DEVELOPMENT AND TESTING OF NEUTRON CROSS-SECTION COVARIANCE DATA FOR SCALE 6.2

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ABSTRACT

Neutron cross-section covariance data are essential for many sensitivity/uncertainty and uncertainty quantification assessments performed both within the TSUNAMI suite and more broadly throughout the SCALE code system. The release of ENDF/B-VII.1 included a more complete set of neutron cross-section covariance data: these data form the basis for a new cross-section covariance library to be released in SCALE 6.2. A range of testing is conducted to investigate the properties of these covariance data and ensure that the data are reasonable. These tests include examination of the uncertainty in critical experiment benchmark model k_{eff} values due to nuclear data uncertainties, as well as similarity assessments of irradiated pressurized water reactor (PWR) and boiling water reactor (BWR) fuel with suites of critical experiments. The contents of the new covariance library, the testing performed, and the behavior of the new covariance data are described in this paper.

The neutron cross-section covariances can be combined with a sensitivity data file generated using the TSUNAMI suite of codes within SCALE to determine the uncertainty in system k_{eff} caused by nuclear data uncertainties. The Verified, Archived Library of Inputs and Data (VALID) maintained at Oak Ridge National Laboratory (ORNL) contains over 400 critical experiment benchmark models, and sensitivity data are generated for each of these models. The nuclear data uncertainty in k_{eff} is generated for each experiment, and the resulting uncertainties are tabulated and compared to the differences in measured and calculated results. The magnitude of the uncertainty for categories of nuclides (such as actinides, fission products, and structural materials) is calculated for irradiated PWR and BWR fuel to quantify the effect of covariance library changes between the SCALE 6.1 and 6.2 libraries.

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One of the primary applications of sensitivity/uncertainty methods within SCALE is the assessment of similarities between benchmark experiments and safety applications. This is described by a c_k value for each experiment with each application. Several studies have analyzed typical c_k values for a range of critical experiments compared with hypothetical irradiated fuel applications. The c_k value is sensitive to the cross-section covariance data because the contribution of each nuclide is influenced by its uncertainty; large uncertainties indicate more likely bias sources and are thus given more weight. Changes in c_k values resulting from different covariance data can be used to examine and assess underlying data changes. These comparisons are performed for PWR and BWR fuel in storage and transportation systems.

KEYWORDS
data testing, cross-section uncertainty, cross-section covariances

1. INTRODUCTION

Neutron cross-section covariance data are essential for many sensitivity/uncertainty and uncertainty quantification assessments performed both within the TSUNAMI suite and more broadly throughout the SCALE code system and the criticality safety community. The release of ENDF/B-VII.1 [1] included a more complete set of neutron cross-section covariance data. These data form the basis for a new cross-section covariance library to be released in SCALE 6.2. A range of testing is conducted to investigate the properties of these covariance data and ensure that the data are reasonable. These tests include examination of the uncertainty in critical experiment benchmark model and application model k_{eff} values due to nuclear data uncertainties, as well as similarity assessments of irradiated pressurized water reactor (PWR) and boiling water reactor (BWR) fuel with suites of critical experiments. The contents of the new covariance library, the testing performed, and the behavior of the new covariance data are described in this paper.

The neutron cross-section covariances can be combined with a sensitivity data file generated using the TSUNAMI suite of codes within SCALE to determine the uncertainty in system k_{eff} caused by nuclear data uncertainties [2]. The Verified, Archived Library of Inputs and Data (VALID) maintained at ORNL contains over 400 critical experiment benchmark models, and sensitivity data are generated for each of these models [3]. The nuclear data uncertainty in k_{eff} is generated for each experiment, and the resulting uncertainties are tabulated and compared to the differences in measured and calculated results. The magnitude of the uncertainty for categories of nuclides (such as actinides, fission products, and structural materials) is calculated for irradiated PWR and BWR fuel to quantify the effect of covariance library changes between the SCALE 6.1 and 6.2 libraries. The irradiated fuel cases are drawn from benchmarking studies performed for PWR and BWR burnup credit [4].

One of the primary applications of sensitivity/uncertainty methods within SCALE is the assessment of similarity between benchmark experiments and safety applications, as described by the c_k value for each experiment with each application [2]. Several studies have analyzed typical c_k values for a range of critical experiments compared with hypothetical irradiated fuel applications [4, 5]. The c_k value is sensitive to the cross-section covariance data because the contribution of each nuclide is influenced by its uncertainty; large uncertainties indicate more likely bias sources and are thus given more weight. Changes in c_k values resulting from different covariance data can be used to examine and assess underlying data changes. These comparisons are performed for PWR and BWR fuel in storage and transportation systems.

This paper not only summarizes the tests performed to examine the new SCALE covariance library, but it also describes the differences that criticality safety practitioners are likely to encounter when using the new library. A summary of the most important nuclide and reaction changes is also presented to provide a context for assessing the reasonableness of changes observed in particular application systems.

