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Abstract. An assessment was previously performed to evaluate modeling capabilities and quantify preliminary biases and uncertainties associated with the modeling methods and data utilized in designing a nuclear reactor such as a beryllium-reflected, highly-enriched-uranium (HEU)-O_2 fission surface power (FSP) system for space nuclear power. The conclusion of the previous study was that current capabilities could preclude the necessity of a cold critical test of the FSP; however, additional testing would reduce uncertainties in the beryllium and uranium cross-section data and the overall uncertainty in the computational models. A series of critical experiments using HEU metal were performed in the 1960s and 1970s in support of criticality safety operations at the Y-12 Plant. Of the hundreds of experiments, three were identified as fast-fission configurations reflected by beryllium metal. These experiments have been evaluated as benchmarks for inclusion in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE). Further evaluation of the benchmark experiments was performed using the sensitivity and uncertainty analysis capabilities of SCALE 6. The data adjustment methods of SCALE 6 have been employed in the validation of an example FSP design model to reduce the uncertainty due to the beryllium cross section data.

Keywords: benchmark, beryllium, fission surface power, HEU, TSUNAMI, SCALE.

INTRODUCTION

Previously an assessment was performed to evaluate modeling capabilities and quantify biases and uncertainties associated with methods and data utilized in designing a space nuclear reactor system. The evaluated baseline fission surface power (FSP) system was a sodium-potassium (NaK) cooled, fast spectrum reactor with highly-enriched-uranium (HEU)-O_2 fuel, stainless steel (SS) cladding, and beryllium reflectors with B_4C control drums. The conclusion of the previous study was that current capabilities could preclude the necessity of a cold critical test of the FSP; however, additional testing would aid in the reduction of uncertainties in the beryllium and uranium cross-section data, thus reducing the overall uncertainty in the computational design models.[1]

Four important critical experiments from the Zero Power Plutonium Reactor (ZPPR)-20 were initially selected for comparison with the FSP model. These experiments represented mockups of a small space reactor.[2] These experiments were previously evaluated as benchmarks and made available through the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE).[3] Use of the four ZPPR experiments as a validation set in the previous study indicated that the dominant uncertainty in computation of the FSP eigenvalue due to cross section covariance data was the Be(n,n) reaction.[1] A significant amount of work was previously performed on the qualification of physics tools for the design of the Jupiter Icy Moons Orbiter (JIMO) reactor, in which intermediate and thermal spectrum experiments were considered.[4,5]

Recently three additional critical experiments have been identified as fast-fission configurations of HEU metal reflected by beryllium metal. These experiments have been evaluated for inclusion in the IHECSBE and further evaluated using the sensitivity and uncertainty analysis capabilities of SCALE 6.[6] The data adjustment methods of SCALE 6 have been employed in the validation of an example FSP design model to reduce the uncertainty due to beryllium cross section data.

BERYLLIUM-REFLECTED HEU EXPERIMENTS

A variety of critical experiments were constructed of enriched uranium metal, oralloy (Oak Ridge Alloy consisting of a ^{235}U enrichment >93%), during the 1960s and 1970s at the Oak Ridge Critical Experiments Facility (ORCEF) in support of criticality safety operations at the Y-12 Plant. The purposes of these experiments included the evaluation of storage, casting, and handling limits, and provision of data for verification of calculation methods and cross sections for nuclear criticality safety applications. The bulk of these experiments included solid cylinders of various diameters, annuli of various inner and outer diameters, two and three interacting cylinders of various diameters, and graphite- and polyethylene-reflected cylinders and annuli.[7-9]

Of the hundreds of delayed critical experiments, three were performed that consisted of HEU reflected by beryllium. Two experiments consisted of uranium metal annuli surrounding a solid beryllium metal core. The outer diameter of the annuli was approximately 33.02 or 38.1 cm (13 or 15 in.) with an inner diameter of 17.78 cm (7 in.). The diameter of the beryllium was 17.78 cm (7 in.). The critical height of the configurations was approximately 12.7 and 10.16 cm (5 and 4 in.), respectively. The uranium annulus consisted of multiple stacked rings, each with radial thicknesses of 2.54 cm (1 in.) and varying heights.[10] The third experiment was comprised of a stack of approximately 17.78-cm-(7-in.)-diameter metal discs. The bottom of the stack consisted of uranium with an approximate height of 10.4775 cm (4-1/8 in.). The top of the stack consisted of beryllium with an approximate height of 14.12875 cm (5-9/16 in.).[11]

