

SCALE 6.2.4 Validation for Light Water Reactor Decay Heat Analysis

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Energy release from the decay of radionuclides in nuclear fuel after its discharge from reactor is a critical parameter for design, safety, and licensing analyses of used nuclear fuel storage, transportation, and repository systems. Well-validated computational tools and nuclear data are essential for decay heat prediction. This paper summarizes the validation of the SCALE nuclear analysis code system version 6.2.4, used with ENDF/B-VII.1 libraries, for decay heat analysis of light water reactor used fuel. The experimental data used for validation include full-assembly decay heat measurements that cover assembly burnups of 5–51 GWd/MTU, cooling times after discharge in the 2 to 27-year range, and initial fuel enrichments up to 4 wt% ²³⁵U. The comparison between calculated (C) and experimental (E) decay heat showed very good agreement, with an average C/E over all considered measurements of 1.006 ($\sigma=0.016$) for PWR and 0.984 ($\sigma=0.077$) for BWR assembly measurements. The effect of using assembly-average versus axially varying modelling data on the calculated decay heat, important to thermal analyses for used fuel transportation and storage systems, is discussed.

Keywords: decay heat; validation; SCALE; ORIGEN; LWR

I. Introduction

Energy release from the decay of radionuclides in nuclear fuel after its discharge from reactor, commonly termed “decay heat,” is a critical parameter for design, safety, and licensing analyses of used nuclear fuel storage, transportation, and repository systems. Well-validated computational tools and associated nuclear data are essential for calculation of the decay heat used in these analyses. This paper summarizes a study

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to validate the SCALE [1] nuclear analysis code system version 6.2.4, used with evaluated nuclear data ENDF/B-VII.1, for decay heat analysis of light water reactor (LWR) used fuel assemblies. The current study is an extension of decay heat validation studies for previous SCALE releases, 5.1 and 6.1, which used different nuclear data libraries, based on ENDF/B-V and ENDF/B-VII.0 evaluations. [2-4] It also discusses the effect of using assembly-average versus axially varying modelling data in the decay heat calculation—which is of consequence to thermal analyses for used fuel transportation and storage systems—as well as the effect on the calculated decay heat of the nuclear data used in modelling the fuel transmutation and decay.

II. Experimental Data

The full-assembly decay heat experimental data used for validation are summarized in Table I. They include 91 decay heat measurement data for 52 pressurized water reactor (PWR) assemblies (there were multiple measurements for an assembly) and 145 measurements for 83 boiling water reactor (BWR) assemblies. The measurements cover a large range of assembly burnups (5.3–51.0 GWd/MTU) and cooling times after discharge from the reactor (2.3–26.7 years). The experiments on fuel assemblies discharged from the Turkey Point reactor were performed at the Hanford Engineering Development Laboratory (HEDL), using a boil-off calorimeter; experiments on Cooper, Dresden, Monticello, and San Onofre assemblies were carried out using a pool calorimeter at the General Electric Morris (GE-Morris) Operations facility [2]. The experiments at HEDL and GE-Morris were conducted in the 1980s. The reported relative uncertainties for the measured decay heat were in the 5–10% range for the HEDL and 4.7–5.9% for the GE-Morris measurements [2], with the reported uncertainties decreasing with increasing decay heat value.

The measurements listed in Table I for the Ringhals and Oscarshamn assemblies were performed by the Swedish Nuclear Fuel and Waste Management Company, SKB, at the Swedish Central Interim Storage Facility for Spent Nuclear Fuel, Clab, in the 2000s, using a pool calorimeter [5,6]. The reported uncertainties for these measurements were in the approximate range of 2–4% for the PWR and 2–8% for the BWR assemblies. The decay heat experiments at Clab go well beyond those used as a validation basis herein. Other experimental programs are ongoing [7] to meet the needs for spent fuel characterization, particularly to include modern assembly designs and short cooling times; these more recent Clab measurement data have limited distribution at this time and are not publicly available. Their availability to the user community will be of great value, as they will fill existing data gaps and needs for modern designs and short cooling times [8].

Table I. Summary of Full-Assembly Experimental Data

Reactor type	Reactor name	Assembly lattice	Enrichment (wt % ²³⁵ U)	Burnup (GWd/MTU)	Cooling time (year)	No. of assemblies	No. of measurements
PWR	Point Beach	14×14	3.4	31.9–39.4	4.5	6	6
	Ringhals 2	15×15	3.1 – 3.3	34.0–51.0	15.9–26.7	18	33
	Ringhals 3	17×17	2.1 – 3.4	19.7–47.3	12.9–25.9	16	38
	San Onofre	15×15	3.9 – 4.0	26.5–32.4	3.0–8.2	8	8
	Turkey Point	14×14	2.6	18.4–28.4	2.4–5.7	4	6
BWR	Cooper	7×7	1.1 – 2.5	11.7–28.0	2.3–7.2	54	81
	Dresden	7×7	2.1	5.3	8.1	1	1
	Monticello	7×7	2.3	9.2–21.0	9.7–11.2	6	13
	Oskarshamn 2	8×8	2.2	14.5–24.5	20.3–26.7	5	5
	Ringhals 1	8×8	2.3 – 2.9	21.3–44.7	12.6–23.6	17	45

III. Analysis

The assembly irradiation and decay history was simulated using capabilities in SCALE 6.2.4 [1]. The primary driver for these simulations is the ORIGEN nuclear transmutation and decay code, used worldwide for a variety of applications that require the calculation of nuclide inventories, decay heat, or neutron and gamma radiation emission rate and energy spectra in used nuclear fuel [9]. The analysis methodology,

illustrated in Fig. 1 [11], is discussed in detail elsewhere [3,4,10]. The first step to provide best-estimate models for decay heat calculation consists of generating burnup-dependent ORIGEN reactor libraries (including cross sections, fission yields, and decay data) that are representative of the measured fuel assemblies. These libraries enable fast (seconds) simulations with ORIGEN to determine nuclide inventories, decay heat, and other used fuel metrics. Selected assembly models used to generate ORIGEN reactor libraries are illustrated in Fig.2, for two BWR assembly designs, 7x7 and 8x8, and for a PWR 17x17 design.

