

ORNL METHODOLOGY FOR COVARIANCE GENERATION FOR SENSITIVITY/UNCERTAINTY ANALYSIS

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Abstract

Nuclear data uncertainties as well as covariance data are required to assess nuclear criticality safety margins of nuclear systems. At Oak Ridge National Laboratory (ORNL), data evaluation is performed in the resonance region, both resolved and unresolved, using the computer code SAMMY. Data fitting of the cross sections is based on the generalized least-squares formalism (Bayes' theory) together with the resonance formalism described by the R-matrix theory. The least-squares fitting method allows the evaluator to generate uncertainty and data covariance information for the resonance parameters directly from the experimental data. To illustrate the ORNL methodology for covariance generation, the evaluation of the covariance data for the ^{238}U isotope will be presented.

Introduction

Recently a resonance parameter evaluation of ^{238}U was obtained [1] from a SAMMY [2] 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 ^{238}U was also determined via SAMMY.

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 section are obtained by propagating the uncertainties from the resonance parameters. For reactor applications, 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 derived from uncertainties in the resonance parameters.

To understand how uncertainties in the resonance parameters are calculated, 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. Both systematic and statistical uncertainties in the experimental data are incorporated directly into the fitting procedure, which then determines the long-range correlations in the RPCM. The experimental uncertainties come from a variety of sources, such as normalization, background, neutron time-of-flight, sample thickness, etc. Such an approach is used in the computer code SAMMY for analyses of available experimental data. It is important that the evaluator understand and include the uncertainties associated with the experimental data in order to assess the impact of these uncertainties in the evaluation process.

For use in sensitivity analysis in criticality safety applications, the RPCM is processed into multigroup form by codes such as ERRORJ [3] and PUFF-IV [4]. Uncertainty in the multiplication factor due to uncertainty in the resonance parameters is then computed with the sensitivity analysis code TSUNAMI [5].

1. Covariance Data

1.1 Covariance Evaluation

A detailed description of the cross-section evaluation for ^{238}U can be found in Ref. 1. The ^{238}U resonance parameters are available in the ENDF/B-VII library [6]. The evaluation resulted in 3312 resonances in the energy range from 0 to 20 keV, 22 negative-energy resonances, and 9 resonances above 20 keV— for a total of 3343 resonances. Because the fission cross section is negligible below 20 keV, each resonance of ^{238}U in the Reich-Moore formalism can be described by only three parameters: the resonance energy E_r , the gamma width Γ_γ , and the neutron width Γ_n .

A total of nine experimental sets of differential data were used in the cross-section evaluation up to 20 keV. Four high-resolution transmission measurements, with the length of the neutron flight path ranging from 26.5 to 200 m, were used to obtain the evaluated total cross sections and their corresponding uncertainties. Three sets of capture cross-section data were used, one of which was taken at a 8.7-m flight path to cover the thermal energy range. The second capture measurement was taken at a 26.5-m flight path; the third was a high-resolution measurement at a 150.0-m flight path. Also included in the data used for the evaluation were one fission measurement, one capture measurement at 0.0253 eV (which used the activation measurement technique), and the resonance integral.

The evaluation was performed in the energy range from 0 to 20 keV using the computer code SAMMY [2]. This code calculates the various cross sections via R-matrix theory (Reich Moore approximation), includes corrections for experimental conditions (Doppler and resolution broadening, multiple scattering corrections, backgrounds, etc.), and determines the best fit of theoretical calculation to experimental data by means of a generalized least-squares fitting procedure. Experimental uncertainties may be incorporated directly into the evaluation process in order to propagate those uncertainties into the resonance parameter results.

Uncertainties treated during the ^{238}U evaluation process included statistical and systematic uncertainties for each of the differential data sets plus the quoted uncertainties for the resonance integral and thermal cross section.

The result of the present evaluation is a complete RPCM matrix associated with the set of parameters obtained in Ref. 1. In that work, the SAMMY fits of the experimental data were performed in partial energy ranges; therefore, only partial covariance matrices were obtained. In the present work, a sequential SAMMY fitting of the experimental data was performed in the entire energy range 0 to 20 keV by varying all the parameters of the 3343 resonances (10,029 parameters), thus generating a complete covariance file of 800 megabytes when written in binary format.