Summary of Benchmark Evaluation

Comprehensive evaluation of the three Be-reflected HEU experiments are available in the IHECSBE in the report identified as HEU-MET-FAST-059 and -069.[3] It should be noted that there was precise measurement of the dimensions and physical properties of the metals used in these experiments, such that the uncertainties in the experimental reproducibility and reactivity worth measurement of the experimental assembly, which are traditionally insignificant compared to other uncertainties, contribute to the total uncertainty. The other two significant uncertainties include impurities in the beryllium metal discs and the measurement uncertainty of the stacked height of the uranium parts (which governs the uncertainty in the neutron leakage paths between the small gaps of each experimental component). Simplification of benchmark experiments by homogenizing metallic parts into solid cylinders or annuli had a more significant modeling impact due to the change in neutron leakage from a near ideal model to one with the general dimensions described in the previous section. For example, the stacked height of annuli in the first two experiments was less than the approximate heights used to describe the experimental configurations.

A summary of the calculated results for these three benchmarks, compared against the benchmark eigenvalues, is shown in Table 1. Calculations were performed using Monte Carlo N-Particle (MCNP)[12] version 5.1.51 with ENDF/B-VII.0,[13] JEFF-3.1,[14] and JENDL-3.3[15] neutron cross section libraries. It is important to note that there is a difference of up to ~0.67 %$\Delta k/k_{eff}$ between the eigenvalues calculated using MCNP5. Additional calculations using KENO-V.a[16] with ENDF/B-VII.0 were also performed using the simple benchmark models, in preparation for sensitivity analysis calculations.

TABLE 1. Summary of Calculations and Benchmark Analysis of Be-Reflected HEU Experiments.

Benchmark Configuration	Model	Analysis Code	Neutron Cross Section Library	Calculated k_{eff}	±	1σ	Benchmark k_{eff}	±	1σ	$\frac{C-E}{E}(\%)$
13" Annulus	Detailed	MCNP5	ENDF/B-VII.0	0.99711	±	0.00002	1.0005	±	0.0005	-0.34
			JEFF-3.1	0.99519	±	0.00002				-0.53
			JENDL-3.3	1.00193	±	0.00002				0.14
	Simple	MCNP5	ENDF/B-VII.0	0.98953	±	0.00002	0.9929	±	0.0028	-0.34
			JEFF-3.1	0.98772	±	0.00002				-0.52
			JENDL-3.3	0.99401	±	0.00002				0.11
		KENO-V.a	ENDF/B-VII.0 (238-group)	0.98902	±	0.00005				-0.39
15" Annulus	Detailed	MCNP5	ENDF/B-VII.0	0.99680	±	0.00002	0.9994	±	0.0003	-0.26
			JEFF-3.1	0.99451	±	0.00002				-0.49
			JENDL-3.3	1.00125	±	0.00002				0.19
	Simple	MCNP5	ENDF/B-VII.0	0.99257	±	0.00002	0.9952	±	0.0016	-0.26
			JEFF-3.1	0.99027	±	0.00002				-0.49
			JENDL-3.3	0.99699	±	0.00002				0.18
		KENO-V.a	ENDF/B-VII.0 (238-group)	0.99216	±	0.00005				-0.31
Top-Reflected	Detailed	MCNP5	ENDF/B-VII.0	0.99802	±	0.00004	0.9998	±	0.0004	-0.18
			JEFF-3.1	0.99578	±	0.00004				-0.40
			JENDL-3.3	1.00217	±	0.00004				0.24
	Simple	MCNP5	ENDF/B-VII.0	0.99781	±	0.00004	0.9994	±	0.0004	-0.16
			JEFF-3.1	0.99531	±	0.00004				-0.41
			JENDL-3.3	1.00166	±	0.00004				0.22
		KENO-V.a	ENDF/B-VII.0 (238-group)	0.99726	±	0.00005				-0.23

SENSITIVITY ANALYSIS OF CROSS-SECTION COVARIANCE DATA

Oak Ridge National Laboratory developed TSUNAMI-3D (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation in Three Dimensions)[17] as part of their SCALE package to automate the analysis procedure of uncertainties and sensitivities in cross section data for a given model. The core model of an example FSP model was investigated previously.[1] The KENO models of the three Be-reflected HEU benchmarks were also analyzed using the TSUNAMI-3D code.

