VALIDATION OF SCALE 6.2 CRITICALITY CALCULATIONS USING KENO V.A AND KENO-VI

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ABSTRACT

SCALE 6.2 provides enhancements for criticality calculations relative to SCALE 6.1, especially with updated nuclear data libraries, resonance self-shielding options for multigroup (MG) calculations, and problem-dependent temperature treatments for continuous-energy (CE) calculations. Benchmark experiments from the International Criticality Safety Benchmark Evaluation Project that are available in the Oak Ridge National Laboratory Verified, Archived, Library of Inputs and Data (VALID) were applied in this validation effort to examine the impact of the SCALE 6.2 enhancements. Over 300 cases are drawn from the VALID library for testing KENO V.a, and a more limited set of approximately 50 configurations is used for validation of KENO-VI. A total of 401 unique critical experiments are used in this validation effort. In some cases, the KENO V.a models were converted to KENO-VI models so that the performance of both codes could be assessed for the same systems.

Validation results for the SCALE 6.2 ENDF/B-VII.1 nuclear data libraries are presented, including MG neutron data in 56- and 252-group structures as well as CE data. The performance of all three multipurpose neutron libraries in calculating k_{eff} is examined with critical experiment models covering a wide range of fuels, moderators, reflectors, absorbers, and neutron spectra. The SCALE 6.2 ENDF/B-VII.1 coupled neutron-photon library, primarily developed for shielding applications with 200 neutron groups and 47 gamma groups, provides additional energy resolution for fast systems relative to the MG neutron libraries which were developed to produce low biases for thermal neutron systems. The applicability of this library to criticality calculations for fast neutron spectrum systems is not investigated here but will be addressed in the final SCALE 6.2 validation report. The results of these calculations demonstrate that SCALE 6.2 generally provides lower biases than SCALE 6.1 and that the two versions of KENO provide equivalent results on the same suite of problems.

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SCALE 6.2 also includes an updated neutron cross-section covariance library based on the ENDF/B-VII.1 covariance data. The effect of these updated covariances on the uncertainty in k_{eff} due to cross section uncertainties is also presented for some cases. A more thorough investigation of the updated covariance data is presented in a companion paper.

KEYWORDS
validation, KENO, SCALE 6.2

1. INTRODUCTION

Validation is an essential step in the software development process. In criticality safety, validation is performed by comparisons between a number of critical benchmark experiments and calculated k_{eff} results from models of these experiments. A code must be validated using critical experiments similar to a safety analysis model before it and its associated computational methodology can be used for safety-related calculations. Since the KENO V.a and KENO-VI three-dimensional Monte Carlo codes are general-purpose criticality safety codes, validation over a broad range of systems is desired. This paper documents the validation of SCALE 6.2 Beta4 [1] using the suite of over 400 critical experiments in the SCALE Verified, Archived Library of Inputs and Data (VALID) described in Ref. [2]. The results of the validation are presented for multigroup (MG) libraries using 56 and 252 neutron energy groups, as well as an updated continuous-energy (CE) library to be released with SCALE 6.2. All three libraries are based on ENDF/B-VII.1 [3]. These results are compared with the MG and CE results from SCALE 6.1 and its ENDF/B-VII.0 libraries [4]. A comparison of KENO V.a and KENO-VI utilizing an identical set of experiments is also presented.

2. CODE AND DATA DESCRIPTIONS

The SCALE code system contains two three-dimensional Monte Carlo transport codes for solving the k_{eff} eigenvalue problem. Both KENO V.a and KENO-VI are internationally recognized staples of the criticality safety community, and they share a heritage of more than four decades of continuous use and development. The primary difference between the two codes is the geometry description that the user provides as input. KENO V.a uses orthogonal Cartesian coordinates and a set of predefined shapes limited to cubes, cuboids, cylinders, and spheres. KENO-VI integrates the SCALE Generalized Geometry Package (SGGP), which has a wider range of geometry options, with more than 15 predefined shapes as well as generalized planes and quadratics. The SGGP also supports truncation of any shape with a plane parallel to an axis, rotation of any object to any orientation, and translation of shapes to the desired position. Both codes support the use of holes and arrays (repeated structures). KENO V.a uses only rectangular arrays, and KENO-VI supports rectangular, hexagonal, and dodecahedral arrays.

