VALIDATION OF KENO V.A AND KENO-VI IN SCALE 6.3 BETA 3 USING ENDF/B-VII.1 AND ENDF/B-VIII LIBRARIES [1]

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ABSTRACT

In early 2019, internal beta releases of SCALE 6.3 were identified for internal users, as well as a limited number of external users, to apply when testing key features. Recently developed AMPX-formatted libraries based on ENDF/B-VIII have also been generated for use in internal testing. In this effort, a criticality safety validation was performed using nuclear data libraries based on the ENDF/B-VII.1 and ENDF/B-VIII releases to quantify the changes caused by code development and to identify differences caused by the new nuclear data. As with past validations, the primary suite of experiments used is the Verified, Archived Library of Inputs and Data (VALID) maintained in the Reactor and Nuclear Systems Division at Oak Ridge National Laboratory. The VALID suite contains a total of 618 individual configurations, including systems with fast, thermal, mixed, and intermediate neutron spectra. Fissile species include a range of uranium enrichments, plutonium, mixtures of uranium and plutonium, and ^{233}U. Metal, solution, and compound, mostly in pin array fissile forms, are included in the suite. The results presented here include the 252-group general purpose multigroup library based on ENDF/B-VII.1 and the continuous-energy libraries based on ENDF/B-VII.1 and ENDF/B-VIII.

KEY WORDS

SCALE, KENO, Validation

1. INTRODUCTION

Ongoing development of the SCALE code package [1] will lead to the release of SCALE version 6.3 in late 2019 or 2020. Before the final code is released, frozen beta releases are being generated for internal and some external users to apply when testing key features. Broader public beta releases are anticipated but have not been made as of this writing.

This paper documents a criticality safety validation performed with KENO V.a and KENO-VI using the Verified, Archived Library of Inputs and Data (VALID) [[2]] maintained at Oak Ridge National Laboratory (ORNL). VALID contains 618 SCALE inputs for critical benchmark experiments taken from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [[3]]. The inputs have been developed and reviewed by qualified individuals and are therefore of high quality. VALID contains benchmarks covering a range of fissile materials and energy spectra; a summary of the contents of the library are provided in Table I. The complete list of cases available in VALID is reported in the SCALE 6.2.2 validation report [[4]].

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Three nuclear data libraries were used in this validation. Continuous-energy (CE) libraries based on ENDF/B-VII.1 [[5]] and ENDF/B-VIII [[6]] were used, as well as a 252-group multigroup (MG) library based on ENDF/B-VII.1. The two libraries based on ENDF/B-VII.1 were used in the SCALE 6.2.2 validation report [[4]] and are used here to provide a direct comparison of calculated k_{eff} values based on code changes since the release of SCALE 6.2.2. The ENDF/B-VIII library is used as an indication of the new data's performance in the final release of SCALE 6.3. These results are similar to results reported earlier based on a beta release of ENDF/B-VIII [[7]]. The CE ENDF/B-VIII results are also compared to the CE ENDF/B-VII.1 results from the SCALE 6.2.2 validation report to generate an estimate of runtime performance for SCALE 6.3.

Table I. Contents of VALID

Experiment category	Evaluations included	Total number of cases available
KENO V.a Cases		
HEU-MET-FAST	-015, -016, -017, -018*, -019*, -020*, -021*, -025, -030, -038, -040, -052, -065	23†
HEU-SOL-THERM	-001, -013, -014, -016, -028, -029, -030	52
IEU-MET-FAST	-002, -003*, -004*, -005*, -006, -007, -008, -009, -019	11†
LEU-COMP-THERM	-001, -002, -008, -010, -017, -042, -050, -078, -080	140
LEU-SOL-THERM	-002, -003, -004	19
MIX-COMP-FAST	-005, -006	2
MIX-COMP-THERM	-001, -002, -004	21
MIX-SOL-THERM	-002, -007	10
PU-MET-FAST	-001, -002, -005, -006, -008, -010, -018, -022, -023, -024, -025, -026	12
PU-SOL-THERM	-001, -002, -003, -004, -005, -006, -007, -011, -020	81
U233-COMP-THERM	-001	3
U233-MET-FAST	-001, -002, -003, -004, -005, -006	10
U233-SOL-INTER	-001	29
U233-SOL-MIXED	-001, -002	8
U233-SOL-THERM	-001, -002, -003, -004, -005, -008, -009, -011, -012, -013, -015, -016, -017	140
KENO-VI Cases		
HEU-MET-FAST	-005, -008, -009, -010, -011, -013, -024, -080, -086, -092, -093, -094	27
IEU-MET-FAST	-019	2
MIX-COMP-THERM	-008	28
* Both detailed and simplified models included		
† Total includes both detailed and simplified models		

