Summary of First 2 SG39 Deliverables

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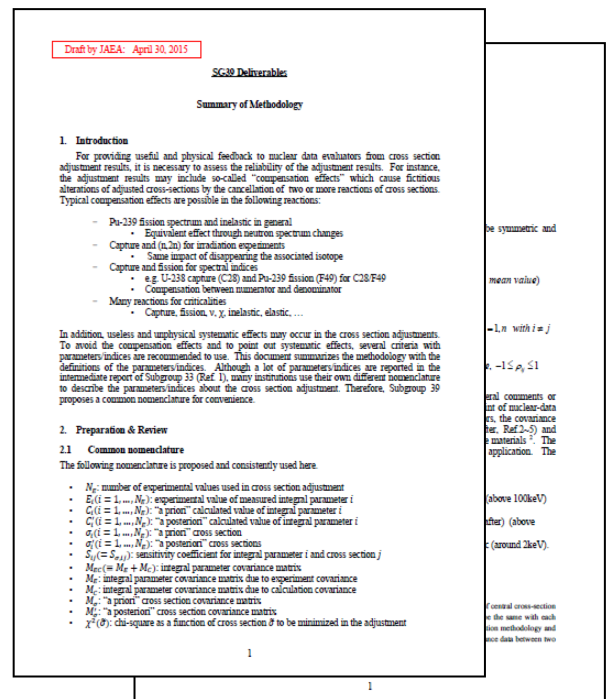
Present Status of Preparing Drafts

- Two drafts of SG39 deliverables are in preparation
- First version of the drafts by JAEA has been distributed to SG39 members at the end of April, 2015
  1. Methodology
  2. Comments on Covariance Data
- Both drafts are based on the presentations in the previous joint SG39 + SG40 meeting held on May 2014



Draft by JAEA: April 30, 2015

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

1

Summary of Draft 1 (Methodology)

- Based on the methodology proposed by INL and JAEA at the moment
  - G. Palmotti, et al., “A-priori and a-posteriori covariance data in nuclear cross section adjustments: issues and challenges,” Joint SG39 + SG40 meeting, May 2014
  - K. Yokoyama, et al., “Revised recommendation from ADJ2010 adjustment,” Joint SG39 + SG40 meeting, May 2014
- Summarized by using common nomenclature proposed and approved by the SG39 members

→ Updating by the SG39 members will be continued

Summary of Draft 2 (Comments on Covariance Data)

- Based on the comments mainly from JAEA
  - M. Ishikawa, “Comments on covariance data of JENDL-4.0 and ENDF/B-VII.1,” Joint SG39+SG40 meeting, May 2014
- On behalf of M. Ishikawa, I have already presented the summary in the previous joint meeting SG39 + SG40 held on May 2014
- The draft was prepared by M. Ishikawa and reviewed by K. Shibata, the top author of JENDL-4.0, before distributing to SG39 members

→ It will be finalized after reflecting a few comments

Summary of Draft 2 (Comments on Covariance Data)

- Comparison of covariance data between JENDL-4.0 and ENDF/B-VII.1
- Comments on the followings:
  - Pu-239: fission (2.5-10keV) and capture(2.5-10keV)
  - U-235: fission (500eV-10keV) and capture (500eV-30keV)
  - U-238: fission (1-10MeV), capture (<20keV, 20-150keV) inelastic (>100keV) and elastic (>20keV)
  - Fe-56: elastic (<850keV) and mu-bar (above 10keV)
  - Na-23: capture (600eV-600keV), inelastic (>1MeV) and elastic (~2keV)

Discussed in the SG39 meeting in Nov. 2014

Methodology studies: summary

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Outline

- Parameters/indices for assessing adjustments
- Premises for valid adjustments
- Assessment of adjustments
- Compensation effects
- Avoiding compensation effects
- Use of “a posteriori” covariance matrix
- Appendix
  - Common nomenclature
  - Adjustment formulas

Parameters for Assessing Adjustments

- Correlation factor between two experiments, E and E'

$$f_{EE'} \equiv \frac{(S_{E'} M_\sigma S_E^T)}{[(S_{E'} M_\sigma S_{E'}^T)(S_E M_\sigma S_E^T)]^{1/2}}$$

- Individual chi-value measured in sigmas (= ratio of |C/E -1| to the total uncertainty):

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

- Ishikawa factor:

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

Parameters for Assessing Adjustments (contd.)

