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SCALE 6.2.4 Validation: Overview

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Nuclear Energy and Fuel Cycle Division

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ABBREVIATIONS

2D	two-dimensional
3D	three-dimensional
BWR	boiling water reactor
CE	continuous energy
DOE	US Department of Energy
ENDF	Evaluated Nuclear Data File
LWR	light-water reactor
NRC	Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor

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ABSTRACT

SCALE is a multi-application code system with tools for reactor physics, criticality safety, radiation shielding, and spent fuel characterization for a range of nuclear systems. The last of the SCALE 6.2 series, version 6.2.4, was released in June 2020 [1]. Validation studies in nuclear criticality safety, reactor physics, and shielding applications were performed to confirm results, assess accuracy, and identify biases from SCALE simulations. Nuclear criticality safety applications yield small code biases for a wide range of systems, generally overestimating cross section uncertainty. Reactor physics applications show improvements in nuclide inventory and full-core eigenvalue predictions, with similar performance in decay heat predictions. Radiation shielding applications yield sufficient agreement in comparisons to measurements and alternate simulations for eight shielding experiments.

1. INTRODUCTION

SCALE is a broad modeling and simulation suite for nuclear safety analysis and design, with applicable tools for reactor physics, criticality safety, radiation shielding, and spent fuel characterization for a range of nuclear systems [2]. It is developed and maintained by Oak Ridge National Laboratory (ORNL) under contract with the US Nuclear Regulatory Commission (NRC), US Department of Energy (DOE), and the National Nuclear Security Administration. SCALE version 6.2.4 was released in June 2020; SCALE version 6.3 is undergoing final reviews before public release.

This volume of the SCALE 6.2.4 validation reports connects all domain-specific validation volumes, describing the data and the tools used and summarizing the simulation results and their comparisons to measurements. The associated volumes contain additional detailed information on SCALE 6.2.4 validation in criticality safety [3], reactor physics [4], and shielding [5] applications. The range of systems, fuels, and materials in these applications is extensive; SCALE 6.2.4 is well validated for a variety of nuclear applications.

Evaluating simulation outcomes against real measured quantities of interest has been a key component of the SCALE code system since its inception. The validation of cross section libraries for criticality safety analyses [6–8] followed soon after the initial release of the SCALE code system in 1980. These studies on the validation of the integral quantity k_{eff} expanded to cover more specific light-water reactor (LWR) applications [9–12]. Other studies expanded these LWR applications, incorporating spent fuel isotopic [13–15] and decay heat [16–18] data for validating reactor physics simulation (i.e., neutron transport and point depletion) results. These studies continued to expand this validation basis to include a variety of available data at different burnups [19–21] and from different reactor systems [22]. More modern advances in computational tools have enabled whole-core reactor startup physics benchmarking with SCALE [23]. SCALE has been refined over the years, and the lineage of criticality safety validation [24–29] has provided a broad and more formalized validation basis for these applications. Iterative reactor physics activities [30–33] also form a strong validation basis in isotopic and full-core predictions. Conversely, shielding application validation is relatively new to the modern SCALE code system. However, these validation activities leverage a long history of research and development at ORNL in deterministic [34] and hybrid methods [35] development and validation [36–40] for shielding applications.

The remainder of this report is divided as follows: Section 1 contains additional information on SCALE nuclear data and codes, Section 2 summarizes the validation results, and Section 3 provides concluding remarks and summarizes future work in these validation subject areas.

1.1 SCALE NUCLEAR DATA

SCALE 6.2.4 leverages ENDF/B-VII.1 [41] and JEFF [42] evaluations to produce its comprehensive nuclear data products for performing neutron transport, decay, and transmutation. Multigroup (MG) and continuous-energy (CE) neutron and coupled neutron–gamma data generated with the AMPX codes [43] provide for applicability across a broad set of criticality safety, reactor physics, and shielding analysis applications. Decay data, reaction cross sections, fission yields, and delayed neutron and gamma information for 2,200 nuclides is amassed from ENDF/B-VII.1 and JEFF evaluations. SCALE also contains neutron cross section covariance data for use in sensitivity and uncertainty analysis tools. This section identifies these nuclear data products and briefly describes their use within SCALE applications.

