

A New Approach for Nuclear Data Covariance and Sensitivity Generation

L. C. Leal^{*}, N. M. Larson^{*}, H. Derrien^{*}, T. Kawano[†] and M.B. Chadwick[†]

^{*}*Oak Ridge National Laboratory*

[†]*Los Alamos National Laboratory*

Abstract. Covariance data are required to correctly assess uncertainties in design parameters in 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 U.S. Evaluated Nuclear Data File, 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. The computer code SAMMY is used in the analysis of the experimental data in the resolved and unresolved resonance energy regions. The data fitting of cross sections is based on generalized least-squares 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, in addition, it also provides the resonance-parameter covariances. For existing resonance-parameter evaluations where no resonance-parameter covariance data are available, the alternative is to use an approach called the "retroactive" resonance-parameter covariance generation. In the high-energy region the methodology for generating covariance data consists of least-squares fitting and model parameter adjustment. The least-squares fitting method calculates covariances directly from experimental data. The parameter adjustment method employs a nuclear model calculation such as the optical model and the Hauser-Feshbach model, and estimates a covariance for the nuclear model parameters. In this paper we describe the application of the retroactive method and the parameter adjustment method to generate covariance data for the gadolinium isotopes.

INTRODUCTION

Over the years, efforts have been made to improve the quality of 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 neutron interaction cross sections, has significantly improved, little information exists on nuclear data uncertainties, and even less exists on nuclear data covariances.

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, and fission cross section are evaluated by taking into account the uncertainties in the experimental data. Various sources of experimental uncertainties must be included when performing a data evaluation. Among these uncertainties are normalization, background, and uncertainty in the time-of-flight; uncertainty in the sample thickness; and temperature uncertainty. All of these uncertainties are included in the evaluation process in or-

der to properly determine the resonance-parameter covariance matrix.

At Los Alamos National Laboratory (LANL), the evaluation of cross sections above the resonance range are performed with nuclear model calculations such as the optical model and the Hauser-Feshbach model. The computer code KALMAN[2] estimates a model parameter covariance by adjusting the parameters to the experimental data available. The covariance matrix of cross sections is given by an error propagation from the model parameter to the cross sections.

COVARIANCE EVALUATION

Covariance Data Generation in SAMMY

The final result of a SAMMY evaluation consists of a parameterization of the neutron cross section. That is, 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 $\langle \delta p_i \delta p_j \rangle$ for the resonance parameters are calculated in SAMMY, as are

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

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

with

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

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

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

Squaring and taking expectation values give the covariance matrix elements as

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

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 of the covariance of the parameters p given as $\langle\delta p_j \delta p_k\rangle$. The sensitivities are calculated either analytically (as in SAMMY) or numerically (as in many processor codes). Covariance matrix elements are available from the SAMMY fitting of the experimental data.

Covariance Data Generation in KALMAN

In the covariance evaluation technique with the KALMAN system[2], the accuracy of model parameters is determined on the basis of the accuracy of experimental data. When the accuracy of measurements is provided, the uncertainties in the model parameters are determined by means of the error propagation

$$P = X - XC^t (CXC^t + V)^{-1} CX, \quad (6)$$

where P is the posterior covariance of the parameters; X , the prior one; V , the covariance of the experimental data; and C , the sensitivity matrix. The accuracy of the

parameters should be determined by the covariance of the experimental data, V , and the prior covariance, X , is unnecessary in principle. However, the matrix X reflects implicit information for the parameters, and it gives a certain upper limit of the uncertainties when reasonable values are given. Such control has the advantage of preventing an unreasonably large uncertainty in a parameter.

The nuclear models considered are the statistical Hauser-Feshbach model, for calculating capture and inelastic scattering cross sections, and the optical model, for the total cross sections. The optical potential parameters, level densities, and γ -ray strength functions are included in this study.

When many experimental data are available, we do not use KALMAN but generate the covariance data directly from those experimental data. This is a model-independent least-squares (LS) technique.

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. There are six stable Gd isotopes, namely, ^{152}Gd , ^{154}Gd , ^{155}Gd , ^{156}Gd , ^{157}Gd , ^{158}Gd , and ^{160}Gd , with percentage abundances of 0.2, 2.18, 14.8, 20.47, 15.65, 24.84, and 21.86, respectively.

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) Generate ‘‘experimental’’ cross sections for total, scattering, and capture cross sections with the NJOY code, for use as ‘‘experimental data’’ in SAMMY.
- (c) Assign a global ‘‘experimental’’ uncertainty to the ‘‘experimental data.’’ (The error magnitude for the cross sections is chosen to be consistent with the authors’ experience in data analysis and evaluations.)
- (d) Run the SAMMY code with the option of generating resonance-covariances retroactively using SAMMY’s new ‘‘propagated uncertainty parameter’’ option to include systematic data uncertainties.[3]
- (e) Convert the resonance-covariance results from SAMMY into the ENDF format for file 32 and MT = 151.