- Initial chi-square value:

$$\chi^2_{init} \equiv (\sigma - \tilde{\sigma})^T M_\sigma^{-1} (\sigma - \tilde{\sigma}) + (E - C(\tilde{\sigma}))^T M_{EC}^{-1} (E - C(\tilde{\sigma}))\Big|_{\tilde{\sigma}=\sigma}$$

$$= (E - C)^T M_{EC}^{-1} (E - C)$$

- Contribution to chi-square value:

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

- Diagonal chi-value measured in sigmas:

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

Indices for Interpreting Adjustments

- Square root of mobility
(= pseudo standard deviation including correlations):

$$\sqrt{D_j} = \mathrm{sgn}(M_{\sigma,j}J)\sqrt{|M_{\sigma,j}|} \quad \text{where} \quad J = [1,1,..,1]^T$$

- Adjustment motive force:

$$F_{i,j} = \frac{\|(\Delta\sigma/\sigma)_{i,j}\|}{\|J\|}\cos\theta \quad \text{where} \quad \begin{aligned} (\Delta\sigma/\sigma)_{i,j} &= M_{\sigma,j}S_{i,j}^T G_{i,j}^{-1}(J - C_i/E_i) \\ \cos\theta &= \frac{(\Delta\sigma/\sigma)_{i,j}\cdot J}{\|(\Delta\sigma/\sigma)_{i,j}\|\cdot\|J\|} \end{aligned}$$

$(\Delta\sigma/\sigma)_{i,j}$ is a special adjustment result, in which only one cross section j is adjusted by using only one integral experiment i

- Adjustment potential
  - This index is calculated with averaged C_I/E_I over a set of core parameters I, which is related to the core parameter i

Premises of Valid 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)

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

- Note:
  - 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
  - Both underestimation and overestimation 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

Assessment of Adjustment

- Before adjustments
  - Some assessments can be performed before adjustments
  - The assessments before adjustment are independent from the set of experiments
- After adjustments
  - Others are done after adjustments with referring to the adjustment results
  - The assessments after adjustment depend on the set of experiments

Assessment of Adjustment (before)

- Selection of experiments
  - Representativity factor: $f_{EE'} << 1$
    - The complementarity of the experiments can be established by looking at the factor among the selected experiments
  - Individual chi-value: $\chi_{ind,i} >> 1$
    - Inconsistency between $|C-E|$ and covariance matrices, $SM_\sigma S$, M_E and M_C
  - Ishikawa factor: IS_i
    - If $IS_i >> 1 \, (S_i M_\sigma S_i^T << (M_{EC})_{ii})$, then $\sigma_j' \approx \sigma_j$ and $S_i M_\sigma' S_i^T \approx S_i M_\sigma S_i^T$
    - If $IS_i << 1 \, (S_i M_\sigma S_i^T >> (M_{EC})_{ii})$, then $S_i M_\sigma' S_i^T \approx (M_{EC})_{ii}$
    - If $IS_i << 1 \, (S_i M_\sigma S_i^T \approx (M_{EC})_{ii})$, then $S_i M_\sigma' S_i^T \approx \frac{1}{2} S_i M_\sigma S_i^T$

Assessment of Adjustment (after)

- 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 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

Assessment of Adjustment (after) (contd.)

- After adjustment if chi-square value is not satisfactory (> 1), experiments can be removed (chi-filtering) based either on diagonal chi-square value (ORNL) or chi-square contribution (INL).
- For instance the "a posteriori" (=minimum) chi-square contribution indicates the integral parameters that contribute more to the final ${\chi_{min}}^2$. 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.

Compensation Effects

- Examples
  - Pu-239 χ 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
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    - Compensation between numerator and denominator
  - Many reactions for criticalities
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Avoiding Compensation Effects (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 (maybe we can find more …)

Avoiding Compensation Effect (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

Use of “A Posteriori” Covariance Matrix

- Not only the standard deviation of the “a priori” covariance matrix, but also the correlations significantly affect the adjustment results
- The “a posteriori” correlation matrix is full and have 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, the “a posteriori” correlations should be reflected to the nuclear data evaluation, otherwise it might be unphysical

APPENDIX

Common Nomenclature

- $E_i(i=1, \ldots, N_E)$: experimental value of measured integral parameter i
- $C_i(i=1, \ldots, N_E)$: "a priori" calculated value of integral parameter i
- $C_i'(i=1, \ldots, N_E)$: "a posteriori" calculated value of integral parameter i
- $\sigma_j\ (j=1, \ldots, N_\sigma)$: "a priori" cross sections
- $\sigma_j'\ (j=1, \ldots, N_\sigma)$: "a posteriori" cross sections
- S_{ij}: sensitivity coefficients for integral parameter i and cross section j
- $M_{EC}=(M_E+M_C)$: 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 function to be minimized in the adjustment
- χ^2_{min} : minimized chi-square value
- $G=(M_{EC}+S\ M_\sigma S^T)$: total integral-parameter covariance matrix (to be inverted in adjustment formulas)

Common Nomenclature (contd.)

- Matrix indexing:

$$A_{ij} = (A)_{ij} = a_{ij}$$

$$A_{i\bullet} = (A)_{i\bullet} = \begin{pmatrix} a_{i1} & a_{i2} & \cdots & a_{in} \end{pmatrix}$$

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

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

Adjustment Formulas

- "A posteriori" cross sections:

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

- "A posteriori" cross section covariance matrix:

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

- Chi-square function to be minimized:

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

- Minimized chi-square value:

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