Validation of the SCALE Criticality Safety Codes and Data Using Reviewed Benchmark Models

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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], require validation of a computer code and the associated data through the calculation of benchmark evaluations that are based on physical experiments. The performance of the code and data are validated through comparison of the calculated and benchmark results. In this process, it is important to model an experiment with the computer code the way it is evaluated into a benchmark so that the performance of the code and the associated cross section libraries may be determined accurately within the uncertainties of the benchmark evaluation and the uncertainties of the computational results. As such, a new SCALE (Standardized Computer Analyses for Licensing Evaluation) [3] procedure has been established for verification and configuration management of benchmark models and derived data.[4] This procedure provides a framework for preparing, peer-reviewing, and controlling models and data sets derived from benchmark definitions so that one can use the models and data with confidence in his/her analyses. 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 gone through the rigorous review process.

The SCALE code system includes Monte Carlo criticality safety codes KENO V.a and KENO-VI. KENO V.a and KENO-VI differ in their treatment of the geometric modeling of the problem; KENO-VI is not the next version of KENO V.a. KENO V.a contains simpler geometric modeling capabilities whereas KENO-VI allows more complex geometric modeling. Both codes can perform neutron transport calculations using either multigroup (MG) or continuous energy (CE) data. The energy treatment is automatically selected based on the cross-section library name if the problem is initiated by one of the corresponding control modules. For KENO V.a, the control module is CSAS5; for KENO-VI, the control module is CSAS6.

The CE cross-section processing software has been added to the AMPX [5] code system that is used to prepare the nuclear data libraries for SCALE. The AMPX code system includes programs that can read the ENDF evaluations; process the data using various ENDF laws; and create reaction cross sections as well as transfer matrices in both MG and CE and store them in appropriate formats for use in the SCALE code system. Production-level CE libraries based on ENDF/B-VI Release 8 and ENDF/B-VII Release 0 evaluations have been prepared and released with SCALE 6.0 for the first time. The SCALE 6.0 release contains the two ENDF/B releases at multiple temperatures: 300, 600, 900, 1200, and 2400 K. In addition, the cross sections for the nuclides with thermal scattering data have been generated at the temperatures that are provided in the corresponding ENDF/B evaluation files. Although temperature interpolation of the cross sections is not yet available in the CE mode of KENO, having multiple temperature cross sections available allows approximate but more accurate analysis of high-temperature systems.

Previous studies [6,7] have reported on the performance of the code and CE cross sections based on ENDF/B-VI Release 8 and ENDF/B-VII Release 0 for a limited number of benchmarks. Another study [8] used a more comprehensive benchmark suite. However, the input models used in those studies were not subjected to a rigorous quality assurance or configuration management plan. Although they were believed to be of good quality, it is not possible to distinguish differences due to errors in the benchmark modelling from differences due to inadequacies in the nuclear data. This paper provides the results of validation efforts for SCALE criticality safety codes and MG and CE cross-section data based on ENDF/B-VII Release 0 for about 220 benchmark models from the QA-controlled library at ORNL. All of the benchmark models used in this study are based on the benchmark definitions in the 2009 *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE).[9] The 2009 IHECSBE contains 170 of the 220 QA-controlled benchmark models used in this study. The additional QA-controlled benchmark models will be released with the 2010 edition. Note that those models and data that have been included with the IHECSBE are no longer QA-controlled under SCALE.

