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SG39 Deliverables

Summary of Methodology

1. Introduction

For providing 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 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 are possible in the following reactions:

- Pu-239 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. U-238 capture (C28) and Pu-239 fission (F49) for C28/F49
    - Compensation between numerator and denominator
- Many reactions for criticalities
    - Capture, fission, ν, χ, inelastic, elastic, …

In addition, useless and unphysical systematic effects may occur in the cross section adjustments. To avoid the compensation effects and to point out systematic effects, several criteria with parameters/indices are recommended to use. This document summarizes the methodology with the definitions of the parameters/indices. Although a lot of parameters/indices are reported in the intermediate report of Subgroup 33 (Ref. 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 & Review

2.1 Common nomenclature

The following nomenclature is proposed and consistently used here.

- N_E: number of experimental values used in cross section adjustment
- $E_i(i = 1, \dots, N_E)$: experimental value of measured integral parameter i
- $C_i(i = 1, \dots, N_E)$: "a priori" calculated value of integral parameter i
- $C_i'(i = 1, \dots, N_E)$: "a posteriori" calculated value of integral parameter i
- $\sigma_i(i = 1, \dots, N_E)$: "a priori" cross section
- $\sigma_i'(i = 1, \dots, N_E)$: "a posteriori" cross sections
- $S_{ij}(= S_{\sigma,ij})$: sensitivity coefficient for integral parameter i and cross section j
- $M_{EC}(\equiv M_E + M_C)$: integral parameter covariance matrix
- M_E: integral parameter covariance matrix due to experiment covariance
- M_C: integral parameter covariance matrix due to calculation covariance
- M_σ: "a priori" cross section covariance matrix
- M_σ': "a posteriori" cross section covariance matrix
- $\chi^2(\tilde{\sigma})$: chi-square as a function of cross section $\tilde{\sigma}$ to be minimized in the adjustment

- χ^2_{min}: minimized chi-square value
- $G(\equiv M_{EC} + SM_\sigma S^T)$: total integral-parameter covariance matrix (to be inverted in adjustment formulas)
- Matrix indexing:

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

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

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

where

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

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

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

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 minimized 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 minimized 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 minimized 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 valid cross section adjustment.

- No missing/underestimation of uncertainty
- Valid nuclear data covariance: M_σ
- Valid experiment covariance: M_E

- Valid calculation covariance: M_C
- Consistency of C/E values and covariance matrices (=chi-square test), i.e., the next 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.
- Underestimation of experiment and/or calculation uncertainty could give unreliable results as well.
- Overestimation of experiment and/or calculation uncertainty does not affect adjustment results because it is equivalent to elimination of the experiment.

4. Assessment of Adjustment

It is possible to classify assessment techniques into two major categories of (1) assessment before adjustment that is independent from the set of experiments, and (2) assessment after adjustment that depends on the set of experiments. Actually, these assessments often applied repeatedly with changing the set of experiments. These repeated assessment procedures can be used for interpreting the adjustment results.

4.1 Assessment before adjustment

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

(1) Representativity factor

Representativity factor between two experiments, i and $i'$is defined as

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

The representativity factor corresponds to the correlation factor. The complementarity of the experiments can be established by looking at the representativity factor $f_{ii'}$ among the selected experiments.

- If the representativity factor $f_{ii'} \ll 1$,
  - there is strong complementarity between experiments i and i'.

(2) Individual chi-value measured in sigmas

Individual chi-value measured in sigmas is defined as

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

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

- If the individual chi-value measured in sigmas $\chi_{ind,i} \gg 1$,
  - 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

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

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

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

(4) Contribution to chi-square value (Ref.2)

Contribution to chi-square value is defined as

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

This value means a contribution 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 points 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.
  - or otherwise, the integral parameter covariance M_{EC} is 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 to 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
    - Cross section variation is larger than one sigma of the "a priori" standard deviation, and no abnormality is observed in "a priori" cross section covariance matrix
  - Physical mechanism should be investigated
    - Large variations of the cross sections are observed in energy ranges, isotopes or reactions that are not the main target
    - Large variations of the cross sections are produced but the "a posteriori" associated standard deviation reductions 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 .
- For instance the "a posteriori" (= minimum) chi-square contribution indicates the integral parameters that contribute more to the final χ^2_{min}. In this way, it is possible to classify in a hierarchical way which experiment should be discarded or reconsidered. It has to be noted that an experiment can give a negative contribution, which means that the corresponding integral parameter is very effective in the adjustment.

4.3 Interpretation of adjustment mechanism

In some cases, it is useful to interpret the adjustment mechanism for validating a specific cross section adjustment result. One can detect the compensation effects by understanding the adjustment mechanism. For this purpose, three indices are recently proposed (Ref.3).