All three data libraries used in SCALE 6.2 Beta4 are based on ENDF/B-VII.1. Two MG libraries are used, including a 56-group broad-group structure and a 252-group fine-group library. The 252-group library has additional groups intended to capture light water reactor (LWR) fuel resonances in more detail than the traditional 238-group structure used in previous versions of SCALE. The 56-group structure has been optimized for LWRs to allow shorter execution times in deterministic transport depletion calculations in TRITON. Problem-dependent cross-section resonance self-shielding and temperature interpolation for both of the multigroup libraries are performed with the new XSProc module, which incorporates similar methodologies to those used in SCALE 6.1 [5]. The CENTRM module has been enhances with a method of characteristics solver that is applied to latticecell geometries, eliminating the Wigner-Seitz approximation to the cell outer boundary. The SCALE CE library has been updated and

improved in multiple areas to reduce biases. The results presented here also use the new in-line Doppler broadening option for the CE calculations. The CE data improvements are described in more detail in Ref. [6] and represent the first significant upgrade to the data since the initial release in SCALE 6.0.

3. VALID LIBRARY CONTENTS

The VALID procedure and library are described in detail in Ref. [2], but a brief discussion is presented here for convenience. The procedure allows for the generation of high-quality models that have been rigorously reviewed to eliminate errors. A range of system types has been added to the library, and the library now spans 10 types of systems with 401 cases, as shown in Table I. The MIX-SOL-THERM category and a total of 21 cases across other categories have been added to the library in the two years since the publication of Ref. [2]. All cases used in this validation are drawn from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (ICSBEP Handbook) [7]. The fissile materials represented in the benchmarks include uranium with a range of enrichments, plutonium, and mixtures of uranium and plutonium. The physical form of the fissile materials includes metal, solution, and lattices of rods or slabs. Fast and thermal systems are included in the library at this time, but there is no coverage for intermediate or mixed spectrum experiments. The number of cases in each class of systems ranges from 2 to 123, so the coverage is uneven. Four categories have fewer than 10 unique cases, and five categories have more than 25 unique cases. Most categories are viewed as having sufficient sample size to provide a reliable indication of code performance for the class of experiments.

Table I. Summary of experiments in VALID used for validation

Experiment category	Evaluations included	Total number of cases
KENO V.a cases		
HEU-MET-FAST	-015, -016, -017, -018, -019, -020, -021, -025, -030, -038, -040, -065	22*
HEU-SOL-THERM	-001, -013, -014, -016, -028, -029, -030	52
IEU-MET-FAST	-002, -003, -004, -005, -006, -007, -008, -009	11*
LEU-COMP-THERM	-001, -002, -010, -017, -042, -050, -078, -080	123
LEU-SOL-THERM	-002, -003, -004	19
MIX-COMP-FAST	-005, -006	2
MIX-COMP-THERM	-001, -002, -004	21
MIX-SOL-THERM	-002	3
PU-MET-FAST	-001, -002, -005, -006, -008, -010, -018, -022, -023, -024	10
PU-SOL-THERM	-001, -002, -003, -004, -005, -006, -007, -011, -020	81
KENO-VI cases		
HEU-MET-FAST	-005, -008, -009, -010, -011, -013, -024, -080, -086, -092, -093	27
IEU-MET-FAST	-019	2
MIX-COMP-THERM	-008	28

*Includes detailed and simple models for the same evaluation in some cases.

4. VALIDATION METHODS

As with prior validation reports, including that for SCALE 6.1 [8], the primary metric is the calculated-to-expected ratio (C/E). This ratio is determined for each case by dividing the KENO calculated k_{eff} result by the expected k_{eff} for the benchmark model defined in the ICSBEP Handbook, thus it is not a ratio to the experimental k_{eff}. The estimated uncertainty in the expected k_{eff} from the ICSBEP Handbook evaluation and the stochastic uncertainty in the Monte Carlo calculation are propagated to determine the uncertainty in the C/E ratio. The stochastic uncertainty is controlled to a small number, typically around 0.00010 Δk but as high as 0.00050 Δk in some cases. The C/E uncertainty is almost always dominated by the experimental uncertainty that is typically a factor of 10–50 times larger than the stochastic uncertainty.

An average C/E value is determined for each experiment category for each cross-section library. A separate average is calculated for each code for cases in which the same category of systems occurs for both KENO V.a and KENO-VI. This average is simply an arithmetic average of the C/E values for all of the cases in the class of systems and is not weighted by uncertainty or any other parameter. The uncertainty in the average C/E is determined as the square root of the sum of squares of the individual C/E uncertainties divided by the number of cases represented in the class of systems. The uncertainty of the average C/E is largely independent of the cross-section library because the same cases are included for all of the libraries, and the individual C/E uncertainties are controlled by the experimental uncertainties. The same cases are considered for all libraries for each class of systems.

