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A Criticality Code Validation Exercise for a LEU Lattice

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INTRODUCTION

In the criticality code validation of common systems, many paths to a correct bias, bias uncertainty, and upper subcritical limit may exist. The challenge for the criticality analyst is to select an efficient, defensible, and safe methodology to consistently obtain the correct values.

One method of testing criticality code validation techniques is to use a sample system with a known bias as a test application and determine if the methods employed can reproduce the known bias. In this summary, a low-enriched uranium (LEU) lattice critical experiment with a known bias is used as the test application, and numerous other LEU experiments are used as the benchmarks for the criticality code validation exercises using traditional and advanced parametric techniques. The parameters explored are enrichment, energy of average lethargy causing fission (EALF), and the TSUNAMI integral index c_k with experiments with varying degrees of similarity.

TEST APPLICATION SYSTEM

For this exercise, the critical experiment identified in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*[1] (IHECSBE) as LEU-COMP-THERM-017 Case 22 was selected as the test application system. This system consists of square-pitched clusters of water-moderated $U(2.35)O_2$ rods with steel reflecting walls. This system has an EALF value of 0.194. With ENDF/B-V cross sections, SCALE/KENO V.a[2] computes a k_{eff} of 0.9901 ± 0.0002. The experimentally measured k_{eff} is 1.0 with a stated uncertainty of 0.28%. The negative code bias of ~1% lies outside three standard deviations of the experimental uncertainty. The exercises reported in this summary are used to account for this bias in an effort to determine of an appropriate upper subcritical limit for safe operation had this been a system with an unknown bias.

BENCHMARK EXPERIMENTS

A key element in a criticality code validation is the selection of appropriate benchmark experiments. For this exercise, 214 thermal LEU benchmark experiments from the IHECSBE were selected for initial evaluation. The benchmarks include fuel-rod lattices as well as solution systems. The solution systems were included because they have similar enrichments to that of the test application, but should be rejected by the parametric techniques for obvious other dissimilarities. Benchmarks are included from evaluations LEU-COMP-THERM-009, -010, -017, -018, -019, -020, -021, -022, -023, -024, -026, -032, -040, and -042, as well as LEU-SOL-THERM-001, -003, -004, -005, -006, -007, -008, -009, -010, -016, -017, -018, -019, 020, and -021. These experiments have ^{235}U enrichments ranging from 2.35 to 10.08 wt % and EALF values ranging from 0.035 to 1.95 eV.

For this exercise, benchmarks are available that contain all of the nuclides present in the test application. For systems where all nuclides are not present in a single benchmark, alternative techniques, beyond the scope of this summary, should be explored.

TRADITIONAL TRENDING ANALYSIS

The first technique employed in this validation exercise is that documented in NUREG/CR-6361[3], which uses a trending analysis of k_{eff} relative to some average system parameter(s). The techniques described in Ref. 3 are well known, and hence not repeated here. Two trending parameters, enrichment and EALF, were selected for this exercise, and ULSTATS[3] was used to compute the bias, bias uncertainty, and USL-1 value. An arbitrary administrative margin of 5% was used for this exercise.

Using all 214 benchmarks, USLSTATS predicts a k_{eff} of 0.9947 with a confidence width of 0.008744 and a USL-1 value of 0.9359 for systems with an enrichment of 2.35 wt % and a k_{eff} of 0.9982 with a confidence width of 0.01049 and a USL-1 value of 0.9377 for systems with an EALF of 0.194 eV. Trend plots for this analysis are shown in Figs. 1 and 2 for enrichment and EALF, respectively. The error bars on the k_{eff} values in the figures represent the quadratically combined experimental and Monte Carlo uncertainties.

* Managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

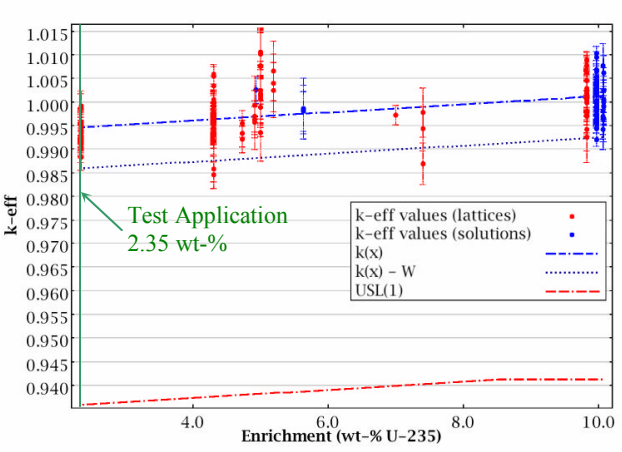

Fig. 1. Trend plot of k_{eff} vs. enrichment for 214 benchmarks.

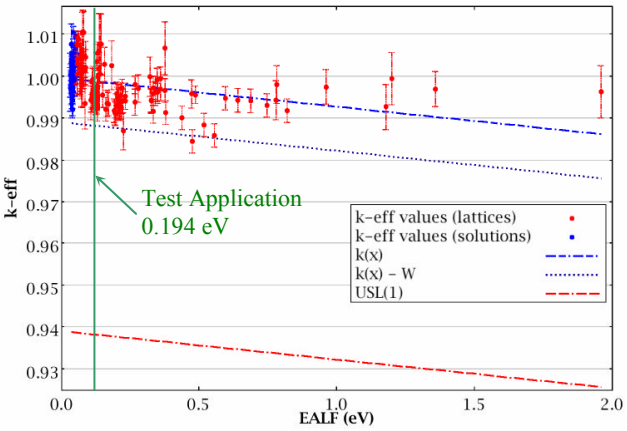

Fig. 2. Trend plot of k_{eff} vs. EALF for 214 benchmarks.

In Fig. 1, the benchmark k_{eff} values at the target enrichment of 2.35 wt % range from ~0.99 to ~1.00, and in Fig. 2, a greater spread of data, ~0.99 to ~1.01, is observed near the target EALF of 0.194 eV. Given the large number of selected benchmarks with parameter values near the target values, a non-parametric analysis could be used to assess a negative 1% bias, consistent with that observed for the test application system. However, it is possible that if some benchmarks were excluded from the analysis, a non-conservative estimate of the true bias could result.

Even when the benchmarks are parsed in parametric space such that only lattice benchmarks with the target enrichment of 2.35% are examined, a 0.5% spread in k_{eff} values near the target EALF value of 0.194 remains, as shown in Fig. 3.

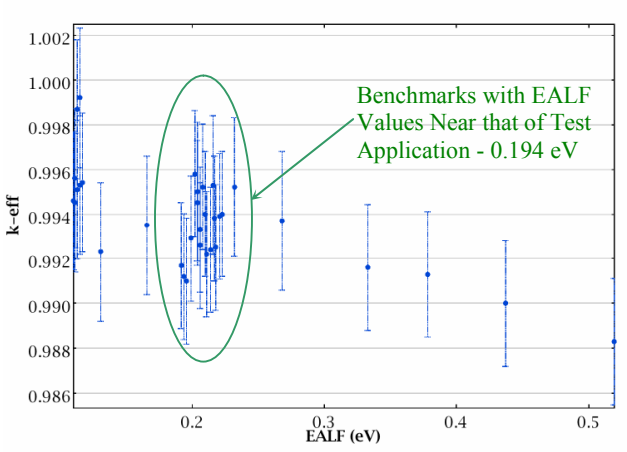

Fig. 3. Plot of k_{eff} vs. EALF for lattice benchmarks with ^{235}U enrichments of 2.35 wt %.

