Covariance Data for ^{232}Th in the Resolved Resonance Region from 0 to 4 keV

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Abstract

This paper reports on the generation and testing of the covariance matrix associated with the resonance parameter evaluation for ^{232}Th up to 4 keV. [1]

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 US Evaluated Nuclear Data Library, ENDF/B. Uncertainty files in the ENDF/B library are obtained from analysis of experimental data and are stored as variance and covariance data. In this paper, we address the generation of covariance data in the resonance region via the computer code SAMMY, which is used in the evaluation of experimental data in the resolved and unresolved resonance energy regions. The resolved resonance parameter covariance matrix for ^{232}Th, obtained using the retroactive approach, is also presented here.

KEYWORDS: Resonance analysis, covariance generation, benchmark calculations

1. Introduction

In the resonance region, pointwise cross sections are reconstructed using the R-matrix cross-section formalism with evaluated resonance parameters. Uncertainties in the reconstructed cross sections are due to uncertainties in the resonance parameters. For reactor applications, energy-group cross sections are produced by weighting the pointwise cross sections with a neutron flux spectrum and integrating over energies within a group. Consequently, uncertainties in the group cross sections are also dependent on uncertainties in the resonance parameters.

To understand how uncertainties arise in the resonance parameters, we must consider the process by which the parameters are determined: resonance parameters are obtained by fitting experimental data using generalized least-squares techniques in conjunction with R-matrix theory. Such an approach is used in the computer code SAMMY [2] for analyses of available experimental data. The evaluator must understand the uncertainties associated with the experimental data in order to assess the impact of these uncertainties in the evaluation process. The uncertainties come from a variety of sources, such as normalization, background, neutron time-of-flight, sample thickness, etc. These uncertainties are included in the evaluation process, in order to properly determine the long-range energy correlation in the resonance-parameter covariance matrix.

Recently an evaluation of the neutron resonance parameters of ^{232}Th was obtained from a SAMMY analysis of high-resolution neutron transmission measurements and high-resolution capture cross sections. In addition to resonance parameters, the associated resonance-parameter covariance matrix (RPCM) for ^{232}Th was also determined via SAMMY, using the retroactive method. The resulting covariance matrix was then processed by the ERRORJ [3] and PUFF-IV [4] into multigroup form. Subsequently, the TSUNAMI code [5, 6] was used to calculate the uncertainty in the multiplication factor due to uncertainty in the resonance parameters.

2. Retroactive Covariance Evaluation

Often there is a need to produce a covariance matrix for a pre-existing set of resonance parameters. For example, resonance parameters for many nuclides are available in ENDF File 2, but the corresponding covariance matrices are not available. Therefore, a retroactive scheme to generate a realistic approximation for the RPCM has been developed within the context of the generalized least squares equations.

Even when performing a new evaluation, it is sometimes convenient to concentrate first on finding a set of resonance parameters that fit the data, and later focus on determining an appropriate associated RPCM. In practice, we have found that covariance matrices determined retroactively are quite similar to covariance matrices produced directly in the course of the evaluation.

The retroactive scheme operates as follows:

First, artificial "experimental data" are generated using R-matrix theory with the already-determined values for the resonance parameters. Transmission, capture, fission, and other data types (corresponding to those used in the actual evaluation) are calculated, assuming realistic experimental conditions: Doppler temperature, resolution function, etc.

Second, realistic statistical uncertainties are assigned to each data point, and realistic values are assumed for data-reduction parameters such as normalization and background. Let D_j represent the "experimental data" and V_{ij} the covariance matrix for those data. Values for V (both on- and off-diagonal) are derived from the statistical uncertainties on the individual data points and from the uncertainties on the data-reduction parameters, in the usual fashion:

$$V_{ij} = v_i \delta_{ij} + \sum_k \left[g_{ik} \, \Delta^2 r_k \, g_{jk} \right] \quad . \tag{1}$$

In this equation, Δr_k represents the uncertainty on the kth data-reduction parameter r_k, and g_{ik} is the partial derivative of the cross section at energy E_i with respect to r_k. The data covariance matrix V_{ij} then describes all the known experimental uncertainties.

Third, the generalized least-squares equations are used to determine the set of resonance parameters P' and associated covariance matrix M' that fit these data. If P is the original set of resonance parameters (for which we wish to determine the covariance matrix), and T is the

theoretical curve generated from those parameters, then, in matrix notation, the least-squares equations are

$$P' = P + M' G^t V^{-1}(D - T) \quad \text{and} \quad M' = \left(G^t V^{-1} G\right)^{-1} \quad . \tag{2}$$

Here G is the set of partial derivatives of the theoretical values T with respect to the resonance parameters P; G is sometimes called the "sensitivity matrix."