5. RESULTS

A range of results is presented here relating primarily to performance of KENO V.a and KENO-VI in SCALE 6.2 Beta4. Some comparisons are shown demonstrating improvements in performance relative to SCALE 6.1, and additional results are presented comparing KENO V.a and KENO-VI using identical experiments. A more complete set of results, including updated TSUNAMI-3D results, will be published in the complete KENO validation report subsequent to the final release of SCALE 6.2.

New cross-section uncertainty data are also implemented in SCALE 6.2 Beta4. Although not a primary focus of this paper, they are presented in some figures shown in this section. A companion paper presented at this conference [9] provides details on the generation and testing of these new data, including comparisons of the SCALE 6.1 and 6.2 Beta4 results for some categories of experiments within the VALID library used for KENO validation. The impact of the new covariance data on c_k values is also addressed in Ref. [9].

5.1. Average C/E Results

As stated in Section 4, an average C/E is calculated for each category of experiments for each code. The average C/E for each category of experiments for all three libraries is provided for KENO V.a in Table II and for KENO-VI in Table III. The SCALE 6.2 Beta4 results are plotted along with SCALE 6.1 results for the 238-group and CE libraries in Fig. 1 for KENO V.a and in Fig. 2 for KENO-VI.

The results in Tables II and III show that the average C/E values for SCALE 6.2 Beta4 for most categories are near 1.0. The 56-group calculations perform relatively poorly for fast uranium systems, with the average C/E more than 0.5% from unity. This is neither surprising nor alarming since the group structure was designed for thermal reactor systems, so there is likely insufficient fidelity in the group structure in the fast energy range to yield accurate results. The library does perform well for the pin array systems for which it was optimized. The 252-group results show significant improvements in both uranium fuelled (high- and intermediate-enriched) fast metal system categories compared to the

SCALE 6.1 238-group library. These results also show that the biases for the fine-group MG library are generally improved with the additional groups in the 252-group structure. The average C/E is closer to unity for many systems, with notable improvements for fast systems. The bias is smaller for the SCALE 6.1 238-group library, however, than for the 56-group or 252-group library for uranium solution systems, and it appears that this effect is magnified for the high-enrichment cases. For the high-enriched solutions, this may be an unintended result of the multigroup processing. Even though the bias to a C/E of unity is lower for this library than for the ENDF/B-VII.1 libraries, the difference from the CE library is larger. The agreement between multigroup and CE libraries is better for the low-enriched solution for the ENDF/B-VII.0 libraries than for the ENDF/VII.1 libraries, and the bias also has a smaller magnitude. More investigation is needed to explain the differences between the ENDF/B-VII.1 MG and CE libraries. The C/E values for all low-enriched uranium lattice systems are shown in Fig. 3 for the 56-group, 252-group, and CE libraries. The results indicate the biases between the MG libraries and the CE library are generally consistent, with differences typically less than 0.1% Δk. In Figs. 3 and 4, the experimental uncertainties reported in the ICSBEP Handbook are shown with the dotted line, and the cross-section induced uncertainty in k_{eff} calculated with TSUNAMI is shown with the dashed line.

The new 252-group library provides a significant reduction in bias compared to the 238-group library for low-enriched uranium water-moderated lattice systems. This is an expected result since the target application for the library is LCT systems. The C/E values for all these lattice systems are shown in Fig. 4. The general trend is clear, with the 252-group results having a less negative bias in almost all cases than the 238-group library. The 252-group library also provides significant improvement for plutonium solution systems and more modest improvements for the uranium metal systems. As discussed above and shown in Fig. 1, the 252-group library exhibits a larger magnitude bias for uranium solution systems of both high and low enrichments.

The performance of the new CE library is generally improved with smaller biases for water-moderated lattice systems, particularly those fueled with mixed uranium and plutonium. The C/E values for mixed oxide lattice systems modeled in KENO V.a are shown in Fig. 5. The results using the CE library are now in better agreement with the two MG libraries; the bias evident in this library in SCALE 6.1, shown in Fig. 1, has clearly been removed. The performance of the new CE library appears to be slightly worse for the plutonium solution systems. The poor performance for plutonium solution systems is not a SCALE issue but is largely due to the underlying evaluated nuclear data for ^{239}Pu as has been observed for a wide range of code and cross-section library combinations [10]. The KENO V.a high-enriched fast metal systems seem to indicate a performance change between the two CE libraries, but the difference is not consistent with results for the KENO-VI systems. These results reinforce the need to establish that KENO V.a and KENO-VI generate the same results for the same systems. This issue is examined in detail in Section 5.3.

