Criticality Safety Validation of SCALE 6.1 with ENDF/B-VII.0 Libraries

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INTRODUCTION

ANSI/ANS-8.1-1998;2007, *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors* [1], and ANSI/ANS-8.24-2007, *Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations* [2], require validation of a computer code and the associated data through benchmark evaluations based on physical experiments. The performance of the code and data are validated by comparing the calculated and the benchmark results. A SCALE [3] procedure has been established to generate a Verified, Archived Library of Inputs and Data (VALID) [4,5]. This procedure provides a framework for preparing, peer reviewing, and controlling models and data sets derived from benchmark definitions so that the models and data can be used with confidence. The procedure ensures that the models and data were correctly generated using appropriate references with documented checks and reviews. Configuration management is implemented to prevent inadvertent modification of the models and data or inclusion of models that have not been subjected to the rigorous review process. VALID entries for criticality safety are based on critical experiments documented in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE) [6]. The findings of a criticality safety validation of SCALE 6.1 [7] utilizing the benchmark models vetted in the VALID library at Oak Ridge National Laboratory are summarized here.

CODE DESCRIPTIONS

The SCALE code system contains two Monte Carlo transport codes that solve the *k*-effective (k_{eff}) eigenvalue problem in three dimensions and are used primarily for nuclear criticality safety analyses: KENO V.a and KENO-VI. KENO V.a can describe complicated systems fairly simply and use repeating Cartesian array structures and holes to facilitate system description; however, each geometry object must be oriented along a coordinate axis, and objects are not allowed to intersect. KENO-VI has capabilities similar to those of KENO V.a but, by incorporating the SCALE Generalized Geometry Package (SGGP), can represent systems that are significantly more complicated geometrically. A predefined set of geometry objects can be specified to define regions. In addition, generalized quadratic surfaces can be supplied to define regions of space that are not well described by any of the predefined shapes. KENO-VI also supports rotation, allowing bodies to be oriented in directions that are not parallel to the major coordinate axes. KENO-VI provides hole and array capabilities, but the types of arrays available are expanded to include hexagonal and dodecahedral arrays. Intersecting geometry definitions can be supplied to precisely model such features as pipe junctions.

VALID LIBRARY CONTENTS

The VALID library contains over 300 individual benchmark experiment configurations covering eight IHECSBE categories of experiments. Most of these cases use KENO V.a, but 45 cases use KENO-VI. No cases are currently archived in the VALID library using both codes, so each code is validated separately. KENO V.a cases are available for all eight categories represented in the library: high-enriched uranium fast metal systems (HMF), high-enriched uranium thermal solution systems (HST), intermediate enrichment uranium fast metal system (IMF), low-enriched uranium thermal compound systems (LCT), low-enriched uranium thermal solution systems (LST), plutonium fast metal systems (PMF), and plutonium thermal solution systems (PST). KENO-VI cases are available for only three categories: HMF, IMF, and MCT. The evaluations used are listed by code and category in Table I.

VALIDATION METHODS

The validation report [7] demonstrates the general performance of the KENO V.a and KENO-VI codes and ENDF/B-VII.0 data in continuous energy and 238 energy groups across a wide range of systems. The performance of the codes and data is reported in terms of the calculated-to-expected (C/E) ratio. The expected k_{eff} value for each benchmark model configuration is provided in the IHECSBE evaluation for each experiment [6]. An estimated uncertainty is also supplied for this expected value for calculated k_{eff}. The C/E ratio and its uncertainty can be calculated from these two values in the evaluation and the calculated k_{eff} and uncertainty from KENO. The relative uncertainty in the C/E ratio is the square root of the sum of the squares of the relative calculation and evaluation uncertainties. The absolute uncertainty in the C/E ratio is thus simply the relative uncertainty multiplied by the C/E ratio. The uncertainty in the evaluated k_{eff} value is on the order of 10 to 50 times

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Table I. Results by Category

Code	Category	238-Group Calculations		Continuous Energy Calculations	
		Average C/E	Average C/E Uncertainty	Average C/E	Average C/E Uncertainty
KENO V.a	HEU-MET-FAST	1.00422	0.00041	1.00004	0.00041
	HEU-SOL-THERM	0.99904	0.00072	0.99777	0.00072
	IEU-MET-FAST	1.00868	0.00083	1.00284	0.00083
	LEU-COMP-THERM	0.99851	0.00025	0.99944	0.00025
	LEU-SOL-THERM	0.99871	0.00083	0.99842	0.00083
	MIX-COMP-THERM	0.99847	0.00087	0.99654	0.00087
	PU-MET-FAST	1.00035	0.00068	1.00013	0.00068
	PU-SOL-THERM	1.00430	0.00056	1.00142	0.00056
KENO-VI	HEU-MET-FAST	0.99848	0.00066	0.99664	0.00066
	IEU-MET-FAST	1.00765	0.00275	1.00534	0.00275
	MIX-COMP-THERM	0.99443	0.00078	0.99215	0.00078

the KENO standard deviation, so the primary driver in the C/E uncertainty is the uncertainty from the evaluation.