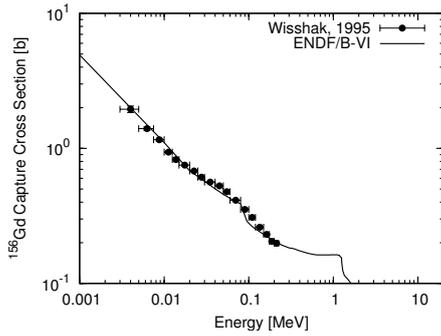


FIGURE 1. Comparison of ^{156}Gd capture cross sections in ENDF/B-VI and experimental data of Wisshak et al.[4]

The covariance data above the resonance region are evaluated as follows:

- The total cross section of ^{152}Gd and ^{154}Gd in ENDF is the optical model calculation. We adopted the KALMAN code to evaluate the covariances. For the other isotopes, the cross section evaluation is based on the experimental data of the natural element. The LS method is utilized for them.
- Covariances of the neutron capture and inelastic scattering cross sections, obtained from nuclear theory, are evaluated with the KALMAN code. The statistical Hauser-Feshbach model is used to calculate cross sections and their model parameter covariances.

The covariance evaluation in the higher-energy region is also “retroactive,” because our evaluation is for an existing data file found in ENDF/B-VI. First we compare the ENDF cross section and the recent capture measurement of Wisshak et al.[4] The experimental uncertainties are about 1–2% in the 10 to 200 keV energy range. Our covariance evaluation includes this experimental accuracy and a deviation of the ENDF/B-VI data from the experimental data.

The evaluated data library with covariance data obtained by the above procedure was processed with the ERRORJ code.[5] 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 is generated on the basis of the Single-Level Breit Wigner formalism.

To illustrate the generation of group covariance data, Table 1 and Figures 2 and 3 show the multigroup covariance data generated with the ERRORJ code in the

TABLE 1. Capture cross sections calculated with ERRORJ

Group	Lower Energy Group Boundary (eV)	Group Flux	σ_{capt} (b)
1	10^{-5}	0.0395	8.54
2	0.03	0.180	4.80
3	0.075	0.146	3.72
4	0.01	1.23	2.66
5	0.0253	0.408	2.10
6	0.03	0.817	1.87
7	0.04	0.706	1.65
8	0.05	1.04	1.44
9	0.07	0.828	1.22
10	0.1	0.486	1.01

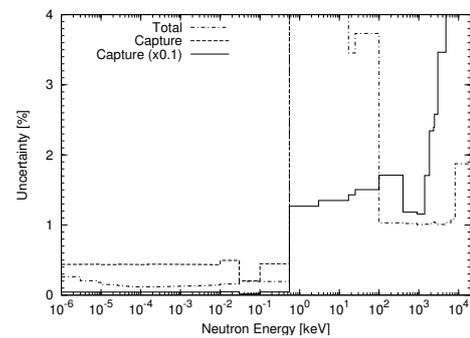


FIGURE 2. Uncertainties in the ^{156}Gd total and capture cross sections, calculated with ERRORJ.

SCALE[6] 44-group neutron structure. The first ten groups of energies for ^{156}Gd , which are in the resonance region, are shown in Table 1. The average of the capture cross section was performed with a $1/E$ plus fission and fusion weighting spectrum. The generated multigroup uncertainties in the total and capture cross sections are shown in Figure 2, and the correlation matrix (scaled by factor of 1000) is plotted in Figure 3. The evaluated uncertainties (processed with ERRORJ) in the 3 to 100 keV range are about 1%, which is consistent with the experimental accuracy we can obtain.

CONCLUSION

In summary, ORNL has developed a methodology 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 generate approximate but realistic resonance parameter covariance data without modifying the existing resonance parameter values.

At LANL, the covariance data are generated with

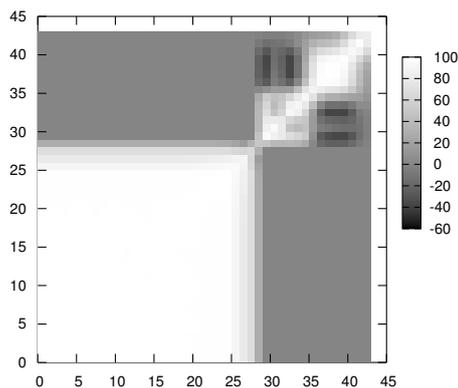


FIGURE 3. Correlation matrix of the ^{156}Gd capture cross section, calculated with ERRORJ.

KALMAN. The data given by KALMAN are basically a representation of experimental data available and a goodness of fitting. The final covariance data are a combination of the data evaluation developed at ORNL and that developed at LANL.

The evaluated covariance data can then be used to generate multigroup covariance data for reactor, shielding, and other applications.

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