2. RESULTS WITH ENDF/B-VII.1 LIBRARIES

The average calculated-to-evaluation (C/E) ratio for each category of experiments with each code, based on ENDF/B-VII.1, is provided in Table II for the MG library and in

Table III for the CE library. These are the same data libraries that were distributed with SCALE 6.2 [[1]], so this comparison isolates the impact of code changes between SCALE 6.2.2 and SCALE 6.3 Beta 3. Only the Monte Carlo calculation uncertainties are considered here, because this is a code-to-code comparison, and the experimental uncertainties are therefore not relevant.

Small but statistically significant differences are evident for the MG KENO calculations for many categories of experiments. The impact of the code changes is significantly less for fast systems than for intermediate, mixed, or especially thermal systems. This change was caused by a difference in the mass lumping treatment in CENTRM. The CENTRM module is used to perform a slowing down calculation to determine the flux present in the unit cells used to flux-weight the MG cross sections. The mass lumping is performed to accelerate the calculation, and the change that was made was intended to improve the accuracy of the approximation. The CENTRM lumping treatment is planned to be reverted to the SCALE 6.2.2 method in future beta releases and in the production release of SCALE 6.3. The lumping treatment can be deactivated by specifying the parameter *alump*=0 in the CENTRM DATA block within the CELLDATA block. The methodology reversion should eliminate the majority of the differences noted in Table II, as would disabling the lumping treatment.

The agreement in the average C/E values for each category of experiments for the CE library based on ENDF/B-VII.1 is quite good. Most categories have a difference of less than 1 standard deviation, and several others are less than 2 standard deviations. The average difference of all 18 average C/E values is 0.00002 ± 0.00001 Δk.

There are noticeable differences between the biases for HMF and MCT cases between KENO V.a and KENO-VI, and a much smaller difference in the biases for IMF systems. These differences were examined in the SCALE 6.2.2 validation report [4] by converting all the KENO V.a models to KENO-VI models and running the KENO-VI models. The purpose of this exercise was to examine the performance of both codes using the same set of experiments. The CE library based on ENDF/B-VII.1 was the only one used for these comparisons. The results presented in Tables 23 and 24 of [4] show that all the calculated k_{eff} values from KENO V.a and KENO-VI for all HMF and IMF systems are within 2 standard deviations of each other. The MCT systems also show excellent agreement, with 95.2% of the models within 2 standard deviations of each other. Only the Monte Carlo calculational uncertainties were considered in these comparisons and not the experimental uncertainties. The conclusion of this study was that KENO V.a and KENO-VI provide equivalent results for the same experiments, and that the apparent differences in bias are a result of different experiments considered in the two codes in the VALID library. This direct comparison was not performed again for this paper but will likely be repeated for the final SCALE 6.3 validation report.