2. COVARIANCE LIBRARIES

The cross-section covariance library included in SCALE 6.1 was originally developed for SCALE 6. Because no single source was available with high-fidelity covariance evaluations, the data were drawn from a range of sources, including ENDF/B-VI, JENDL, and JEFF. These high-fidelity covariance evaluations are generated as part of the cross-section evaluation process, and contain significant detail of the covariance data as a function of energy. As mentioned previously, ENDF/B-VII.1 contains a significantly larger number of high-fidelity evaluations and is the starting point for the new SCALE 6.2 covariance library. The original intention was to supplement these data with other sources as necessary, but, as discussed later, some replacements of ENDF data appear to be warranted. Significant changes to cross-section covariance data have also been included in the new data that appear to be applicable. The contents and development of both of these libraries within SCALE is summarized in this section.

2.1 SCALE 6.1 Library

The generation and contents of the SCALE 6.1 covariance library are described in Section M19 of the SCALE 6.1 Manual [6]. A total of 401 materials have covariance data tabulated in 44 energy groups in this library. The manual describes the sources of high-fidelity evaluations, including ENDF/B-VII.0, ENDF/B-VI, and JENDL 3.3, which are used to generate covariance data for more than 50 nuclides. Many important nuclides, including ^{235}U, ^{1}H, and several Pu isotopes, have high-fidelity evaluations. The remaining isotopes have low-fidelity evaluations generated using procedures described in Ref. [7]. Furthermore, several isotopes have covariance data adjusted, generally to improve consistency with the *Atlas of Neutron Resonances: Resonance Parameters and Thermal Cross-sections* [8] as this is a well-established reference for cross-section uncertainty information. Most of these adjustments bring the uncertainty in line with the thermal uncertainty provided in the *Atlas*, but the resonance integral uncertainties are also used in some cases for covariance data at higher energies. The fission spectrum (χ) covariance data are taken from the SCALE 5.1 library [9]. The list of all covariance data in the library and the sources of the data are provided in Table M19.4.1 of the SCALE 6.1 Manual [6].

2.2 SCALE 6.2 Library

The SCALE 6.2 covariance library has incorporated ENDF/B-VII.1 covariance data for over 180 nuclides. These evaluations are used, with the exception of the data for three isotopes for which the testing discussed later revealed problems in the data: ^{1}H, ^{235}U, and ^{239}Pu. The sources for the covariance data for these nuclides will be discussed later in the paper, as a variety of approaches are taken. A few high-fidelity evaluations from ENDF/B-VI remain in the library. New covariance data are generated for fission spectra based on the data contained in ENDF/B File 35. More discussion of these new spectrum covariances is provided in a companion paper being presented at this conference [10]. As with the SCALE 6.1 library, the remaining covariance data provided are the low-fidelity evaluations documented in Ref. [7]. The SCALE 6.2 covariance data are tabulated in 56 groups instead of the 44 used in the SCALE 6.1 library. The fine group cross-section library in SCALE 6.1 has 238 groups, but this number has been increased to 252 in SCALE 6.2 to improve performance for light-water reactor systems. The 56 energy groups used for the covariance library are a subset of the new 252-group multigroup library structure, as the 44 group structure was a subset of the 238 group library. TSUNAMI-IP [6] has been modified to allow use of existing 238-group sensitivity data files (SDFs) with the new 56-group uncertainty data, so existing SDFs can still be used with the new library.

2.3 Major Changes

As discussed in the previous section, there are significant changes to the covariance evaluations for several of the most important and common nuclides in nuclear systems. Two of the changes that have extensive impacts on many experiments are the changes made to the covariance data for nu-bar for ^{235}U and ^{239}Pu. The uncertainty in ^{235}U nu-bar is shown in Fig. 1. The uncertainty in the thermal range increases from approximately 0.31% to 0.39%. Conversely, the uncertainty in ^{239}Pu decreases dramatically across the entire energy range, as shown in Fig. 2. These changes are responsible for many of the differences exhibited in the covariance testing described in the next section of the paper.

