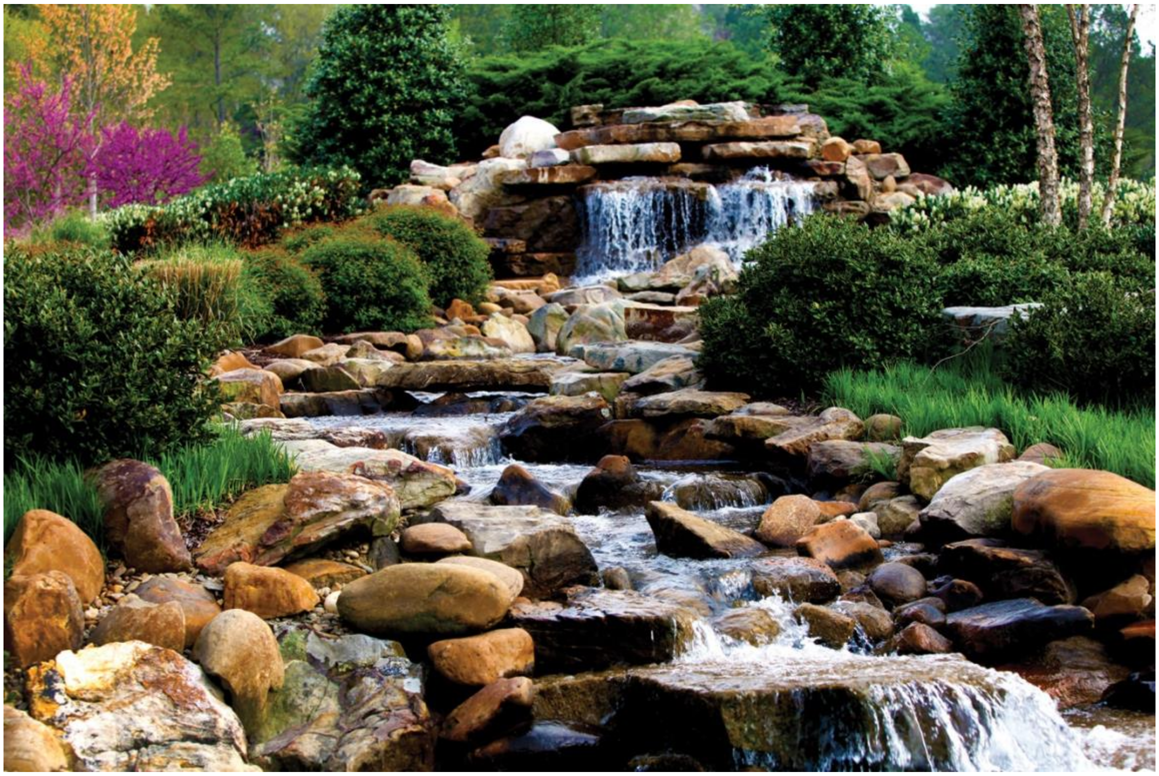
ORNL/SPR-2022/2692

Review of SCALE Validations Applicable to Spent Nuclear Fuel Shielding Calculations



Georgeta Radulescu
Arzu Alpan

December 2022

ORNL IS MANAGED BY UT-BATTELLE LLC FOR THE US DEPARTMENT OF ENERGY

ORNL/SPR-2022/2692

Nuclear Energy and Fuel Cycle Division

REVIEW OF SCALE VALIDATIONS APPLICABLE TO SPENT NUCLEAR FUEL SHELDING CALCULATIONS

Georgeta Radulescu
Arzu Alpan

December 2022

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831
managed by
UT-BATTELLE LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

CONTENTS

LIST OF TABLES

ABBREVIATIONS

ATM	approved testing material
BWR	boiling water reactor
C/E	calculated-to-experimental
DOE	U.S. Department of Energy
ENDF	Evaluated Nuclear Data File
ICSBEP	International Criticality Safety Benchmark Evaluation Project
JAERI	Japan Atomic Energy Research Institute
MAVRIC	Monaco with Automated Variance Reduction using Importance Calculations
MCNP	Monte Carlo N-Particle
NEA	Nuclear Energy Agency
NRC	U.S. Nuclear Regulatory Commission
OECD	Organisation for Economic Co-operation and Development
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor
RCA	radiochemical assay
SD	standard deviation
SFCOMPO	Spent Fuel Isotopic Compositions (Database)
SINBAD	Shielding Integral Benchmark Archive and Database
SNF	spent nuclear fuel

ABSTRACT

This report presents a review of publicly available documents providing validations of SCALE code system capabilities for depletion and shielding calculations. The validation studies primarily used information available in the Spent Fuel Isotopic Composition Database, the Shielding Integral Benchmark Archive and Database, and the International Criticality Safety Benchmark Evaluation Project Handbook. Validation results based on radiochemical assay data and shielding benchmark experiments relevant to spent nuclear fuel shielding applications are summarized in this report. The information summarized in this report supports pressurized water reactor and boiling water reactor spent fuel storage and transportation safety analyses.

