Recent use of covariance data for criticality safety assessment

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The TSUNAMI codes of the Oak Ridge National Laboratory SCALE code system were applied to a burnup credit application to demonstrate the use of sensitivity and uncertainty analysis with recent cross-section covariance data for criticality safety code and data validation. The use of sensitivity and uncertainty analysis provides for the assessment of a defensible computational bias, bias uncertainty, and gap analysis for a complex system that otherwise could be assessed only through the use of expert judgment and conservative assumptions.

I. Introduction

The *American National Standards for Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*, ANSI/ANS-8.1-1998 [1], and the *American National Standard for Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations*, ANSI/ANS-8.24-2007 [2], allow the use of calculations in the determination of subcritical limits for the design of fissionable material systems. The standards require validation of the analytical methods and data used in nuclear criticality safety calculations to quantify any computational bias and the uncertainty in the bias. The validation procedure must be conducted through comparison of the computed results with experimental data, and the design system for which the subcritical limit is established must fall within the area of applicability of the experiments chosen for validation. The 8.1 standard defines the area (or areas) of applicability as "the limiting ranges of material compositions, geometric arrangements, neutron energy spectra, and other relevant parameters (e.g., heterogeneity, leakage, interaction, absorption, etc.) within which the bias of a computational method is established."

In compliance with the standards, the nuclear criticality safety community in the United States typically evaluates the computational biases and uncertainties of its computational methods and nuclear data through the use of trending analyses, usually a linear regression with a statistical confidence band. For a traditional trending analysis, a suite of experimental benchmarks is selected with physical characteristics that are similar to the corresponding values in the design system for which the subcritical limit is to be established.[3] Some physical characteristics used to evaluate system similarity are fissile element(s), fissile concentration, moderator type, geometrical configuration, hydrogen-to-fissile atom ratios (H/X), average neutron-energy group causing fission, and energy of average neutron lethargy causing fission (EALF). Typically, the trending parameters are calculated as averages for each benchmark experiment.

Each of the experiments in the benchmark suite is modeled with the same code and neutron cross-section data that will be used in the criticality safety analysis of the design system. The difference between the measured and calculated values of k_{eff}, the effective neutron multiplication factor, of a critical experiment is considered to be the computational bias for that experiment. The expected computational bias of the design system is established through a trending analysis of the bias for all of the selected critical experiments as a function of their physical characteristics (e.g., H/X, EALF). The uncertainty in the bias is established through a statistical analysis of the trend, taking into account the uncertainty in each k_{eff} data point and the distribution of the data.

The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) software developed at Oak Ridge National Laboratory (ORNL) provides a unique means of determining the similarity of nuclear criticality experiments to safety applications.[4] Instead of using one or more average physical parameters to characterize a system, correlation coefficients are developed by propagating the uncertainties in neutron cross-section data to uncertainties in the computed neutron multiplication factor for experiments and safety applications through sensitivity coefficients. The bias in the experiments, as a function of correlation with the intended application, is extrapolated to predict the bias and bias uncertainty in the application.

Even with advanced tools to identify benchmark experiments, criticality safety analysts occasionally find that the safety analysis models include some feature or material for which adequately similar, well-defined critical experiments do not exist to support validation. For example, the analyst may want to take credit for the presence of fission products in spent nuclear fuel. In such cases, analysts sometimes rely on "expert judgment" to select an additional administrative margin to cover the validation weakness or to conclude that the impact on the calculated bias and bias uncertainty is negligible. As a result of advances in computer programs and the evolution of cross-section covariance data, analysts can use the sensitivity and uncertainty analysis tools in the TSUNAMI codes to estimate the potential impact on the application-specific bias and bias uncertainty resulting from nuclides not represented in the critical experiments. This paper presents the application of methods described in a companion paper [5] to develop a methodology for producing a defensible upper subcritical limit for a burnup credit model.