A comprehensive sensitivity study of each model determined the relative standard deviation in k_{eff} due to cross-sections in the neutron library. A summary of the uncertainty in k_{eff} and major sources of uncertainty is provided for each of the Be-reflected HEU benchmarks in Table 2. Previously calculated data for the FSP model is also provided in Table 2 for comparison. Only uncertainty components greater than 0.1 $\%\Delta k/k_{eff}$ are included in this report. As cross-section errors, as bounded by their uncertainties, are the most significant sources of computational bias, the data shown in Table 2 represent a ranked list of the most likely bias sources. The component uncertainty from the (n,γ) reactions in ^{235}U are greater than the uncertainty in the (n,f) reactions. Although the FSP is more sensitive to the (n,f) reaction, the uncertainty of the (n,γ) cross section far exceeds that of (n,f), especially at fast energies, leading to a greater uncertainty in k_{eff} due to (n,γ) than for (n,f). The contribution to the total covariance uncertainty due to beryllium reactions is approximately an order-of-magnitude less in the Be-reflected benchmark experiments than in the FSP model. Where cross-section uncertainties are not available, a uniform uncertainty of 5% was used. Note that some uncertainties are represented as a negative Δk/k. These values represent anticorrelations between two reactions that are present in the covariance data. As some component of the uncertainty is shared between the two reactions, the presence of both sources of uncertainty together represent a net *decrease* in the system uncertainty relative to what would be observed if the system were sensitive to one reaction but not the other.

TABLE 2. Cross-Section Covariance Uncertainty in TSUNAMI-3D Analysis.

Model	Total Uncertainty (%$\Delta k/k_{eff}$)	Major Components	Component Uncertainty (%$\Delta k/k_{eff}$)
13" Annulus	1.1153	^{235}U(n,γ)	1.0045 ± <0.00001
		^{235}U(n,n,) to ^{235}U(n,γ)	0.2765 ± <0.00001
		^{235}U(n,n')	0.2590 ± <0.00001
		^{235}U(n,f)	0.2516 ± <0.00001
		^{235}U(n,n) to ^{235}U(n,n')	-0.2172 ± <0.00001
		^{235}U(χ)	0.1515 ± <0.00001
		^{235}U(ν-bar)	0.1458 ± <0.00001
		^{234}U(n,f)	0.1278 ± <0.00001
		^{235}U(n,n)	0.1217 ± <0.00001
15" Annulus	1.0520	^{235}U(n,γ)	0.9545 ± <0.00001
		^{235}U(n,f)	0.2522 ± <0.00001
		^{235}U(n,n,) to ^{235}U(n,γ)	0.2162 ± <0.00001
		^{235}U(n,n')	0.2066 ± <0.00001
		^{235}U(n,n) to ^{235}U(n,n')	-0.1659 ± <0.00001
		^{235}U(χ)	0.1563 ± <0.00001
		^{235}U(ν-bar)	0.1468 ± <0.00001
		^{234}U(n,f)	0.1304 ± <0.00001
Top-Reflected	1.0902	^{235}U(n,γ)	0.9929 ± <0.00001
		^{235}U(n,n')	0.2940 ± <0.00001
		^{235}U(n,f)	0.2526 ± <0.00001
		^{235}U(n,n) to ^{235}U(n,n')	-0.2344 ± <0.00001
		^{235}U(n,n,) to ^{235}U(n,γ)	0.2000 ± <0.00001
		^{235}U(ν-bar)	0.1467 ± <0.00001
		^{235}U(χ)	0.1283 ± <0.00001
		^{234}U(n,f)	0.1282 ± <0.00001
		^{235}U(n,n)	0.1101 ± <0.00001
FSP	2.0872	^{235}U(n,γ)	1.9576 ± 0.0006
		^{235}U(ν-bar)	0.5651 ± 0.0000
		Be(n,n)	0.3559 ± 0.0023
		^{235}U(n,n')	0.2261 ± 0.0009
		^{235}U(n,f)	0.1864 ± 0.0000
		^{235}U(n,n,) to ^{235}U(n,γ)	-0.1297 ± 0.0003