1. INTRODUCTION

Publicly available measurement data for validating spent nuclear fuel (SNF) radiation source term and shielding calculations are identified in ORNL/SPR-2022/2518 [1]. The sources of the measurement data are the Spent Fuel Isotopic Composition (SFCOMPO) Database [2], the Shielding Integral Benchmark Archive and Database (SINBAD) [3], and the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [4]. This report summarizes existing validation results for the SCALE code system [5] that are relevant to SNF storage/transportation shielding applications. Section 2.1 presents a summary of the radiochemical assay (RCA) data used in SCALE depletion validation studies and the bias and bias uncertainty values associated with the calculated nuclide concentrations in fuel, for nuclides important to radiation source terms and dose rates. Section 2.2 provides a summary of SCALE shielding validation studies. Conclusions are provided in Section 3.

2. VALIDATION STUDIES

2.1 RADIOCHEMICAL ASSAY DATA FOR SPENT NUCLEAR FUEL

This section provides a summary of Oak Ridge National Laboratory (ORNL) publications [6,7,8] that document the validation of spent fuel nuclide concentrations calculated with 1) SCALE 6.2.4 and nuclear cross sections based on Evaluated Nuclear Data File (ENDF)/B-VII.1 [9] and 2) SCALE 6.1 and nuclear cross sections based on ENDF/B-VII.0 [10]. The nuclide inventory validation is based on comparisons with RCA data. Only nuclides important to radiation source terms and dose rates are discussed in this report. These radionuclides have been identified in previous studies based on cask shielding calculations [11, 12, 13]. The cooling times analyzed in those studies are 1 to 40 years, 100 years, and 10,000 years. Principal gamma emitters in SNF include ^{144}Ce ($T_{1/2}$=284.89 days)/^{144}Pr ($T_{1/2}$=17.29 min), ^{106}Ru ($T_{1/2}$=1.02 years)/^{106}Rh ($T_{1/2}$=2.18 hours), ^{134}Cs ($T_{1/2}$=2.0652 years), ^{154}Eu ($T_{1/2}$=8.593 years), and ^{137}Cs ($T_{1/2}$=30.1 years)/^{137m}Ba ($T_{1/2}$=2.6 min). ^{90}Sr ($T_{1/2}$=28.78 years)/^{90}Y ($T_{1/2}$=64 hours) contributes bremsstrahlung radiation. Principal neutron emitters in the SNF currently in dry storage include ^{244}Cm ($T_{1/2}$=18.1 years) and ^{242}Cm ($T_{1/2}$=163 days). Other transuranic nuclides important for SNF source terms at long cooling times (100 years or longer) include ^{238}Pu, ^{241}Am, ^{246}Cm, ^{240}Pu, ^{239}Pu, and ^{242}Pu.

Table 1 summarizes the main characteristics of pressurized water reactor (PWR) fuel samples that were used in SCALE validations. For each nuclide of interest, Table 2 provides the number of PWR fuel samples used in the validation studies, the average values of calculated-to-experimental (C/E) nuclide concentrations, and the standard deviations (SDs) of the C/E values. These data are provided in Table 3 and Table 4 for boiling water reactor (BWR) fuel. The SCALE and ENDF/B-VII versions, and the lattice physics code used in the validation studies (i.e., either TRITON or Polaris) are indicated in Table 2 and Table 4.

Nuclide concentrations in SNF samples and sample burnup measured by RCA methods are affected by uncertainties. The uncertainties reported by measurement laboratories vary considerably among the evaluated experimental programs depending on the experimental technique, radiochemical procedures, and uncertainty analysis used for each nuclide. Bias and bias uncertainty associated with calculated nuclide concentrations in SNF are also affected by modeling assumptions that may be necessary due to unavailability of fuel design and operating data. Therefore, nuclide concentration bias and bias uncertainty based on comparisons with RCA data are the result of RCA measurement uncertainties, uncertainties in the modeling data, uncertainties associated with nuclear cross-section data, and the intrinsic uncertainties and approximations used in the numerical solutions. The isotopic measurement uncertainties for the evaluated PWR fuel samples are provided in Table 2. The measurement uncertainties for the evaluated BWR fuel samples used in SCALE 6.2.4 validations were not readily available. However, these uncertainties are analyzed in greater detail in other ORNL publications (as listed in ORNL/TM-2020/1500/v3 [6]). It is beyond the scope of this report to state the range of uncertainties for RCA data used in previous BWR validation studies. The primary ORNL publications [6,7,8] provided mean C/E values and the SD associated with the C/E values, but the effects on the C/E values of the various experiment and modeling uncertainties were not evaluated in these publications. An effort of the SFCOMPO Technical Review Group is underway to publish first isotopic evaluations of individual assay data using a standard data evaluation format, which includes uncertainty analyses. A mean C/E value is referred to as bias and the SD associated with the individual C/E values used in mean C/E calculations is referred to as bias uncertainty in this report.