TSUNAMI METHODS

The Tools for Sensitivity and UNcertainty Analysis Methodology Implementation (TSUNAMI) [4,5] computational sequences within the SCALE code system use first-order eigenvalue perturbation theory to predict the response of a system k_{eff} value to changes in each constituent group-wise cross-section-data value. These sensitivity data can be coupled with energy-dependent cross-section-covariance data to give an uncertainty in the computed k_{eff} value due to uncertainties in the cross-section data. The TSUNAMI-IP[6] code utilizes the sensitivity and uncertainty data from an application and a benchmark to quantify system similarity with numerical indices, including the integral index c_k. The c_k index is a correlation coefficient that quantifies the amount of shared uncertainty in the k_{eff} values of an application and a benchmark due to cross-section uncertainties. A c_k value of 1.0 means that the uncertainties for the application and the benchmark are all generated from the same nuclides and reactions at the same energies, whereas a c_k value of 0.0 means that uncertainties of the two systems are completely unrelated.

A premise of the TSUNAMI validation concept is that computational biases originate with the cross-section data. If the cross-section uncertainties are correctly tabulated, then computational biases should be bounded by the uncertainties. For the current application system, TSUNAMI gives the uncertainty in k_{eff} due to uncertainties in the cross section data of 0.85%. When combined quadratically with the experimental (0.28%) and statistical (0.02%) uncertainties for this system, a total uncertainty of 0.90% results. Recall that the computed k_{eff} of this system is 0.9901 ± 0.0002. Thus, this computed k_{eff} lies just outside one standard deviation of the measured value of 1.0.

USE OF TSUNAMI FOR SIMILARITY ASSESSMENT

The sensitivity data for the test application and the benchmarks were drawn from an existing database of TSUNAMI sensitivities computed with the KENO V.a-based TSUNAMI-3D sequence using the SCALE 238-group ENDF/B-V cross-section data library. These sensitivity data were processed through the TSUNAMI-IP code to produce the c_k of each benchmark relative to the test application.

A scatter plot of k_{eff} vs. c_k for all 214 benchmarks is shown in Fig. 4. All experiments have c_k values above 0.8, with some as high as 0.999. This indicates that the minimum correlation of the uncertainties for the selected benchmarks is 80% and the maximum correlation is 99.9%. As c_k approaches 1.0, the k_{eff} values of the most similar benchmarks converge towards the k_{eff} of the test application. The TSUNAMI methods provide a convenient means of automatically selecting experiments that are most similar to the test application. The c_k values for 2.35 wt % benchmarks are shown in Fig. 5 as a function of EALF. The benchmarks with EALF values closest to that of the test application, 0.194 eV, have c_k values near 1.0. The c_k value decreases for benchmarks with increasing or decreasing EALF values relative to the test application. Thus, the TSUNAMI methods have automatically selected the benchmarks that are most similar to the test applications in terms of multiple traditional trending parameters.

Examining the k_{eff} values of only the 2.35 wt % benchmarks with c_k values ≥ 0.98 shown in Fig. 6, the trend of the benchmarks towards a k_{eff} of 0.99 where c_k = 1.0 is further emphasized.

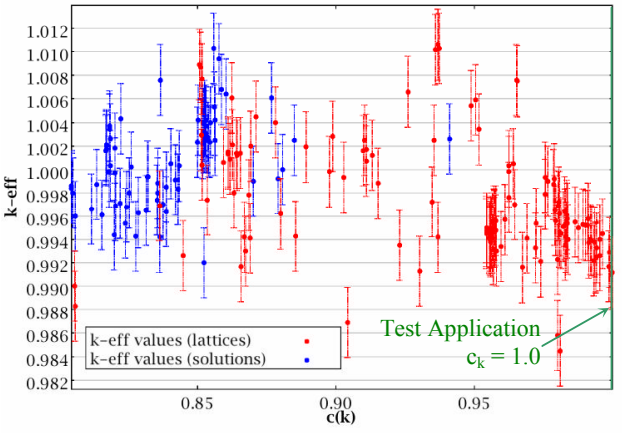

Fig. 4. Scatter plot of k_{eff} vs. c_k for 214 benchmarks.