An average C/E value is determined for each category of experiment for each code. The average value reported is an arithmetic average of the individual C/E values. The uncertainty in the average C/E value is determined as the square root of the sum of the individual C/E uncertainties for a given category of experiments divided by the number of experiments in that category.

The results for each case and category of experiments are generated and reported for each library, allowing comparison of the multigroup and continuous energy performance of the KENO codes based on the same benchmark models.

RESULTS

The average C/E value and its uncertainty for each category of experiments are provided in Table I for both the 238-group and continuous-energy cross-section libraries for both KENO V.a and KENO-VI. The results show that the average C/E values are near 1.0. The absolute differences from an average C/E of unity are plotted for both cross-section libraries for KENO V.a in Fig. 1 and for KENO-VI in Fig. 2.

For the 238-group calculations in KENO V.a, the largest deviation from unity on an absolute basis occurs for the intermediate enrichment fast metal systems and is approximately 0.87% Δk_{eff}. The largest deviation on a relative error basis also occurs for the IMF systems and is more than 10 standard deviations from unity. It is worth noting that four of the eight categories have an average C/E difference from unity of less than 2 standard deviations. Both IMF and HMF systems show a greater than 10 sigma deviation from unity for average C/E. Two other categories, LCT and PST systems, show discrepancies of 6 to 8 sigma. The LCT experiments form the only category showing significant deviations that exhibit a negative bias with this cross-section library.

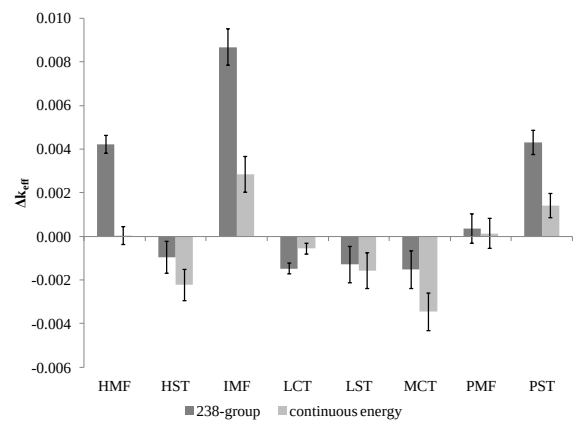

Fig. 1. Difference from unity of average C/E value by category for KENO V.a (Δk_{eff}).

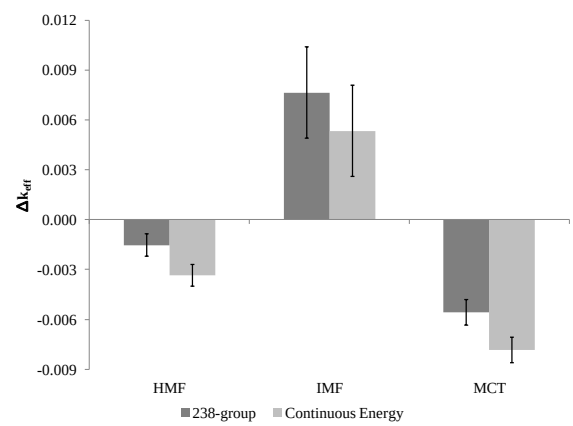

Fig. 2. Difference from unity of average C/E value by category for KENO-VI (Δk_{eff})

For the KENO V.a continuous-energy calculations, the largest deviation from unity on an absolute basis

occurs for the MCT systems and is about -0.35% Δk_{eff}. The largest deviation on a relative error basis also occurs for the MCT systems and is just under 4 standard deviations from unity. Only three of the eight categories have an average C/E within 2 standard deviations of unity indicating that the modest biases observed are statistically significant for the other five categories.

For the 238-group calculations in KENO-VI, the largest deviation from unity on an absolute basis occurs for the IMF systems and is approximately 0.77% Δk_{eff}. The largest deviation on a relative error basis occurs for the MCT systems and is more than 7 standard deviations from unity. All three categories of experiments with KENO-VI data show deviations of more than 2 standard deviations from unity. The IMF systems appear to be overpredicted, while the HMF and MCT cases show average C/E values less than unity.