Bias and bias uncertainty values are available for all nuclides of interest except for ^{242}Cm in PWR fuel and ^{246}Cm in BWR fuel. The number of evaluated PWR fuel samples varies as a function of nuclide from 14 (^{246}Cm) to 92 (^{240}Pu and ^{239}Pu) [6]. The SCALE 6.2.4/ENDF/B-VII.1 validation study [6] for BWR fuel provides bias and bias uncertainty values for ^{137}Cs and most actinides of interest (i.e., this validation does not provide bias and bias uncertainty values for most fission products of interest). However, a SCALE 6.1/ENDF/B-VII.0 validation study [8] using a relatively small number of BWR fuel samples provides bias and bias uncertainty values for fission products ^{144}Ce, ^{106}Ru, ^{134}Cs, ^{154}Eu, and ^{90}Sr, but not for actinides ^{244}Cm and ^{242}Cm.

The concentrations of ^{106}Ru and ^{154}Eu are overpredicted on average and the concentrations of ^{144}Ce, ^{134}Cs, ^{90}Sr, ^{137}Cs, ^{244}Cm, and ^{242}Pu are underpredicted on average for both PWR and BWR fuel with SCALE 6.2.4/ENDF-B/VII.1 and SCALE 6.1/ENDF-B/VII.0. The nuclides whose concentrations are underpredicted on average are highlighted in Table 2 and Table 4.

For the PWR fuel, the bias values associated with nuclide concentrations from SCALE 6.2.4/TRITON /ENDF-B/VII.1 and SCALE 6.1/TRITON/ENDF-B/VII.0 depletion calculations are less than approximately 10%. The associated bias uncertainty values are less than approximately 11% for all nuclides of interest except for ^{106}Ru, ^{241}Am, and ^{246}Cm. For these nuclides, the bias uncertainty values vary from 20% to approximately 26%.

For the BWR fuel, bias values associated with nuclide concentrations from SCALE 6.2.4/Polaris/ENDF-B/VII.1 depletion calculations are less than approximately 10%. The bias uncertainty values vary from 6% for ^{137}Cs to 68% for ^{244}Cm in the BWR fuel. The SCALE 6.1/TRITON/ENDF/B-VII.0 validation results using six GE14 fuel samples show an isotopic bias of less than approximately 14% and bias uncertainty values less than 18%.

Comparison of code predictions to experimental measurements for high quality experimental data [14] for one PWR UO_2 fuel sample shows that SCALE nuclide concentration predictions are in good agreement with the measured values for most of the measured nuclides and these predictions are similar to nuclide concentrations calculated with other depletion codes. For example, the differences between SCALE/TRITON isotopic inventory predictions and measurement values varied from 0.3% for ^{235}U to -12.5% for ^{241}Pu. Differences among different lattice code predictions were attributed to the differences in the computational method (Monte Carlo-based depletion vs. deterministic-based depletion) and various nuclear data used in the simulations (JEFF-3.2, JEFF-3.3, ENDF/B-VII.1, ENDF/B-VIII.0).

Table 1. Summary of SNF samples for PWR fuel

Reactor[a]	**Country**	**Assembly design**	**Number of samples**	**Enrichments (wt % ^{235}U)**	**Sample burnup (GWd/MTU)**	**Experimental program**
Calvert Cliffs-1	U.S.	14 × 14	3	3.038	27.4–44.3	ATM-104[b]
		14 × 14	3	2.72	18.7–33.2	ATM-103
		14 × 14	3	2.453	31.4–46.5	ATM-106
GKN II	Germany	18 × 18	1	3.8	54.1	REBUS[c]
Gösgen	Switzerland	15 × 15	3	3.5, 4.1	29.1–59.7	ARIANE[c]
		15 × 15	3	4.3	47.2–70.4	MALIBU[c]
H. B. Robinson-2	U.S.	15 × 15	4	2.561	16.0–31.7	ATM-101
Obrigheim	Germany	14 × 14	15	2.83, 3.00	15.6–37.5	EUR[d]
		14 × 14	5	3.13	27.0–29.4	ICE[e]
Takahama-3	Japan	17 × 17	13	2.63, 4.11	17.4–47.3	JAERI[f]
TMI-1	U.S.	15 × 15	8	4.657	22.8–29.9	DOE YMP[g]
Trino Vercellese	Italy	15 × 15	15	2.719, 3.13, 3.897	7.2–17.5	EUR
		15 × 15	16	3.13	12.8–25.3	EUR
Turkey Point-3	U.S.	15 × 15	13	2.556	19.9–31.6	NWTS

[a]Data in this table are from ORNL/TM-2021/1500/v3 [6].
[b]Approved testing material.
[c]International Experimental Programs coordinated by Belgonucleaire, Belgium, currently managed by Studiecentrum voor Kernenergie – Centre d'étude de l'Énergie Nucléaire.
[d]European research program.
[e]Isotopic Correlation Experiment.
[f]Japan Atomic Energy Research Institute (now Japan Atomic Energy Agency).
[g]U.S. Department of Energy Office of Civilian Radioactive Waste Management Yucca Mountain Project.