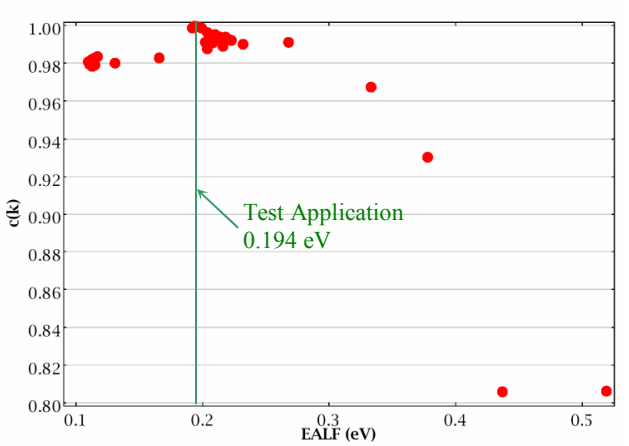

Fig. 5. Plot of c_k vs. EALF for benchmarks with ^{235}U enrichments of 2.35 wt %.

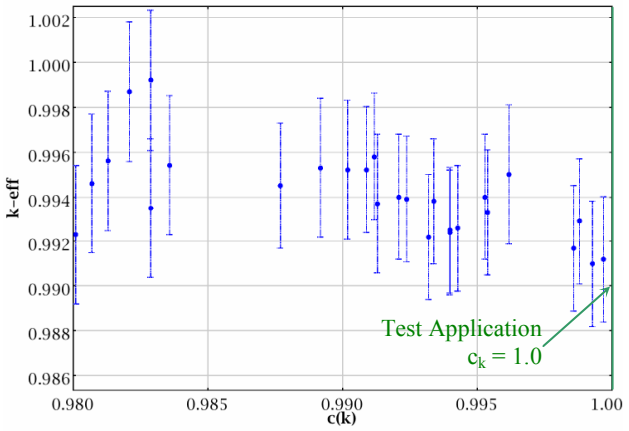

Fig. 6. Plot of k_{eff} vs. c_k for benchmarks with ^{235}U enrichments of 2.35 wt %.

USE OF TSUNAMI FOR BIAS DETERMINATION

TSUNAMI was used to predict the bias, bias uncertainty, and USL-1 for the test application. If k_{eff} is trended from low to high values of c_k, then extrapolating to the k_{eff} value where c_k is 1.0 gives the predicted bias of the application system. With extrapolations, the confidence band is non-linear, and an enhanced version of USLSTATS was developed to output a quadratic confidence band.

When c_k trending is applied to the test application with all 214 benchmarks, and with the extrapolation to c_k = 1.0, USLSTATS predicts a k_{eff} of 0.9953 with a confidence width of 0.009205 and a USL-1 value of 0.9361. The trend plot of this analysis is shown in Fig. 7.

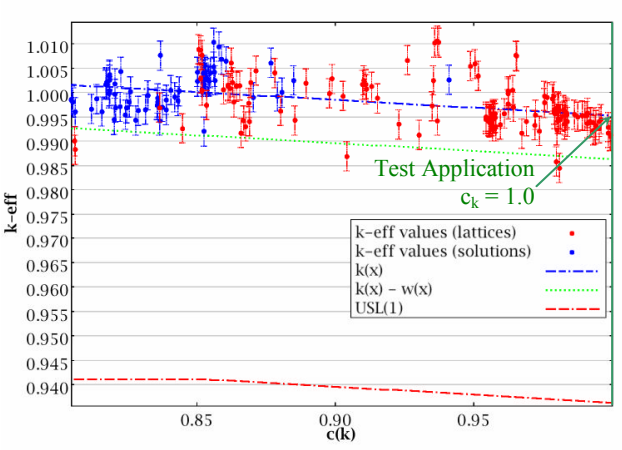

Fig. 7. Trend plot of k_{eff} vs. c_k for 214 benchmarks.