1.1.1 ENDF/B-VII.1 Continuous Energy

The CE cross section library (see Figure 1) released with SCALE 6.2.4 is provided for general-purpose neutron, gamma, and coupled neutron/gamma calculations. It is generated with AMPX using ENDF/B-VII.1 evaluation data. This neutron cross section library is used in all validation volumes with the CSAS, TRITON, and MAVRIC applications.

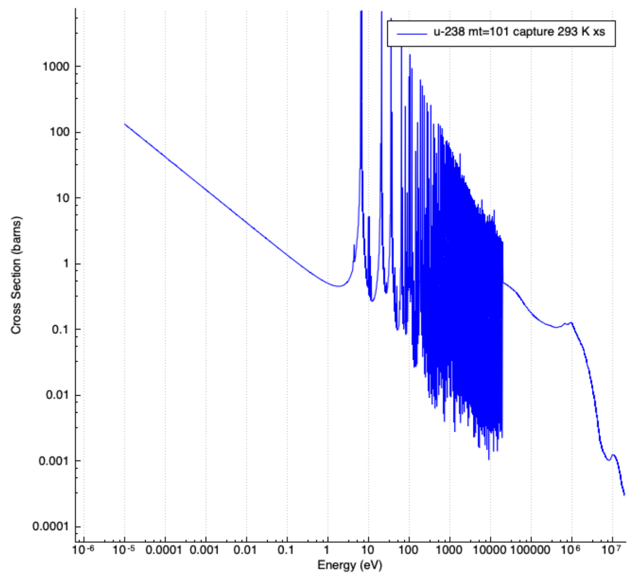

Figure 1. U-238 continuous energy capture cross section.

1.1.2 ENDF/B-VII.1 252-group Thermal System

The 252-group (see Figure 2) ENDF/B-VII.1 AMPX-generated library is a general-purpose fine-group library first released with SCALE 6.2. It reduces biases in LWR applications from the previous 238-group libraries using a more detailed representation of the ^{238}U resonance structure. As such, it is optimized for thermal systems. This neutron cross section library is used in reactor physics [4] and nuclear criticality safety [3] validation with the CSAS, TRITON, and Polaris applications.

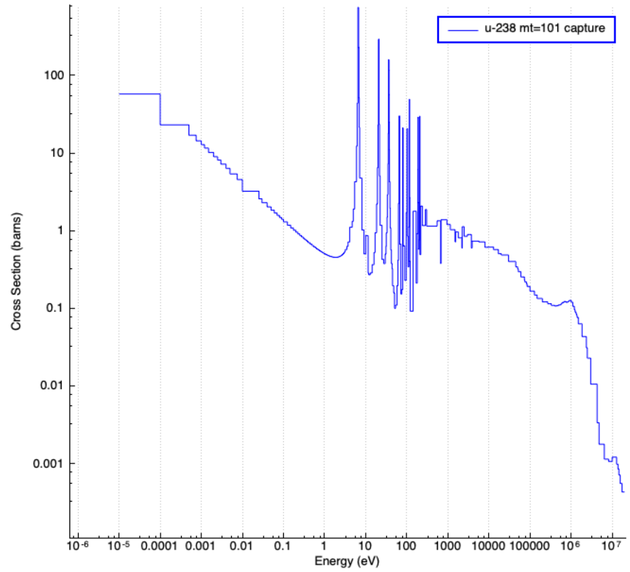

Figure 2. U-238 252-group capture cross section.

1.1.3 ENDF/B-VII.1 56-group Thermal System

The 56-group (see Figure 3) ENDF/B-VII.1 AMPX-generated library is an optimized broad-group library first released with SCALE 6.2. It is intended for rapid scoping analyses for LWR and other thermal system applications, sacrificing accuracy for calculation speed. It is optimized for thermal systems. This neutron cross section library is used in reactor physics [4] and nuclear criticality safety [3] validation with the CSAS, TRITON, and Polaris applications. However, it should not be relied upon for criticality safety analyses.