Table 2. SCALE bias and bias uncertainty for PWR SNF nuclide concentrations

				SCALE 6.2.4/TRITON ENDF/B-VII.1		SCALE 6.1/TRITON ENDF/B-VII.0	
Nuclide	**$T_{1/2}$ (years)**	**Number of samples**	**Reported measurement uncertainty (%)**	**Mean C/E[a]**	**SD[b]**	**Mean C/E**	**SD**
^{144}Ce	0.78	32	1.7 – 10.0	0.968	0.075	0.979	0.081
^{106}Ru	1.02	31	3.0 – 12.2	1.059	0.218	1.079	0.227
^{134}Cs	2.065	59	1.5 – 5.0	0.898	0.070	0.930	0.071
^{154}Eu	8.59	44	1.7 – 11.9	1.066	0.107	1.042	0.104
^{90}Sr	28.9	15	1.5 – 8.0	0.991	0.066	0.991	0.069
^{137}Cs	30.07	73	1.3 – 3.5	0.989	0.032	0.993	0.031
^{242}Cm	0.446	–	–	–	–	–	–
^{244}Cm	18.1	57	0.9 – 28.0	0.987	0.113	0.956	0.111
^{238}Pu	87.81	77	0.3 – 14.3	0.959	0.074	0.883	0.059
^{241}Am	433	39	1.8 – 20.0	1.043	0.192	1.102	0.207
^{246}Cm	4.73×10^{3}	14	5.0 –10.1	0.930	0.224	0.956	0.255
^{240}Pu	6.56×10^{3}	92	0.3 – 2.7	1.005	0.035	1.022	0.034
^{239}Pu	2.41×10^{4}	92	0.3 – 2.4	1.019	0.034	1.041	0.035
^{242}Pu	3.75×10^{5}	91	0.3 – 5.3	0.959	0.064	0.941	0.061

[a]Average value of the ratio between calculated and experimental nuclide concentrations and [b]associated standard deviation.

Table 3. Summary of SNF samples for BWR fuel

Reactor	Country	Assembly design	Number of samples	UO_2 sample enrichment (wt% ^{235}U)	$UO_2 – Gd_2O_3$ sample enrichment (wt% ^{235}U–wt% Gd_2O_3)	Sample burnup (GWd/MTU)	Experimental program	Reference
Dodewaard	Belgium	6 × 6	1	4.94	–	55.5	ARIANE	[6,15]
Forsmark 3	Sweden	10 × 10 (SVEA-96)	1	3.97	–	55.8	Studsvik	
Forsmark 3	Sweden	10 × 10 (GE14)	8	3.95	–	38.3–51.1	CSN[b]	
Fukushima Daini 1	Japan	9 × 9 – 9[a]	13	2.1; 4.9	3.0–5.0	35.6–68.4	JNES[c]	
Fukushima Daini 2	Japan	8 × 8 – 4[a]	25	3.4; 4.5	3.4–4.5	9.4–59.1	JAERI	
Fukushima Daini 2	Japan	8 × 8 – 2[a]	17	3.91	3.4–4.5	4.2–44.0	JAERI	
Leibstadt 3	Switzerland	10 × 10 (SVEA-96)	3	3.9	–	58.4–65	MALIBU[d]	
Limerick 1	U.S.	9 × 9 (GE11)	8	3.95	3.6–5.0	37.0–65.5	DOE YMP	
Forsmark 3	Sweden	10 × 10 (GE14)	6	3.95	–	38.3–51.1	CSN[b]	[8]

[a]Assembly lattice size followed by the number of lattice locations occupied by the water rod.
[b]Consego de Securidad Nuclear (Spanish Nuclear Safety Council). Data not publicly available [16].
[c]Japan Nuclear Energy Safety (now Japan Nuclear Regulation Authority).
[d]Data not publicly available [17,18].

Table 4. SCALE bias and bias uncertainty for BWR SNF nuclide concentrations

SCALE version, ENDF/B version	Nuclides and their half-lives (years)														Description
	^{144}Ce	**^{106}Ru**	**^{134}Cs**	**^{154}Eu**	**^{90}Sr**	**^{137}Cs**	**^{242}Cm**	**^{244}Cm**	**^{238}Pu**	**^{241}Am**	**^{246}Cm**	**^{240}Pu**	**^{239}Pu**	**^{242}Pu**	
	0.78	**1.02**	**2.065**	**8.59**	**28.9**	**30.07**	**0.446**	**18.1**	**87.81**	**433**	**4.73×10^3**	**6.56×10^3**	**2.41×10^4**	**3.75×10^5**	
SCALE 6.2.4 / Polaris, ENDF/B-VII.1 [6]						42	48	51	76	62	–	76	76	76	Number of samples
						0.968	0.906	0.983	1.063	0.941	–	0.999	0.974	0.985	Mean (C/E)[a]
						0.061	0.679	0.456	0.206	0.114	–	0.088	0.085	0.168	SD[b]
SCALE 6.1 / TRITON, ENDF/B-VII.0 [8]	6	6	6	6	6	6	–	–	6	6	–	6	6	6	Number of samples
	0.861	1.051	0.883	1.124	0.900	0.954	–	–	0.860	1.075	–	1.073	0.980	0.997	Mean (C/E)
	0.177	0.032	0.052	0.079	0.026	0.032	–	–	0.048	0.021	–	0.032	0.018	0.059	SD
	16.9	17.8	1.5	4.8	11.6	2.2			4.1	15.7		3.2	3.0	4.0	Measurement uncertainty (2σ) %

[a]Average value of the ratio between calculated and experimental nuclide concentrations and [b]associated standard deviation. Range of measurement uncertainty not provided by the SCALE 6.2.4 validation study [6].

