

Covariance and Sensitivity Data Generation at ORNL

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Abstract

Covariance data are required to assess uncertainties in design parameters in several nuclear applications. The error estimation of calculated quantities relies on the nuclear data uncertainty information available in the basic nuclear data libraries, such as the US Evaluated Nuclear Data Library, ENDF/B. The uncertainty files in the ENDF/B library are obtained from the analysis of experimental data and are stored as variance and covariance data. In this paper we will address the generation of covariance data in the resonance region done with the computer code SAMMY. SAMMY is used in the evaluation of the experimental data in the resolved and unresolved resonance energy regions. The data fitting of cross sections is based on the generalized least square formalism (Bayes' theory) together with the resonance formalism described by R-matrix theory. Two approaches are used in SAMMY for the generation of resonance-parameter covariance data. In the evaluation process SAMMY generates a set of resonance parameters that fit the data, and, it provides the resonance-parameter covariances. For resonance parameter evaluations where there are no resonance-parameter covariance data available, the alternative is to use an approach called the "retroactive" resonance-parameter covariance generation. In this paper we will describe the application of the retroactive covariance generation approach for the gadolinium isotopes.

Covariance Data Generation in SAMMY

Over the years, efforts have been made to improve the quality of the basic nuclear data. Thermal reactor designs and applications have been the driving force for new data evaluations in the low-energy range. Data evaluations in the high energy region have been accomplished primarily in support of shielding applications and fast reactor design. Although the accuracy of the nuclear data, such as the neutron interaction cross sections, has significantly improved, little information exists on nuclear data uncertainties, i.e., nuclear data covariance. The uncertainty files in the ENDF/B library are obtained from analyses of experimental data and are stored as covariance and sensitivity data.

At Oak Ridge National Laboratory (ORNL), data evaluations in the resolved and unresolved resonance energy regions are performed with the computer code SAMMY.¹ In a SAMMY evaluation, experimental data such as transmission data (total cross section), capture cross section, fission cross section, etc., are evaluated by taking into account the uncertainties in the experimental data. Various sources of experimental uncertainties exist that have to be accounted for when performing a data evaluation. These uncertainties include normalization, background, uncertainty in the time-of-flight, uncertainty in the sample thickness, temperature uncertainty, and others. All of these uncertainties are included in the evaluation process in order to properly determine the resonance parameter covariance matrix.

The SAMMY evaluation in the resolved resonance region uses the R-matrix formalism; and in the unresolved range, the evaluation is based on the Hauser-Feshbach theory. Resonance parameters are obtained by fitting the experimental data using the generalized-least-squares technique, from which the parameter covariance matrix is determined.

The final result of a SAMMY evaluation consists of a parameterization of the neutron cross section, i.e., if p_1, p_2, \dots, p_n are resonance parameters, a reaction cross section is written as

$$\sigma_x = \sigma_x(p_1, p_2, \dots, p_n) . \quad (1)$$

The covariance matrix elements for the resonance parameters $\langle \delta p_i \delta p_j \rangle$ are calculated in SAMMY, as well as the derivatives of the cross section with respect to the resonance parameters, i.e., the sensitivity coefficients $\partial \sigma_x / \partial p_i$.

Average Cross Section and Uncertainties

Flux-weighted group cross sections are defined for a reaction cross section, e.g., σ_x , as

$$\bar{\sigma}_{xg} \Phi_g = \int_{E_g}^{E_{g+1}} \sigma_x(E) \Phi(E) dx \quad (2)$$

with

$$\Phi_g = \int_{E_g}^{E_{g+1}} \Phi(E) dx . \quad (3)$$

Here Φ_g is the energy-dependent neutron flux in the energy group g , and $\bar{\sigma}_{xg}$ is the flux-weighted group cross section. The covariance matrix for the group cross section is obtained by taking small increments in $\bar{\sigma}_{xg}$ with respect to the resonance parameters as

$$\delta \bar{\sigma}_{xg} = \sum_j \frac{\partial \sigma_{xj}}{\partial p_j} \delta p_j . \quad (4)$$

The group covariance matrix elements are then obtained by taking expectation values as

$$\langle \delta \bar{\sigma}_{xg} \delta \bar{\sigma}_{xg'} \rangle = \sum_{jk} \frac{\partial \sigma_{xj}}{\partial p_j} \langle \delta p_j \delta p_k \rangle \frac{\partial \sigma_{xk}}{\partial p_k} . \quad (5)$$

The covariance of $\bar{\sigma}_{xg}$ obtained from Eq. (5) is a function of the derivative of the cross sections with respect to the parameters p_j (sensitivities) and the covariance of the parameters p given as $\langle \delta p_j \delta p_j \rangle$. These quantities are available from the SAMMY fitting of the experimental data.

Covariance Generation for Gadolinium Isotopes

To generate resonance covariance data for gadolinium (Gd) isotopes in the resolved and unresolved resonance regions, the resonance parameters in the basic data libraries, ENDF and the Japanese Evaluated Nuclear Data Library (JENDL), were used. The uncertainties in the resonance parameters were obtained from the open literature.² There are seven stable Gd isotopes, namely, ¹⁵²Gd, ¹⁵⁴Gd, ¹⁵⁵Gd, ¹⁵⁶Gd, ¹⁵⁷Gd, ¹⁵⁸Gd, and ¹⁶⁰Gd, with percentage abundances of 0.2, 2.18, 14.8, 20.47, 15.65,

24.84, and 21.86, respectively. The energy limits for the resolved and unresolved energy regions and the basic nuclear data library which were used are shown in Table 1.