II. Basis for Validation Assumption

The basis of the TSUNAMI validation techniques is that computational biases are primarily caused by errors in the cross-section data, which are quantified and bounded by the cross-

section-covariance data. To provide credence to this claim, sensitivity data for 1378 critical benchmark experiments were generated with TSUNAMI-3D, and the cross-section-covariance data were propagated to uncertainties in the computed values of k_{eff}. In this exercise, k_{eff} and sensitivity data for the benchmark experiments were drawn from those available from a variety of previous studies. As a result of this agglomeration of existing data, results were computed with ENDF/B-V, ENDF/B-VI, and some ENDF/B-VII cross-section data. The cross-section covariance data used for this analysis are the most recent data available for public use from SCALE 5.1, the 44GROUPV6RECU233 library, available for download from the SCALE website, which consists of all ENDF/B-VI covariance data, prerelease ENDF/B-VII covariance data for ^{233}U, some covariance data from other sources such as JENDL, and the low-fidelity covariance data for thermal and intermediate energies for > 200 nuclides.[6]

Application of these covariance data to 1378 benchmark experiments, consisting of a variety of fuel types and moderation levels, results in the k_{eff} plots shown in Figs. 1–6 for ^{233}U, high-enriched uranium (HEU) and intermediate-enriched uranium (IEU), low-enriched uranium (LEU), Pu, mixed-oxide (MOX), and haut taux de combustion (HTC) or high burnup [7–10] systems, respectively. With the exception of the HTC systems, most of these experiment configurations are available in the International Criticality Safety Benchmark Experiment Project Handbook.[11] All systems were modeled and computed using the multigroup Monte Carlo code KENO V.a from SCALE 5.1 with 238-group cross sections. In Figs. 1–6, the actual computational biases of the benchmarks are the differences between the computed data points and k_{eff} = 1.0. For this exercise, a uniform experimental uncertainty of 0.3% is assumed for each critical configuration. In an actual criticality safety assessment, the true experimental uncertainty for each configuration should be determined, and consistency should be observed in the selection of the cross-section and cross-section-covariance data libraries for all benchmark experiments and safety applications. However, for the purposes of this manuscript, the conveniently available values were used. Analysis of the distribution of data in Figs. 1–6 reveals that computed and experimental values agree within one standard deviation for 81% of the experiments, within two standard deviations for 98%, and within three standard deviations for 99.6%. Thus, the initial assumption that biases are bounded by the uncertainties is supported by the results.

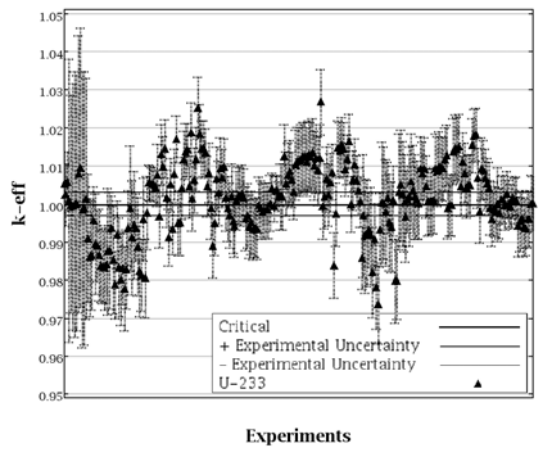

FIG. 1: k_{eff} and uncertainty for ^{233}U systems.

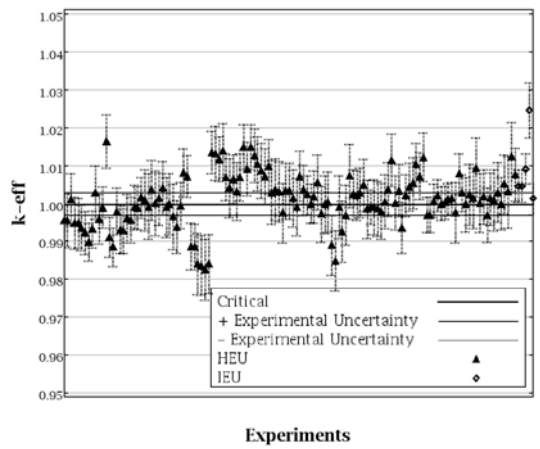

FIG. 2: k_{eff} and uncertainty for HEU and IEU systems.