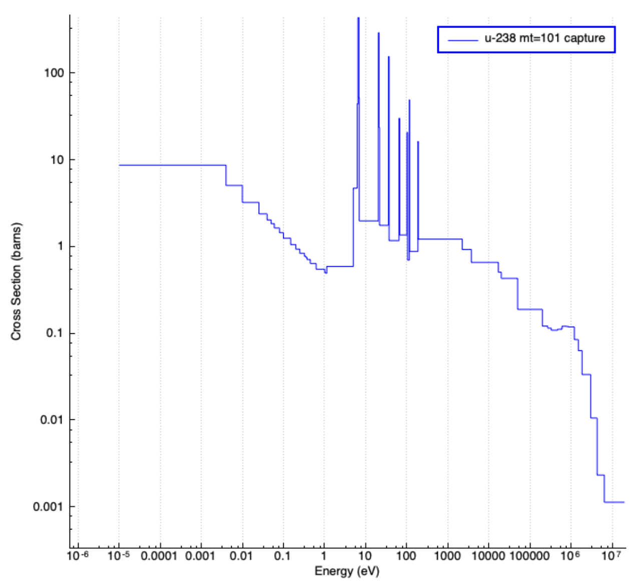

Figure 3. U-238 56-group capture cross section.

1.1.4 ENDF/B-VII.1 200-group Shielding

The coupled neutron–gamma ENDF/B-VII.1 AMPX-generated shielding library has 200 neutron energy groups (see Figure 4) and 47 gamma energy groups. It was first released in SCALE 6.1 and has a group structure tuned to cover the fast energy range for shielding and fast reactor applications. This cross-section library is used in shielding validation [5] with the MAVRIC application.

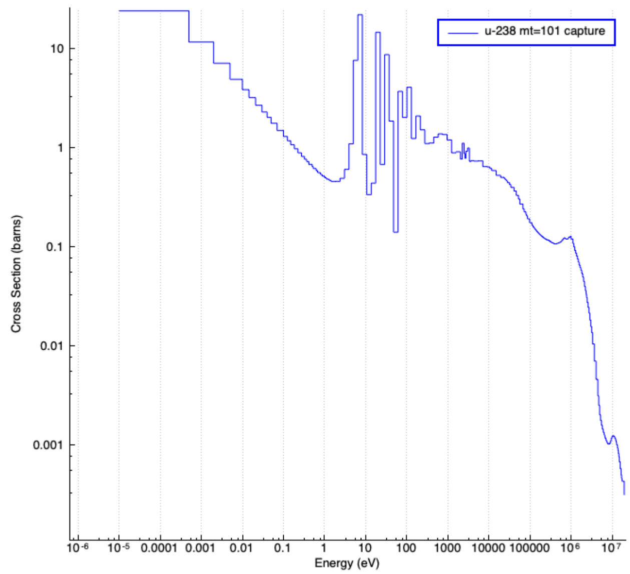

Figure 4. U-238 200-group capture cross section.

1.1.5 ENDF/B-VII.1 Decay and Yield Data

Nuclear decay data, fission product yields, and gamma ray emission data are developed from ENDF/B-VII.1 evaluations using AMPX. Decay data include ground and metastable state nuclides with half-lives greater than 1 millisecond. SCALE 6.2 uses these data to track 174 actinides, 1,149 fission products, and 974 activation products. These data are used in reactor physics validation [4] with the ORIGEN[1] and ORIGAMI applications.

1.1.6 JEFF/3.1-A Reaction Data

Cross section data for materials and reaction processes not available in ENDF/B-VII.1 are incorporated from the JEFF-3.1-A special-purpose activation library [42]. This library contains over 700 materials and 12,000 neutron-induced reactions below 20 MeV. These data are used in reactor physics validation [4] with the ORIGEN and ORIGAMI applications.

1.2 SCALE APPLICATIONS

Validation of SCALE 6.2.4 is performed for several applications spanning the criticality safety, reactor physics, and shielding subject matter areas. This section provides a brief description of each application and their use in validation volumes.

[1] The reactor physics tools Polaris and TRITON natively integrate ORIGEN simulations.

1.2.1 CSAS

The CSAS5 and CSAS6 applications perform 3D Monte Carlo eigenvalue and criticality search simulations with MG or CE cross sections. These applications run the KENO V.a and KENO-VI Monte Carlo codes to generate the neutron transport random walks required to estimate integral quantities. MG cross sections are processed to generate problem-specific libraries to account for self-shielding effects. Transport is performed on a constructive solid geometry (CSG) defined with the SCALE general geometry package (see Figure 5). CSAS5 and CSAS6 are used in the criticality safety validation volume [3].

