Impact of the ^{235}U covariance data in benchmark calculations

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Abstract

The error estimation for calculated quantities relies on 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 (covariance matrices) in the ENDF/B library are generally obtained from analysis of experimental data. In the resonance region, the computer code SAMMY is used for analyses of experimental data and generation of resonance parameters. In addition to resonance parameters evaluation, SAMMY also generates resonance parameter covariance matrices (RPCM). SAMMY uses the generalized least-squares formalism (Bayes' method) together with the resonance formalism (R-matrix theory) for analysis of experimental data. Two approaches are available for creation of resonance-parameter covariance data. (1) During the data-evaluation process, SAMMY generates both a set of resonance parameters that fit the experimental data and the associated resonance-parameter covariance matrix. (2) For existing resonance-parameter evaluations for which no resonance-parameter covariance data are available, SAMMY can retroactively create a resonance-parameter covariance matrix. The retroactive method was used to generate covariance data for ^{235}U. The resulting ^{235}U covariance matrix was then used as input to the PUFF-IV code, which processed the covariance data into multigroup form, and to the TSUNAMI code, which calculated the uncertainty in the multiplication factor due to uncertainty in the experimental cross sections. The objective of this work is to demonstrate the use of the ^{235}U covariance data in calculations of critical benchmark systems.

1. Covariance evaluation

At Oak Ridge National Laboratory (ORNL), data evaluations in the resolved and unresolved resonance energy regions are performed with the computer code SAMMY (Larson, 2003). In a SAMMY evaluation, the uncertainties in the data, such as statistical and systematic uncertainties, are incorporated in the evaluation procedure. Various sources of experimental uncertainties must be included; among these are normalization, background, neutron time-of-flight, sample thickness, and temperature. Uncertainties in all of these are included in the evaluation process in order to properly determine the resonance-parameter covariance matrix. As reported elsewhere (Leal et al., 1997), a Reich-Moore resonance evaluation (ENDF/B-VI) for ^{235}U has been performed in the energy range 0 to 2250 eV using the computer code SAMMY (i.e., same as ENDF/B-VII.0 resonance evaluation). A total of 3193 resonances, including the external levels, were used. At the time the evaluation was performed, the resonance-parameter covariance matrix was generated; however, this matrix is no longer available. Therefore, an approach was developed within SAMMY to

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retroactively generate approximate covariance matrices for resonance parameters. This procedure has been used to generate the covariance matrix for the ^{235}U parameters. Each resonance of ^{235}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 15965 parameters. The large number of resonance parameters leads to major issues regarding data storage for the covariance file. The required storage for the ^{235}U RPCM in the ENDF/B format is 1.76 Gigabytes (Arbanas et al., 2006). The computer code PUFF-IV (Wiarda and Dunn, 2006) was used to process the ^{235}U evaluation in the ENDF/B format. Changes were made to the PUFF-IV code to reduce the processing time of the covariance data. A great reduction in processing time was achieved. Computation of the cross-section covariance matrices (CSCM) was optimized by utilizing Basic Linear Algebra Subprograms (BLAS) to perform matrices multiplications (Dongarra et al., 1990). This optimization was crucial for computation of CSCM for actinides on energy grids with many points, since multiplication of very large matrices is required in this case. The CPU time used to compute CSCM for ^{235}U on 238-group energy grid decreased from more than a month to only 16 hours of CPU time after the optimization. The covariance evaluations above 2250 eV and for the number of neutrons per fission (ν-bar) were done at Los Alamos National Laboratory (Talou, 2007).

2. Conversion of the ^{235}U RPCM from FILE32 into FILE33

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's disk space required to store the data. In the ENDF format the ^{235}U RPCM representation requires 1.76 Gigabytes of computer storage. The size of the whole ^{235}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 in the FILE32 representation with reduced computer storage. A procedure was developed and implemented in the code PUFF-IV to convert the RPCM representation into the ENDF FILE33 representation. The FILE33 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.