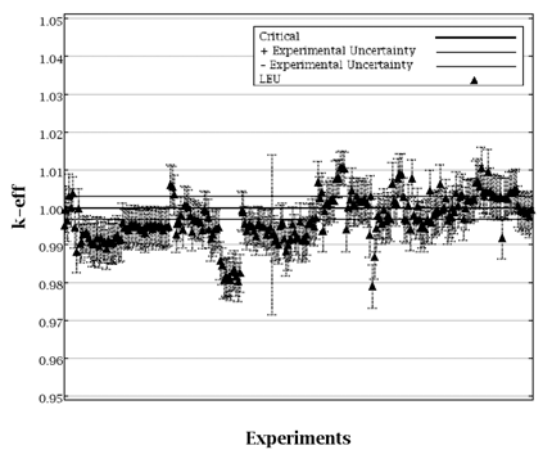

FIG. 3: k_{eff} and uncertainty for LEU systems.

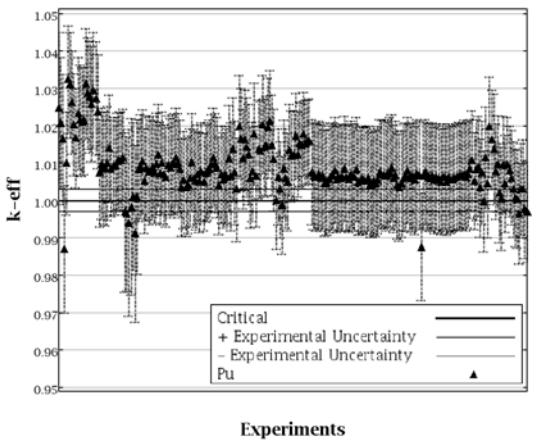

FIG. 4: k_{eff} and uncertainty for Pu systems.

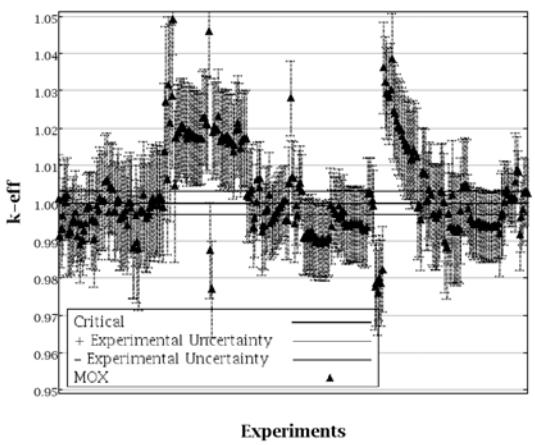

FIG. 5: k_{eff} and uncertainty for MOX systems.

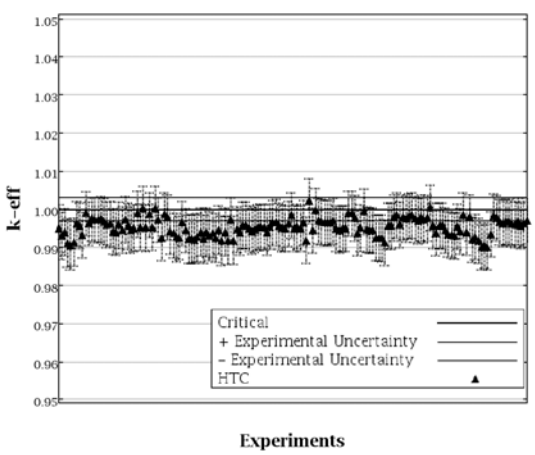

FIG. 6: k_{eff} and uncertainty for HTC systems.

III. Application System

The application system selected for analysis is the Transportation, Aging, and Disposal (TAD) canister designed for Yucca Mountain.[12] The TAD canister is a stainless steel vessel used for the transportation, cooling (aging), and disposal of spent nuclear fuel. At Yucca Mountain, the TAD canister is removed from the shipping cask and placed into either an aging package, which allows the spent fuel to further cool prior to placement inside the repository, or a disposal package for placement in the repository.

The computational model represents 21 pressurized-water-reactor spent fuel assemblies in a TAD canister inside a disposal package flooded with water and surrounded by earthen materials called tuff, simulating burial in the Yucca Mountain repository. The 21 fuel assemblies are Babcock and Wilcox 15 × 15 bundles that have been burned to 40 GWd/MTU. There are seven axial zones in the fuel, but only one radial zone. A stainless steel sheath surrounds each of the fuel bundles, which are also separated by borated steel plates. Cutaway views of the TAD canister, fuel, and disposal package and a 15×15 fuel bundle section are shown in Fig. 7. In this model of the TAD canister, the fuel burnup analysis tracked 14 actinides and 15 fission products. The nuclides present in each major component of the TAD, except for water, are shown in Table I.