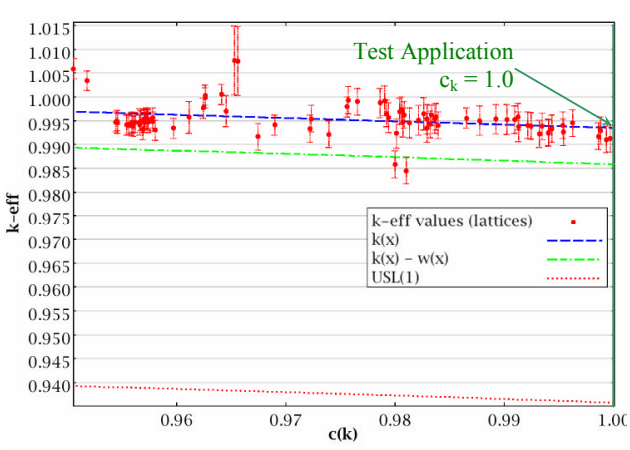

Fig. 8. Trend plot of k_{eff} vs. c_k for benchmarks with $c_k \geq 0.95$.

HOW TO DETERMINE IF YOU HAVE SUFFICIENT BENCHMARKS

For this test application, the availability of several benchmarks with c_k values above 0.99 allows for an accurate determination of the code bias. In fact, the use of only a few systems with c_k values above 0.99 should lead to an accurate assessment of the computational bias. However, in general, such highly correlated benchmarks are not always available. To determine how similar the benchmarks must be to the test application to obtain the correct bias, several other bias determinations were conducted with various subsets of benchmarks, each with varying degrees of correlation. Initially, three subsets of benchmarks were included:

- only those with $c_k \geq 0.95$,
- those $c_k \geq 0.90$,
- and those with $0.80 \geq c_k \geq 0.90$.

Trend plots with $c_k \geq 0.95$, $c_k \geq 0.90$ and $0.80 \geq c_k \geq 0.90$ are shown in Figs. 8, 9, and 10, respectively. The results of each of the trending analyses are summarized in TABLE I, along with the results of the traditional trending analysis. The resulting bias, confidence width, and USL-1 values with all benchmarks and those with $c_k \geq 0.95$ and $c_k \geq 0.90$ are quite similar. However, when the benchmarks with the highest c_k values are omitted in the $0.80 \geq c_k \geq 0.90$ case, the bias increases non-conservatively by 1.5%. However, the USL-1 value only increases by ~0.5% due to the positive-bias adjustment of USLSTATS.

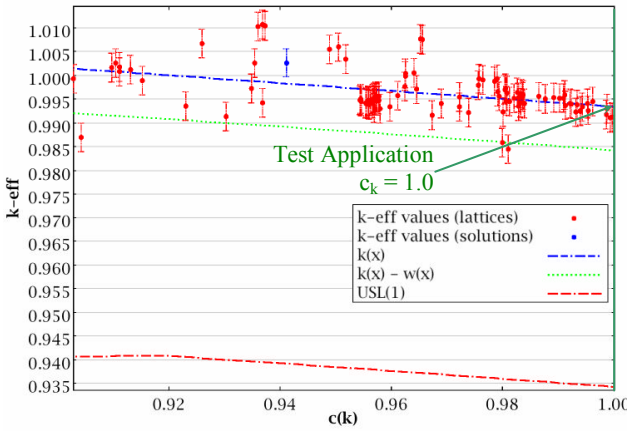

Fig. 9. Trend plot of k_{eff} vs. c_k for benchmarks with $c_k \geq 0.90$.

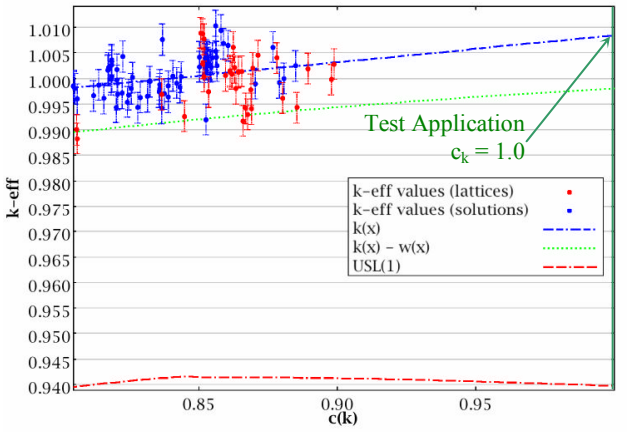

Fig. 10. Trend plot of k_{eff} vs. c_k for benchmarks with $0.80 \geq c_k \geq 0.90$.