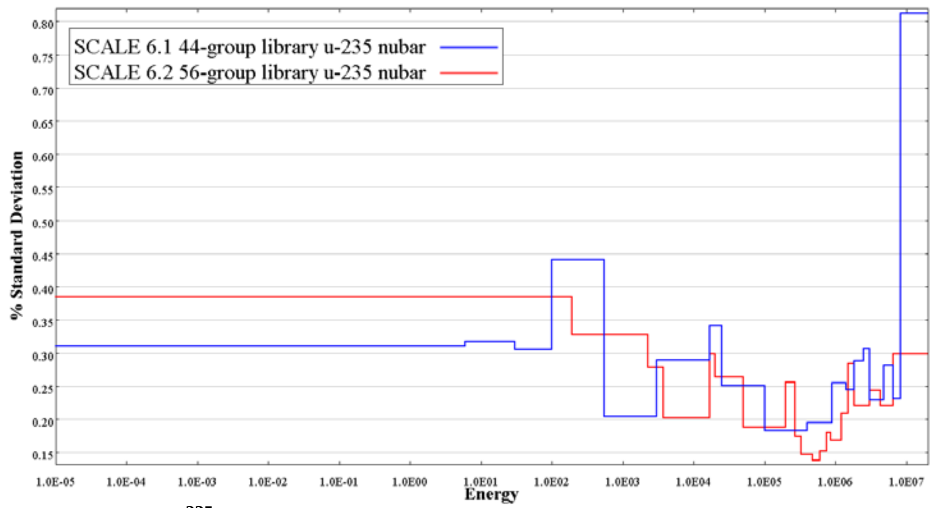

Figure 1. ^{235}U Nu-Bar Uncertainty in Both Covariance Libraries.

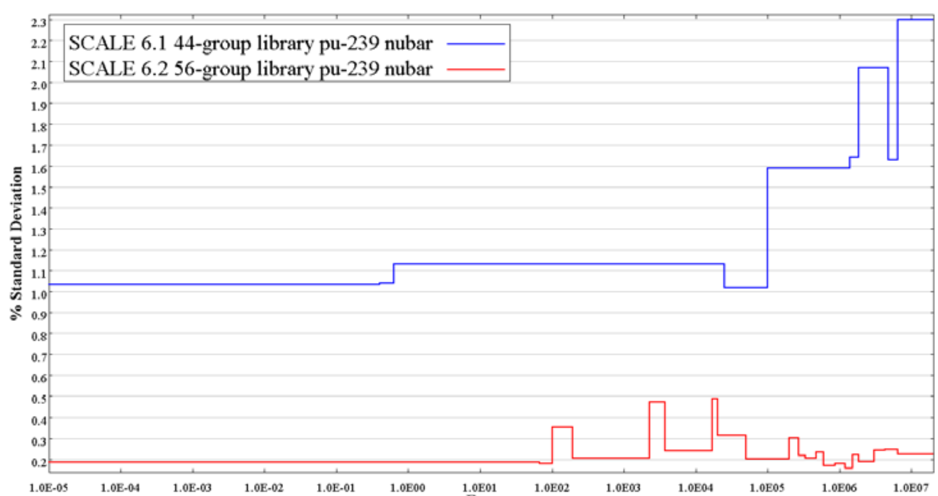

Figure 2. ^{239}Pu Nu-Bar Uncertainty in Both Covariance Libraries.

3. COVARIANCE DATA TESTING

A range of different tests is performed to investigate the new covariance data. Covariance data cannot be directly validated because they represent uncertainties, but several different applications can shed light on the veracity of the data. These applications examine the cross-section–induced uncertainty in k_{eff} globally and by isotope or isotope set, as well as the c_k parameter quantifying similarity of applications and experiments.

3.1 Nuclear Data–Induced Uncertainty in VALID Model k_{eff} Values

The first test method considers the predicted uncertainty in k_{eff} for critical benchmark experiment models resulting from cross-section uncertainty. In this work, this uncertainty is determined through the use of TSUNAMI-IP [6] and available SDFs from VALID [3]. The existing sensitivities are propagated with the new covariance data to the uncertainty in k_{eff}; the details of the method are described in Ref. [2]. A comparison of the distribution of the calculated-to-experiment (C/E) ratios to this uncertainty band for these experiments provides an indication of the accuracy of the cross-section–induced k_{eff} uncertainty.

Examination of both mixed uranium/plutonium pin array (MCT) systems and low-enriched, water moderated uranium oxide pin array (LCT) systems using the preliminary covariance libraries revealed problems with the uncertainty data for ^{235}U, ^{239}Pu, and ^{1}H. The ^{235}U nu-bar uncertainty had increased by a factor of more than two. The ^{1}H capture uncertainty increased by a factor of five, making it significantly larger than the Ref. [8] value. Updated versions of the covariance data for ^{235}U and ^{1}H were generated and committed to the repository maintained at the National Nuclear Data Center (NNDC) after these testing results were shared with the ENDF/B evaluators. Furthermore, it was noted that the ^{239}Pu nu-bar uncertainty was zero for some low energy groups. The JENDL-3.3 and -4.0 evaluations both contain an uncertainty of approximately 0.18% from 0.01 eV to the bottom of the evaluated energy range, and this value is used in the library. The updated evaluations for all three isotopes have been implemented in the SCALE 6.2 covariance library.