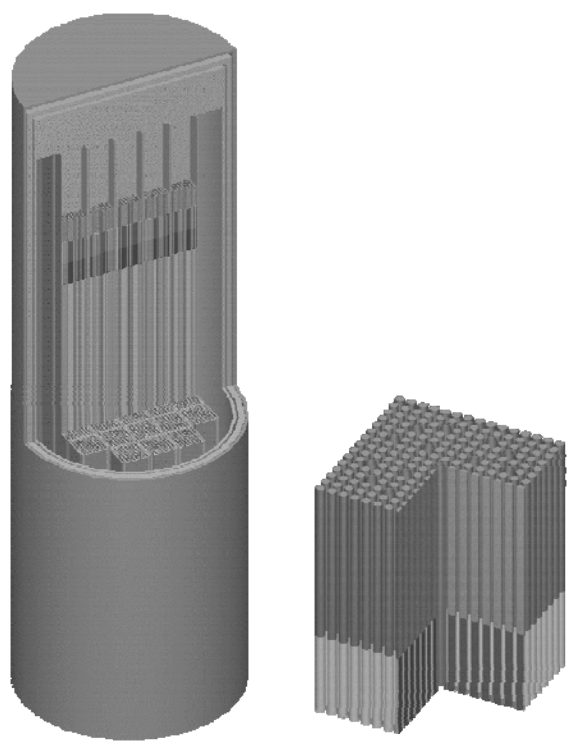

FIG. 7: Cutaway views of TAD canister and 15×15 fuel bundle.

TABLE I: Nuclides in TAD model.

Spent Fuel		Clad	Steel Sheaths	Borated Steel	Tuff
^{16}O	^{233}U	^{16}O	C	^{10}B	^{16}O
^{95}Mo	^{234}U	^{50}Cr	^{14}N	^{11}B	^{23}Na
^{99}Tc	^{235}U	^{52}Cr	Si	C	Mg
^{101}Ru	^{236}U	^{53}Cr	^{31}P	^{14}N	^{27}Al
^{103}Rh	^{238}U	^{54}Cr	^{32}S	Si	Si
^{109}Ag	^{237}Np	^{54}Fe	^{50}Cr	^{31}P	^{31}P
^{143}Nd	^{238}Pu	^{56}Fe	^{52}Cr	^{32}S	K
^{145}Nd	^{239}Pu	^{57}Fe	^{53}Cr	^{50}Cr	Ca
^{147}Sm	^{240}Pu	^{58}Fe	^{54}Cr	^{52}Cr	Ti
^{149}Sm	^{241}Pu	Zr	^{55}Mn	^{53}Cr	^{55}Mn
^{150}Sm	^{242}Pu	^{112}Sn	^{54}Fe	^{54}Cr	^{54}Fe
^{151}Sm	^{241}Am	^{114}Sn	^{56}Fe	^{55}Mn	^{56}Fe
^{152}Sm	^{242m}Am	^{115}Sn	^{57}Fe	^{54}Fe	^{57}Fe
^{151}Eu	^{243}Am	^{116}Sn	^{58}Fe	^{56}Fe	^{58}Fe
^{153}Eu		^{117}Sn	^{58}Ni	^{57}Fe	
^{155}Gd		^{118}Sn	^{60}Ni	^{58}Fe	
		^{119}Sn	^{61}Ni	^{59}Co	
		^{120}Sn	^{62}Ni	^{58}Ni	
		^{122}Sn	^{64}Ni	^{60}Ni	
		^{124}Sn	Mo	^{61}Ni	
				^{62}Ni	
				^{64}Ni	