Table II. Average C/E values for each category of experiments for the MG ENDF/B-VII.1 library

Category	SCALE 6.2.2		SCALE 6.3 Beta 3		Comparison		
	Avg. C/E	Uncert.	Avg. C/E	Uncert.	Difference	Uncert.	Diff./Uncert.
KENO V.a cases							
HMF	1.00316	0.00002	1.00304	0.00002	-0.00012	0.00003	-4.2
HST	0.99696	0.00002	0.99614	0.00002	-0.00082	0.00002	-37.5
IMF	1.00567	0.00003	1.00565	0.00003	-0.00002	0.00004	-0.4
LCT	0.99899	0.00001	0.99876	0.00001	-0.00023	0.00002	-13.3
LST	0.99777	0.00006	0.99744	0.00006	-0.00033	0.00009	-3.6
MCF	1.00721	0.00007	1.00730	0.00007	0.00009	0.00010	0.9
MCT	0.99878	0.00002	0.99813	0.00002	-0.00065	0.00003	-21.4
MST	0.99803	0.00003	0.99759	0.00003	-0.00044	0.00004	-9.9
PMF	1.00015	0.00003	1.00013	0.00003	-0.00002	0.00004	-0.4
PST	1.00222	0.00001	1.00159	0.00001	-0.00063	0.00002	-40.5
UCT	1.00104	0.00006	1.00033	0.00006	-0.00070	0.00008	-8.7
UMF	0.99877	0.00003	0.99866	0.00003	-0.00011	0.00004	-2.4
USI	0.98273	0.00002	0.98187	0.00002	-0.00086	0.00003	-30.1
USM	0.97885	0.00004	0.97788	0.00004	-0.00097	0.00005	-18.1
UST	0.99947	0.00001	0.99851	0.00001	-0.00096	0.00001	-75.3
KENO-VI cases							
HMF	0.99847	0.00002	0.99836	0.00002	-0.00012	0.00003	-4.6
IMF	1.00536	0.00007	1.00539	0.00007	0.00003	0.00010	0.3

MCT	0.99408	0.00002	0.99374	0.00002	-0.00035	0.00003	-13.3

Table III. Average C/E values for each category of experiments for the CE ENDF/B-VII.1 library

Category	SCALE 6.2.2		SCALE 6.3 Beta 3		Comparison		
	Avg. C/E	Uncert.	Avg. C/E	Uncert.	Difference	Uncert.	Diff./Uncert.
KENO V.a Cases							
HMF	1.00201	0.00002	1.00196	0.00002	-0.00004	0.00003	-1.5
HST	0.99779	0.00002	0.99773	0.00002	-0.00006	0.00002	-2.6
IMF	1.00276	0.00003	1.00281	0.00003	0.00004	0.00004	1.0
LCT	0.99962	0.00001	0.99959	0.00001	-0.00003	0.00002	-1.8
LST	0.99819	0.00007	0.99821	0.00007	0.00002	0.00009	0.2
MCF	1.00248	0.00007	1.00257	0.00007	0.00009	0.00010	0.9
MCT	0.99919	0.00002	0.99922	0.00002	0.00002	0.00003	0.8
MST	0.99813	0.00003	0.99843	0.00003	0.00030	0.00004	6.7
PMF	0.99970	0.00003	0.99970	0.00003	0.00000	0.00004	-0.1
PST	1.00296	0.00001	1.00302	0.00001	0.00006	0.00002	4.1
UCT	1.00068	0.00006	1.00065	0.00006	-0.00003	0.00008	-0.4
UMF	0.99846	0.00003	0.99849	0.00003	0.00002	0.00004	0.5
USI	0.98271	0.00002	0.98269	0.00002	-0.00002	0.00003	-0.7
USM	0.97901	0.00004	0.97898	0.00004	-0.00003	0.00005	-0.5
UST	1.00019	0.00001	1.00015	0.00001	-0.00004	0.00001	-2.9
KENO-VI cases							
HMF	0.99863	0.00002	0.99858	0.00002	-0.00005	0.00003	-2.2
IMF	1.00572	0.00007	1.00579	0.00007	0.00008	0.00010	0.8
MCT	0.99422	0.00002	0.99419	0.00002	-0.00004	0.00003	-1.4

3. RESULTS WITH ENDF/B-VIII LIBRARIES

The average C/E values for each category of experiments is provided in Table IV for the CE libraries based on ENDF/B-VIII and ENDF/B-VII.1. The difference between the average C/E values is also provided in the table. In this case, the uncertainty reported for the average C/E values includes the evaluation uncertainty. The average C/E results are also plotted in Figure 1, including the results for the MG ENDF/B-VII.1 library, for systems modeled in KENO V.a, and in Figure 2 for systems modeled in KENO-VI. The results are similar to previously reported results based on SCALE 6.2 and a beta version of ENDF/B-VIII [[7]].

