Covariance Representation in the Resonance Region: Application to ^{233}U Data

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INTRODUCTION

As reported elsewhere [1], a Reich-Moore resonance evaluation for ^{233}U has been performed in the energy range 0 to 600 eV using the computer code SAMMY.[2] 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. 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. In addition to the evaluated resonance parameters, the code SAMMY also provides the associated uncertainties given as the resonance parameter covariance matrix (RPCM). While the resonance parameters are converted to the evaluated nuclear data file (ENDF) format in the so called FILE2 representations the RPCM is converted to the ENDF FILE32 representation. One major drawback for the RPCM is the computer size required to store the data. The ^{233}U RPCM in the ENDF format is a file of 100 MB. The size of the whole ^{233}U cross section library in the ENDF format is about 3 MB. Therefore it is worthwhile to look for an alternative to represent the covariance data in the ENDF format that can still capture all the features inherent of the FILE32 representation with reduced computer storage. The purpose of this paper is to describe a procedure to convert the RPCM representation into the ENDF FILE33 representation. The FILE33 cross section covariance matrix (CSCM) representation is intended to characterize the variances of the cross sections within a specified energy region, and the correlation between cross sections of adjacent energy regions. The choice of CSCM over the RPCM is expected to lead to a reduction in computer storage.

AVERAGE CROSS SECTION AND UNCERTAINTIES

Flux-weighted group cross sections are defined for a reaction cross section, example, σ_x, as

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

with

$$\Phi_g = \int_{E_g}^{E_{g+1}} \Phi(E)\, dx\,. \qquad (2)$$

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

$$\delta\bar{\sigma}_{xg} = \sum_j \frac{\partial\bar{\sigma}_{xgj}}{\partial p_j}\,\delta p_j\,. \qquad (3)$$

Squaring and taking expectation values give the covariance matrix elements as

$$<\delta\bar{\sigma}_{xg}\ \delta\bar{\sigma}_{xg'}> = \sum_{jk} \frac{\partial\bar{\sigma}_{xgj}}{\partial p_j} <\delta p_j\ \delta p_k> \frac{\partial\bar{\sigma}_{xgk}}{\partial p_k}\,. \qquad (4)$$

The covariance of $\bar{\sigma}_{xg}$ obtained from Eq. (4) 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 $<\delta p_j\ \delta p_k>$. The SAMMY generated covariance of the parameters p is converted in the ENDF FILE32 representation.

Alternatively, the group covariance cross section can also be obtained from Eq. 1 as

$$<\delta\bar{\sigma}_{xg}\ \delta\bar{\sigma}_{xg'}> = \frac{1}{\Phi_g\Phi_{g'}} \int_{E_g}^{E_{g+1}}\int_{E_{g'}}^{E_{g'+1}} \Phi(E)\Phi(E')\, COV(\sigma)\, dE dE'\,. \qquad (5)$$

$COV(\sigma)$ is the covariance representation for the pointwise cross section, that is, the ENDF FILE33 representation.

RESULTS AND CONCLUSIONS

A procedure has been developed at Oak Ridge National Laboratory (ORNL) to allow converting FILE32 covariance representation into FILE33 included in the PUFF-IV code.[3] The task is to find an energy group boundary that can be used to represent $COV(\sigma)$ such that the uncertainty in the group cross section calculated with Eq. (5) reproduces the same as that calculated with Eq. (1)

(4). In the energy range 0 to 600 eV it was found that 380 energy boundaries are needed for representing $COV(\sigma)$. These numbers of energies are roughly half of the number of resonances up to 600 eV. The size of the ENDF library using the FILE33 representation is about 8 times smaller than that using FILE32. Cross section uncertainties and covariance were calculated and compared with the PUFF-IV code [3] using the FILE32 and FILE33 ENDF representation of the covariance matrix. To do so, the 44-energy group structure of the SCALE system [4] was used. Average total, capture, and fission cross sections were calculated with the PUFF-IV code using Eq. (4) and Eq. (5) for a constant neutron flux. The results using both representations are identical up to four significant digits. The computer time needed to process the FILE33 covariance information is about 750 times smaller than that using FILE32. The covariance for the capture cross section using the FILE33 representation is shown in Fig. 1. The results displayed in Fig. 1 indicate that the uncertainty in the capture cross section in the resolved and unresolved resonance region up to 40 keV varies from 2% to 10%. In the high energy above 40 keV, the uncertainty in the capture cross section can be as high as 60%. It is concluded that the FILE33 can be used to represent the resonance covariance for ^{233}U. Reduction in the covariance storage and processing time for the ^{233}U evaluation was achieved by converting FILE32 to FILE33 representation. While computer speed and storage have constantly been improving, it is worthwhile to have small sized data evaluations. The evaluations are stored in nuclear data banks, and are retrieved by users worldwide who may have limited network and processing capabilities to download and process the data. The U.S. National Nuclear Data Center (NNDC) [5] has expressed concern about the size of the FILE32 matrices, and NNDC has requested smaller covariance files.