The general conclusion from the full data set is that the updated data libraries in SCALE 6.2 Beta4 provide better performance, as manifested in average C/E values closer to unity, than SCALE 6.1. The new 252-group library provides a performance improvement in the targeted application systems, and the significant bias for water-moderated mixed oxide lattice systems has been removed from the CE results. The new 56-group library yields good k_{eff} results for the thermal lattice systems for which it was optimized.

Table II. Average C/E values for KENO V.a

Category	56-group		252-group		Continuous energy	
	Average C/E	Uncertainty	Average C/E	Uncertainty	Average C/E	Uncertainty
HMF	1.00610	0.00041	1.00285	0.00041	1.00197	0.00041
HST	0.99669	0.00072	0.99719	0.00072	0.99805	0.00072
IMF	1.00906	0.00083	1.00566	0.00083	1.00293	0.00083
LCT	0.99981	0.00020	0.99915	0.00020	0.99970	0.00020
LST	0.99647	0.00083	0.99724	0.00083	0.99777	0.00083
MCF	1.00220	0.00158	1.00730	0.00159	1.00241	0.00158
MCT	0.99855	0.00087	0.99870	0.00087	0.99931	0.00087
MST	1.00182	0.00139	1.00147	0.00139	1.00128	0.00139
PMF	1.00041	0.00068	0.99985	0.00068	1.00025	0.00068
PST	1.00176	0.00056	1.00232	0.00056	1.00307	0.00056

Table III. Average C/E Values for KENO-VI

Category	56-group		252-group		Continuous energy	
	Average C/E	Uncertainty	Average C/E	Uncertainty	Average C/E	Uncertainty
HMF	1.00067	0.00044	0.99835	0.00044	0.99872	0.00044
IMF	1.00879	0.00276	1.00548	0.00275	1.00607	0.00275
MCT	0.99458	0.00078	0.99456	0.00078	0.99428	0.00078

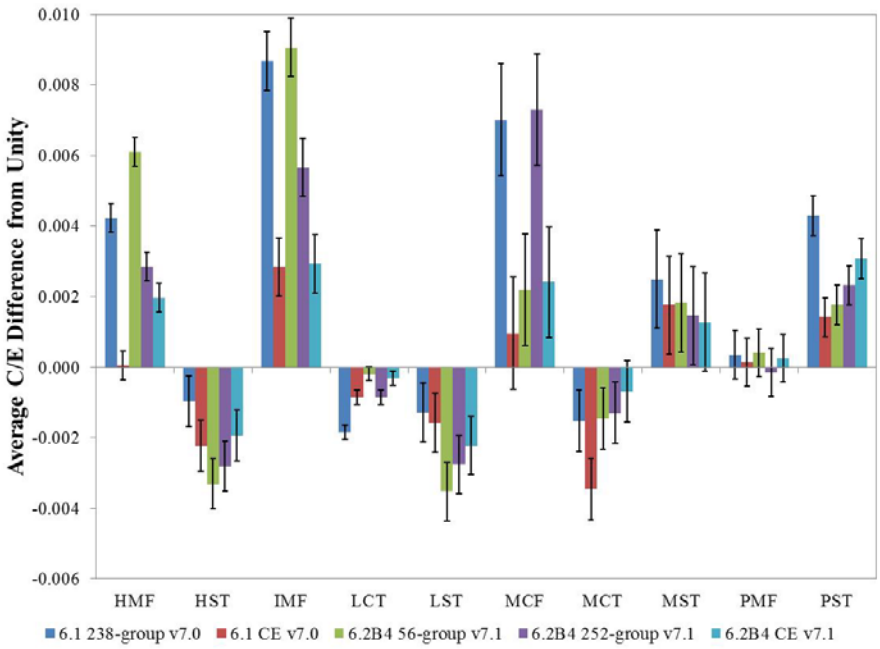

Figure 1. Average C/E Difference from Unity by Category for KENO V.a.