2.2 SHIELDING BENCHMARKS

A summary of shielding validations for SCALE is provided in Section 2.2.1. Code-to-code comparison between SCALE and MCNP (Monte Carlo N-Particle) [19] is discussed in Section 2.2.2.

2.2.1 SCALE Validation for Shielding Applications

Validation of the Monaco with Automated Variance Reduction using Importance Calculations (MAVRIC) shielding sequence in SCALE 6.2.4 is documented in a report by Celik et al. [20]. Either continuous-energy AMPX cross-section libraries generated from ENDF/B-VII.1 nuclear data or ENDF/B-VII.0 multigroup (200 neutron groups and 47 gamma groups) were used in the validation study. Eight benchmarks were selected from the ICSBEP Handbook, SINBAD, and other publicly available shielding validations. Typical experimental results analyzed from those benchmarks include leakage neutron fluxes, detector count rates, detector energy response functions, neutron and gamma doses, foil neutron activation rates and activities, and skyshine dose rates. Thousands of points of comparison between experiment and calculation are documented in the validation report. MAVRIC agrees well with the experimental results for most of the measurement datapoints. However, large disagreements are also observed for certain energy ranges of the neutron flux spectrum. Some of these discrepancies could be the result of large experimental uncertainties or missing information details on the experiment conditions, material, or dimensions not incorporated into the validation models. It was noted that quality of information for measured reaction rates is likely much higher than that of measured spectra, which depends on the quality of the processing of pulse-heights through unfolding algorithm [21]. A comparison between MAVRIC validation calculations and measurement data is further provided for each of the analyzed benchmark experiments:

1) Experiment providing neutron flux spectrum measurements at a set distance from an iron sphere with a ^{252}Cf source placed at the center of the sphere [22]. The purpose of the experiment was to assess iron neutron inelastic cross sections. Measurement uncertainties varied significantly depending on the energy region of the neutron spectrum, from 3% for energies above 1 MeV to 100% for the energy range below 0.1 MeV. The relative difference between the measured and calculated spectra is mostly less than 50% for the neutron energy range 100 keV to 1 MeV, and less than ~ 10% for neutron energies between 1 MeV and 6 MeV. Larger discrepancies between calculations and measurements were observed around resonance peaks in the cross sections for neutron energies below 0.1 MeV. The authors of the shielding validations attributed these discrepancies to high uncertainty in cross sections and low resolution of the measurement detectors for the lower neutron energy range (i.e., < 0.1 MeV). The relative difference between the measured and calculated integral flux was less than 0.1%.

2) Neutron leakage measurements [50 keV to 11 MeV] of ^{252}Cf neutrons through a heavy water shield [23]. Simulations were performed for two different source configurations. The measurement uncertainty varied from 1% to 30%, depending on neutron energy. The fractions of simulated values within one standard deviation of the measurement error are 53% and 52%, within two standard deviations are 79% and 73%, and within three standard deviations are 91% and 86%.

3) Measurements of Am-Be neutrons leaking through spherical shells of beryllium, polyethylene, lead, niobium, molybdenum, tantalum, tungsten, and air [24], including corrections for background neutrons. Measurement data are available for the absolute leakage

neutron flux at 2 m after passing through the various materials for about 70 energy bins covering the range of 0.4–12 MeV. Reported measurement error was generally less than 15%, except for several measurement data near the 12 MeV energy that had higher measurement errors (up to 40%). Overall, the simulations match the measured shape of the leakage energy distributions. Underpredictions up to ~50% were reported for energy bins below approximately 3 MeV for bare source, beryllium, niobium, molybdenum, tantalum, and tungsten. Some of the observed discrepancy between simulations and measurements were attributed to the fact that no detector resolution function was applied to the energy-dependent flux calculated with MAVRIC.

4) Measurement of leakage neutron spectrum from a Deuterium-Tritium source contained in an iron spherical shell. This is the University of Illinois Iron Sphere Benchmark available in SINBAD [3]. The evaluated uncertainties associated with the measurements varied from a few percent to 83% for a few measurement data within the energy range 8-11 MeV. MAVRIC simulations underestimated the neutron flux below approximately 5 MeV, but matched the measured peak flux values for neutron energies above approximately 10 MeV within measurement uncertainty.