2.1. *Average cross section and uncertainties*

Flux-weighted group cross sections are defined by

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

with

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

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 for reaction x. The covariance matrix for the group cross section is obtained by taking small increments in $\bar{\sigma}_{xg}$ with respect to the j resonance parameters p_j as

$$\delta\bar{\sigma}_{xg} = \sum_j \frac{\partial \bar{\sigma}_{xgj}}{\partial p_j} \delta p_j \ . \tag{3}$$

Squaring and taking expectation values give the covariance matrix elements as

$$\left\langle \delta\bar{\sigma}_{xg}\ \delta\bar{\sigma}_{xg'} \right\rangle = \sum_{jk} \frac{\partial \bar{\sigma}_{xgj}}{\partial p_j} \left\langle \delta p_j\ \delta p_k \right\rangle \frac{\partial \bar{\sigma}_{xgk}}{\partial p_k} \ . \tag{4}$$

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 p_k is given as $\left\langle \delta p_j \delta p_k \right\rangle$. The SAMMY-generated covariance of the parameters p is converted to the ENDF FILE32 representation.

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

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

$COV(\sigma)$ is the covariance representation for the pointwise cross section, that is, the ENDF FILE33 representation. A procedure has been developed and included in the PUFF-IV code at ORNL to allow converting FILE32 covariance representation into the FILE33 format. 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. (4). In the energy range 0 to 2250 eV, it was found that 580 energy boundaries are needed for representing $COV(\sigma)$. The size of the ENDF library using the FILE33 representation is reduced to about 30 Megabytes, that is, 57 times smaller than that using FILE32. Cross section uncertainties and covariance were calculated and compared with the PUFF-IV code using the FILE32 and FILE33 ENDF representation of the covariance matrix. To do so, the 44-neutron energy group structure of the SCALE system (SCALE, 2004) 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. 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.

3. Application of data uncertainty in benchmark calculations

The impact of data uncertainty in calculations for benchmark systems for which ^{235}U isotope is a major component has been investigated. The ^{235}U covariance data were processed with the PUFF-IV code in the COVERX format (Drischler 1980) for use in the calculations with the TSUNAMI code (Rearden, 2003). The covariances were processed into the SCALE 44-group neutron structure. As an example, the capture cross section covariance data processed with PUFF-IV code in the 44-group structure are shown in Fig. 1. The average uncertainty in the capture cross section as displayed in Fig. 1 is about 1% in the resolved resonance energy region (energies smaller than 2250 eV) and 10% above the resonance region.

The TSUNAMI-3D sequence in SCALE uses the KENO V.a Monte Carlo neutron transport code to produce the sensitivity of multiplication factor (k_{eff}) to the cross-section data on an energy-dependent, nuclide-reaction-specific basis. In this calculation, the sensitivities of k_{eff} to the problem-dependent multigroup cross-section data are produced with adjoint-based perturbation theory.

The benchmarks used in the calculations are ten thermal benchmarks, five intermediate energy benchmarks, and three fast systems. The k_{eff} KENO

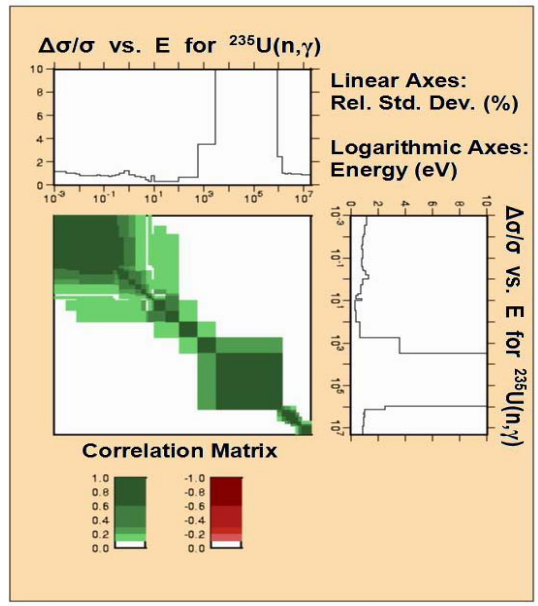

Fig. 1. Correlation matrix for the ^{235}U capture cross section in the 44-neutron energy group structure.

calculations were done with cross section data from the ENDF/B-VI release eight based on the 238-energy group structure of the SCALE system. The benchmark-model k_{eff} and uncertainties for the thermal, intermediate, and fast benchmark systems used in the calculations throughout this paper are listed in Table 1. The quoted values are from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) (International, 2006).