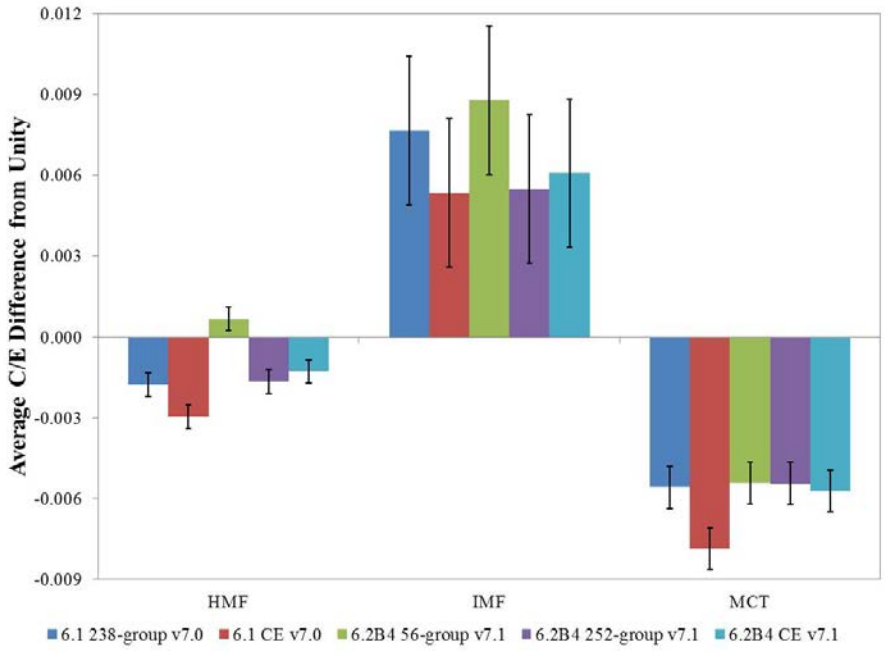

Figure 2. Average C/E Difference from Unity by Category for KENO-VI.

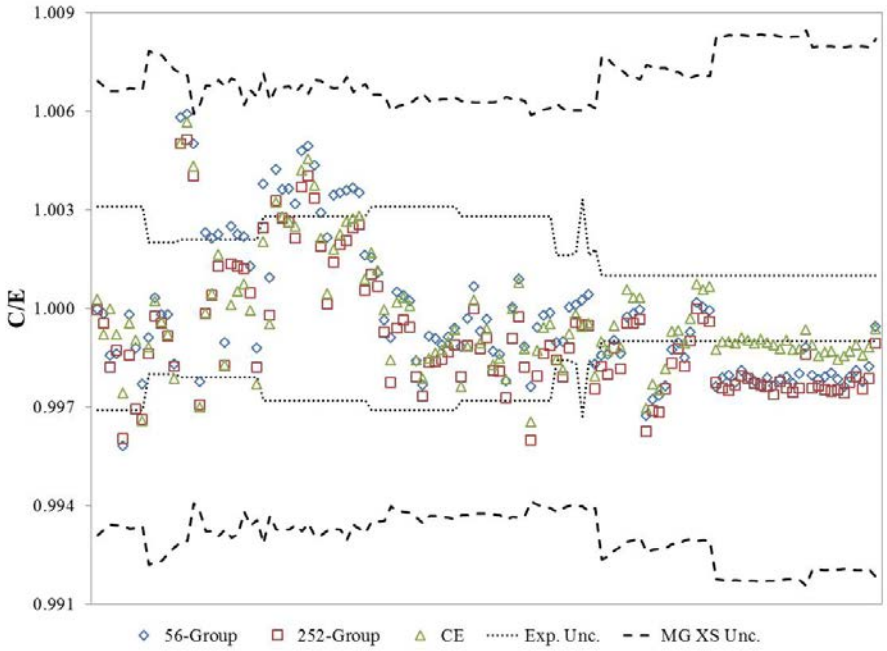

Figure 3. C/E Values for All LEU-COMP-THERM Systems Using SCALE 6.2 Beta4 and ENDF/B-VII.1 Data.