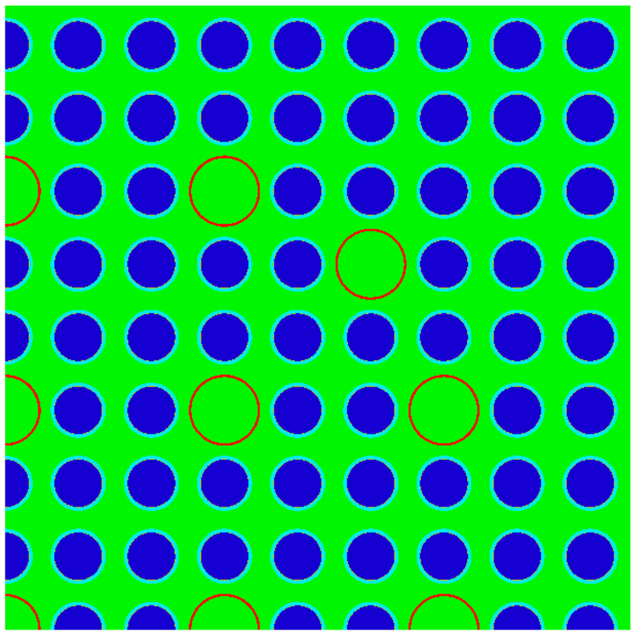

Figure 5. KENO-VI 2D geometry of a PWR fuel assembly.

1.2.2 TRITON

The TRITON application manages coupled neutron transport–point depletion simulations with a selected SCALE neutron transport application and the point depletion solver ORIGEN (see § 1.2.4). It is a general-purpose reactor physics tool applicable to many reactor system types and geometries. Neutron transport applications include 1D, 2D, and 3D geometries defined per the selected neutron transport application. The most common applications for TRITON include (1) LWR lattice physics with the NEWT 2D discrete-ordinates application [44] that uses the extended step characteristic method (see Figure 6) and (2) 3D reactor or assembly depletion with the KENO Monte Carlo codes. NEWT is restricted to the use of MG cross sections. TRITON is used in the reactor physics validation volume [4].

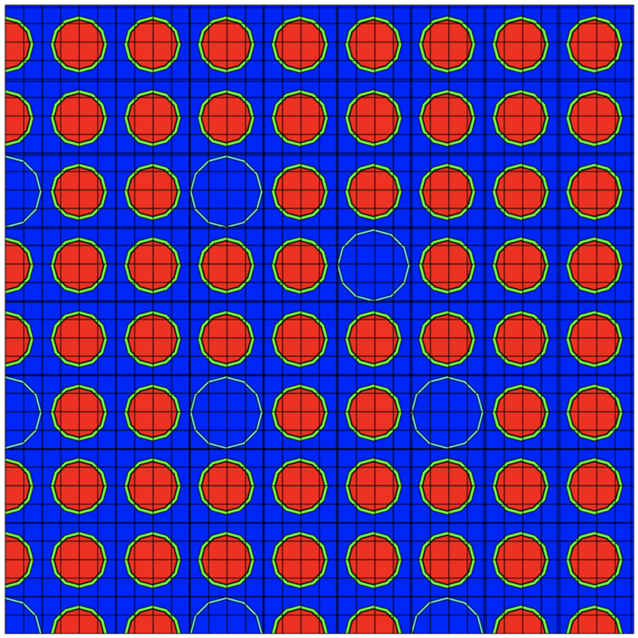

Figure 6. NEWT 2D geometry of a PWR fuel assembly showing the transport mesh.

1.2.3 Polaris

The Polaris [45] application was first released in SCALE 6.2 to provide a more optimized application for boiling water reactor (BWR) and pressurized water reactor (PWR) lattice physics assessments relative to the more general-purpose TRITON application. Polaris employs the embedded self-shielding method and a 2D method of characteristics (MOC) transport solver (see Figure 7). Polaris can solve LWR problems in much less computational time compared to TRITON and the input files tend to be significantly shorter. Like TRITON, Polaris uses the point depletion solver ORIGEN to simulate nuclide transmutation and decay. Polaris is used in the reactor physics validation volume [4].