Table 1. Resonance energy regions and nuclear data library

| | ¹⁵² Gd | ¹⁵⁴ Gd | ¹⁵⁵ Gd | ¹⁵⁶ Gd | ¹⁵⁷ Gd | ¹⁵⁸ Gd | ¹⁶⁰ Gd |
|--------------------------|--------------------------------|--------------------------------|---------------------------------|--------------------------------|---------------------------------|--------------------------------|--------------------------------|
| Data Library | ENDF | ENDF | ENDF | JENDL | ENDF | JENDL | JENDL |
| Resolved Energy Region | 10 ⁻⁵ eV to 2660 eV | 10 ⁻⁵ eV to 2680 eV | 10 ⁻⁵ eV to 183.3 eV | 10 ⁻⁵ eV to 2214 eV | 10 ⁻⁵ eV to 306.6 eV | 10 ⁻⁵ eV to 6580 eV | 10 ⁻⁵ eV to 4224 eV |
| Unresolved Energy Region | 2660 eV to 50 keV | 2680 eV to 50 keV | 183.3 eV to 60.4 keV | 2214 eV to 100 keV | 306.6 eV to 54.8 keV | 6580 eV to 100 keV | 4224 eV to 100 keV |

The procedure used to generate the resolved and unresolved resonance covariance data for Gd with the SAMMY code is summarized as follows:

- a) Select the best available evaluation from the nuclear data libraries;
- b) Convert the resolved resonance parameters from the Multi-Level Breit-Wigner formalism to the Reich Moore formalism;
- c) Retrieve resonance parameter uncertainties from the literature;²
- d) Generate “experimental” cross section for total, scattering, and capture cross sections with the NJOY code which will be used as “experimental data” in SAMMY;
- e) Assign a global “experimental” uncertainty to the “experimental data.” The error magnitude on the cross sections is chosen to be consistent with the authors’ experiences in data analysis and evaluations;
- f) Run SAMMY code with the option to generate resonance-covariances retroactively;
- g) Convert the resonance-covariance results from SAMMY into the ENDF format for file 32 and MT=151.

The evaluated data library with covariance data obtained by the above procedure was processed with the ERRORJ code.³ ERRORJ is a tool developed to process the ENDF error files in a multigroup form usable in reactor, shielding, and other applications. The present version of ERRORJ generates the temperature-dependent infinitely dilute multigroup covariance. Presently, ERRORJ is the only tool that can process resolved resonance covariance data in the Reich Moore formalism. The covariance data in the unresolved resonance region are generated based on the Single-Level Breit Wigner formalism.

To illustrate the generation of group covariance data, Tables 2 and 3 show the multigroup covariance data generated with the ERRORJ code in the SCALE⁴ 44-group neutron structure for the first 10 groups of energies for ¹⁵⁶Gd. The average of the capture cross section was performed with a 1/E plus fission and fusion weighting spectrum. The relative capture multigroup covariance is shown in Table 3.

Table 2. Capture Cross Section Calculated with ERRORJ

| Group Number | Lower Energy Group Boundary (eV) | Group Flux | Capture Cross Section (barns) |
|--------------|----------------------------------|------------|-------------------------------|
| 1 | 1.0000E-05* | 3.9472E-02 | 8.5432E+00 |
| 2 | 3.0000E-03 | 1.7980E-01 | 4.7980E+00 |
| 3 | 7.5000E-03 | 1.4613E-01 | 3.7243E+00 |
| 4 | 1.0000E-02 | 1.2295E+00 | 2.6588E+00 |
| 5 | 2.5300E-02 | 4.0794E-01 | 2.0977E+00 |
| 6 | 3.0000E-02 | 8.1743E-01 | 1.8703E+00 |
| 7 | 4.0000E-02 | 7.0600E-01 | 1.6488E+00 |
| 8 | 5.0000E-02 | 1.0385E+00 | 1.4381E+00 |
| 9 | 7.0000E-02 | 8.2817E-01 | 1.2168E+00 |
| 10 | 1.0000E-01 | 4.8601E-01 | 1.0110E+00 |

*Read as 1.0×10^{-5}

Table 3. Relative Group Covariance Data Calculated with ERRORJ for Capture Cross Section

| Group Number | Group Number | Relative Group Covariance for Capture Cross Section |
|--------------|--------------|---|
| 1 | 1 | 7.860E-02 |
| 1 | 2 | 2.004E-03 |
| 1 | 3 | 2.003E-03 |
| 1 | 4 | 2.001E-03 |
| 1 | 5 | 2.001E-03 |
| 1 | 6 | 2.001E-03 |
| 1 | 7 | 1.998E-03 |
| 1 | 8 | 1.995E-03 |
| 1 | 9 | 1.993E-03 |
| 1 | 10 | 1.988E-03 |

Conclusion

In summary, a methodology exists at ORNL to generate covariance data in the resolved and unresolved energy regions using the computer code SAMMY. The retroactive covariance generation option in SAMMY permits one to combine the resonance parameter uncertainties and existing resonance parameter evaluations to generate approximate but realistic resonance parameter covariance data. The evaluated covariance data can then be used to generate multigroup covariance data for reactor, shielding, and other applications.

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