Table IV. Average C/E values for each category of experiments for the CE libraries

Category	ENDF/B-VII.1		ENDF/B-VIII		Comparison		
	Avg. C/E	Uncert.	Avg. C/E	Uncert.	Difference	Uncert.	Diff./Uncert.
KENO V.a cases							
HMF	1.00196	0.00039	1.00180	0.00039	-0.00017	0.00055	-0.3
HST	0.99773	0.00072	0.99862	0.00072	0.00089	0.00102	0.9
IMF	1.00281	0.00083	1.00058	0.00082	-0.00223	0.00116	-1.9
LCT	0.99959	0.00018	0.99915	0.00018	-0.00044	0.00026	-1.7
LST	0.99821	0.00083	0.99847	0.00083	0.00025	0.00118	0.2
MCF	1.00257	0.00158	0.99797	0.00157	-0.00460	0.00222	-2.1
MCT	0.99922	0.00087	0.99810	0.00087	-0.00111	0.00123	-0.9
MST	0.99843	0.00158	0.99358	0.00157	-0.00485	0.00222	-2.2
PMF	0.99970	0.00062	0.99939	0.00062	-0.00031	0.00088	-0.3
PST	1.00302	0.00056	0.99772	0.00055	-0.00530	0.00078	-6.8
UCT	1.00065	0.00141	0.99808	0.00140	-0.00257	0.00198	-1.3
UMF	0.99849	0.00051	0.99860	0.00051	0.00012	0.00072	0.2
USI	0.98269	0.00124	0.97942	0.00123	-0.00327	0.00174	-1.9
USM	0.97898	0.00215	0.97548	0.00214	-0.00350	0.00302	-1.2
UST	1.00015	0.00052	0.99750	0.00052	-0.00265	0.00074	-3.6
KENO-VI cases							
HMF	0.99858	0.00044	0.99836	0.00044	-0.00022	0.00062	-0.4
IMF	1.00579	0.00275	1.00407	0.00274	-0.00173	0.00388	-0.4
MCT	0.99419	0.00078	0.99366	0.00078	-0.00053	0.00110	-0.5