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CALCULATIONS AND RESULTS

Calculations reported in this study have been performed until a calculated standard deviation of 0.0001 is achieved. Percent differences between the calculated (C) values and benchmark values (B) are determined for each modeled case. For most of the cases, MG and CE mode calculations yield k_{eff} values that are within a few tenths of a percent of the benchmark values. For the remainder of the cases, CE mode calculations generally yield k_{eff} values that are closer to the benchmark values. Figure 1 shows the benchmark k_{eff} values with 2σ error bars. Calculated k_{eff} values are also shown in Fig. 1. Since the standard deviations of the calculated values are very small, they are not shown in the figure. The IHECSBE identifiers have been shortened to the first letters. For example, HMF stands for HEU-METAL-FAST, LST stands for LEU-SOL-THERM, etc. Benchmark series that have been analyzed with KENO V.a are HMF series 016, 017, 018, 019, 020, 021, 030, 038; HST series 001, 013, 014, 016, 028, 029, 030; IMF series, 002, 003, 004, 005, 006, 008, 009; LCT series 001, 002, 050; LST series 002, 003, 004; MCT series 001, 002, 004; PMF series 001, 002, 005, 006, 008, 010, 018, 022, 023, 024; and PST 001, 002, 003, 004, 005, 006. Benchmark series that have been analyzed with KENO-VI are HMF series 005, 008, 009, 010, 011, 013, 024, 080 and IMF series 019.

Table I lists the maximum of the percent deviations for each set of calculations. The first eight rows in Table I correspond to the KENO V.a cases, whereas the last two rows in the table correspond to the KENO-VI cases.

Table I also lists the maximum differences in units of numbers of combined standard deviations (benchmark and statistical) [(C-B)/σ]. The worst case in both CE and MG calculations is for HST series 016 case 3. For this case, the calculated and benchmark k_{eff} values are about 3σ apart, which indicates a high benchmark value for a high k_{eff} percent difference value. Indeed, the benchmark uncertainty for this case is 0.0079. Calculated k_{eff} values reported in IHECSBE also differ from the benchmark value on the order of several percent. The other outlier is PMF series 005 case 1 with about 0.9% difference that is more than 7σ apart from the benchmark. Calculated k_{eff} values reported in IHECSBE for this case are also about 0.8% different and about 5σ apart. The worst cases in each of the other series show absolute percent differences between ~0.3 and ~1.3. However, the numbers of sigma differences are about 3, indicating the benchmark and calculated k_{eff} values are within 3σ of each other.

MG and CE calculation results show similar trends. Although generally MG calculation results are very good, for some cases (e.g., IEU systems) the MG mode does not perform as well as the CE mode due to the limitations in generating problem-dependent MG cross sections.

Table I. Maximum Deviations

	CE			MG		
	(C-B)/B%	(C-B)/σ	Case	(C-B)/B%	(C-B)/σ	Case
HMF	0.72	2.41	HMF-019-001S	0.78	2.60	HMF-019-001
HST	2.64	3.33	HST-016-003	2.48	3.13	HST-016-003
IMF	0.78	2.45	IMF-004-001	1.32	5.75	IMF-005-001S
LCT	-0.33	3.24	LCT-050-008	-0.46	4.58	LCT-050-008
LST	-0.72	1.95	LST-002-002	-0.69	1.63	LST-003-004
MCT	-0.75	1.64	MCT-004-001	-0.44	0.96	MCT-004-001
PMF	0.92	7.09	PMF-005-001	0.96	7.37	PMF-005-001
PST	0.70	1.49	PST-002-005	1.06	2.12	PST-001-003
HMF	-1.10	3.04	HMF-005-004	-0.94	2.61	HMF-005-004
IMF	0.58	1.66	IMF-019-001	0.72	2.05	IMF-019-001