Table 1
Benchmark-model k_{eff} and uncertainties (1 σ)

Benchmark	k_{eff}
HST-001-01	1.0004 ± 0.0060
HST-001-02	1.0021 ± 0.0072
HST-001-03	1.0003 ± 0.0035
HST-001-04	1.0008 ± 0.0053
HST-001-05	1.0001 ± 0.0049
HST-001-06	1.0002 ± 0.0046
HST-001-07	1.0008 ± 0.0040
HST-001-08	0.9998 ± 0.0038
HST-001-09	1.0008 ± 0.0054
HST-001-10	0.9993 ± 0.0054
ZEUS 1	0.9976 ± 0.0008
ZEUS 2	0.9997 ± 0.0008
ZEUS 3	1.0010 ± 0.0009
HISS/HUG	1.0000 ± 0.0004
Godiva	1.0000 ± 0.0010
Flattop-25	1.0000 ± 0.0030
Big-Ten	0.9948 ± 0.0013

3.1. *Thermal benchmark systems*

The thermal benchmark systems for which the uncertainty in the k_{eff} was investigated consist of critical experiments involving a tank of highly enriched uranyl nitrate. This series of experiments was performed in the 1970s at the Rocky Flats Plant. These experiments are included in the ICSBEP and are identified as HEU-SOL-THERM-001.

The sensitivity S of the calculated multiplication factor to the cross section is defined as

$$S = \frac{\sigma_x}{k}\frac{\partial k}{\partial \sigma_x} \quad , \tag{6}$$

where k is the calculated multiplication factor and σ_x is the reaction cross section. If the covariance C matrix evaluated from the experimental data is known, the variance V (or the standard deviation $\sqrt{V}$) of the calculated multiplication factor is given by

$$V = S\,C\,S^t \quad , \tag{7}$$

where S^t is the transpose of S, a neutron energy-dependent array of sensitivity coefficients. The experimental covariance matrix C used in the calculations here is that of the ^{235}U isotope.

The sensitivities of the multiplication factor to the ^{235}U ν-bar, fission, and capture cross sections for the HEU-SOL-THERM-001-01 benchmark are shown in Fig. 2, which indicates that k_{eff} is very sensitive to ν-bar. The KENO calculation of the k_{eff} for this system using the ENDF/B-VI release 8 cross section library is 0.9989 ± 0.0004. The quoted uncertainty is due to the stochastic aspect of the Monte Carlo calculation. As calculated by TSUNAMI, the uncertainty in k_{eff} due to the ^{235}U covariance data is 0.7213 ± 0.0002 percent $\Delta k/k$. The contributions to the uncertainty in k_{eff} due to individual cross sections, ν-bar, and their correlations are shown in Table 2. The relative standard deviation (% $\Delta k/k$ in k_{eff}) is computed from individual values by adding the square of the positive values, subtracting the square of the negative values, and taking the square root. As can be seen from Fig. 2, the sensitivity in the k_{eff} is significant in the energy region below 2250 eV.

Table 2
Relative percent standard deviation of k_{eff} due to ^{235}U uncertainty data for the HEU-SOL-THERM-001-01 benchmark system

	(n,γ)	(n,f)	(n,n)	(n,n')	(n,2n)	ν-bar
(n,γ)	$2.0057 \times 10^{-1} \pm 6.7745 \times 10^{-5}$					
(n,f)	$1.1572 \times 10^{-1} \pm 8.3693 \times 10^{-5}$	$8.5765 \times 10^{-2} \pm 9.1514 \times 10^{-5}$				
(n,n)	$1.4599 \times 10^{-2} \pm 3.8936 \times 10^{-6}$	$-6.4656 \times 10^{-3} \pm 2.9765 \times 10^{-6}$	$3.2326 \times 10^{-3} \pm 3.7405 \times 10^{-6}$			
(n,n')			$-6.1170\ 10^{-3} \pm 1.0276 \times 10^{-5}$	$1.0497 \times 10^{-2} \pm 1.2372 \times 10^{-5}$		
(n,2n)			$-6.4745\ 10^{-5} \pm 1.1040 \times 10^{-7}$		$5.6611 \times 10^{-4} \pm 5.2855 \times 10^{-7}$	
ν-bar						$6.7756 \times 10^{-1} \pm 5.2886 \times 10^{-5}$
Relative standard deviation % $\Delta k/k$ in k_{eff} 0.7213 ± 0.0002						

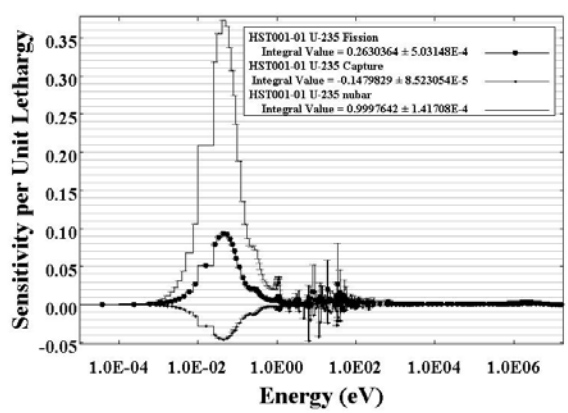

Fig. 2. Sensitivity of the multiplication factor to ν-bar, fission, and capture cross sections for ^{235}U for the HEU-SOL-THERM-001-01 benchmark system.