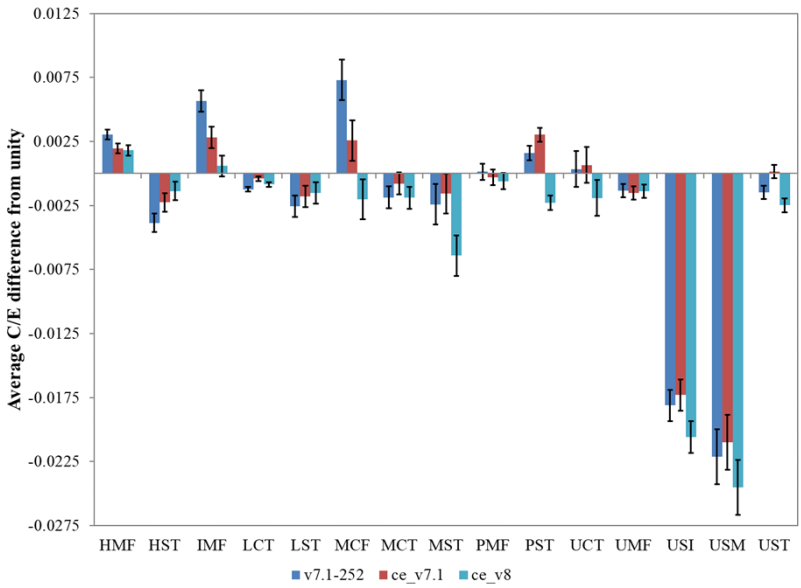

Figure 1. Average C/E values for each system category modeled in KENO V.a

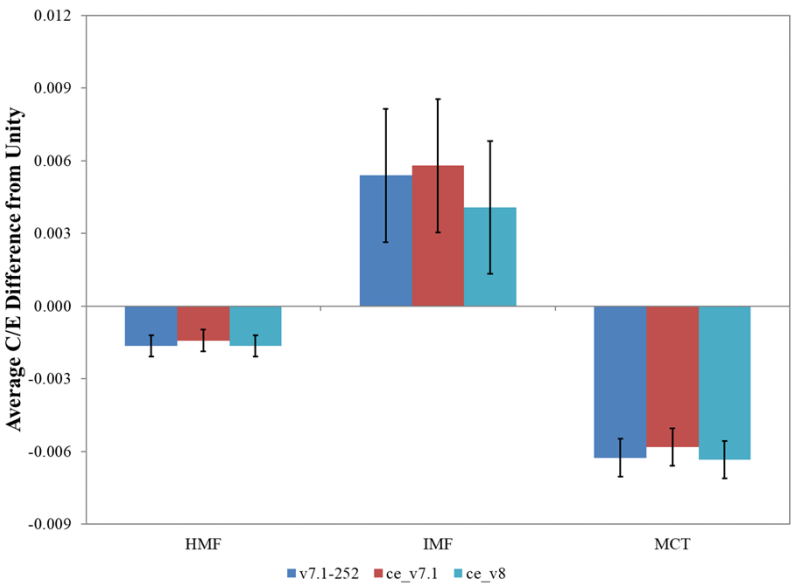

Figure 2. Average C/E values for each system category modeled in KENO-VI

Most categories of experiments perform quite well with both ENDF/B-VII.1 and ENDF/B-VIII libraries. The intermediate enrichment fast uranium metal (IMF) systems show a much lower bias with the ENDF/B-VIII library than the ENDF/B-VII.1 library. More IMF systems are needed to improve the statistical reliability of this conclusion, especially since several of the IMF benchmarks in VALID are detailed and simplified models of the same experiment. More noticeably, the thermal plutonium solution (PST) systems have a much lower average C/E value. The average C/E drops over 0.5% Δk, from 1.00302 to 0.99772, with both average C/E values having an uncertainty of ±0.00055 Δk. The bias—that is, the difference from an average C/E of unity—changed from +0.00302 Δk to -0.00228 Δk; the magnitude of the bias is thus only marginally smaller, by less than 1 standard deviation. The adjustment of the PST benchmarks was the primary goal of the Working Party on International Nuclear Data Evaluation Co-operation (WPEC), subgroup 34 [[8]]. As shown in Figure 3, the reactivity reduction in the PST benchmarks is fairly consistent for all systems included in VALID.