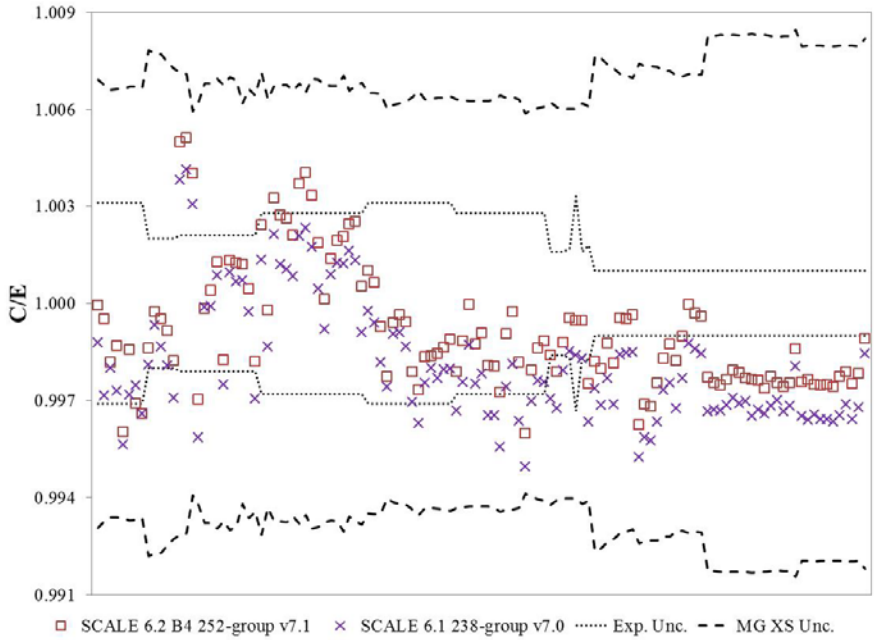

Figure 4. C/E Values for All LEU-COMP-THERM Systems Using SCALE 6.1 and 6.2 Beta4.

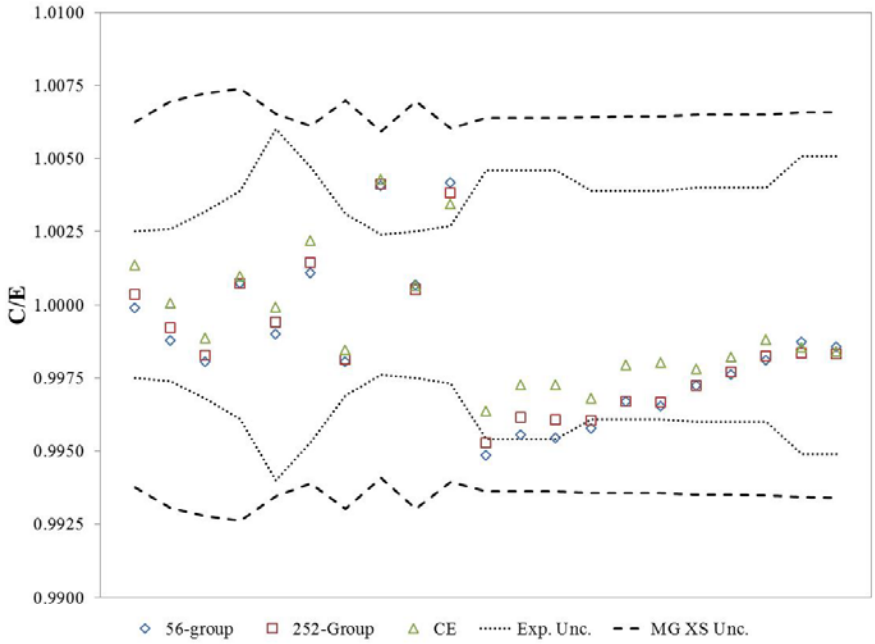

Figure 5. C/E Values for KENO V.a MIX-COMP-THERM Systems Using SCALE 6.2 Beta4 and ENDF/B-VII.1 Data.

5.2. Outlier Cases

Outlier cases can occur for a wide range of different reasons including errors in the nuclear data, experiment description, code, model, or any combination of the four. The probability of modeling errors has been reduced by using benchmark models from the ICSBEP Handbook and by using only models that

are part of the VALID library and have been vetted by independent reviews. The use of sensitivity data generated using TSUNAMI-3D and the cross-section uncertainty data can in some cases eliminate nuclear data as a cause for an outlier, or it can indicate that the most likely cause for the outlier is the nuclear data [8, 11]. Results of validation studies like this one have identified errors in all four areas in the past.

The largest outlier for each category of experiments is determined as the individual C/E value that is farthest from unity in terms of standard deviations. The uncertainty in each C/E value is determined as described in Section 4 at the one-sigma level. The difference of each C/E value from unity can then be divided by this uncertainty to determine the number of standard deviations from unity. The C/E value and its associated difference from unity, in standard deviations, are shown for each category of experiments for KENO V.a in Table IV and for KENO-VI in Table V.