Correlation Analysis and Data Adjustment

The sensitivity data generated by the TSUNAMI-3D analyses for the various experiment models and the core model can be compared using TSUNAMI-IP (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation – Indices and Parameters).[17] The TSUNAMI-IP code uses the sensitivity data generated by the TSUNAMI-3D analysis with the cross-section covariance data to compute various relational parameters and indices. The parameters can be used to determine the degree of similarity between two systems. Where two systems show a high degree of similarity in terms of uncertainties due to cross-section-covariance data, the systems are expected to have similar computational biases.

The primary global integral indices generated in TSUNAMI-IP include the correlation coefficient index, c_k, which measures the similarity of two systems in terms of related uncertainty.[17] The integral index c_k

can be used as a trending parameter in criticality safety analysis validation studies to determine computational uncertainties and biases.[18] Utility of this application in the analysis of space power reactor design has been previously discussed and demonstrated.[1]

The FSP model was compared against the three Be-reflected HEU benchmark models using SCALE 6 ENDF/B-VII cross-section covariance data. A summary of the correlation coefficient and cross-section uncertainties for both libraries is provided in Table 3. General guidance is that c_k values greater than 0.9 demonstrate similarity between two experiments or models, and c_k values between 0.8 and 0.9 demonstrate moderate similarity. Values closer to zero indicate systems that are totally dissimilar. All three Be-HEU benchmarks have c_k values greater than 0.9 and thus exhibit similarity with the FSP model. The c_k values are similar to those found for the ZPPR benchmark series used in previous assessments (also shown in Table 3).

TABLE 3. Correlation Coefficient and Cross-Section Uncertainties Comparison.

Model	C_k	**Cross-Section Uncertainty (%)**
13" Annulus	0.9448 ± 0.0003	1.116
15" Annulus	0.9347 ± 0.0003	1.053
Top Reflected	0.9443 ± 0.0003	1.091
ZPPR-20C(105)	0.9732 ± 0.0004	1.995
ZPPR-20D(129)	0.9489 ± 0.0003	1.609
ZPPR-20D(136)	0.9435 ± 0.0003	1.531
ZPPR-20E(160)	0.9619 ± 0.0005	1.446

The initial assessment of uncertainty in the FSP model using the four ZPPR benchmarks yielded an uncertainty of 2.09% δk/k. TSUNAMI-IP was then used to develop a penalty assessment for the model, which provides additional margins of uncertainty where sufficient experimental information is unavailable. This additional uncertainty component can be included with the calculated k_{eff} of the system to provide an added measure of safety where validation coverage might be lacking. An analysis of the nuclides that make important contributions to this penalty can also help to identify what benchmark problems could be added to the analysis to potentially reduce the uncertainty. The initial penalty was calculated to be 0.29% δk/k. Of this, 0.28% δk/k resulted from the Be(n,n) reaction, indicating that this reaction was not covered sufficiently by the four ZPPR benchmarks.

Since beryllium was not sufficiently assessed by the initial calculations, it was determined that adding the three Be-reflected HEU benchmarks would potentially reduce the overall uncertainty of the FSP model. However, it was discovered that these benchmarks also do not sufficiently cover the Be(n,n) reaction. This is illustrated in Figure 1, which plots the sensitivity of the FSP model and the three Be-reflected HEU benchmarks to the Be(n,n) reactions. The much smaller sensitivities in the benchmarks indicate that they cannot be used to validate the FSP sensitivity to this reaction. TSUNAMI-IP results using both the four ZPPR and the three Be-HEU benchmarks also indicate that the three Be-HEU benchmarks make very little contribution to uncertainty reduction. Using all seven benchmarks, overall uncertainty of the FSP model was calculated to be 2.02%, and the penalty remained at 0.29% δk/k with 0.28% δk/k continuing to result from the Be(n,n) reaction.