5) ^{252}Cf neutron transmission measurements through slab layers of different shielding materials, as well as combinations of various thicknesses of steel and polyethylene, known as Ueki Shielding Measurements [25]. Single-material measurements used polyethylene, NS-4-FR, Resin-F, KRAFTON-HB, and stainless steel (304). Reported measurements are neutron and photon dose rates in μSv/h, with an associated measurement uncertainty of 15%. The measurement values were available as plotted data. Therefore, the measurement data used in comparisons between simulation and measurement results include uncertainty associated with reading points from semi-logarithmic plots. Among five different response functions that were analyzed, the ANSI 1977 flux-to-dose-rate conversion factors [26] provided the best agreements with the experimental values. For single-material measurements, MAVRIC simulations matched Ueki's measurements within about ±20%, except for polyethylene. For polyethylene slabs varying from 15 cm to 30 cm, MAVRIC overpredicted neutron dose rate by 25% to 60%. There are also poor agreements with the experimental dose rate for experiments involving a steel plate followed by large amounts of polyethylene. The disagreements typically increase with increasing thickness. It is noted that simulations using MCNP have shown similar difficulty matching Ueki's measurements that involve polyethylene [27].

6) Neutron flux measurements with Bonner sphere neutron spectrometers in a large three-section concrete labyrinth [4]. A ^{252}Cf source, in a bare configuration or covered by a thin layer of cadmium, was used at the entrance of the labyrinth. Measurement data are available for various labyrinth configurations and wall lining materials such as polyethylene, cadmium plates, and borated concrete plates. Experimental relative uncertainties were between 5% and 30%. Overall, the MAVRIC calculations were within 30% of the measurement values for all measurement locations, except for a measurement location that was farthest away from the source. For this location, the maximum difference between calculated and measured values was 70%.

7) Photon skyshine experiment performed at Kansas State University in 1977, which is available in SINBAD [3]. In this experiment, the direct radiation from a ^{60}Co source was completely shielded by a silo, and photon dose rates were measured at various distances up to 700 m from the source. The estimated total measurement uncertainty was 7%. The agreement between MAVRIC and benchmark experimental data for the close-range (less than 300 m from source) and far-range measurement locations (beyond 500 m from source) was within measurement 2σ uncertainty, and a disagreement of approximately 25% between the

calculated and measured dose rates was observed for mid-range locations (300 m to 500 m from source).

8) Neutron activation measurements for SILENE Pulse 1 (unshielded configuration), Pulse 2 (configuration shielded by lead) and Pulse 3 (configuration shielded by polyethylene). The selected SILENE benchmark experiments are described in the ICSBEP Handbook as ALARM-TRAN-AIR-SHIELD-001, ALARM-TRAN-PB-SHIELD-001, and ALARM-TRAN-CH2-SHIELD-001, respectively. Only foil activation measurements were simulated with MAVRIC. Most of the simulation results agree with the benchmark measurements within the experimental uncertainties, which were approximately 7%. Maximum difference between the calculated and measured activities was 18%.

2.2.2 Code-to-Code Comparisons

A shielding benchmark suite is distributed with MCNP [28]. A summary of the fission shielding benchmarks in SINBAD for which MCNP models exist and a quality review of these benchmarks is available [21]. These benchmarks currently include experiments conducted at the Activation and SPectroscopy in Shields and Ispra shielding facilities, which tested radiation attenuation in individual shielding materials, skyshine benchmarks, and the VENUS-3 reactor shielding benchmark. MCNP models also exist for ICSBEP criticality alarm experiments relevant to shielding. A brief description of these benchmarks is provided in ORNL/SPR-2022/2518 [1], and detailed information is available in SINBAD and the ICSBEP handbook. Code-to-code comparisons between available MCNP and MAVRIC calculations agree within 40% relative error [20].

3. CONCLUSIONS

This report provides a summary of 1) nuclide inventory validations that used SCALE 6.2.4/ENDF/B-VII.1 or SCALE 6.1/ENDF/B-VII.0, and 2) SCALE/MAVRIC shielding validation results, which were published in various ORNL reports.

Comparisons between calculated and measured nuclide concentrations in SNF samples, as taken from the various reviewed validation publications, are provided for nuclides important to radiation source terms and dose rates. The nuclide concentration bias and bias uncertainty that are based on validation against RCA measurement data are affected by uncertainties in the measurement data, uncertainties in the modeling data (e.g., fuel operating history and assembly characteristics), uncertainties associated with nuclear cross-section data, and intrinsic uncertainties and approximations associated with the computational methods used for simulations.

Bias and bias uncertainty values are available for all nuclides of interest except for ^{242}Cm in PWR fuel and ^{246}Cm in BWR fuel. The number of evaluated PWR fuel samples varies as a function of nuclide from 14 (^{246}Cm) to 92 (^{240}Pu and ^{239}Pu) [6]. The SCALE 6.2.4/ENDF/B-VII.1 validation study [6] for BWR fuel provides bias and bias uncertainty values for ^{137}Cs and most actinides of interest (i.e., bias and bias uncertainty values for most fission products of interest were unavailable). However, a SCALE 6.1/ENDF/B-VII.0 validation study [8] using a relatively small number of BWR fuel samples provides bias and bias uncertainty values for fission products ^{144}Ce, ^{106}Ru, ^{134}Cs, ^{154}Eu, and ^{90}Sr.