1.2 Covariance Testing

Covariance matrices of evaluated data are used for applications such as data adjustment of group constants, evaluation of design accuracy, etc. To prepare for that type of use, tests were done to verify that all the required properties for covariance matrices are followed (positive definite, positive eigenvalues, etc). Additionally, the SAMMY ^{238}U covariance matrix was used to calculate the uncertainty on the average cross section with a constant neutron flux. The covariance matrix of the group cross section $\bar{\sigma}_{xg}$ is obtained by first taking small increments in the cross section,

$$\delta\bar{\sigma}_{xg} = \sum_j \left(\partial\bar{\sigma}_{xj} / \partial p_j \right) \delta p_j \quad , \quad (1)$$

and then squaring and taking expectation values to give

$$\langle \delta\bar{\sigma}_{xg} \delta\bar{\sigma}_{x'g'} \rangle = \sum_{jk} \left(\partial\bar{\sigma}_{xj} / \partial p_j \right) \langle \delta p_j \delta p_k \rangle \left(\partial\bar{\sigma}_{x'k} / \partial p_k \right) \quad . \quad (2)$$

Equation (2) shows that the group covariance matrix $\langle \delta\bar{\sigma}_{xg} \delta\bar{\sigma}_{x'g'} \rangle$ is a function of the sensitivities of the cross section to the resonance parameters $(\partial\bar{\sigma}_{xj} / \partial p_j)$ and of the covariance matrix of the resonance parameters $\langle \delta p_j \delta p_k \rangle$.

The ^{238}U evaluation, including the covariance matrix, was processed with SAMMY using the 44-group structure of the SCALE system [7]. Thirty-two energy groups of the 44-group structure are in the energy range below 20 keV. Group-averaged capture cross sections and uncertainties generated using the resonance parameter covariance data are shown in Table 1. The energy boundary of the energy group 13 was changed to 20 keV.

Table 1. Group-averaged capture cross section in the 44-group structure

Group	Energy Range (eV)	Cross Section (b)	Rel.s.d	Std.dev
13	20000.000–17000.000	0.517430	0.144000	0.074509
14	17000.000–3000.0000	0.812190	0.044108	0.035824
15	3000.0000–550.00000	2.278900	0.022072	0.050300
16	550.00000–100.00000	11.205000	0.021179	0.237300
17	100.00000–30.00000	45.044998	0.023170	1.043700
18	30.00000–10.00000	60.556999	0.019940	1.207500
19	10.00000–8.10000	0.783020	0.015348	0.012018
20	8.10000–6.00000	424.470001	0.011897	5.050100
21	6.00000–4.75000	2.874800	0.010169	0.029232
22	4.75000–3.00000	0.779960	0.019184	0.014963
23	3.00000–1.77000	0.471900	0.031793	0.015003
24	1.77000–1.00000	0.474280	0.030767	0.014592
25	1.00000–0.62500	0.548210	0.025677	0.014076
26	0.62500–0.40000	0.654120	0.021826	0.014277
27	0.40000–0.37500	0.726340	0.020433	0.014841
28	0.37500–0.35000	0.748110	0.020130	0.015059
29	0.35000–0.32500	0.772380	0.019840	0.015324
30	0.32500–0.27500	0.815530	0.019434	0.015849
31	0.27500–0.25000	0.864830	0.019104	0.016522
32	0.25000–0.22500	0.905830	0.018894	0.017115
33	0.22500–0.20000	0.954110	0.018712	0.017853
34	0.20000–0.15000	1.050100	0.018491	0.019417
35	0.15000–0.10000	1.253900	0.018307	0.022954
36	0.10000–0.07000	1.501500	0.018302	0.027480
37	0.07000–0.05000	1.770600	0.018333	0.032461
38	0.05000–0.04000	2.025100	0.018390	0.037241
39	0.04000–0.03000	2.295300	0.018424	0.042288
40	0.03000–0.02530	2.573600	0.018448	0.047478
41	0.02530–0.01000	3.257000	0.018509	0.060285
42	0.01000–0.00750	4.555800	0.018570	0.084601
43	0.00750–0.00300	5.869300	0.018585	0.109080
44	0.00300–0.00001	10.44500	0.018612	0.194400

1.3 Conversion of SAMMY Covariance into ENDF Format and Processing

In the ENDF format, the RPCM matrix is found in File 32 (MT = 151); the specific form for File 32 is designated by the flag LCOMP. If LCOMP = 1, the entire covariance matrix may be listed; if LCOMP = 2, the compact format is used [2,8]. In either case, File 32 can be generated by SAMMY. In the present work, the ^{238}U covariance matrix was generated using option LCOMP = 1. This file was then merged into the latest ^{238}U ENDF/B-VII evaluation [6].