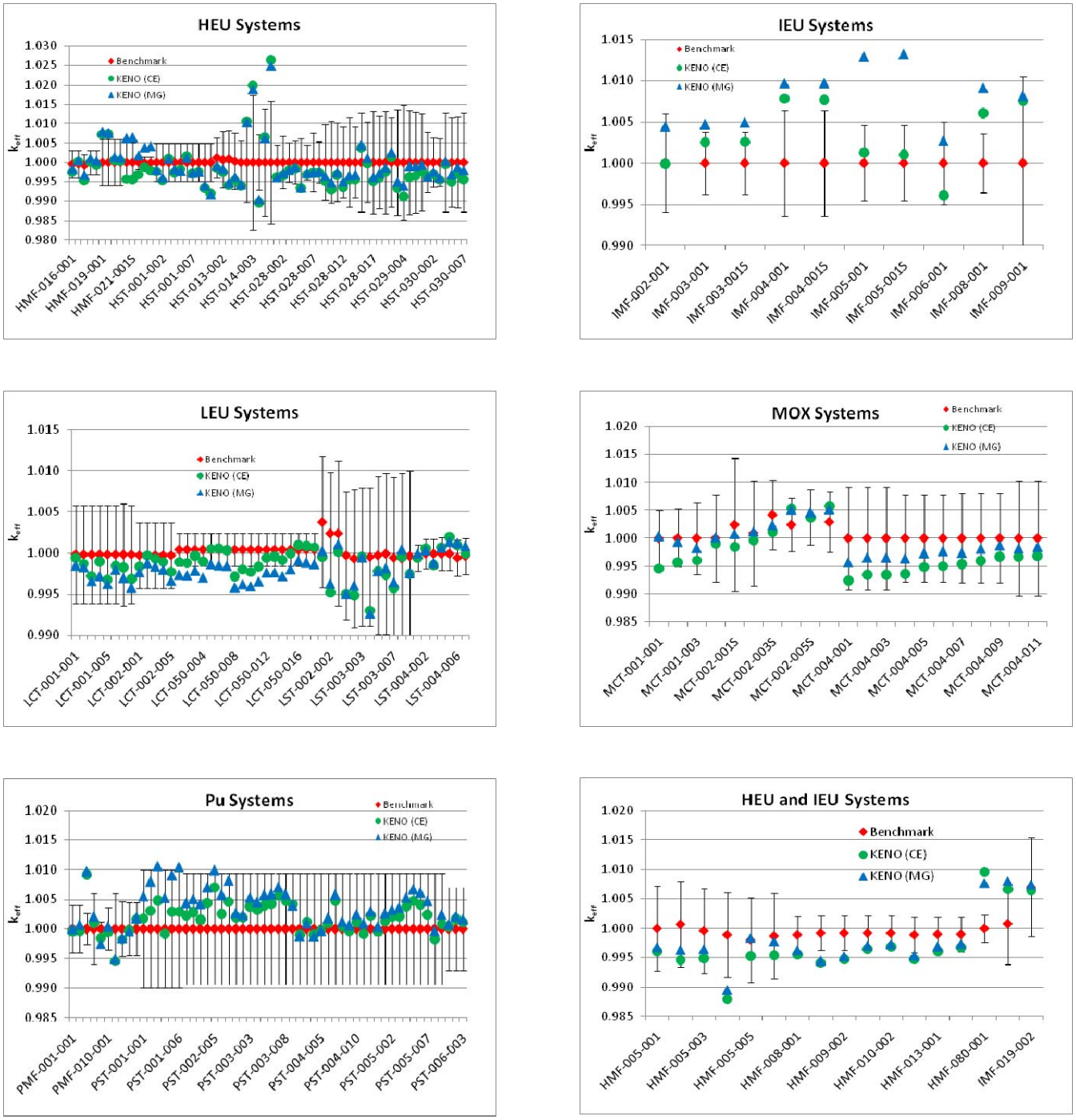

Fig. 1. Benchmark and calculated k_{eff} values.

CONCLUSIONS

The performance of the SCALE Monte Carlo criticality safety codes has been assessed using peer-reviewed, QA-controlled and verified models of benchmark experiments from the IHECSBE. With these QA-verified models of IHECSBE benchmark experiments, differences observed between the computed and benchmark values are generally due either to inadequacies in the computational tools or, more likely, weaknesses in the ENDF/B nuclear data.

MG and CE calculations generally produce the same results for both KENO V.a and KENO-VI. Although the CE mode calculations generally take longer to perform, they are not subject to an analyst's expertise in determining and setting up unit cell data that may be needed in the MG mode and therefore may be easier to set up.

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