

Covariance Data for ^{233}U in the Resolved Resonance Region for Criticality Safety Applications

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Uncertainties in nuclear data play an important role in determining the uncertainties in criticality safety calculations. This paper addresses the evaluation of a physically reasonable covariance matrix for the resonance parameters in the resolved energy region for ^{233}U (0 to 600 eV) to be used for criticality safety applications. Resonance parameters are obtained by fitting experimental data using generalized least-squares techniques in conjunction with a resonance formalism (e.g., R-Matrix theory). Such an approach is used in the computer code SAMMY [1]. The result of a SAMMY evaluation performed on one or more sets of experimental data is a set of resonance parameters that describes all of the fitted experimental data. As an integral part of the evaluation process, SAMMY also provides the covariance matrix for those resonance parameters.

In general, covariance matrices for resonance parameters have not been reported in the current evaluated data files because the dimension of the matrix can be very large and because, until recently, formats in the Evaluated Nuclear Data Files (ENDF) were inadequate. These obstacles have been eliminated with the advent of the new “compact” resonance-parameter covariance matrix format proposed by these authors and adopted by the Cross Section Evaluation Working Group in 2004 for ENDF/B-VII [2].

As reported elsewhere [3], a Reich-Moore resonance evaluation for ^{233}U has been performed in the energy range 0 to 600 eV using the computer code SAMMY. A total of 769 resonances, including the external levels, were identified. At the time the evaluation was performed, the resonance parameter covariance matrix was generated. However, this matrix is no longer available. Unfortunately, this is also true for most existing evaluations. Therefore, an approach was developed within SAMMY to retroactively generate covariance matrices for resonance parameters. This procedure has been used to generate the covariance matrix for the ^{233}U parameters. Each resonance of ^{233}U in the Reich-Moore formalism is described by five parameters (the resonance energy E_r , the gamma width Γ_γ , the neutron width Γ_n , and the two fission widths Γ_{f1} , and Γ_{f2}), for a total of 3845 parameters. The resulting covariance matrix, converted into the original ENDF format, resulted in a file of 100 megabytes. Conversion of the ^{233}U covariance matrix into the new compact format results in a file of only 2 megabytes. This remarkable reduction in the storage space will permit the processing of SAMMY-generated covariance data and the subsequent generation of covariance matrices for groupwise cross sections using computer codes such as ERRORJ [4].

The flux-weighted group cross sections, based on the Bondarenko narrow resonance weighting scheme and the associated uncertainties, were calculated with the SAMMY code using the 44-group structure of the SCALE system. In the Bondarenko scheme, the flux-weighted group cross section is given as

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

where subscript x indicates the reaction type. In this approach $\Phi(E)$ is defined as

$$\Phi(E) = \frac{C(E)}{\sigma_0 + \sigma_t(E,T)} \quad (2)$$

where $C(E)$ is a smooth function of energy, σ_0 is the background cross section, and $\sigma_t(E, T)$ is the energy- and temperature-dependent total 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

$$\delta \bar{\sigma}_{xg} = \sum_j \frac{\partial \sigma_{xj}}{\partial p_j} \delta p_j \quad (3)$$

Squaring and taking expectation values give the covariance matrix elements as

$$\langle \delta \sigma_{xg} \delta \sigma_{xg'} \rangle = \sum_{jk} \frac{\partial \sigma_{xj}}{\partial p_j} \langle \delta p_j \delta p_k \rangle \frac{\partial \sigma_{xk}}{\partial p_k} \quad (4)$$

The covariance of $\bar{\sigma}_{xg}$ obtained from Eq. 4 is a function of (1) the derivative of the cross sections with respect to the parameters p_j (sensitivities), and (2) the parameter covariance $\langle \delta p_j \delta p_k \rangle$.

Twenty-nine energy groups of the 44-group structure are in the energy region below 600 eV. The 29 group boundaries are shown in Table 1. Average total, capture, and fission cross sections were calculated with SAMMY for 500 barns background cross section using Eq. 1 with constant $C(E)$. The group covariance and uncertainties of the group cross sections were also calculated with SAMMY. The results for the average fission cross sections are shown Figure 1. In general, the uncertainties in the fission cross sections are on the order of 2 to 3%. In the full paper we will present and discuss the results of multiplication-factor calculations for the benchmark system containing ^{233}U . The computer code TSUNAMI [5] will be used to assess the impact of the multigroup cross section uncertainties in the multiplication-factor calculations.

Table 1. Twenty -nine energy groups of the 44-group structure

Group Number	Lower Boundary (eV)	Upper Boundary (eV)
1	1.00000E-05	3.00000E-03
2	3.00000E-03	7.50000E-03
3	7.50000E-03	1.00000E-02
4	1.00000E-02	2.53000E-02
5	2.53000E-02	3.00000E-02
6	3.00000E-02	4.00000E-02
7	4.00000E-02	5.00000E-02
8	5.00000E-02	7.00000E-02
9	7.00000E-02	1.00000E-01
10	1.00000E-01	1.50000E-01
11	1.50000E-01	2.00000E-01
12	2.00000E-01	2.25000E-01
13	2.25000E-01	2.50000E-01
14	2.50000E-01	2.75000E-01
15	2.75000E-01	3.25000E-01
16	3.25000E-01	3.50000E-01
17	3.50000E-01	3.75000E-01
18	3.75000E-01	4.00000E-01
19	4.00000E-01	6.25000E-01
20	6.25000E-01	1.00000E+00
21	1.00000E+00	1.77000E+00
22	1.77000E+00	3.00000E+00
23	3.00000E+00	4.75000E+00
24	4.75000E+00	6.00000E+00
25	6.00000E+00	8.10000E+00
26	8.10000E+00	1.00000E+01
27	1.00000E+01	3.00000E+01
28	3.00000E+01	1.00000E+02
29	1.00000E+02	5.50000E+02

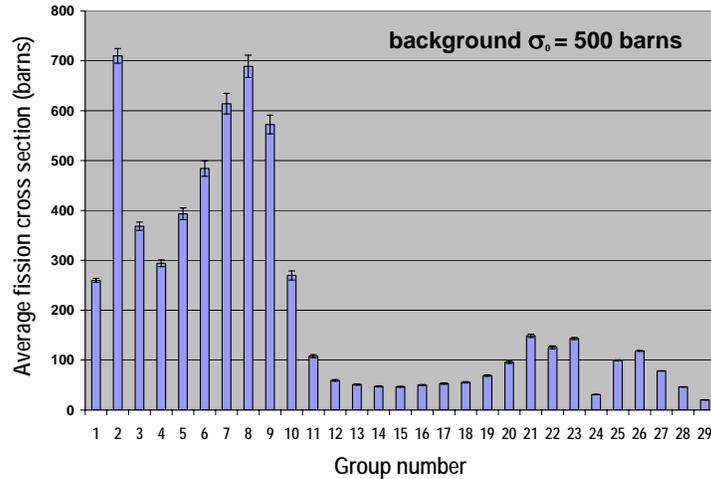


Figure1. Average fission cross section calculated for a background cross section of 500 barns

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