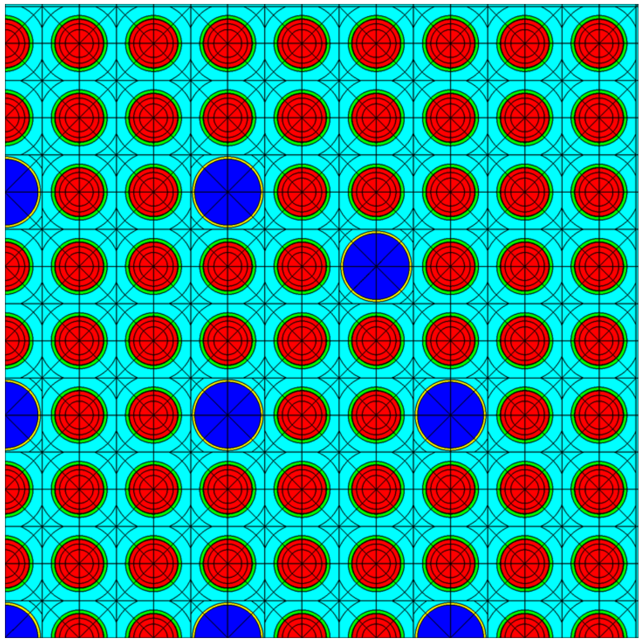

Figure 7. Polaris 2D geometry of a PWR fuel assembly showing the transport mesh.

1.2.4 ORIGEN

The ORIGEN application solves the set of coupled Bateman equations defining the depletion, activation, and decay of a material under irradiation. Two solvers are available: a solver based on the Chebyshev Rational Approximation Method (CRAM) and a traditional matrix power series–based solver; both solvers introduce computational errors less than 0.1% compared to analytic solutions of the governing equations. ORIGEN generates time-dependent concentrations for the 2,200 nuclides tracked within the ORIGEN data. These nuclide compositions are used in comparison to radioisotope concentration measurements and decay heat measurements; the latter uses ORIGEN to calculate the time-dependent heat generation of the material. ORIGEN is used in the reactor physics validation volume [4].

1.2.5 ORIGAMI

The ORIGAMI application was introduced in SCALE 6.2 for computing detailed isotopic compositions for LWR assemblies with UO_2 fuel. It uses assumed assembly power distributions and pre-generated ORIGEN reactor libraries, interfacing with the ORIGEN application to perform burnup calculations for the distributed regions. This results in discretized decay heat sources and isotopic compositions for LWR fuel assemblies that can be used in follow-on fuel assembly operations. ORIGAMI is used in the reactor physics validation volume [4].

1.2.6 MAVRIC

The MAVRIC application performs 3D Monte Carlo fixed-source simulations with MG or CE cross sections with automated variance reduction. SCALE 6.2 introduced an improved solution fidelity with the CE treatment. It uses a Consistent Adjoint Driven Importance Sampling (CADIS) methodology [35] to generate weight windows and bias the fixed source to generate fluxes and dose rates with low uncertainties in a reasonable amount of run time. MAVRIC automatically performs a coarse-mesh 3D discrete ordinates transport calculation with Denovo to determine the position- and energy-dependent adjoint flux for importance weighting. MAVRIC is used in the shielding validation volume [5].

2. SUMMARY OF VALIDATION RESULTS

A summary of SCALE 6.2.4 validation is presented in the following section. SCALE users are encouraged to consult the individual validation volumes for additional details, Greene et al. [3] for criticality safety validation, Ilas et al. [4] for reactor physics validation, and Celik et al. [4] for radiation shielding validation.

2.1 CRITICALITY SAFETY VALIDATION

The average calculated-to-experimental (C/E) values for CSAS-KENO V.a are shown in Figure 8 for the four transport cross section libraries deployed in SCALE 6.2.4 [3], across a number of benchmark categories. The CE results are based on ENDF/B-VII.1 (ce_v7.1) and may be regarded as the maximum fidelity "truth" according to SCALE. The other three MG cross section libraries have implicit assumptions as to the neutron energy spectrum of the problem and will achieve the CE-level accuracy only if the benchmark problem spectrum is reasonably close to the assumed MG library spectrum.

For example, for thermal spectrum systems (e.g., those categories ending with "T"), the 252-group library shows excellent agreement with CE (note MG calculations will typically be a factor of 2 or more faster than CE). We generally do not recommend the broad-group library (56-groups) or the activation/shielding library (200-groups) for criticality safety; however, for completeness, results from those libraries have been generated. The 200-group library does have more energy groups in the fast range and will have better agreement with CE than the 252-group for fast-spectrum problems (e.g., those categories ending with "F").