TABLE I. Results of trending analyses with benchmarks set with differing ranges of c_k

Trending Parameter	Benchmarks Included	Predicted k_{eff}	Confidence Width	USL-1
Enrichment	All	0.9947	0.0087	0.9359
EALF	All	0.9982	0.0105	0.9377
c_k	All	0.9953	0.0092	0.9361
	$c_k \geq 0.95$	0.9935	0.0077	0.9358
	$c_k \geq 0.90$	0.9934	0.0092	0.9342
	$0.80 \geq c_k \geq 0.90$	1.0084	0.0104	0.9396

Lowest Correlated Benchmarks

To further explore the variation of the bias and the resulting USL-1 values, a series of USLTATS calculations was conducted. First, a USLSTATS analysis was conducted using only benchmarks with the lowest c_k values. Then benchmarks with increasing c_k values were incrementally added to form a cumulative benchmark set including all benchmarks with a certain c_k and below, and the USLSTATS analysis was repeated. The results of this series of USLSTATS calculations are shown in Fig. 11. For example, the k(1.0) curve at the "Maximum c_k" value 0.90 is the predicted k_{eff} for the test application using a cumulative set of all benchmarks with c_k values of 0.90 and lower. This particular 0.90 data point corresponds to the trending analysis shown in Fig. 10. Thus, Fig. 11 represents the data from 214 trend plots like Fig. 10 but with increasing numbers of benchmarks moving from low to high c_k values. The k(1.0) line represents the extrapolation of each trend line to $c_k = 1.0$.

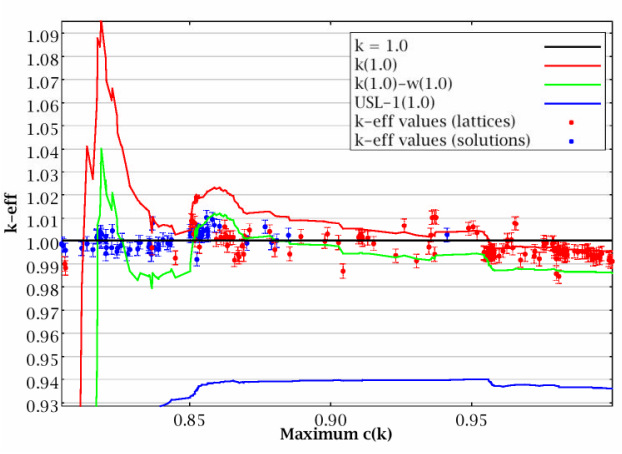

Fig. 11. Results of USLSTATS analyses for cumulative benchmarks sets with increasing c_k values.

The wide variation of the predicted values for benchmark sets including only low c_k values, as shown in Fig. 11, is due to a lack of information included in the initial steps of this analysis. Once sufficient benchmarks are included, the solution begins to converge. In Fig. 11 the predicted k_{eff} value does not drop below 1.0 until the benchmark set includes experiments with $c_k \geq 0.95$. However, the predicted k_{eff} less the confidence width, shown as the k(1.0) – w(1.0) curve, does drop below 1.0 when c_k values ≥ 0.90 are included in the benchmark set. Because of the positive bias adjustment, the USL-1 value for all sets never exceeds 0.94.

Highest Correlated Benchmarks

An alternative approach is to repeat this procedure starting with only the benchmarks with the highest c_k values and incrementally adding benchmarks with decreasing c_k values. The results of this series of analyses are shown in Fig. 12. Here, the predicted k_{eff} value remains below 1.0 for all benchmark sets, and the trending procedure converges with only a few benchmarks included. Also, the USL-1 values remain below 0.94.