Therefore the uncertainty in the k_{eff} is predominantly due to the uncertainty in the resonance region of the ^{235}U.

The k_{eff} results for the ten cases of the HEU-SOL-THERM-001 benchmark systems are presented in Table 3. The uncertainty in k_{eff} due to data uncertainty of ^{235}U is also listed. The average uncertainty in k_{eff} due to ^{235}U data is about 0.7%.

Table 3
Uncertainties in k_{eff} and % $\Delta k/k$ due to ^{235}U covariance data for thermal systems

Case	k_{eff}	% $\Delta k/k$ due to ^{235}U covariance data
HST-001-01	0.9989 ± 0.0004	0.7213 ± 0.0002
HST-001-02	0.9952 ± 0.0003	0.6938 ± 0.0001
HST-001-03	1.0025 ± 0.0004	0.7219 ± 0.0002
HST-001-04	0.9987 ± 0.0004	0.6932 ± 0.0001
HST-001-05	0.9999 ± 0.0003	0.7415 ± 0.0002
HST-001-06	1.0033 ± 0.0003	0.7403 ± 0.0002
HST-001-07	0.9987 ± 0.0004	0.7229 ± 0.0002
HST-001-08	0.9998 ± 0.0003	0.7213 ± 0.0002
HST-001-09	0.9948 ± 0.0004	0.6930 ± 0.0001
HST-001-10	0.9939 ± 0.0003	0.7390 ± 0.0001

3.2. *Intermediate-energy benchmark*

The intermediate-energy benchmark systems for which the uncertainty in the k_{eff} was investigated are the following.

a) Three critical experiments of highly enriched uranium platters moderated by graphite and reflected by copper. This series of experiments was performed at the Los Alamos National Laboratory. The experiments are included in the ICSBEP and are identified as HEU-MET-INTER-006 and are referred to as ZEUS.
b) One uranium hydride cylinder reflected by depleted uranium. The experiments were performed at the Los Alamos National Laboratory. They are included in the ICSBEP and are identified as HEU-COMP-INTER-003 and referred to as the UH_3 experiment.
c) One k_∞ experiment in intermediate-energy neutron spectra for ^{235}U identified in the ICSBEP as HEU-COMP-INTER-004 and referred to as HISS/HUG.

The sensitivities of the multiplication factor to the ^{235}U, fission, and capture cross sections for the HEU-MET-INTER-006 (ZEUS case 2) benchmark are shown in Fig. 3. It can be seen that the covariance in the fast region (energy above 2250 eV) also contributes to the uncertainty in the intermediate-energy region. Above the resonance region, the covariance data used were evaluated at the Los Alamos National Laboratory.

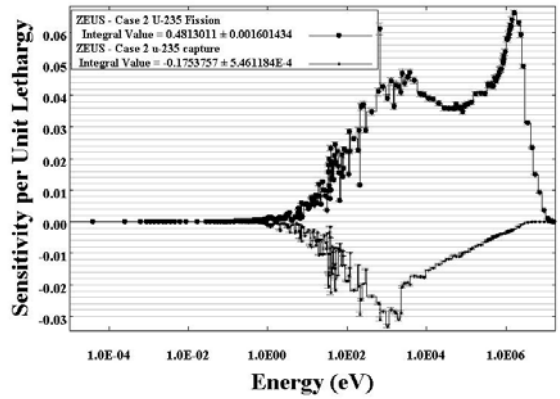

Fig. 3. Sensitivities of the multiplication factor to fission and capture cross sections for ^{235}U for the HEU-MET-INTER-006 (ZEUS case2) benchmark system.