As discussed in a companion paper being presented at this conference on the validation of KENO in SCALE 6.2 Beta4 [11], all the cases from VALID have been executed and the C/E values tabulated for k_{eff} predictions. A plot is generated for each category of experiments showing the C/E value, the experimental uncertainty, and the cross-section–induced k_{eff} uncertainty for each case. These results include the covariance adjustments and corrections described above. The uncertainty in k_{eff} calculated by TSUNAMI-IP due to cross-section uncertainty represents a one sigma level of uncertainty, and as such, it is expected that approximately 68% of cases fall within the uncertainty band presented. As shown in Table I, however, a much larger percentage of cases are within the cross-section uncertainty band. This likely indicates that the cross-section uncertainties are too large on average, as has been observed previously [12]. A smaller percentage of plutonium-fueled cases is within the uncertainty band, indicating that the plutonium uncertainties may be more accurate than the uranium uncertainties. It is also worth noting that all of the MCT cases outside the one sigma band come from a single evaluation, so there may be a problem with the experiments in that series or, more likely, there may be a problem with the description of the experiments.

Table I. Percentage of VALID cases within one sigma uncertainty band

Category	Cases in band	Total cases	Percentage in band
HMF	45	49	91.8
HST	49	52	94.2
IMF	13	13	100.0
LCT	123	123	100.0
LST	17	19	89.5
MCF	1	2	50.0
MCT	32	49	65.3
MST	3	3	100.0
PMF	10	10	100.0
PST	74	81	91.4

A series of comparisons of the new and old cross-section uncertainty band is shown in Figs. 3 through 6. The k_{eff} C/E and its uncertainty, dominated by the experimental uncertainty, are shown for each case. Figure 3 shows results for high-enriched uranium fast metal (HMF) systems, and it illustrates that only small changes have been made to the covariance data impacting this type of system.

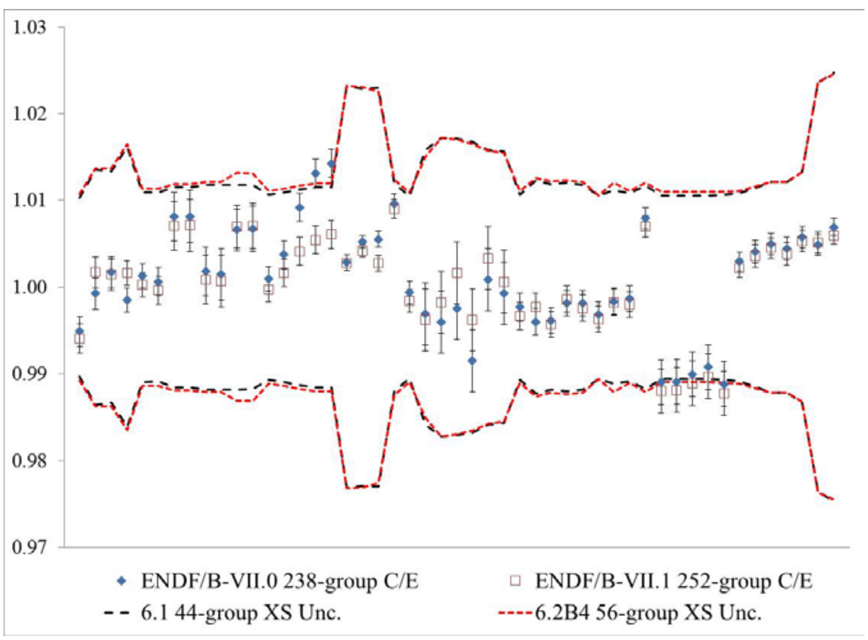

Figure 3. C/E Ratios and Uncertainty Bands for HMF Systems.

Figure 4 shows LCT systems and the uncertainty in system k_{eff} is noticeably larger for these systems using the SCALE 6.2 covariance data than with the SCALE 6.1 data. This change is largely caused by an increase in the uncertainty of ^{235}U nu-bar.