For the PWR fuel, the bias values associated with nuclide concentrations from SCALE 6.2.4/ENDF-B/VII.1 and SCALE 6.1/ENDF-B/VII.0 depletion calculations are less than approximately 10%. The associated bias uncertainty values are less than approximately 11% for all nuclides of interest except for ^{106}Ru, ^{241}Am, and ^{246}Cm. For these nuclides, the bias uncertainty values vary from 20% to approximately 26%.

For the BWR fuel, bias values associated with nuclide concentrations from SCALE 6.2.4/ENDF-B/VII.1 depletion calculations are less than approximately 10%. The bias uncertainty values vary from 6% for ^{137}Cs to 68% for ^{244}Cm in the BWR fuel. The SCALE 6.1/ENDF/B-VII.0 validation results using six GE14 fuel samples show an isotopic bias of less than approximately 14% and bias uncertainty values less than 18%. The concentrations of ^{106}Ru and ^{154}Eu were overpredicted on average and the concentrations of ^{144}Ce, ^{134}Cs, ^{90}Sr, ^{137}Cs, ^{244}Cm, and ^{242}Pu were underpredicted on average for both PWR and BWR fuel.

SCALE 6.2.4/MAVRIC validation was based on four types of shielding experiments, which are briefly summarized below. Shielding validations based on comparisons with measurement data are affected by uncertainties in the measurement data, uncertainties in the modeling data, uncertainties associated with nuclear cross-section data, and intrinsic uncertainties and approximations associated with the computational methods used for radiation transport simulations. Thousands of points of comparison between experiment and calculation were documented in the validation report [20]. Generally, MAVRIC calculations and the experimental values agreed within measurement uncertainty.

(1) A series of shielding experiments testing radiation attenuation in individual shielding materials (e.g., iron, steel, polyethylene, polyethylene, lead, and tungsten) as well as combinations of various thicknesses of steel and polyethylene. Either leakage neutron spectra, detector count rates, or detector energy response functions were measured in these experiments. The measurement uncertainty greatly varied, from 1% to 100%, as a function of neutron energy among the leakage neutron spectrum measurements. SCALE shielding calculations generally agreed with the experimental results within 50%, except for rare outliers. Outliers with discrepancies were commonly attributed to unknown materials or dimensions from the benchmark description.

(2) An experiment involving neutron streaming through ducts. For this experiment, the MAVRIC calculations were within 30% of the measurement values for all measurement locations, except for a measurement location that was farthest away from the source. For this location, the experimental neutron count was low and the maximum difference between calculated and measured values was 70%. Experimental relative uncertainties for this experiment varied between 5% and 30%.

(3) A skyshine experiment using ^{60}Co sources. The agreement between MAVRIC and benchmark experimental data for the close-range measurement locations (less than 300 m from source) and far-range measurement locations (beyond 500 m from source) was within 2σ measurement uncertainty (14%) and a disagreement of approximately 25% between the calculated and measured dose rates was observed for mid-range measurement locations (300 m to 500 m from source).

(4) A criticality alarm experiment providing foil activation measurements. The simulation results agreed mostly within the experimental uncertainties of the benchmark measurements, which were approximately 7%. Maximum difference between the calculated and measured activities was 18%.

ACKNOWLEDGMENTS

The work described in this report was accomplished with funding provided by the U.S. Nuclear Regulatory Commission. The authors acknowledge review and useful comments by Lucas Kyriazidis of the Office of Nuclear Regulatory Research, Division of Systems Analysis, and Andrew Barto of the Office of Nuclear Material Safety and Safeguards, Division of Spent Fuel Management. The technical review and helpful comments of Germina Ilas and Ugur Mertyurek from Oak Ridge National Laboratory are much appreciated.