The results for the five intermediate-energy benchmark cases are displayed in Table 4. The uncertainty in k_{eff} due to data uncertainty of ^{235}U is also listed. The average uncertainty in k_{eff} due to ^{235}U data for the ZEUS benchmarks is about 2.5%. The larger uncertainties in k_{eff} for the ZEUS benchmarks are driven by the uncertainties in the cross sections in the high-energy region, which are larger than the cross section uncertainties in the resonance region.

Table 4
Uncertainties in k_{eff} and % $\Delta k/k$ due to ^{235}U covariance data for intermediate energy systems

Case	k_{eff}	$\Delta k/k$ % due to ^{235}U covariance data
ZEUS 1	0.9909 ± 0.0004	2.3511 ± 0.0020
ZEUS 2	0.9942 ± 0.0003	2.6266 ± 0.0039
ZEUS 3	0.9982 ± 0.0003	2.9497 ± 0.0041
UH_3	0.9976 ± 0.0010	1.6829 ± 0.0076
HISS/HUG	1.0098 ± 0.0027	1.0119 ± 0.0027

3.3. *Fast-energy benchmark systems*

Calculations were done for the following three benchmark systems in the fast energy range:

a) the Godiva benchmark, which consists of a bare sphere of highly enriched (94 wt %) uranium identified in the ICSBEP as HEU-MET-FAST-001);
b) the Flattop-25 benchmark, a highly enriched (93 wt %) uranium sphere surrounded by a thick reflector of uranium referred to as HEU-MET-FAST-028; and
c) the Big-Ten, a large mixed-uranium-metal cylindrical core with 10% average ^{235}U enrichment, surrounded by a thick reflector of depleted uranium identified as IEU-MET-FAST-007.

The sensitivities of the multiplication factor to the ^{235}U, fission, and capture cross sections for the Godiva benchmark are shown in Fig. 4.

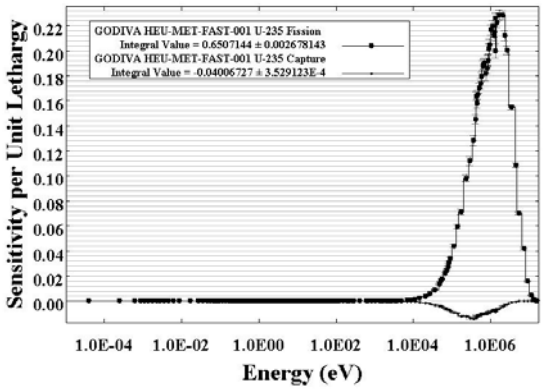

Fig. 4. Sensitivities of the multiplication factor to fission and capture cross sections for ^{235}U for the Godiva benchmark system.

The results for the three fast-energy benchmark cases are displayed in Table 5. The uncertainty in k_{eff} due to data uncertainty of ^{235}U is also listed. The average uncertainty in k_{eff} due to ^{235}U data for these benchmark system ranges from 1 to 3% with the smaller uncertainty for the Godiva benchmark.

Table 5
Uncertainties in k_{eff} and % $\Delta k/k$ due to ^{235}U covariance data for fast systems

Case	k_{eff}	$\Delta k/k$ % due to ^{235}U covariance data
Godiva	0.9956 ± 0.0005	1.1828 ± 0.0026
Flattop-25	1.0010 ± 0.0005	1.3164 ± 0.0031
Big-Ten	1.0199 ± 0.0005	2.1767 ± 0.0020

4. Conclusions and recommendations

Covariance data for ^{235}U resonance parameters in the resonance region 0 to 2250 eV was evaluated at ORNL with the computer code SAMMY using the Reich-Moore resonance formalism. It has been shown that the large size of the covariance matrix will not be a concern. The option of translating the ENDF covariance from the FILE32 into the FILE33 representation leads to a great decrease in computer storage while still capturing all the features inherent in the FILE32. The covariance data can be processed with the PUFF-IV code to obtain group cross section uncertainty data on any user-defined neutron group structure. In particular, the calculations presented here are for the 44-group structure of the SCALE system. The ^{235}U covariance data were used in the TSUNAMI code to assess the uncertainty in k_{eff} for thermal, intermediate-energy, and fast-energy benchmark systems. In conclusion, the benchmark calculations indicate the uncertainties in k_{eff} due to ^{235}U covariance data for thermal systems are less than 1%. For the intermediate and high energy benchmarks the uncertainties varies in between 1 % and 3 %. Further studies are needed to assess these uncertainty results.

5. Acknowledgement

This work was sponsored by the U.S. Department of Energy Nuclear Criticality Safety Program (NCSP), under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

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