IV. TSUNAMI Analysis of TAD Canister

A sensitivity and uncertainty analysis of the TAD canister model was performed with TSUNAMI-3D using ENDF/B-VI cross-section data from the SCALE 5.1 238-group library.[13] Resonance self-shielding calculations with implicit sensitivity coefficient generation were performed with BONAMIST, CENTRMST, and PMCST for each fuel composition and structural component in the model. Forward and adjoint neutron transport calculations were performed with KENO V.a, and the sensitivity coefficients were computed with the SAMS module. The energy-dependent sensitivity data for some important nuclides and reactions are shown in Fig. 8, in which it can be observed that the k_{eff} of the TAD canister is most sensitive to cross sections at thermal and intermediate energies. The cross-section covariance data from the SCALE 44GROUPV6RECU233 library were propagated to uncertainties in k_{eff} for the TAD canister using the TSUNAMI-IP module of SCALE. TSUNAMI-IP provides options to append user-defined covariance data to supplement shortcomings in the library. In this case, a 5% uncertainty was assigned to the fast energies for low-fidelity covariances, with a full correlation across the energy region. The overall uncertainty of k_{eff} for the TAD canister due to cross-section covariances is 0.60% Δk/k. The largest uncertainties for the TAD canister are shown in Table II, ordered in decreasing magnitude. As biases are caused by errors in the cross sections and are bounded by the uncertainties, the data in Table II provide a ranked list of nuclides and reactions that should be the top contributors to the computational bias for the TAD canister. Based on the top contributors to uncertainty, critical experiments that are most likely to produce similar bias will contain ^{239}Pu and ^{238}U in a thermal spectrum. Fission products and structural materials are of secondary importance in bias determination.

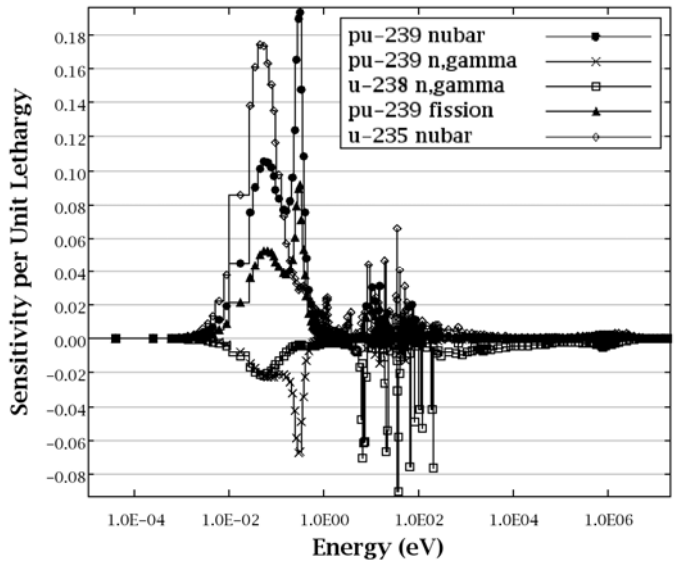

FIG. 8: Sensitivity profiles for important nuclide reactions in TAD.

TABLE II: Top contributors to uncertainty in k_{eff} for TAD canister.

Covariance Matrix		% Δk/k
^{239}Pu nubar	^{239}Pu nubar	4.0032E-01
^{239}Pu n,gamma	^{239}Pu n,gamma	2.2350E-01
^{238}U n,gamma	^{238}U n,gamma	2.2281E-01
^{239}Pu fission	^{239}Pu fission	1.5511E-01
^{235}U nubar	^{235}U nubar	1.3980E-01
^{239}Pu chi	^{239}Pu chi	1.1627E-01
^{235}U fission	^{235}U fission	8.3958E-02
^{235}U n,gamma	^{235}U n,gamma	8.1041E-02
^{238}U elastic	^{238}U n,gamma	-7.7056E-02
^{56}Fe n,gamma	^{56}Fe n,gamma	6.5059E-02
^{239}Pu nubar	^{241}Pu nubar	6.2339E-02
^{239}Pu fission	^{239}Pu n,gamma	5.6603E-02
Zr n,gamma	Zr n,gamma	4.7340E-02
^{1}H elastic	^{1}H elastic	4.6046E-02
^{240}Pu n,gamma	^{240}Pu n,gamma	4.5968E-02
^{143}Nd n,gamma	^{143}Nd n,gamma	4.1819E-02

V. Similarity and Bias Assessment

The similarity of each of the 1378 critical experiments described in Section II relative to the TAD canister was determined using the c_k integral index from TSUNAMI-IP. The results of this analysis are presented in Fig. 9, which shows that the least similar experiments are ^{233}U systems with increasing similarity for HEU, LEU, Pu, MOX, and HTC systems.