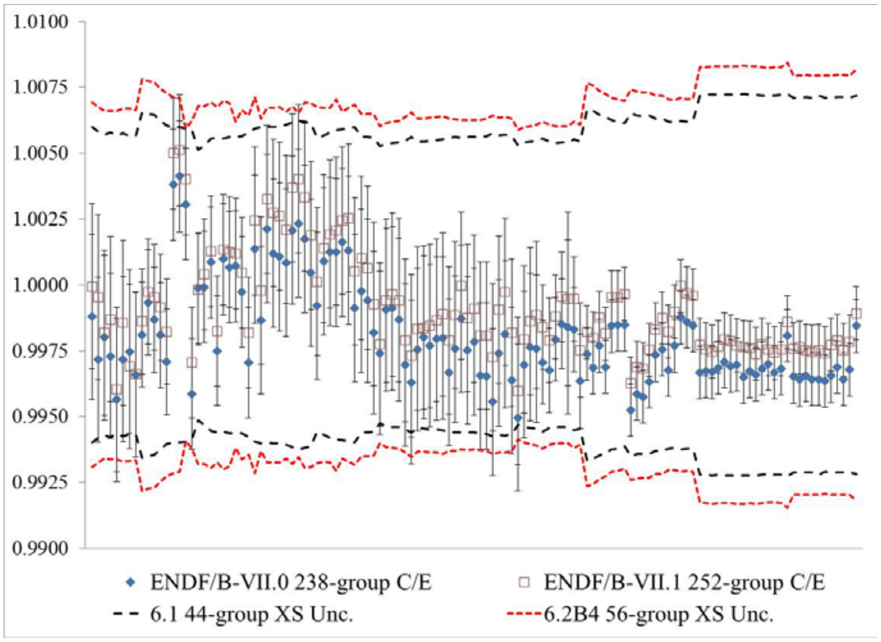

Figure 4. C/E Ratios and Uncertainty Bands for LCT Systems.

Figure 5 shows MCT systems, and Fig. 6 shows systems of plutonium solutions with a thermal neutron spectrum (PST). The uncertainties in system k_{eff} are dramatically smaller for the SCALE 6.2 covariance library than for the SCALE 6.1 covariance library, primarily because of a decrease in the ^{239}Pu nu-bar uncertainty.

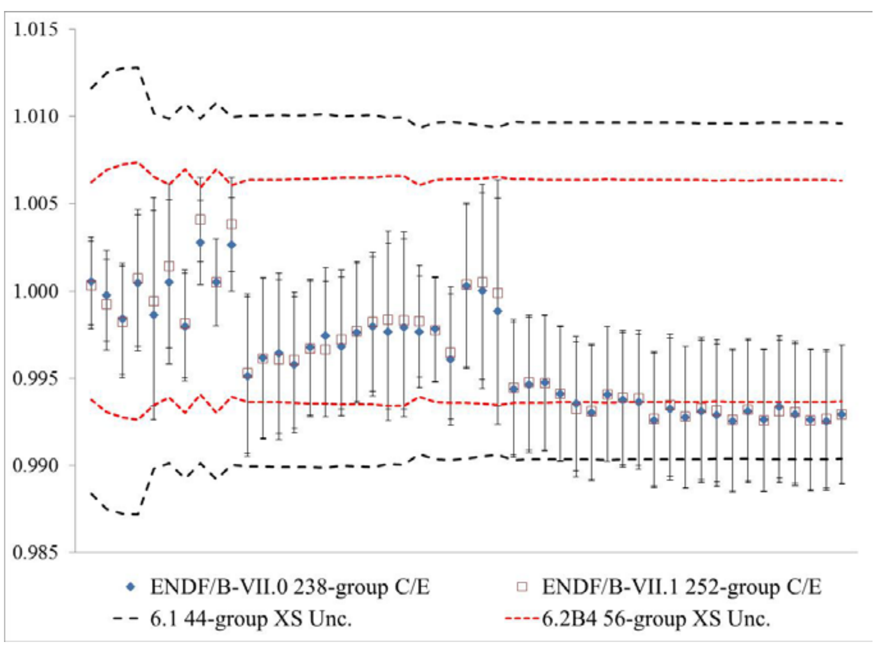

Figure 5. C/E Ratios and Uncertainty Bands for MCT Systems.

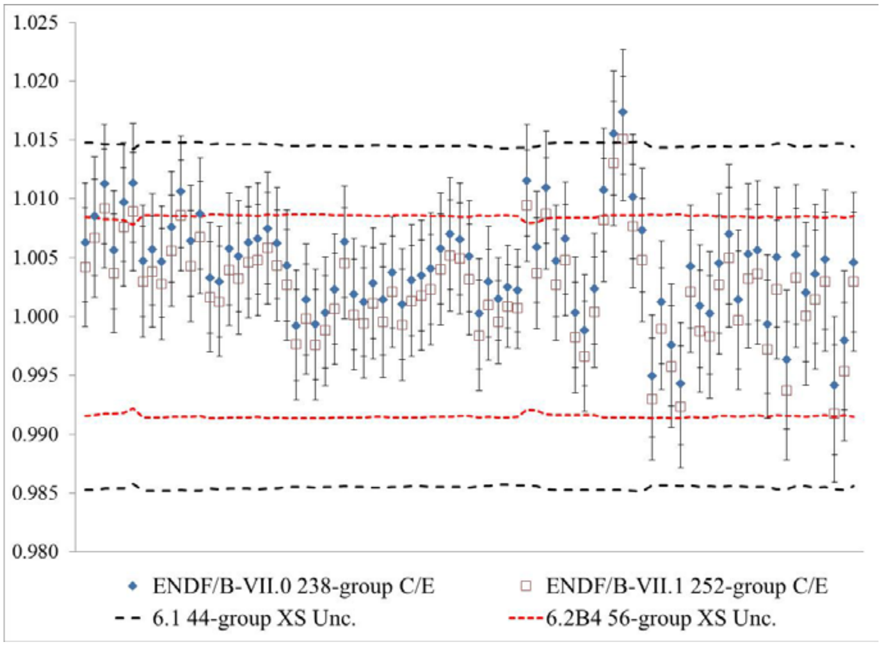

Figure 6. C/E Ratios and Uncertainty Bands for PST Systems.