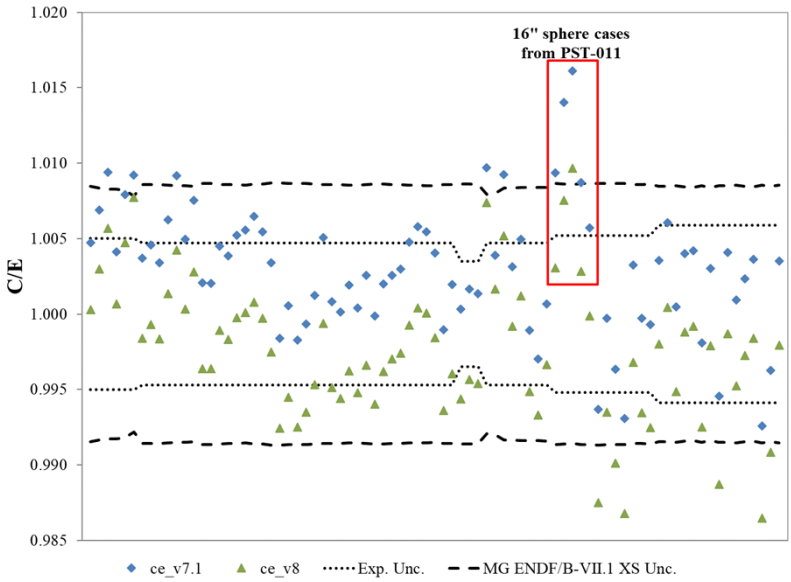

Figure 3. C/E values for all 81 PST systems using both CE libraries

The performance of some categories of systems is worse with the ENDF/B-VIII library than with the ENDF/B-VII.1 library. Many thermal systems that include plutonium, such as the thermal systems containing mixed uranium/plutonium compounds (MCT) and solutions (MST), are negatively impacted by the reactivity adjustment applied to fix the PST systems. A large difference is also noted for the mixed compound fast spectrum (MCF) systems, but this indication is unreliable, as it is based on only two systems and is not consistently reflected by the fast plutonium metal (PMF) systems.

A small decrease is also evident in the average performance of the low-enriched uranium compound thermal (LCT) systems. A detailed examination of the differences in the C/E values as a function of the energy of the average lethargy causing fission (EALF) is provided in Figure 4. A clear trend is evident, with ENDF/B-VIII becoming more negative with increasing EALF. Further investigation is needed to determine the root cause of this change. Some of the higher EALF cases come from the smaller pitch experiments in LCT-010 and have relatively large positive biases. The reactivity reduction for these cases improves agreement. Other harder spectrum cases come from LCT-078 and LCT-080, which have negative biases. The magnitude of the biases obviously increases for these cases.

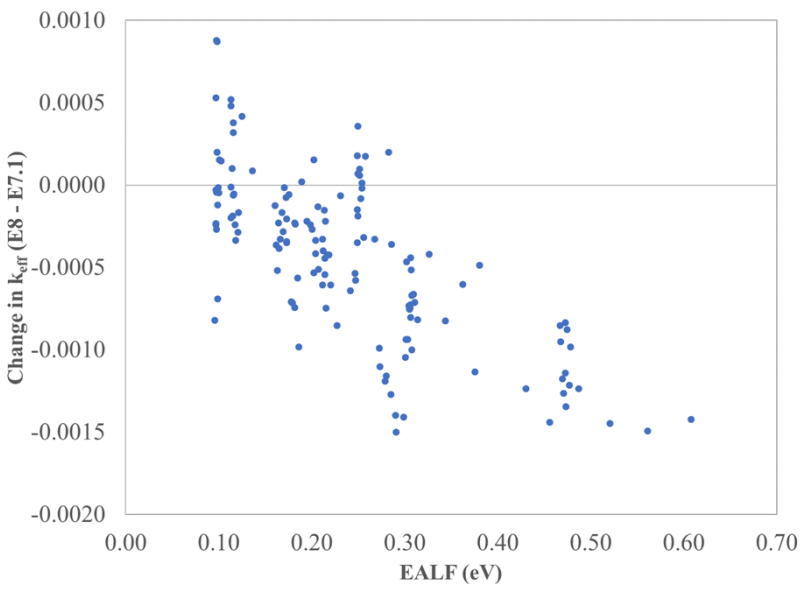

Figure 4. Change in calculated k_{eff} for LCT systems between ENDF/B-VII.1 and ENDF/B-VIII

The average C/E values for the ^{233}U solution systems with intermediate (USI), mixed (USM), and thermal (UST) neutron spectra are lower with the ENDF/B-VIII library than with the ENDF/B-VII.1 library. The ^{233}U-fueled pin array (UCT) systems also have lower reactivity, but the fast metal ^{233}U (UMF) systems appear to be unchanged. As indicated in the data, there are no clear trends as a function of energy, although the larger differences appear to be due to beryllium- or wax- (carbon and hydrogen) reflected systems. The largest differences lower reactivity by slightly more than 0.5% Δk, while other systems see increases of up to almost 0.1% Δk. The average C/E for all UST systems is reduced from 1.00015 with ENDF/B-VII.1 to 0.99750 with ENDF/B-VIII. The reactivity change for the UCT systems is of a similar magnitude, while the USM and USI systems are impacted more significantly.