The ORNL Upper Subcritical Limit STATistical Software (USLSTATS) package [3] was applied to determine the computational bias, bias uncertainty and upper subcritical limit (USL) based on trends in calculated k_{eff} values as a function of their similarity to the TAD canister as determined by the

integral index, c_k. In this assessment, only critical experiments that are highly correlated to the safety application are included in the statistical analysis. In this case, only experiments with c_k values of 0.90 or higher are included, indicating that at least 90% of the uncertainty in the safety application is shared by the selected benchmark experiments. Through the definition of the c_k correlation coefficient, extrapolation of the linear regression to a c_k of 1.0 indicates full correlation with the uncertainties in the safety application, and thus the bias in the safety application is predicted. For this example exercise, the predicted k_{eff} is 0.993, indicating a computational bias of -0.7% Δk/k, as shown by the k(x) curve in Fig. 10. The singled-sided quadratic confidence band, w(x), computed to a 0.95/0.95 confidence gives an uncertainty in this bias of 0.7% Δk/k at c_k = 1.0. However, it should be noted that the critical experiments used in this bias determination exercise had c_k values ranging from 0.90 to 0.97, but not extending to 1.0. Thus, a portion of the bias in the TAD canister is not accounted for in the critical experiments selected for this exercise. In particular, no critical experiments contain fission products, resulting in a gap in the validation. In the absence of additional interpretation, the impact of the fission products on the computational bias and uncertainty is unquantified.

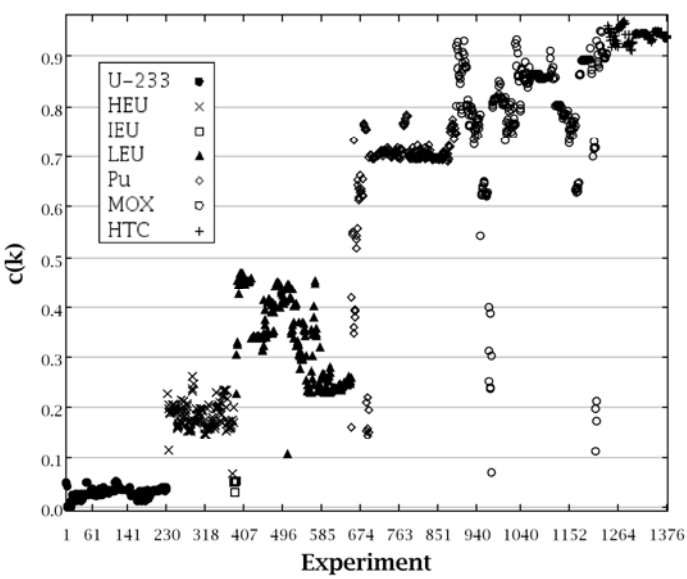

FIG. 9: Values of c_k for 1378 experiments relative to TAD.

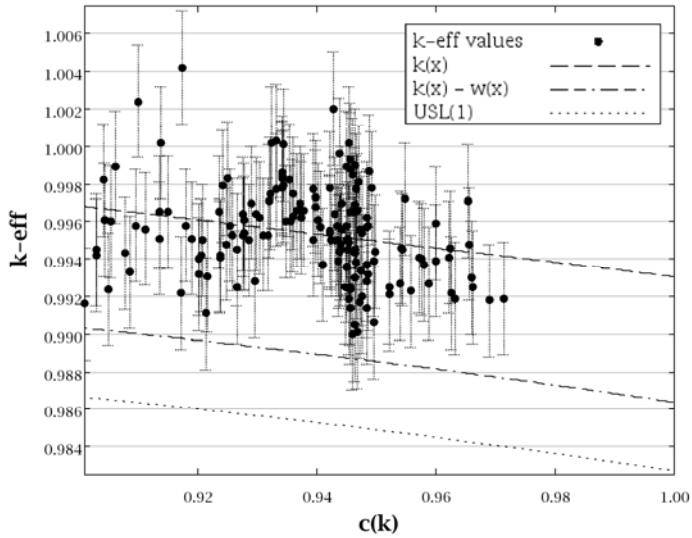

FIG. 10: Bias, bias uncertainty, and USL results.