The solutions of Eq. (2) provide the "new" parameter values P' and the associated resonance parameter covariance matrix M', fitting all of the artificial data simultaneously and using the full off-diagonal data covariance matrix for each data set.

If we were analyzing measured data, P' would be different from P. However, because we are analyzing artificially-created data, P' is very nearly identical to P; this follows directly from Eq. (2) when $D = T$. The matrix M', which was derived as the covariance matrix associated with the updated parameters P', is therefore an appropriate representation for the resonance parameter covariance matrix associated with the original set of resonance parameters P.

3. Covariance Evaluation

Recently a Reich-Moore resonance evaluation for ^{232}Th was performed in the energy range from 0 to 4 keV using the computer code SAMMY. The resonance parameters are available in the ENDF/B-VIIbeta2 library. The evaluation resulted in 911 resonances in the energy range from 0 to 4 keV, 8 negative resonances, and 8 resonances above 4 keV, for a total of 927 resonances. Because the fission cross section is negligible below 4 keV, each resonance of ^{232}Th in the Reich-Moore formalism is described by only three parameters: the resonance energy E_r, the gamma width Γ_γ, and the neutron width Γ_n.

The ENDF format available for representing the covariance matrix for resonance parameters in the resolved resonance region is the LCOMP = 1 format, in which the entire covariance matrix is listed. In the newer LCOMP = 2 format, the covariance matrix is represented in a compact form, permitting a reduction in the size of the of the covariance matrix at the expense of accuracy. For the case of ^{232}Th, the LCOMP=1 format was used; the resulting file size is 50 megabytes.

The final ^{232}Th evaluation, including the covariance matrix, was processed using the 44-group ENDF/B-V library structure in SCALE. The results of the processing codes ERRORJ and PUFF-IV were cross-checked in the resolved-resonance region with results obtained from a similar calculation with SAMMY. No major differences were found.

The covariance matrix in the group form is obtained according by first taking small increments in the cross section,

$$\delta\overline{\sigma}_{xg} = \sum_j \frac{\partial \sigma_{xj}}{\partial p_j} \delta p_j \quad , \tag{3}$$

then multiplying $\delta\overline{\sigma}_{xg}$ by $\delta\overline{\sigma}_{x'g'}$ and taking expectation values to give

$$< \delta\bar{\sigma}_{xg} \; \delta\bar{\sigma}_{xg'} > = \sum_{j\,k} \frac{\partial \sigma_{xj}}{\partial p_j} < \delta p_j \; \delta p_k > \frac{\partial \sigma_{xk}}{\partial p_k} \quad . \tag{4}$$

Equation (4) shows that the group covariance matrix is a function of the sensitivities (derivative of the cross sections with respect to the resonance parameters) and of the covariance of the resonance parameters.

Thirty-one of the energy groups in the 44-group structure of the SCALE system [6] are in the energy range below 4 keV. Group-average cross sections and uncertainties generated using the resonance covariances are given in Table 1. Note the effect of the large resolved-resonance levels greater than 10 eV in the magnitude of the cross section. The correlation matrix for the capture cross section is shown in Fig. 1.

Fig. 1. Correlation matrix for the capture cross section for the thirty-one energy groups