4. PRELIMINARY TIMING RESULTS

When a new version of a code is being developed and released, calculation time is always of interest to existing users. A limited assessment of the KENO V.a and KENO-VI runtimes in SCALE 6.3 beta 3 was performed in comparison with SCALE 6.2.2. Unfortunately, SCALE 6.2 was noticeably slower than SCALE 6.1 [[9]]. The calculations used to perform this assessment were run on a shared compute cluster at ORNL in a production environment. The performance of any or all jobs in both SCALE 6.2.2 and in SCALE 6.3 beta 3 may have been impacted by other calculations being performed on the cluster or on a specific node at a specific time. As such, these results are prototypic of running in a production environment instead of a clean, isolated development environment.

The results presented here for VALID with the CE library based on ENDF/B-VIII were generated on the same compute cluster that was used to generate the results for the SCALE 6.2.2 validation report [[4]]. In almost all cases, results with SCALE 6.3 beta 3 used a different number of generations to reach the desired uncertainty target as compared to the results in SCALE 6.2.2. The total execution time for each case was thus divided by the number of generations run to generate a runtime per generation. This runtime per generation was then compared between SCALE 6.3 beta 3 and SCALE 6.2.2. There are no obvious trends based on neutron energy spectrum or fissile material in the KENO V.a results. Overall, KENO V.a appears to be about 4% slower in SCALE 6.3 than in SCALE 6.2.2. KENO-VI; however, it is approximately 13% faster and may see higher speed-ups for fast systems than for thermal ones.

5. CONCLUSIONS

VALID was used to perform a criticality safety validation of SCALE 6.3 beta 3 using the KENO V.a and KENO-VI codes. This assessment included a comparison of the calculations with a prior release of SCALE using the same nuclear data and a comparison of ENDF/B-VII.1 libraries with new libraries based on ENDF/B-VIII. The ENDF/B-VIII libraries are available for internal testing at ORNL and are expected to be available for wider beta testing in future SCALE 6.3 beta releases. The ENDF/B-VIII libraries are also expected to be released for production use in the full release of SCALE 6.3.

Both MG and CE libraries based on ENDF/B-VII.1 were used to isolate code changes from SCALE 6.2.2 based on comparisons to the SCALE 6.2.2 validation report [[4]]. This comparison shows that the thermal, intermediate, and mixed spectrum systems have been impacted by a change in the lumping treatment with CENTRM, but this change is planned to be reverted prior to the full release of SCALE 6.3. Systems with fast spectra were largely not impacted by this change. Also, the CE results are in good agreement between SCALE 6.3 beta 3 and SCALE 6.2.2.

Continued testing of the ENDF/B-VIII-based CE library shows similar results to those generated based on a beta-release of ENDF/B-VIII [[7]]. The reactivity of PST systems has been reduced by nearly 0.5% Δk, potentially at the cost of larger biases for mixed uranium and plutonium compound and solution systems. The magnitude of the bias for PST systems was not reduced greatly, from approximately +0.30% Δk to -0.23% Δk. The PMF systems do not appear to be significantly impacted by these adjustments. Incorporation of the CIELO isotopes has increased the magnitude of the negative bias associated with LCT systems. This impact also increases in magnitude with increased neutron energy spectrum. Further investigation is needed to understand the cause of this energy-dependent behavior. ^{233}U-fueled solution systems also exhibit lower reactivity with

ENDF/B-VIII than with ENDF/B-VII.1. It is not immediately obvious that this shift has a common cause with the LCT systems.

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