An alternative method for uncertainty quantification is the code TSURFER.[19] Like TSUNAMI-IP, TSURFER uses sensitivity data calculated by TSUNAMI-3D and cross-section covariance data to determine uncertainty, but unlike TSUNAMI-3D also employs the measured k_{eff} values of the benchmark experiments. The initial estimates for the computed and measured responses are improved by adjusting the experimental values and the nuclear data – taking into account correlated uncertainties – so that the most self-consistent set of data is obtained. Consolidation of the original experimental data and calculated results reduces the prior uncertainty in the response estimates because additional information has been incorporated.

TSURFER analysis was performed using only the four ZPPR experiments and using both the ZPPR and Be-reflected HEU experiments. Correlations between experiments, which may result from such things as experiments using the same materials or the same measurement devices, are included in a TSURFER analysis. Since these correlations are difficult to quantify, a parametric study using a variety of coefficients was implemented. It was assumed that correlations existed between the four ZPPR experiments and the three Be-HEU experiments, but no correlations existed between the two sets.

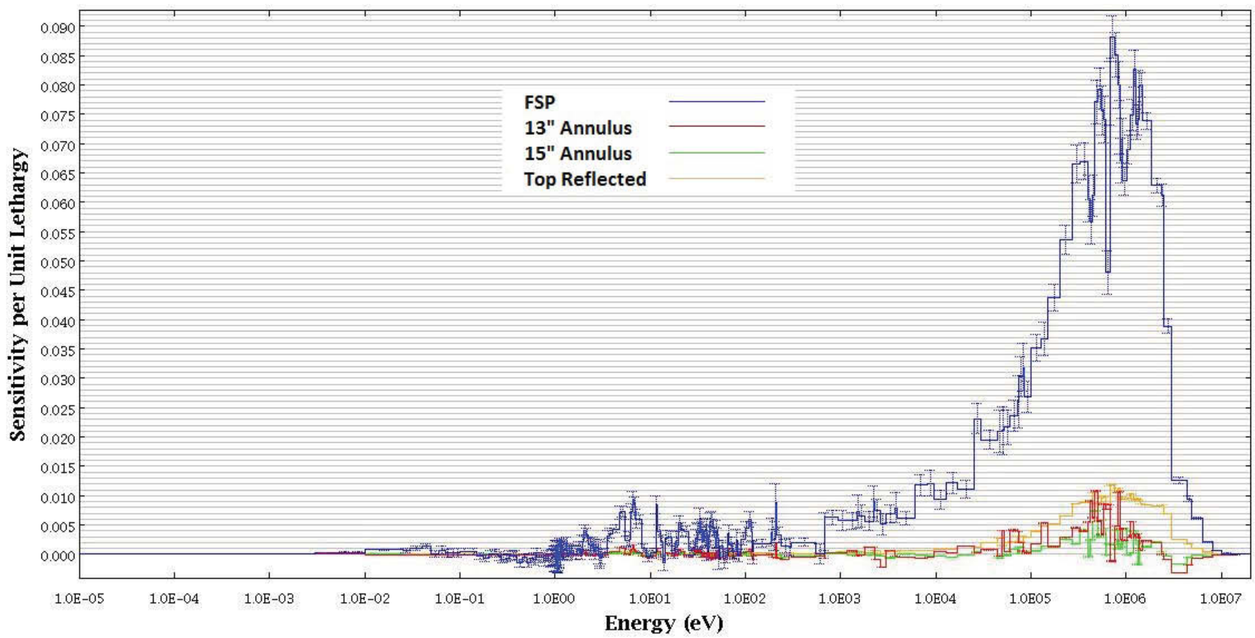

FIGURE 1. Sensitivity profiles of the FSP model and the 13” Annulus, 15” Annulus, and Top Reflected Be-reflected HEU benchmarks

Table 4 shows the final calculated uncertainties of the FSP model for a set of experimental correlation coefficients when FSP was compared to the ZPPR experiments only. The final calculated uncertainty ranges from 0.53% for correlation coefficients less than 0.5 to 0.45% for full correlation between experiments. The addition of the three Be-HEU experiments tends to reduce the final overall uncertainty calculated by TSURFER, as illustrated in Table 5. Aside from an outlier of 2.36% uncertainty for full correlation in both experiment sets, the final calculated uncertainty ranges from 0.20% (for correlation coefficients of 0.9 in both experiment sets) to 0.47% (for correlation coefficients of 0.0 or 0.1 in both experiment sets). Therefore it appears that the additional information provided by the three Be-HEU experiments provides a benefit in the TSURFER calculation of final overall uncertainty.