3.2 Nuclear Data–Induced Uncertainty in Spent Fuel Model k_{eff} Values

The second aspect of the testing also uses the nuclear data–induced uncertainty in k_{eff} generated by TSUNAMI-IP, but in addition it also examines isotopes in spent PWR and BWR fuel in a storage/transportation configuration. Here the uncertainty contribution for each isotope and group of isotopes is compared with results obtained using the SCALE 6.1 covariance data. Differences between the libraries are examined to identify the cause and to determine if the difference is reasonable.

Extensive work quantifying the uncertainty in k_{eff} resulting from cross-section uncertainty in spent fuel systems was presented in Ref. [4], Table 6.10. The SDFs for all five application models were used with the new covariance library to generate the same information, with the only difference being the use of the new library. A summary of these results is shown in Table II for PWR systems and Table III for the BWR spent fuel pool (SFP) application model.

Table II. Summary of k_{eff} uncertainty resulting from cross-section uncertainty data, PWR systems (Δk_{eff})

App.	SFP				Cask			
Burnup	**10 GWd/MTU**		**40 GWd/MTU**		**10 GWd/MTU**		**40 GWd/MTU**	
Library	**6.1**	**6.2**	**6.1**	**6.2**	**6.1**	**6.2**	**6.1**	**6.2**
Major act.	0.00463	0.00469	0.00476	0.00416	0.00455	0.00449	0.00466	0.00406
Minor act.	0.00007	0.00007	0.00027	0.00022	0.00007	0.00007	0.00025	0.00022
Major FP	0.00022	0.00036	0.00052	0.00070	0.00024	0.00036	0.00052	0.00068
Other act.	0.00003	0.00006	0.00003	0.00006	0.00000	0.00000	0.00001	0.00001
Other FP	0.00015	0.00032	0.00034	0.00083	0.00008	0.00017	0.00024	0.00050
Else	0.00081	0.00123	0.00073	0.00102	0.00106	0.00145	0.00104	0.00127
Total	0.00471	0.00488	0.00486	0.00442	0.00468	0.00473	0.00481	0.00434

Table III. Summary of k_{eff} uncertainty resulting from cross-section uncertainty data, BWR SFP (Δk_{eff})

Burnup	11 GWd/MTU	
Library	6.1	6.2
Major Act.	0.00393	0.00447
Minor Act.	0.00013	0.00011
Major FP	0.00023	0.00032
Other Act.	0.00000	0.00000
Other FP	0.00014	0.00045
Else	0.00080	0.00099
Total	0.00402	0.00461

The results show that the total uncertainty changes are small—less than 15% in all cases—and are dominated by the uncertainty contribution from the major actinides. It is also evident that at low burnups, the uncertainty is higher with the SCALE 6.2 library, and the uncertainty is lower at high burnups. These changes are driven by the increase in ^{235}U uncertainty at low burnup and ^{239}Pu uncertainty at high burnup. These results are consistent with those shown in Figs. 3 through 6 in Section 3.1. Minor actinide uncertainty decreases slightly at high burnup with the new data, and major fission product uncertainty increases. A comparison of the individual isotope contributions for the major fission products in the PWR cask model at 40 gigawatt days per metric ton of uranium (GWd/MTU) is shown in Table IV. The detailed data reveal that the uncertainty contribution from most of the major fission products changes only slightly, but large increases are evident for ^{151}Sm and ^{155}Gd. These particular differences will be investigated further prior to the final release of SCALE 6.2.

Table IV. Major fission product contribution to k_{eff} uncertainty, PWR cask, 40 GWd/MTU (% Δk_{eff}/k)

Isotope	6.1	6.2
mo-95	5.19E-03	4.99E-03
tc-99	7.14E-03	9.90E-03
ru-101	7.79E-03	7.88E-03
rh-103	2.06E-02	2.35E-02
ag-109	2.27E-03	2.32E-03
cs-133	1.67E-02	1.69E-02
sm-147	5.48E-03	5.49E-03
sm-149	2.05E-02	2.05E-02
sm-150	5.20E-03	5.21E-03
sm-151	1.23E-02	4.31E-02
sm-152	6.15E-03	6.17E-03
nd-143	3.38E-02	3.51E-02
nd-145	1.68E-02	1.82E-02
eu-151	2.38E-04	2.38E-04
eu-153	7.08E-03	8.05E-03
gd-155	3.84E-03	1.24E-02
total	5.48E-02	7.20E-02