Many of the outlier cases are the same as those identified in the SCALE 6.1 validation report [8], and discussion of these outliers is provided in the referenced document. Some of the cases, such as HMF-025-005 and HST-016-003, are discussed at length because these discrepancies have been investigated. For cases such as PMF-008-001 and PST-011-003, the same case is the outlier with all three libraries. This may indicate a problem with the experiment or, more likely, its description. A comparison of the outlier cases for the CE library in this work and the CE results in Ref. [8] supports the observation in Section 5.1 that the updated data provide lower biases for water-moderated lattices.

Table IV. C/E values for the most significant outlier case for each category, KENO V.a

Category	56-group			252-group			CE		
	Case	C/E	Δ ($\sigma_{C/E}$)	Case	C/E	Δ ($\sigma_{C/E}$)	Case	C/E	Δ ($\sigma_{C/E}$)
HMF	040-001	1.01266	11.3	040-001	1.00903	8.1	015-001	0.99511	2.9
HST	016-001	0.98913	3.0	016-001	0.98886	3.1	016-003	1.02419	3.0
IMF	005-001S	1.01758	7.5	005-001S	1.01253	5.4	004-001	1.00787	2.6
LCT	010-002	1.00590	2.8	010-002	1.00511	2.4	010-002	1.00565	2.7
LST	003-004	0.99106	2.1	002-002	0.99204	2.2	002-002	0.99240	2.1
MCF	006-001	1.00775	3.6	006-001	1.01175	5.5	006-001	1.00589	2.8
MCT	002-006S	1.00416	1.5	002-004S	1.00410	1.7	002-004S	1.00428	1.8
MST	002-002	1.00208	0.9	002-002	1.00154	0.6	002-002	1.00146	0.6
PMF	008-001	0.99698	5.0	008-001	0.99663	5.6	008-001	0.99812	3.1
PST	011-003	1.01422	2.7	011-003	1.01508	2.9	011-003	1.01618	3.1

Table V. C/E values for the most significant outlier case for each category, KENO-VI

Category	56-group			252-group			CE		
	Case	C/E	Δ ($\sigma_{C/E}$)	Case	C/E	Δ ($\sigma_{C/E}$)	Case	C/E	Δ ($\sigma_{C/E}$)
HMF	094-002	1.01303	12.8	080-001	1.00701	5.8	080-001	1.00966	8.0
IMF	019-001	1.00931	2.6	019-001	1.00561	1.6	019-001	1.00607	1.7
MCT	008-026	0.99240	1.9	008-023	0.99260	1.8	008-021	0.99233	1.9

5.3. KENO V.a and KENO-VI Comparisons

Two validation reports exist for KENO-VI [12, 13], but neither is recent, and they do not contain models that have been checked as rigorously as those that are in VALID. Some comparisons were made as part of the recent validation of SCALE 6.1 [8], but these comparisons are problematic because different systems are used in the KENO V.a and KENO-VI validations. Generally, KENO-VI is only used for cases in which generalized geometry or hexagonal array capabilities are needed. As discussed in Ref. [8], the more complicated experiments are likely more difficult to describe accurately and thus may result in larger apparent biases. A more complete comparison of the two codes using models of the same experiments is thus desired. SCALE contains a utility module to convert a CSAS5 model to a CSAS6 model (C5toC6) [4], so the entire library of KENO V.a models could be converted to KENO-VI models for a direct comparison and validation effort. A preliminary evaluation with three categories of experiments was presented in Ref. [14], but a more complete analysis has been completed and is presented here. The results presented only considered the ENDF/B-VII.1 252-group library executed within SCALE 6.2 Beta4.

The average k_{eff} value for each of the classes of systems differs by less than the one standard deviation uncertainty if the experimental uncertainty is included. In this case, the experimental uncertainty is not necessarily relevant because both the KENO V.a and KENO-VI models contain the same materials and geometry. In the more restrictive case in which only the Monte Carlo stochastic uncertainty is considered, the average KENO V.a and KENO-VI k_{eff} values for 7 of the 10 categories of experiments are still within one standard deviation of each other. As discussed in Section 4, the one-sigma stochastic uncertainty ranges between 0.00010 Δk and 0.00050 Δk. The average k_{eff} values and associated uncertainties are provided for each category of experiments in Table VI. The average of the individual case differences is $3.3 \times 10^{-5}\ \Delta k$ with a standard deviation of $18 \times 10^{-5}\ \Delta k$. The number of cases compared in each category of experiments is shown in Table VII, along with the number of individual cases with k_{eff} differences more than two times the root-sum-squared Monte Carlo uncertainties for the case. Only 12 of the 326 cases, or 3.68%, have this level of disagreement; if the differences were normally distributed, it would be expected that 4.55%, or about 15, of the cases would disagree by more than two standard deviations. A histogram of the differences is shown in Fig. 6, with an imposed normal distribution with the same average and standard deviation shown as a solid red line. The actual results appear to be skewed slightly to the high side, and there are more differences near the center of the distribution than would be expected. The distribution of the differences fails a Shapiro-Wilks normality test.