In addition to the resonance parameter covariance matrix, ENDF files require covariance information for the higher energy ranges. For ranges above 20 keV, covariance information was generated at Los Alamos National Laboratory [9]. The final ^{238}U ENDF evaluation, including all pieces of the covariance matrix, was then processed by the cross-section processing codes AMPX (for which the covariance-processing module is PUFF-IV) and NJOY (for which the code ERRORJ is used to process the covariance information). Results from ERRORJ and PUFF-IV were cross-checked in the resolved-resonance region with results obtained from a similar calculation by SAMMY; no major differences were found. Capture cross section correlations for the 44-neutron energy groups calculated with the ERRORJ code are shown in Fig. 1. Uncertainties in the capture cross section in the resonance region (up to 20 keV) range from 1 to 15% (see Table 1). Above 20 keV the uncertainty can be as high as 25%.

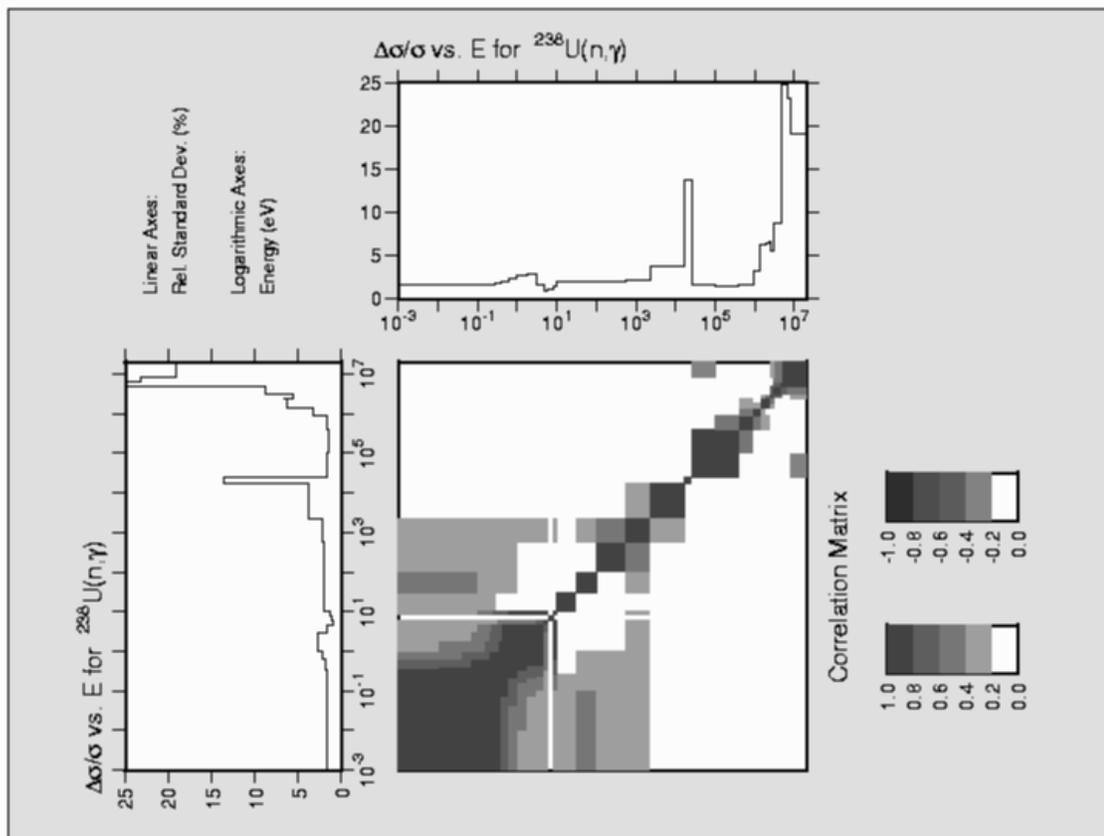


Fig. 1. Correlation matrix for the ^{238}U capture cross section for the energy groups up to 20 MeV

2. Benchmark Calculations and Data Uncertainty

Covariance data generated with the PUFF-IV code in the COVERX [10] format were used in benchmark calculations with the code TSUNAMI. The calculations were done with the SCALE 238-group ENDF/B-V cross-section data library, for which the ^{238}U evaluation in the SCALE library was replaced by the new ^{238}U ENDF/B-VII cross-section evaluation. The AMPX code [11] was used to process the cross sections in the 238-group structure.

The benchmark system for which the uncertainty in the multiplication factor k_{eff} was investigated is the LEU-SOL-THERM-001 unreflected assembly, fueled with aqueous solution of approximately 5% enriched uranyl fluoride, also known as SHEBA-II (Solution High Energy Burst Assembly-II) included in the International Criticality Safety Benchmark Evaluation Project [12]. The sensitivity of the multiplication factor to the ^{238}U capture cross section for the SHEBA-II benchmark is shown in Fig. 2. Also shown in Fig. 2 is the sensitivity to the ^{235}U capture cross section. This illustrates the importance of the contribution of the ^{238}U cross section in determining the uncertainty on k_{eff} .

