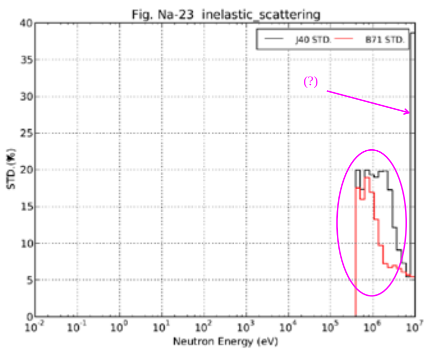
(a) JENDL-4.0



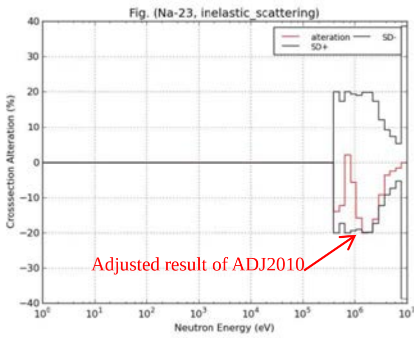
(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



(d) Alteration of Na-23 inelastic cross-section by the adjustment based on JENDL-4.0



As can be seen in Figure 12, the STD values of E-7.1 monotonously decrease from 17% at 1 MeV to 5% at 6 MeV, on the other hand, those of J-4.0 keep a constant value of 20% until 3 MeV, and monotonously decrease to 5% at 6 MeV. Consequently, the STD differences of the two libraries are more than double in the 2~3 MeV region.

The cross-sections of E-7.1 were evaluated with the EMPIRE code using the RIPL library [33], while those of J-4.0 adopted the results of the TNG code (1986), and the first excitation level was multiplied by a factor of 1.25 [4], according to an analytical result of an integral experimental related to neutron penetration in thick sodium layers at ORNL. The covariance data of both libraries were evaluated with KALMAN [4,8], but there is no information related to the large STD differences between J-4.0 and E-7.1. The adjusted result of ADJ2010 shown in Figure 12 (d) indicates the large decrease of ^{23}Na inelastic cross-section.

Recommendations

J-4.0 and E-7.1 evaluators should be consulted about the physical reason for the large STD differences.

3.13. ^{23}Na elastic

The energy region discussed here is around 2 keV with a giant resonance peak. Figure 13 shows the covariance data, the STD comparison and the adjusted result in ADJ2010.

In J-4.0, the STD values at the resonance peak take the maximum value of 17%, on the other hand, those of E-7.1, the minimum value of 1%. Further, the correlations with other energy region at the peak energy can be seen in J-4.0, but not in E-7.1.

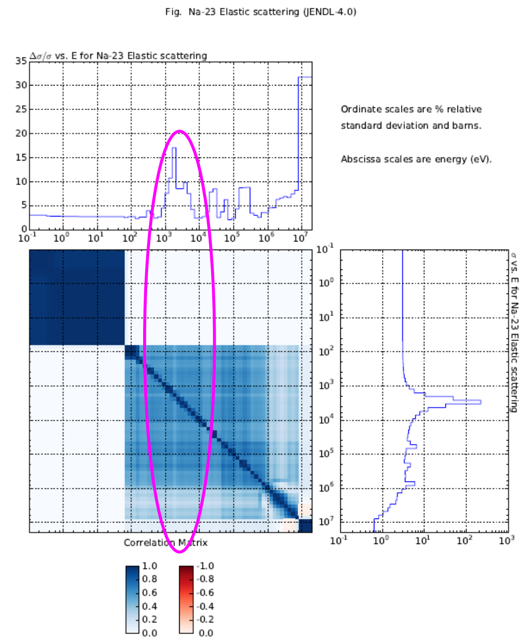
The physical reason for the large covariance differences between the two libraries was interpreted as follows [34]: In this energy range, there appears a giant resonance peak which significantly affects the sodium-voiding reactivity in sodium-cooled fast reactor cores. As shown in Figure 13, the STD values are rather different between the two libraries, that is, the minimum STD value occurs at the cross-section peak energy in E-7.1, in contrast, the maximum appears there in J-4.0. It can be concluded that the trend of E-7.1 seems more natural, since the larger cross-sections would be more accurate due to the small statistical error in the measurement. The correlations are also quite different. In the E-7.1 covariance, the peak around 2 keV has no correlations with other energy, while J-4.0 is partially positive everywhere above 100 eV. The covariance of E-7.1 was evaluated by the EMPIRE/KALMAN combination, where the prior resonance model parameter uncertainties are derived from Mughabghab [9], on the other hand, J-4.0 applies the GMA code with some corrections to meet the measured cross-sections with the evaluated ones of J-4.0, which is based on the multi-level Breit-Wigner formula with rather old resonance parameter values recommended by BNL in 1981 [32]. The central cross-section differences between E-7.1 and J-4.0 are -17~+4% around 2 keV, therefore, the differences of the STD values could be reasonable taking into account the corrections given to the J-4.0 covariance data. Only for information, the adjusted result of ADJ2010 is shown in Figure 13 (d).