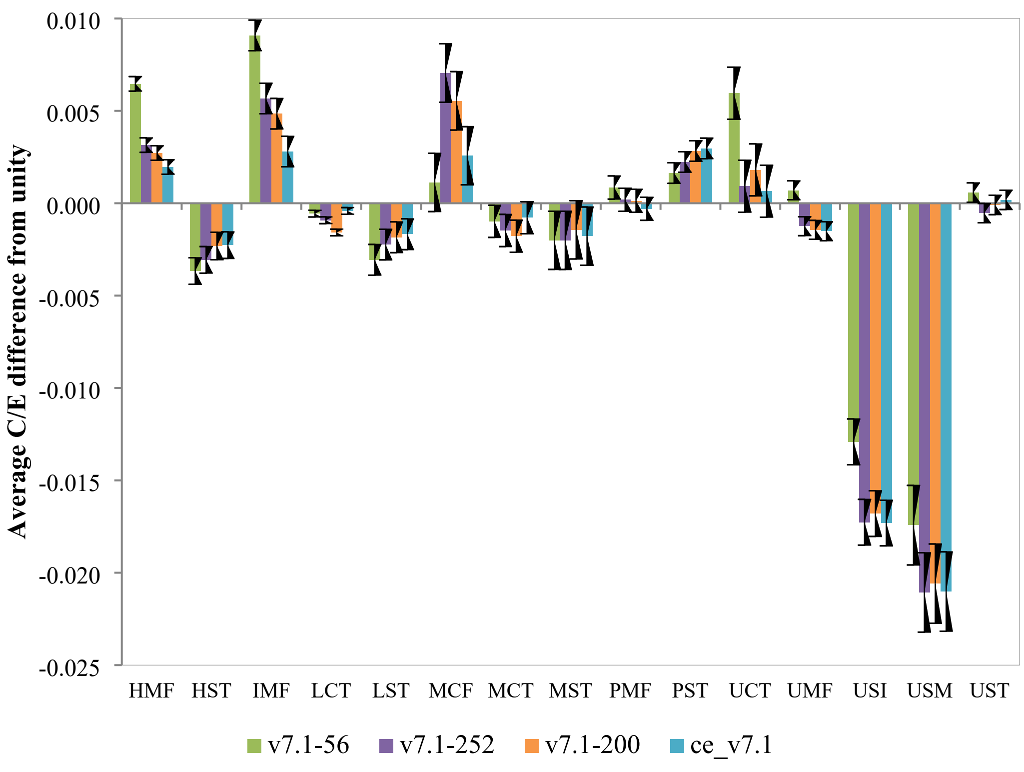

Figure 8. Average C/E bias for CSAS-KENO V.a criticality safety validation.

The criticality safety code bias for a wide range of systems is fairly small. When considering all categories of systems examined, the bias is less than 2.2% Δ*k*. After removing the USI and USM systems due to evidence of performance problems, the bias for KENO V.a is less than 0.91% Δ*k*, and it is less than 0.5% Δ*k* for almost all categories in KENO V.a. The biases in KENO-VI appear to be larger, but this may be the result of the increased geometric complexity of the benchmark experiments, which require the use of the generalized geometry capabilities. Comparisons have been performed where KENO V.a cases were converted to KENO VI. There was no statistically significant bias between the codes for that comparison [25].

2.2 REACTOR PHYSICS VALIDATION

Reactor physics validation currently contains cases for PWR and BWR spent fuel destructive assay for 169 samples, and decay heat. In addition, validation results are reported for a full-core analysis of Watts Bar 1 PWR and two non-LWR cases, HTR-10 and HTTR [4]. Table 1 shows just the spent fuel destructive assay results for PWR and BWR. The average bias is shown as the calculation divided by measurement (i.e., C/E) minus one in percent. Note that each average C/E-1 is calculated from many independent comparisons to measurement. For some nuclides, there may be ~10 measurements—for others close to 100. Any average bias over 5% is colored lightly in orange, up to a dark orange at 10%. The standard deviation in the bias is shown in the next column and gives an idea of how much variation is present in the distribution of biases. For example, one could say the bias in ^{239}Pu for PWRs is for example 2% ± 3%. Note the large biases in ^{109}Ag and ^{125}Sb are typical as these are difficult-to-measure nuclides and, as evidenced by a large uncertainty in the bias, indicate that the underlying measurements themselves are varying and have high uncertainty. See the report for additional details on the nuclide inventory validation as well as decay heat and other reactor physics quantities of interest.