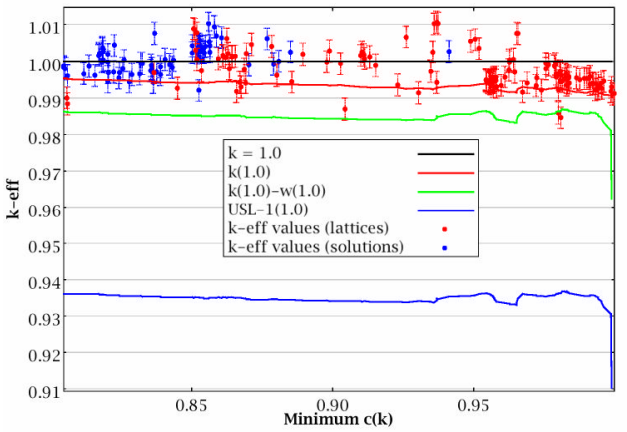

Fig. 12. Results of USLSTATS analyses for cumulative benchmarks with decreasing c_k values.

From Figs. 11 and 12, it is clear that the inclusion of higher quality benchmarks, those with higher c_k values, lead to an improved estimate of the actual bias. In Fig. 11, the predicted k_{eff} less the confidence band bounds the computed k_{eff} of the test application when benchmarks with c_k values ≥ 0.95 are included in the analysis. However, this value should not be treated as a general cutoff criterion, as it may not be generally applicable for all systems. Note that for this test application, there is a scarcity of data between c_k of 0.90 and 0.95. Only 19 experiments have c_k values in this range, and the computed k_{eff} values for these benchmarks range from 0.99 to 1.01. The use of 19 experiments with the wide

variation of k_{eff} values is not sufficient for a reliable prediction using the parametric methods of USLSTATS.

Sufficient Number of Benchmarks

Another process for determining sufficient benchmarks is to examine the number of benchmarks with $c_k \geq 0.90$ required to obtain a correctly predicted k_{eff} value. The convergence of the USLSTATS calculation as a function of incrementally adding benchmarks with increasing c_k values of 0.90 and above is shown in Fig. 13. Here, the USLSTATS results are shown as a function of the number of experiments included, not the maximum c_k of the experiments. For this case, when 25 experiments are included in the analysis, the predicted k_{eff} less the confidence band bounds the actual k_{eff} of the test application. Thus, the inclusion of more benchmarks with c_k values between 0.90 and 0.95 could lead to the correct prediction of k_{eff} without including experiments with c_k values exceeding 0.95. Also note that for this series of USLSTATS calculations, the USL-1 value remains below 0.935 for the entire series of calculations.

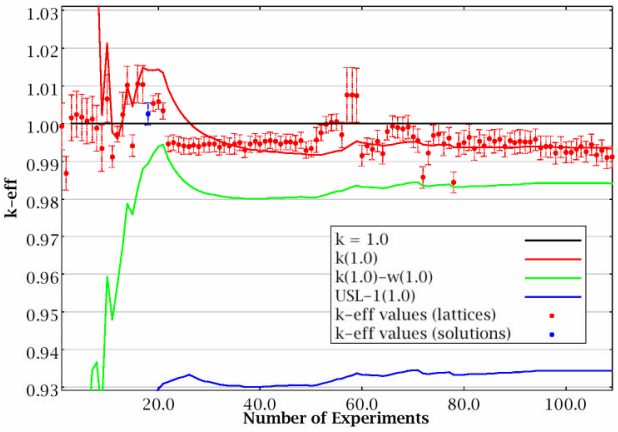

Fig. 13. Results of USLSTATS analyses for cumulative benchmarks with increasing c_k values from 0.90.

CONCLUSIONS

This code validation exercise has demonstrated that the known bias of an actual system can be accurately bounded through the use of parametric analysis and applicable critical experiments. The TSUNAMI integral index c_k was shown to identify benchmarks that are most similar to the test application, consistent with those identified through the use of multiple traditional parameters, enrichment, and EALF. As the c_k value of the most similar benchmarks increases, the k_{eff} values trend towards that of the test application. For each trending analysis, the USL-1 value remains below 0.94. It was demonstrated that, for this test application with benchmarks that contain all of its nuclides, trending based on benchmarks with c_k values ≥ 0.95 bounds the true computational bias with only a few benchmarks. It was also demonstrated that trending with 25 or more benchmarks with $c_k \geq 0.90$ bounds the true computation bias.

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