It should also be noted that the TSURFER results for post-adjustment uncertainty are larger than those generated from the TSUNAMI-IP penalty calculation. The penalty calculation only accounts for remaining uncertainty due to under-coverage of the application sensitivity data. The TSURFER post adjustment uncertainty assessment quantifies uncertainties due to lacking or inconsistent data present from multiple benchmark experiments.

With TSURFER, it may be possible to further reduce uncertainties by including benchmark experiments with beryllium, but with different fuel types. A small, compact, unmoderated critical assembly consisting of HEU-O_2 reflected by beryllium was performed at ORCEF was developed for space reactor design analysis.[20] It would be beneficial to benchmark and include this experiment in the analysis of the FSP model. As the results indicate, the inclusion of additional experimental data using existing benchmarks or new experiments would be necessary to further reduce the uncertainty due to the Be(n,n) reaction.

TABLE 4. Experimental correlation coefficients and calculated uncertainty in the FSP model; 4 ZPPR experiments only

Correlation	Uncertainty(%)
0.1	0.53
0.2	0.53
0.3	0.53
0.4	0.53
0.5	0.52
0.6	0.52
0.7	0.51
0.8	0.50
0.9	0.48
1.0	0.45

TABLE 5. Experimental correlation coefficients and calculated uncertainty in the FSP model; 4 ZPPR experiments and 3 Be-Reflected HEU experiments

Be-HEU Correlation	ZPPR Correlation	Uncertainty(%)
0.0	0.0	0.47
0.1	0.1	0.47
0.2	0.2	0.46
0.3	0.3	0.45
0.4	0.4	0.44
0.5	0.5	0.42
0.6	0.6	0.40
0.7	0.7	0.37
0.8	0.8	0.31
0.9	0.9	0.20
1.0	1.0	2.36
0.2	0.4	0.46
0.2	0.6	0.45
0.2	0.8	0.43
0.4	0.2	0.45
0.4	0.6	0.43
0.4	0.8	0.41
0.6	0.2	0.42
0.6	0.4	0.42
0.6	0.8	0.37
0.8	0.2	0.39
0.8	0.4	0.38
0.8	0.6	0.36

CONCLUSION

An uncertainty analysis of the fission surface power (FSP) system was recently performed using a comparison to four ZPPR benchmark experiments. While this study indicated that current capabilities could preclude the necessity of a cold critical test of the FSP, a reduction in the uncertainty of beryllium and uranium cross-section data, which would reduce the overall uncertainty in the computed FSP design model, is still desired. In an effort to reduce these uncertainties, three more critical benchmark experiments, all containing HEU with beryllium reflectors, were added to the FSP analysis. Despite the presence of uranium and beryllium in these benchmarks, however, TSUNAMI-IP analysis indicated that the sensitivity of the benchmarks to the beryllium elastic scatter cross section (the dominant contributor to overall uncertainty) was much smaller than the sensitivity of the FSP model to this cross section, indicating that these experiments are not useful for quantifying the Be(n,n) bias. TSUNAMI-IP produced nearly the same uncertainty using the both the three Be-HEU benchmarks and the four ZPPR benchmarks as when only the four ZPPR benchmarks were used.

Another method for uncertainty quantification, the code TSURFER, was also used to study FSP model. TSURFER employs an adjustment methodology to maximize consistency between calculated and experimental values, thus reducing overall uncertainty. For its analysis, TSURFER also incorporates correlations between the critical benchmarks experiments used in the comparison to the FSP system. A parametric study of final calculated uncertainties in k_{eff} as a function of correlation coefficients indicates that the addition of the three new critical benchmark experiments is beneficial for reducing uncertainty. The inclusion of these three experiments results in an approximately 0.1% reduction in the final uncertainty calculated by TSURFER.

With TSURFER, it may be possible to further reduce uncertainties by including benchmark experiments with beryllium, but with different fuel types.

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