Calculations with TSUNAMI using the ^{238}U ENDF/B-V 238-group cross section give $k_{\text{eff}} = 1.008398 \pm 0.000296$. The quoted uncertainty is due to the stochastic aspect of the Monte Carlo calculation. Replacing the ^{238}U ENDF/B-V cross section with the ENDF/B-VII cross section and keeping everything else the same produced a value for k_{eff} of 1.004371 ± 0.000314 . The purpose of the present work is to assess the uncertainty in the k_{eff} due to the ^{238}U nuclear data. The TSUNAMI-calculated percentage uncertainty in k_{eff} due to the ^{238}U data is 0.202191 ± 0.00001 . The percentage contribution to the uncertainty in k_{eff} due to various cross sections is shown in Table 2. As can be seen, the uncertainties in k_{eff} are due mainly to the capture and inelastic cross sections. Values in this Table positive and negative indicate correlated and uncorrelated data, respectively. The total uncertainty of 0.202191 ± 0.00001 is obtained by squaring each component of Table 2 and adding (correlated data) or subtracting (uncorrelated data).

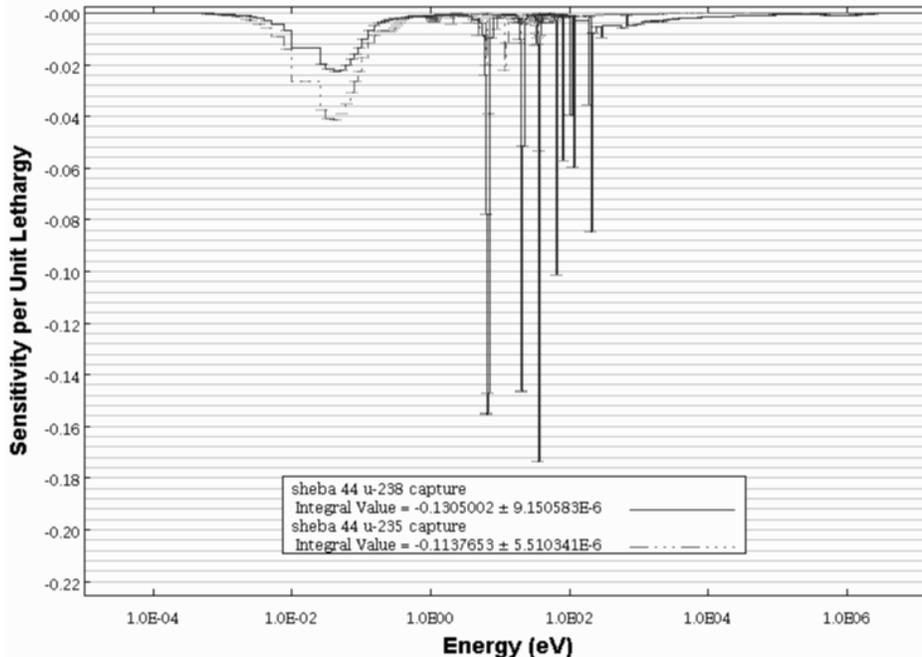


Fig. 2. Sensitivity of the multiplication factor to the capture cross section of ^{238}U and capture cross section of ^{235}U , for the LEU-SOL-THERM-001 benchmark system (i.e., SHEBA-II).

Table 2. Contribution to uncertainty in k_{eff} by individual components or cross-correlations of the various ^{238}U cross sections, in units of % $\Delta k/k$

	n,n'	n,gamma	elastic	nubar	n,2n	fission
n,n'	0.15102 ± 0.00008					
n,gamma		0.14788 ± 0.000005				
elastic	- 0.073720 ± 0.000044	0.0049657 ± 0.0000231	0.033494 ± 0.000020			
nubar				0.020799 $\pm .000001$		
n,2n			- 0.00080726 ± 0.00000032		0.0072928 $\pm .0000032$	
fission		0.00052855± 0.00000002	- 0.00085442 ± 0.00078239			0.0064727 $\pm .0000004$

3. Conclusion

Covariance generation for ^{238}U resonance parameters in the resonance region 0 to 20 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 matrix, it is possible to use uncertainty processing codes such as ERRORJ and PUFF-IV to obtain group cross sections on any user-defined neutron group structure. In particular, the calculations presented here are for the 238-group structure of the SCALE system. An example of the application of the uncertainty data was presented for the SHEBA-II benchmark system. The uncertainty calculations were done with the TSUNAMI code.

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