Table 1. Destructive Assay Validation Summary.

Nuclide	PWR		BWR	
	C/E-1 (%)	std. dev. (%)	C/E-1 (%)	std. dev. (%)
^{234}U	13%	17%	4%	13%
^{235}U	1%	4%	3%	11%
^{236}U	2%	3%	2%	5%
^{238}U	0%	0%	0%	0%
^{238}Pu	4%	7%	6%	21%
^{239}Pu	2%	3%	3%	9%
^{240}Pu	0%	4%	0%	9%
^{241}Pu	2%	5%	6%	11%
^{242}Pu	4%	6%	2%	17%
^{237}Np	2%	20%	1%	12%
^{241}Am	4%	19%	1%	17%
^{243}Am	7%	13%	5%	34%
^{242}Cm	-	-	9%	68%
^{244}Cm	1%	11%	2%	46%
^{245}Cm	1%	15%	-	-
^{246}Cm	7%	22%	-	-
^{95}Mo	-	-	2%	8%
^{90}Sr	1%	7%	1%	7%
^{99}Tc	16%	16%	26%	16%

Table 1. Destructive Assay Validation Summary (continued).

Nuclide	PWR		BWR	
	C/E-1 (%)	std. dev. (%)	C/E-1 (%)	std. dev. (%)
^{101}Ru	6%	11%	6%	13%
^{106}Ru	6%	22%	-	-
^{103}Rh	12%	11%	7%	9%
^{109}Ag	76%	68%	34%	39%
^{125}Sb	99%	45%	-	-
^{133}Cs	2%	2%	3%	7%
^{134}Cs	10%	7%	-	-
^{135}Cs	2%	4%	-	-
^{137}Cs	1%	3%	3%	6%
^{143}Nd	1%	2%	4%	4%
^{145}Nd	0%	1%	2%	3%
^{146}Nd	-	-	0%	3%
^{148}Nd	0%	0%	0%	3%
^{144}Ce	3%	8%	3%	8%
^{147}Sm	1%	3%	1%	8%
^{149}Sm	1%	6%	8%	12%
^{150}Sm	1%	3%	3%	7%
^{151}Sm	3%	4%	3%	12%
^{152}Sm	1%	4%	5%	7%
^{151}Eu	11%	19%	12%	21%
^{153}Eu	4%	3%	4%	3%
^{154}Eu	7%	11%	-	-
^{155}Eu	2%	8%	1%	16%
^{155}Gd	6%	14%	5%	11%

2.3 SHIELDING VALIDATION

The shielding validation report considers benchmarks with measured neutron fluxes, detector count rates, detector energy response functions, neutron and gamma doses, foil neutron activation rates and activities, neutron leakage fluxes, and skyshine dose rates [5]. Thousands of points of comparison between experiment and calculation are presented. Other than rare outliers typically explained by either a lack of information or large uncertainties in the experiment conditions, material, or dimensions, MAVRIC agrees well with the experiment results. As an example of radiation shielding validation, see Figure 9, which shows the comparison of MAVRIC to a leakage measurement of ^{252}Cf neutrons through a heavy water shield.