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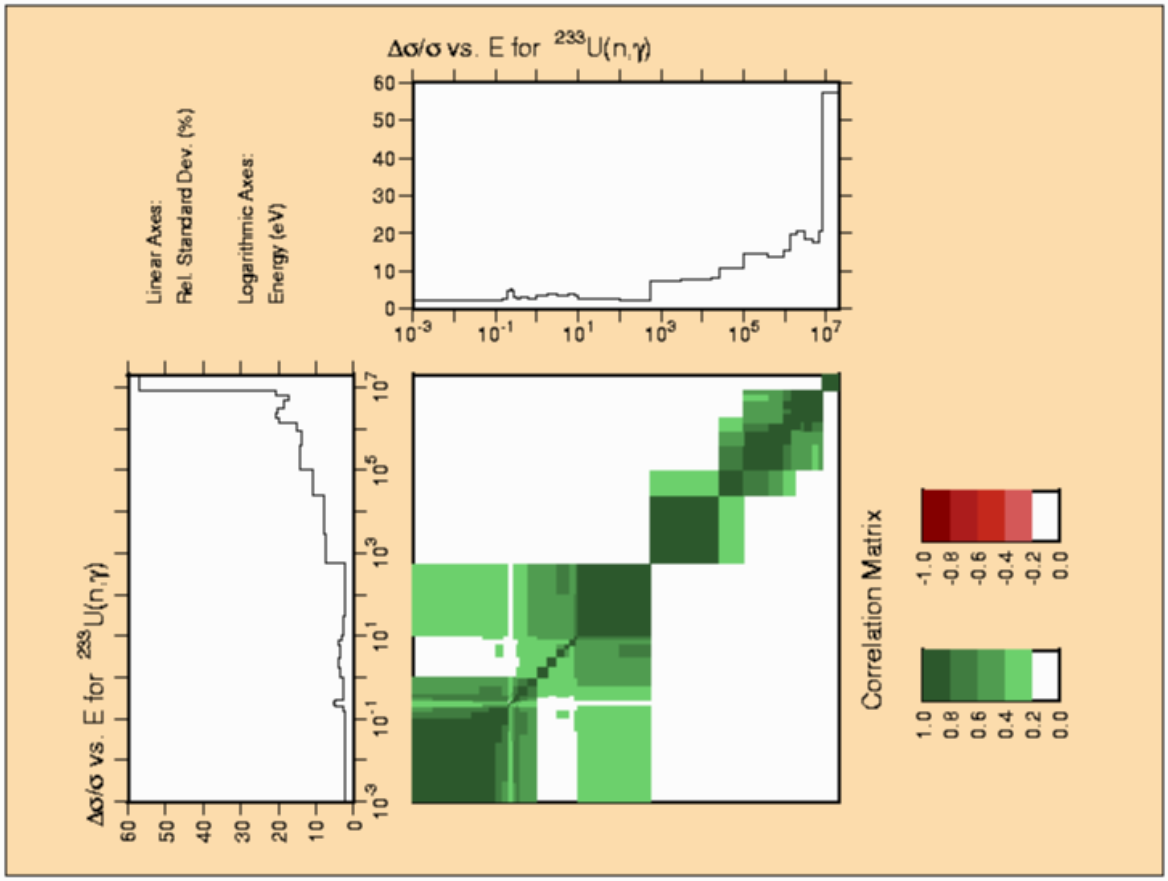

Fig. 1. Uncertainty in the capture cross section calculated with FILE33 representation.