REFERENCES

1. G. Radulescu and P. Stefanovic, Review of Experimental Data for Validating Spent Fuel Shielding Calculations, ORNL/SPR-2022/2518, Oak Ridge National Laboratory, Oak Ridge, TN (2022).
2. Organisation for Economic Co-operation and Development (OECD)-Nuclear Energy Agency (NEA), SFCOMPO 2.0, Database of Measured Isotopic Concentrations of Spent Nuclear Fuel, with Operational Histories and Design Data (2017).
3. SINBAD-2022, Shielding Integral Benchmark Archive and Database, available from Radiation Safety Information Computational Center as DLC-237.
4. International Handbook of Evaluated Criticality Safety Benchmark Experiments NEA/NSC/DOC(95)03, NEA Nuclear Science Committee (2016).
5. W. A. Wieselquist, R. A. Lefebvre, and M. A. Jessee, Eds., SCALE Code System, ORNL/TM-2005/39, Version 6.2.4, Oak Ridge National Laboratory, Oak Ridge, TN (2020).
6. G. Ilas, J. R. Burns, B. D. Hiscox, and U. Mertyurek, SCALE 6.2.4 Validation: Reactor Physics, ORNL/TM-2020/1500/v3, Oak Ridge National Laboratory, Oak Ridge, TN (2022).
7. G. Ilas and B. Hiscox, Validation of SCALE 6.2.4 and ENDF/B-VII.1 Data Libraries for Nuclide Inventory Analysis in PWR Used Fuel, Transactions of the American Nuclear Society, 2021 ANS Virtual Annual Meeting, June 14-16, 124: 552-554.
8. H. J. Smith, I.C. Gauld, and U. Mertyurek, Analysis of Experimental Data for High Burnup BWR Spent Fuel Isotopic Validation—SVEA-96 and GE14 Assembly Designs, NUREG/CR-7162 (ORNL/TM–2013/18), U.S. Nuclear Regulatory Commission, Washington, D.C. (2012).
9. M. B. Chadwick et al., "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data," *Nuclear Data Sheets* 112(12): 2887-2996 (2011).
10. M. B. Chadwick et al., "ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology." *Nuclear Data Sheets* 107(12): 2931-3060 (2006).
11. B. L. Broadhead et al., Investigation of Nuclide Importance to Functional Requirements Related to Transport and Long-Term Storage of LWR Spent Fuel, ORNL/TM-12742, Oak Ridge National Laboratory, Oak Ridge, TN (1995).
12. I. C. Gauld and J. C. Ryman, Nuclide Importance to Criticality Safety, Decay Heating, and Source Terms Related to Transport and Interim Storage of High-Burnup LWR Fuel, NUREG/CR-6700 (ORNL/TM-2000/284), U.S. Nuclear Regulatory Commission (2000).
13. G. Radulescu and P. Stefanovic, A Study on the Characteristics of the Radiation Source Terms of Spent Fuel and Various Non-Fuel Hardware for Shielding Applications, ORNL/SPR-2021/2373, Oak Ridge National Laboratory, Oak Ridge, TN (2022).
14. J. Eysermans et al., "REGAL International Program: Analysis of experimental data for depletion code validation." *Annals of Nuclear Energy* 172: 109057 (2022).
15. I. C. Gauld and U. Mertyurek, "Validation of BWR spent nuclear fuel isotopic predictions with applications to burnup credit" *Nuclear Engineering and Design* 345: 110-124 (2019).
16. J. Conde, C. Alejano, and J.M. Rey, Nuclear Fuel Research Activities of the Consejo De Seguridad Nuclear, Transactions of the 2006 International Meeting on LWR Fuel Performance, TopFuel 2006, Salamanca, Spain.
17. MALIBU Program, Irradiation Data Report of the MALIBU Extension Program, SCK•CEN report MA 2010/05 (2010).
18. MALIBU Program, Final Report on the Extension Scope. SCK•CEN report MA 2015/20 (2015).
19. T. Goorley et al., "Initial MCNP6 Release Overview." *Nuclear Technology* 180: 298-315 (2012).

20. C. Celik, D. Peplow, M. Dupont, and G. Radulescu, SCALE 6.2.4 Validation: Radiation Shielding. ORNL/TM-2020/1500/v4, Oak Ridge National Laboratory, Oak Ridge, TN (2022).
21. I. A. Kodeli and E. Sartori, "SINBAD – Radiation shielding benchmark experiments." *Annals of Nuclear Energy* 159: 108254 (2021).
22. E. Sajo, M. L. Williams, and M. Asgari, "Comparison of Measured and Calculated Neutron Transmission Through Steel for a 252Cf Source." *Annals of Nuclear Energy* 20(9): 585-604 (1993).
23. B. Janský et al., "Comparison of Measured and Calculated Neutron Transmission Through Heavy Water for 252Cf Source Placed in the Center of 30 cm Diameter Sphere." *Annals of Nuclear Energy* 24(15): 1189-1212 (1997).
24. D. Bogart, D. F. Shook, and D. Fieno, "Transport Analysis of Measured Neutron Leakage Spectra from Spheres as Tests of Evaluated High-Energy Cross Sections." *Nuclear Science and Engineering*, 53(3): 285-303 (1974).
25. K. Ueki et al., "Systematic Evaluation of Neutron Shielding Effects for Materials," *Nuclear Science and Engineering*, 124(3): 455-464 (1996).
26. ANSI/ANS-6.1.1-1977 (N666), Neutron and Gamma-Ray Flux-to-Dose-Rate Factors, American Nuclear Society, La Grange Park, IL (1977).
27. C. J. Solomon, A. Sood, and R. D. Mosteller, A study of a polyethylene and stainless steel composite deep shield benchmark of MCNP. *ANS 14th Biennial Topical Meeting of the Radiation Protection and Shielding Division of the American Nuclear Society*, LA-UR-06-2349, Los Alamos National Laboratory, Los Alamos, NM (2006).
28. B. C. Kiedrowski et al., MCNP6 Shielding Validation Suite: Past, Present, and Future. Transactions of the American Nuclear Society, LA-UR-11-03719, Los Alamos National Laboratory, Los Alamos, NM (2011).