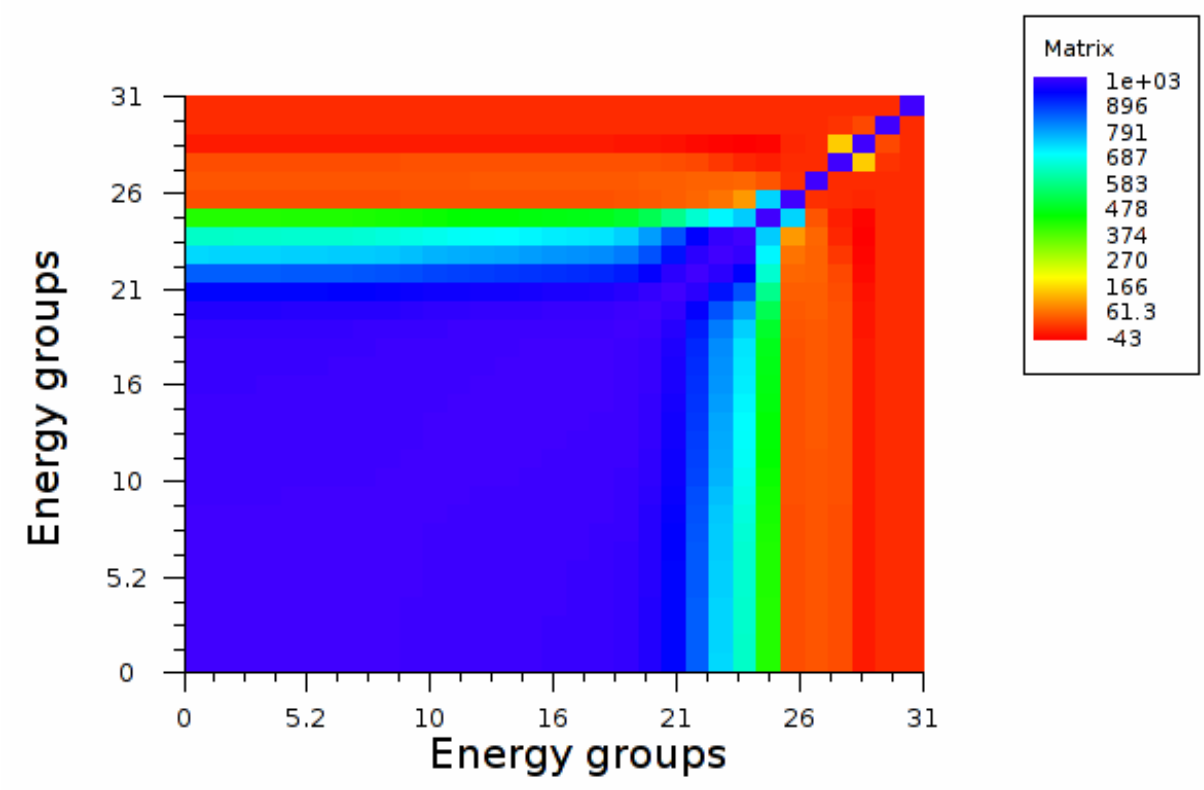


Table 1. Average capture cross section and uncertainty for ^{232}Th calculated with SAMMY

G	E_{min}	E_{max}	σ	δσ
1	0.00001	0.003	40.7465	1.32952
2	0.003	0.0075	16.6662	0.543446
3	0.0075	0.01	12.6052	0.410773
4	0.01	0.0253	9.04371	0.294307
5	0.0253	0.03	7.01618	0.227933
6	0.03	0.04	6.22523	0.202003
7	0.04	0.05	5.45892	0.176858
8	0.05	0.07	4.70415	0.152059
9	0.07	0.1	3.90884	0.125892
10	0.1	0.15	3.16911	0.101518
11	0.15	0.2	2.61193	8.316151E-02
12	0.2	0.225	2.32568	7.374910E-02
13	0.225	0.25	2.17571	6.882891E-02
14	0.25	0.275	2.04701	6.461704E-02
15	0.275	0.325	1.88556	5.935308E-02
16	0.325	0.35	1.74822	5.489914E-02
17	0.35	0.375	1.66923	5.235072E-02
18	0.375	0.4	1.59774	5.005474E-02
19	0.4	0.625	1.33163	4.162456E-02
20	0.625	1.0	0.946675	3.000571E-02
21	1.0	1.77	0.606446	2.080525E-02
22	1.77	3.0	0.357411	1.485115E-02
23	3.0	4.75	0.213502	1.106095E-02
24	4.75	6.0	0.149953	8.793070E-03
25	6.0	8.1	0.118056	8.702677E-03
26	8.1	10.0	0.165135	0.111094
27	10.0	30.0	46.6725	0.875735
28	30.0	100.0	16.1891	0.193321
29	100.0	550.0	8.26973	4.308997E-02
30	550.0	3000.0	3.85223	7.612263E-02
31	3000.0	4000.0	1.15663	3.015903E-02