3.3 c_k Values

The third piece of the covariance data testing is determining the c_k values for a number of experiments compared to PWR and BWR fuel in a storage and transportation system model. The integral index c_k is a correlation coefficient for each experiment with each application based on the sensitivities propagated with the covariance data. It is calculated by determining the amount of nuclear data–induced uncertainty that is shared between two systems. A full description of the calculation of c_k is provided in Ref. [2]. The covariance data effectively act as a weighting function for the sensitivities; the nuclide/reaction pairs with larger uncertainties contribute more strongly to c_k because they are expected to be larger sources of bias since they are more uncertain. Typically, a c_k value of 0.8 or higher indicates sufficient similarity between the experiment and the application to allow the application to be used for validation [2]. This threshold value of 0.8 is shown in Figs. 7 and 8 for reference, although the primary focus of this section is the change in c_k caused by the use of the SCALE 6.2 covariance library.

A collection of SDFs for 1,643 experiments was created for work documented in Ref. [5]. The SDFs are drawn from VALID, cases used in Ref. [4], and SDFs generated by the Nuclear Energy Agency [13]. The set of experiments includes over 1,000 LCT experiments and over 250 MCT experiments. The set also includes the Haut Taux de Combustion (HTC) experiments [14], a series of MCT experiments with the actinide composition designed to match spent fuel, and a collection of low-enriched uranium and mixed uranium/plutonium (MIX) solution cases. The last component of the experiment set is a group of cases categorized as miscellaneous configurations with low-enriched uranium fissile material. A complete list of the experiments is provided in Ref. [5], Appendix C. A PWR cask model from Ref. [4] and a BWR cask model from Ref. [5] are used as the application models for comparison. All experiments are compared to both applications with the SCALE 6.1 44-group covariance library and the SCALE 6.2 56-group library. The results are shown in Fig. 7 for the PWR model and Fig. 8 for the BWR model.

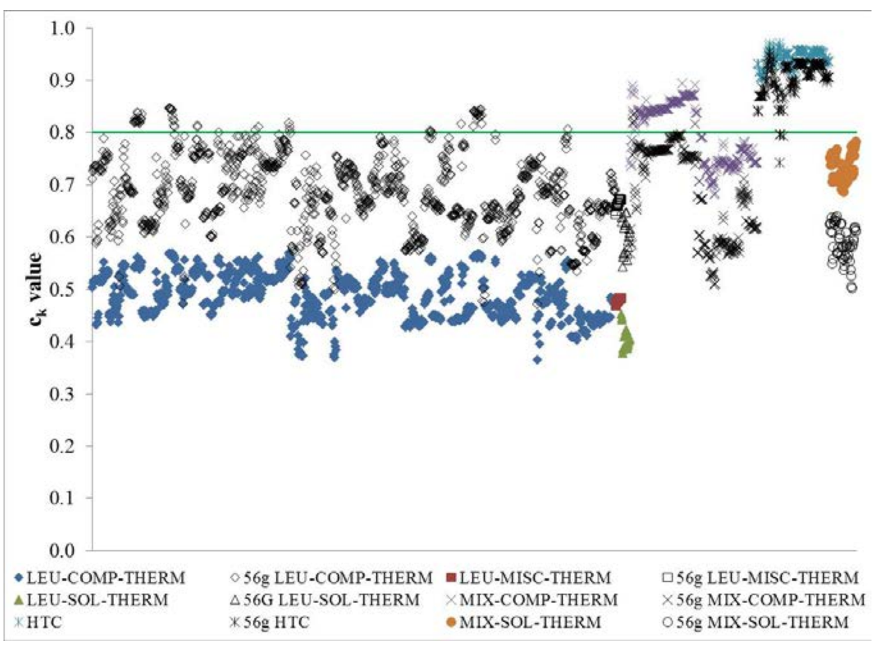

Figure 7. c_k Values with Both Covariance Libraries for the PWR Cask Application.