(1) Mobility in adjustment

Square root of mobility for the reaction j is defeined as

$$\sqrt{D_j} = \mathrm{sgn}\left(M_{\sigma,j} J\right) \sqrt{\left|M_{\sigma,j} J\right|}, \tag{4.6}$$

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

$$J = (1 \quad 1 \quad \cdots \quad 1)^T. \tag{4.7}$$

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 interpreting the adjustment results because it is approximately proportional to cross section alteration. However, it is not always true. In that case, it is recommended to use the square root of mobility.

(2) Adjustment motive force

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

$$F_{i,j} = \frac{\left\| \left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} \right\|}{\|J\|} \cos\theta. \tag{4.8}$$

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

$$\left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} = M_{\sigma,j} S_{i,j}^T G_{i,j}^{-1} \left(J - \frac{C_i}{E_i}\right), \tag{4.9}$$

and

$$\cos\theta = \frac{\left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} \cdot J}{\left\| \left(\frac{\Delta\sigma}{\sigma}\right)_{i,j} \right\| \cdot \|J\|}. \tag{4.10}$$

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 alterations over all energy group. By using the adjustment motive force, one can arrange the experiments in a unique order, and identify the most influential experiment to the alteration of the specific cross section. Note, however, that the discussion with the motive force (and the adjustment potential described later), is limited to the correlations in 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 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 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 considered as a conflict. In this case, the cross section of the reaction is not significantly adjusted. Then, the other freely –adjustable cross sections are altered.

5. Avoiding Compensation Effects

To avoid the compensation effects, Subgroup 39 proposes two major classes of methods, static method and dynamic method, as below.

5.1 Static Method

- Use of specific experiments
  - "Flat" or "steep" adjoint flux reactivity experiments
    - To separate inelastic from absorption cross sections
  - Neutron transmission of leakage experiments
    - Sensitive mostly for inelastic
  - Reaction rate distribution
    - Sensitive mostly for elastic and inelastic
  - Reaction rate ratio
    - Sensitive mostly for specific reactions
  - Sample oscillations

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 reflect the result to nuclear data evaluation. However, we should notice 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 (Ref.4). This section is devoted to review and summarize it.

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:

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

On the other hand, the global “a posteriori” covariance matrix M'_y is rewritten from Eq. (7.2):

$$\begin{aligned} M'_y &= \left(I - M_y S_y^T G^{-1} S_y\right) M_y \\ &= \left(I - \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix} \begin{pmatrix} S_\sigma^T \\ I \end{pmatrix} G^{-1} (S_\sigma \quad I)\right) \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix} \\ &= \left(I - \begin{pmatrix} M_\sigma S_\sigma^T \\ M_{EC} \end{pmatrix} G^{-1} (S_\sigma \quad I)\right) \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix} \\ &= \left(I - \begin{pmatrix} M_\sigma S_\sigma^T G^{-1} S_\sigma & M_\sigma S_\sigma^T G^{-1} \\ M_{EC} G^{-1} S_\sigma & M_{EC} G^{-1} \end{pmatrix}\right) \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix} \\ &= \begin{pmatrix} I - M_\sigma S_\sigma^T G^{-1} S_\sigma & M_\sigma S_\sigma^T G^{-1} \\ M_{EC} G^{-1} S_\sigma & I - M_{EC} G^{-1} \end{pmatrix} \begin{pmatrix} M_\sigma & 0 \\ 0 & M_{EC} \end{pmatrix} \\ &= \begin{pmatrix} M_\sigma - M_\sigma S_\sigma^T G^{-1} S_\sigma M_\sigma & M_\sigma S_\sigma^T G^{-1} M_{EC} \\ M_{EC} G^{-1} S_\sigma M_\sigma & M_{EC} - M_{EC} G^{-1} M_{EC} \end{pmatrix} \end{aligned} \tag{7.2'}$$

By comparing Eq. (7.7) with Eq. (7.2'), one can derive the following equations.

The “a posteriori” cross section covariance matrix:

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

The “a posteriori” integral parameter covariance matrix:

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

The “a posteriori” integral parameter/cross section correlation matrix:

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

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

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

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 raised between the cross section and the integral parameters.

7. Concluding Remarks

The methodology to assess the cross section adjustments are summarized with the proposed common nomenclature. Some of the assessment parameters/indices are well-established and used in many institutions. To achieve a reliable cross section adjustment result, one should make full use of the methodology. In addition, the methodology itself has room for improvement especially for avoiding the compensation effects.

On the other hand, the following remarks on the covariance matrix are noteworthy:

- Not only the standard deviation of the "a priori" covariance matrix but also the correlation significantly affect the adjustment results.
- The "a posteriori" correlation matrix is full and has a significant impact in reducing the "a posteriori" uncertainty.
- The "a posteriori" correlations are useful and physical since they come from combination of two physical data, i.e. differential and integral experiments.
- Once the adjustment is utilized, not only the adjusted cross-sections but the "a posteriori" correlations should be reflected on the nuclear data evaluation, otherwise it might be unphysical.

References

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