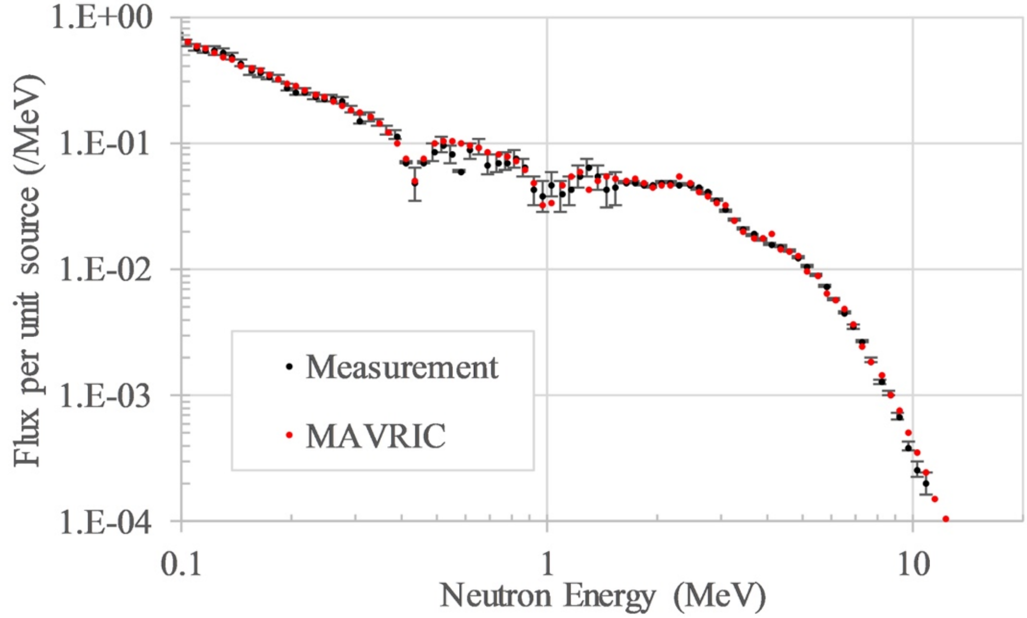

Figure 9. Measured fluxes (per unit source) for the A8 source as a function of neutron energy and MAVRIC-simulated values.

3. CONCLUSIONS AND FUTURE WORK

Overall, SCALE 6.2.4 simulation results compare well with measurements in a variety of criticality safety, reactor physics, and shielding applications.

In nuclear criticality safety applications, SCALE 6.2.4 was validated against 600 critical experiments with a variety of fissile material types and enrichments, energy spectra, and accompanying materials. The apparent biases of the KENO V.a and KENO-VI codes have been reduced in recent years as nuclear data and processing have improved. When considering all categories of systems examined, the bias is less than 2.2% Δk. Removing the USI and USM systems due to evidence of performance problems, the bias for KENO V.a is less than 0.91% Δk, and it is less than 0.5% Δk for almost all categories in KENO V.a. The biases in KENO-VI are less than 0.9% Δk, largely due to geometric complexities.

In reactor physics applications, SCALE 6.2.4 was validated against more than 160 LWR fuel isotopic measurements, 230 decay heat measurements, short cooling time decay heat measurements in six types of fissile nuclides, and initial critical full-core eigenvalue measurements for one LWR and two non-LWRs. SCALE calculations compare well with the 40 measured nuclides of importance to burnup credit, decay heat, and radiation shielding applications. The bias in assembly decay heat is on average less than 1% for PWRs and less than 2% for BWRs for the analyzed assembly experiments. The results for the fissile material experiments at cooling times up to ~100 s, as relevant to loss-of-coolant accident scenarios, show generally good agreement between calculated and measured values of energy release following fission. The eigenvalue bias is less than 50 pcm for WBN1, within the benchmark experiment uncertainty (370 pcm) for HTR-10, and within ~500 pcm of criticality for HTTR.

In shielding applications, SCALE 6.2.4 was validated against eight benchmark shielding experiments, with additional verification against accompanying MCNP results. MAVRIC calculations generally agree with the experimental results within 50% and agree with MCNP results within 20%. Typical experimental results analyzed from those benchmarks include neutron fluxes, detector count rates, detector energy response functions, neutron and gamma doses, foil neutron activation rates and activities, neutron leakage fluxes, and skyshine dose rates. Thousands of points of comparison between experiment and calculation were made.

This validation work forms the basis for future SCALE releases, where the relative performance will be assessed with each release. Further expansion of the validation basis is pertinent to broaden it to support deployments of higher enrichment fuels, higher burnup fuels, and advanced reactors with novel materials and geometries. In criticality safety applications, nuclear data evaluations can be examined in light of the outlier cases, and the number of experiments can be increased to broaden the experimental categories covered. In shielding applications, additional cases can be added from validated benchmarks, such as the SILENE benchmark and fission rate benchmarks from a fission chambers experiment involving platinum. In reactor physics applications, quantifying and evaluating the bias and uncertainty in code predictions of key metrics associated with fuel depletion, such as spent nuclear fuel compositions, are necessary to validate the accuracy of the codes and nuclear data used for reactor safety and licensing calculations.

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