Recommendations

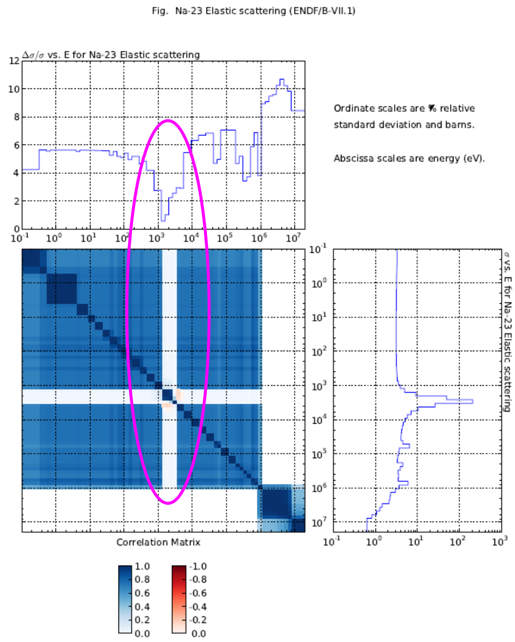
There are no comments for the covariance data of ^{23}Na elastic.

Figure 13. JENDL-4.0 and ENDF/B-VII.1 covariance–^{23}Na elastic

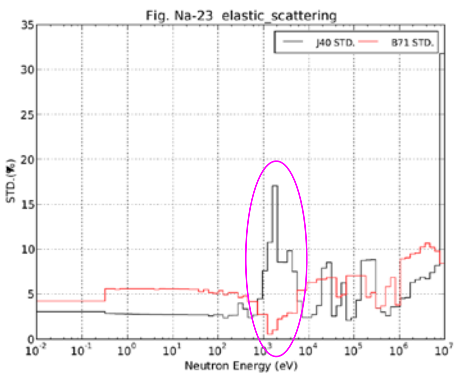
(a) JENDL-4.0



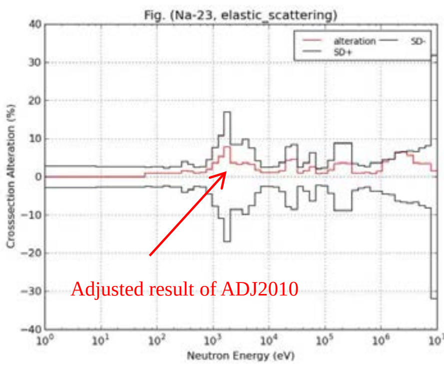
(b) ENDF/B-VII.1



(c) Comparison of Standard Deviation



(d) Alteration of Na-23 elastic cross-section by the adjustment based on JENDL-4.0



4. Conclusion

The latest evaluated nuclear data libraries such as JENDL-4.0, or ENDF/B-VII.1 supply excellent covariance data from the viewpoints of both quality and quantity. However, it is also true that the evaluation of the covariance data has not yet been matured or converged on the satisfactory level in their applications, therefore, the close communication on the evaluation of the covariance data is indispensable between the nuclear data evaluators and users. The recommendations made in the present section are the first trial of WPEC/SG39 to launch such conversations. We believe that the continuous efforts in this field could improve the reliability and accountability of the evaluated covariance data in the near future.

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