VI. Gap Analysis

The TSUNAMI tools include a gap analysis methodology for quantifying an additional USL penalty resulting from uncertainties in the safety application that exceed the area of applicability of the critical experiment suite selected for validation. The penalty calculation determines the uncertainty remaining after the coverage for each group-wise, nuclide-reaction-specific sensitivity from the suite of benchmark experiments is deducted from the sensitivity of the safety application. The penalty procedure is described in detail in the SCALE manual section for TSUNAMI-IP.[13]

For the TAD canister, the penalty calculation reveals that the uncertainty arising from the gap in the area of applicability of the benchmark experiment suite results in a one-standard-deviation additional uncertainty (in the USL) of 0.18% Δk/k. The penalty introduced from each covariance matrix is shown in Table III. Note that some of the top contributors to the overall uncertainty in the TAD are present, but with reduced values relative to Table II. A reduction in uncertainty indicates that the proper materials were present in the critical experiments, but they were either not present in sufficient quantities, or the spectra of the experiments differed from the spectrum of the safety application. For other nuclides, such as the fission products, the penalty quantity listed in Table III is the same as the uncertainty quantity listed in Table II, indicating an absence of the material from the experimental suite.

If a material is lacking or absent from the experimental suite, its bias cannot be determined by direct comparison with experiments as recommended by the standards. However, the standards do allow for extrapolations beyond the area of applicability. The penalty-calculation methodology quantifies the potential impact of this extrapolation from an otherwise complete validation suite. Using a 95% confidence level for this extrapolation, a 0.36% Δk/k penalty is applied to the USL for

the TAD canister, as shown by the USL(1) curve in Fig. 10. Thus, based on this exercise, the maximum allowed computed value for this configuration of the TAD canister to ensure that the actual TAD will be subcritical in the same configuration is 0.983.

It should be noted that the quality of the penalty calculation and resulting USL are only as good as the quality of the covariance data from which they are derived. For complex materials, such as those used here, quality covariance data are needed for many nuclides.

TABLE III: Top contributors to USL penalty for TAD canister.

Covariance Matrix				% Δk/k
^{239}Pu nubar		^{239}Pu nubar		7.0692E-02
^{239}Pu n,gamma		^{239}Pu n,gamma		6.5976E-02
^{239}Pu fission		^{239}Pu fission		6.2445E-02
^{56}Fe n,gamma		^{56}Fe n,gamma		5.1023E-02
^{235}U fission		^{235}U fission		5.0409E-02
^{238}U n,gamma		^{238}U n,gamma		4.7994E-02
^{235}U chi		^{235}U chi		4.4762E-02
^{235}U n,gamma		^{235}U n,gamma		4.2924E-02
^{143}Nd n,gamma		^{143}Nd n,gamma		4.1819E-02
^{239}Pu chi		^{239}Pu chi		4.0166E-02
^{239}Pu fission		^{239}Pu n,gamma		-2.8513E-02
^{103}Rh n,gamma		^{103}Rh n,gamma		2.6863E-02
^{145}Nd n,gamma		^{145}Nd n,gamma		2.2994E-02
^{149}Sm n,gamma		^{149}Sm n,gamma		2.2000E-02
^{236}U n,gamma		^{236}U n,gamma		2.1556E-02
^{101}Ru n,gamma		^{101}Ru n,gamma		2.1286E-02

VII. Conclusions

Through this example exercise, the use of sensitivity and uncertainty analysis to quantify the bias, bias uncertainty, and gap analysis of the described Yucca Mountain TAD canister has been demonstrated. Before the availability of computational tools and data for this sensitivity and uncertainty analysis, the bias, bias uncertainty, and especially gap analysis could be performed only though subjective interpretations and expert judgments. The methodologies employed through the TSUNAMI tools with the best-available covariance data provide a physics-based, defensible approach to establishing bias and k_{eff} prediction due to uncertainties in nuclear data in cases where critical experiment data is lacking or non-existent, which is a very important and real issue in criticality safety analyses. Although this approach has broad and significant implications in the field of criticality safety, its practical usefulness is dependent on the fidelity of the covariance data. Hence, future work is planned to more definitively compare bias predictions from this methodology to bias predictions based on critical experiments for situations in which sufficient critical experiment data are available.

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