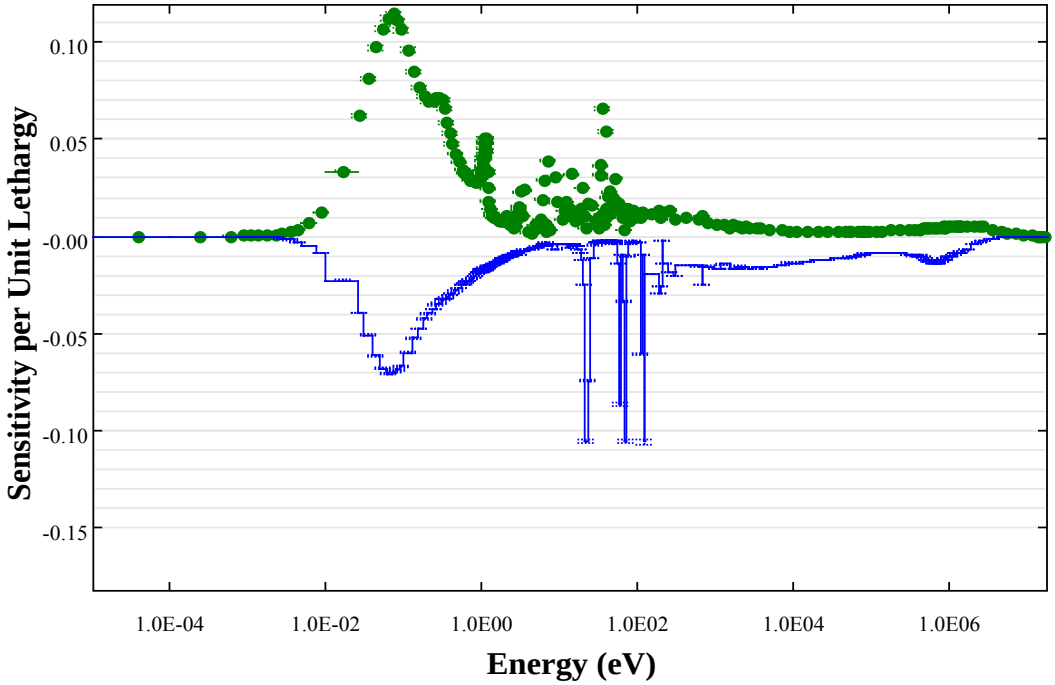
5. Data Uncertainty in Benchmark Calculations

Covariance data generated with the PUFF-IV code in the COVERX [7} format were used in benchmark calculations with the code TSUNAMI. The calculations were done with SCALE 44-group ENDF/B-V cross section data library.[6] The ^{232}Th evaluation in the SCALE library was replaced by the new ^{232}Th cross section evaluation. The AMPX code [8] was used to process problem-dependent shielded cross sections in the 44-group structure. The benchmark system for which the uncertainty in the multiplication factor (k_{eff}) was investigated consists of k_∞

experiments performed at the Institute of Physics and Power Engineering, Obninsk, Russia; these experiments are included in the International Criticality Safety Benchmark Evaluation Project (ICSBEP).[9] Four k_∞ experiments are available with enriched uranium mixed with thorium and polyethylene and the H/^{235}U ratio ranging from 0.0 to approximately 70; these experiments are KBR-18, KBR-19, KBR-20, and KBR-21. Calculations were done for KBR-21 with the ratio H/^{235}U of ~70. The sensitivity of the multiplication factor to the ^{232}Th capture cross section for the KBR-21 benchmark is shown in Fig. 2. Also shown is the sensitivity to the ^{235}U fission cross section. This clearly illustrates the importance of the contribution of the ^{232}Th cross section in determining the uncertainty on k_∞ .

Reference 9 indicates that the experimental k_∞ is 0.964 ± 0.012. Calculations with TSUNAMI give k_∞ = 0.975 ± 0.001. The quoted uncertainty is due the stochastic aspect of the Monte Carlo calculation. The TSUNAMI-calculated uncertainty in k_∞ due to the ^{232}Th data is 0.019. For the KBR-21 system the uncertainty on the ^{232}Th data comes mainly from the capture cross section of ^{232}Th. Work is underway to extend the TSUNAMI calculations to other systems sensitive to the ^{232}Th data.

Fig. 2. Sensitivity of the multiplication factor to the capture cross section of ^{232}Th and fission cross section of ^{235}U, for the KRB-21 benchmark system.



6. Conclusion

Covariance generation for ^{232}Th resonance parameters in the resonance region 0 to 4 keV is presented in this paper. The evaluation was performed with the computer code SAMMY using the Reich-Moore resonance formalism. It has been shown that, despite the large size of the covariance data, it is possible to use uncertainty processing codes such as ERRORJ and PUFF-IV to obtain group cross section on any user-defined neutron group structure. In particular, the calculations presented here are for the 44-group structure of the SCALE system. An example of the application of the uncertainty data was presented for the KBR-21 benchmark system. The uncertainty calculations were done with the TSUNAMI code.

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