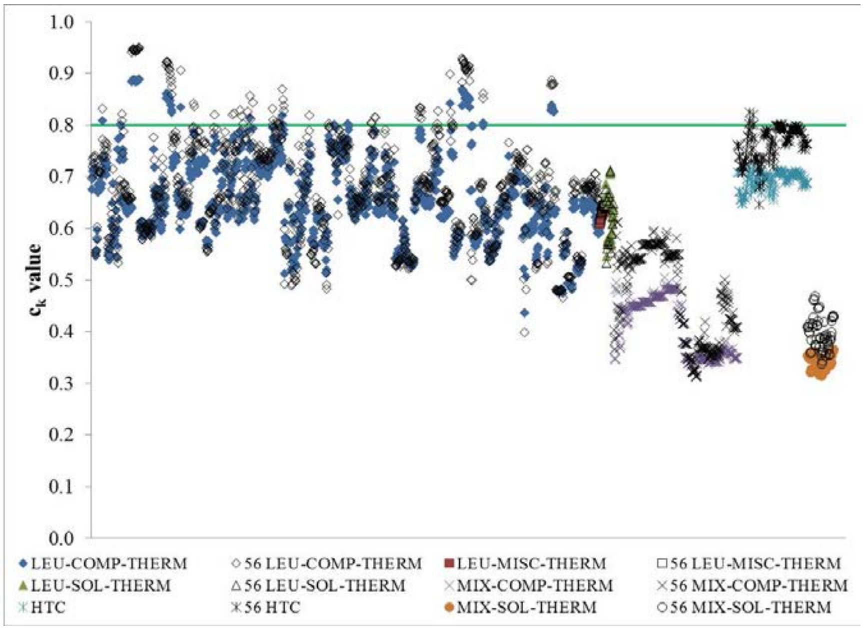

Figure 8. c_k Values with Both Covariance Libraries for the BWR Cask Application.

The PWR cask model contains fuel with a burnup of 40 GWd/MTU, so a significant amount of plutonium is present in the fuel. The c_k contribution from ^{239}Pu is relatively high using the SCALE 6.1 library because of the large uncertainty in ^{239}Pu nu-bar, as shown by the high c_k values for the MCT, HTC, and MST experiments. As shown earlier in Fig. 5, the total uncertainty in MCT systems has dropped with the new covariance data. The reduction in uncertainty in the SCALE 6.2 56-group library indicates that ^{239}Pu nu-bar is a less likely source of bias, causing the contribution to be smaller with the new library. This causes the shift to lower c_k values seen in the experiments with mixed uranium and plutonium fissile material. Conversely, the uncertainty in ^{235}U has increased, so it is now a more likely source of bias. A further relative increase in the importance of ^{235}U is caused by the fact that c_k is a correlation coefficient and thus ranges from -1 to 1. The lower overall uncertainty means that the largest remaining uncertainty source is a more dominant contributor to c_k. The differences shown in Fig. 7 are thus entirely consistent with the known changes in the covariance data.

The BWR cask model contains fuel with a burnup of 7.5 GWd/MTU, so the relative abundances of ^{235}U and ^{239}Pu are very different than in the PWR case. In this case, nearly all the c_k values increase because of the increased uncertainty in ^{235}U nu-bar. The MCT cases that have small changes with the new covariance library are the result of cases with depleted uranium (0.15 wt % ^{235}U) in which the ^{235}U sensitivity is too low for a significant contribution to c_k. Overall, as with the PWR application case, the differences in c_k values shown in Fig. 8 are consistent with known changes in the covariance data.

4. SUMMARY AND FUTURE WORK

4.1 Summary

A new cross-section covariance library has been developed for SCALE 6.2 based on new high-fidelity evaluations provided in ENDF/B-VII.1 [1] for more than 180 isotopes. The remaining isotopes are retained from the SCALE 6.1 library. All covariances in the SCALE 6.2 library are represented in a new 56-group structure which is a subset of the new 252-group structure. TSUNAMI-IP has been modified to correctly apply 56-group covariance data to existing 238-group sensitivity data. All existing SDFs are compatible with the new covariance library.

Extensive testing has been performed to examine the impact of the new covariance data on sensitivity/uncertainty analyses. The first set of tests focus on the uncertainty in system k_{eff} due to nuclear data uncertainty for the more than 400 critical experiments in the VALID library. These results show modest increases in the k_{eff} uncertainty for thermal systems with ^{235}U as the primary fissile material driven by the change in ^{235}U nu-bar uncertainty shown in Fig. 1. The k_{eff} uncertainty in systems with Pu as a primary fissile material, either alone or mixed with uranium, now exhibit lower uncertainties as shown in Figs. 5 and 6. These changes result from the lower ^{239}Pu nu-bar uncertainty shown in Fig. 2. Additional testing utilizing PWR and BWR spent fuel system k_{eff} uncertainties showed mainly small changes that are consistent with the changes in ^{235}U and ^{239}Pu.

Finally, c_k values for PWR and BWR spent fuel applications have been generated in comparisons with over 1,600 critical experiments. The differences across the entire range of experiments for both applications are also consistent with observed changes in ^{235}U and ^{239}Pu nu-bar uncertainty changes. The gross impact of the new covariance library on any specific application system should therefore be straightforward to analyze and understand.

4.2 Future Work

Testing of the new SCALE 6.2 covariance library will continue throughout the summer until the final release of SCALE 6.2 in September 2015. As indicated in Section 3.2, fission product data will be a focus based on the results shown in Table IV. Additional work is needed to vet the complete set of ENDF/B-VII.1 covariance data for isotopes and/or energy ranges that have not been exercised with the testing performed so far. The fission spectrum data for many of the less common actinide isotopes also need further review. The goal of this testing is to ensure that the new covariance library is as complete and correct as possible, especially since it is being applied to additional uncertainty quantification tools such as Sampler which have not previously existed within SCALE.

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