For the continuous-energy calculations in KENO-VI, the largest deviation from unity on an absolute basis occurs for the MCT systems and is about -0.79% Δk_{eff}. The largest deviation on a relative error basis also occurs for the MCT systems and is just over 10 standard deviations from unity. Only the IMF systems have an average C/E within 2 standard deviations of unity, though the uncertainty in the average C/E is quite large because only two systems were considered. As with the multigroup library results, the IMF systems have an average C/E value greater than 1, and the HMF and MCT results have an average C/E less than unity.

The results of all cases are surveyed to determine the greatest difference from a C/E of unity for each category. The case with the largest difference in absolute and relative error is identified and reported in Table II and Table III, respectively.

Table II. Maximum Individual Case Absolute Difference from C/E Ratio of 1.0

Code	Category	238-Group Calculations		Continuous Energy Calculations	
		Maximum Difference (% Δk)	Case	Maximum Difference (% Δk)	Case
KENO V.a	HEU-MET-FAST	1.43	HMF-025-025	0.70	HMF-019-001S
	HEU-SOL-THERM	2.53	HST-016-003	2.64	HST-016-003
	IEU-MET-FAST	1.41	IMF-005-001	0.76	IMF-004-001
	LEU-COMP-THERM	-0.50	LCT-017-026	0.47	LCT-010-002
	LEU-SOL-THERM	-0.63	LST-002-002	-0.72	LST-002-002
	MIX-COMP-THERM	-0.49	MCT-004-001	-0.77	MCT-004-001
	PU-MET-FAST	0.62	PMF-005-001	0.92	PMF-005-001
	PU-SOL-THERM	1.74	PST-011-003	1.48	PST-011-003
KENO-VI	HEU-MET-FAST	0.80	HMF-080-001	-1.09	HMF-005-004
	IEU-MET-FAST	0.80	IMF-019-001	0.53	IMF-019-001
	MIX-COMP-THERM	-0.75	MCT-008-021	-0.98	MCT-008-021

Table III. Maximum Individual Case Relative Deviation from C/E Ratio of 1.0

Code	Category	238-Group Calculations		Continuous Energy Calculations	
		Maximum Deviation ($\sigma_{C/E}$)	Case	Maximum Deviation ($\sigma_{C/E}$)	Case
KENO V.a	HEU-MET-FAST	8.8	HMF-025-025	-3.2	HMF-030-001
	HEU-SOL-THERM	3.1	HST-016-003	3.3	HST-016-003
	IEU-MET-FAST	8.6	IMF-007-001	3.5	IMF-008-001
	LEU-COMP-THERM	-4.8	LCT-050-008	-3.2	LCT-050-008
	LEU-SOL-THERM	2.9	LST-004-005	-2.0	LST-002-002
	MIX-COMP-THERM	1.1	MCT-002-004S	-2.1	MCT-001-001
	PU-MET-FAST	4.7	PMF-005-001	7.0	PMF-005-001
	PU-SOL-THERM	3.3	PST-011-003	2.8	PST-011-003
KENO-VI	HEU-MET-FAST	6.6	HMF-080-001	7.6	HMF-080-001
	IEU-MET-FAST	2.3	IMF-019-001	1.5	IMF-019-001
	MIX-COMP-THERM	-1.9	MCT-008-016	-2.4	MCT-008-012

CONCLUSIONS

The average C/E values shown in Table I, Fig. 1, and Fig. 2 indicate a fairly small code bias for a wide range of potential systems. The bias is less than 1% for all categories of systems examined, and less than 0.5% for almost all categories in KENO V.a. The biases appear to be larger in KENO-VI, but all biases are less than 0.8%. The higher apparent biases for KENO-VI may be a result of the increased geometric complexity of the KENO-VI benchmark experiments, which makes it more difficult to precisely measure and report all geometric details for these experiments. These more complex geometries are more difficult to describe accurately in benchmark definitions, and may therefore have a larger apparent bias. Further investigation of the KENO-VI bias using simple geometry models should be performed to examine this issue. The biases for several categories of experiments are statistically significant. These results indicate that improvements in the cross-section measurements, cross-section processing, or the physics approximations within the AMPX or SCALE code systems could result in smaller biases and also indicate which nuclides and energy regions are most likely to benefit from such improvements in future versions.

The validation studies reported here also compare the 238-group and continuous-energy ENDF/B-VII.0 libraries. The continuous-energy capability generally appears to manifest a smaller bias than the 238-group results. The MCT experiments, and to a smaller degree the HST experiments, do not follow this trend, and the causes are under investigation. Ongoing efforts to improve both CE and MG nuclear data generated from the AMPX code system should result in updated nuclear data libraries which improve the performance of SCALE. These updated libraries will be included in a future release of SCALE..

Overall, the KENO V.a and KENO-VI codes have been shown to provide consistent, low bias results across a range of systems that are commonly encountered in criticality safety applications. Some outlier cases are examined in a companion paper [8].

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