It is evident from the results presented that the differences between the average k_{eff} values for KENO V.a and KENO-VI are extremely small. The differences in the individual case results are also quite small, and more than the expected number of results is nearly equal than would be expected for a normal distribution. While it is important to perform validation with a consistent computational method (i.e., do not validate KENO V.a with KENO-VI), the results provide good confidence that the two codes will predict a statistically equivalent k_{eff} value for the same system.

Table VI. Average k_{eff} values and uncertainties for KENO V.a and KENO-VI

Category	KENO V.a		KENO-VI	
	Average k_{eff}	Uncertainty	Average k_{eff}	Uncertainty
HMF	1.00248	0.00002	1.00250	0.00002
HST	0.99734	0.00002	0.99737	0.00002
IMF	1.00607	0.00003	1.00609	0.00003
LCT	0.99862	0.00001	0.99867	0.00002
LST	0.99737	0.00006	0.99743	0.00006
MCF	0.99733	0.00007	0.99713	0.00007
MCT	0.99822	0.00002	0.99825	0.00002
MST	1.00147	0.00006	1.00154	0.00006
PMF	0.99985	0.00003	0.99986	0.00003
PST	1.00232	0.00001	1.00234	0.00001

Table VII. Number of KENO V.a cases analyzed in KENO-VI

Category	Number of cases	Number of cases that differ by more than 2σ
HMF	22	0
HST	52	1
IMF	11	0
LCT	108	8
LST	19	0
MCF	2	0
MCT	18	2
MST	3	0
PMF	10	0
PST	81	1
Total	326	12

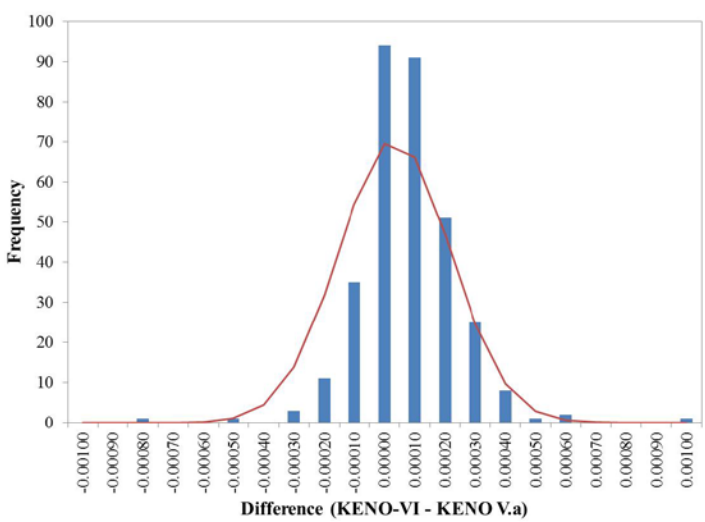

Figure 6. Distribution of Individual Case Differences.

6. CONCLUSIONS

The primary conclusion of this work is that the MG and CE libraries planned for release with SCALE 6.2 provide generally lower k_{eff} biases than the libraries released with SCALE 6.1. The performance of the ENDF/B-VII.1 252-group library provides improvements, especially for light-water–moderated lattices, compared to the ENDF/B-VII.0 238-group library in SCALE 6.1. A new 56-group broad group structure has been developed which provides good results for the water-moderated lattice systems for which it was optimized. Substantial improvements have also been made to the CE library, resulting in significantly improved performance for fuel pin lattice applications.

Results are also presented for an updated validation of KENO-VI using the same experiments as KENO V.a. This allows a direct comparison of the two codes, and results generated to date indicate that the codes produce statistically equivalent estimates of k_{eff} for identical systems.

The work presented in the paper is intended to demonstrate general code performance, and does not eliminate or reduce the requirements of ANSI/ANS-8.24 [15] for application specific validation of computational methods used in criticality safety analyses.

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