For completeness, a summary of the modeling approach [3,4,10] is also provided here. The analyzed fuel assemblies were divided into groups for the purpose of generating ORIGEN libraries, to account for differences in geometry, material data, or assembly layout that would impact the flux spectrum across the assembly and consequently the assembly-average, burnup-dependent, one-group cross section data of the nuclides in the ORIGEN library. Individual two-dimensional (2D) assembly depletion models were developed for each of the assembly groups to generate burnup-dependent ORIGEN cross section libraries with the TRITON depletion sequence in SCALE. These models include the geometry, material, and operation data as available. The assembly modeling groups are generally mapping the reactor and assembly lattices listed in Table I, with at least one assembly depletion model being developed for a reactor and lattice type. In some cases, more depletion models were developed for a given reactor and assembly lattice to account for significant differences in the assembly configuration. For example, for the PWR Ringhals 3 17x17 lattice, two assembly models were used even though the geometry data was similar, to account for the presence of burnable absorber rods in one assembly group, whereas the other group did not contain such rods. For PWR assemblies, the ORIGEN reactor libraries were created

for fuel enrichment values that covered the enrichment range of the measured assemblies in that group and using a core-average value of the water moderator density. The differences between the assembly groups considered for the BWR ORIGIN reactor libraries generation consisted of rod or assembly channel geometry data, number of water or spacer rods, number of burnable absorber (Gd) rods, and enrichment distribution across the assembly. For the BWR assemblies, five values were used for coolant density between 0.1 and 0.9 g/cm³ within each 2D depletion model to encompass the range of axial void values. Control blades were not included in the BWR assembly models, lacking specific information on the assembly exposure to control blades during irradiation.

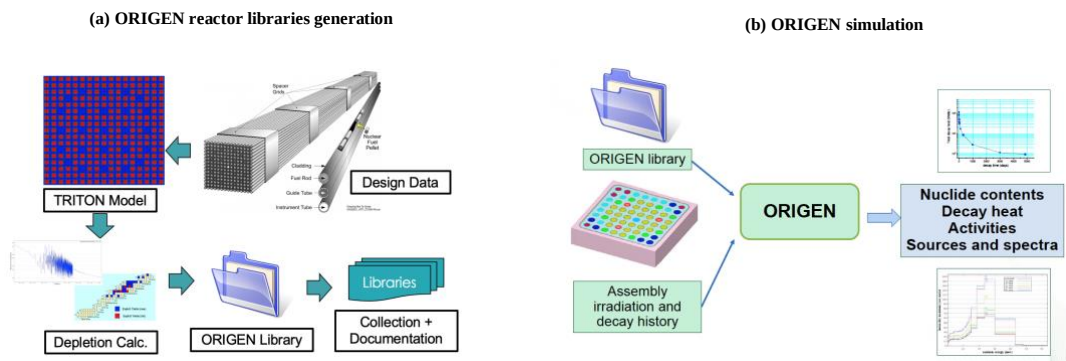


Fig 1. Decay Heat Calculation with SCALE/ORIGIN.

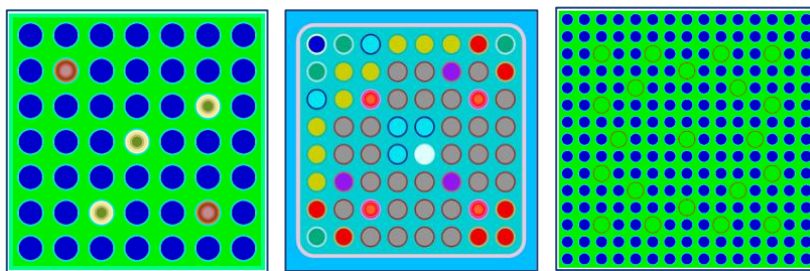


Fig 2. Selected Assembly Models for ORIGIN Libraries Generation (not to scale).

The ORIGIN reactor libraries for each of the considered assembly groups were generated as function of burnup and enrichment for the PWR assemblies, and as function of burnup, enrichment, and coolant density for the BWR assemblies. These

ORIGEN libraries were used in standalone depletion and decay ORIGEN simulations for each individual assembly under the ORIGAMI [12] graphical user interface. These simulations applied assembly-specific irradiation history data (cycle duration and downtime, power, decay time after discharge, coolant density) and assembly characteristics (fuel load and composition, clad load and composition, etc.). The contribution to the assembly decay heat from activation of the structural materials (e.g., spacers) was included in the ORIGEN simulation. Single zone models (assembly-averaged values applied for the coolant density and burnup) were used in the ORIGEN simulations for which results are shown here, unless otherwise specified.

IV. Results

All results presented in this section were obtained with SCALE 6.2.4 and ENDF/B-VII.1 nuclear data, unless otherwise specified. A comparison of the measured and calculated decay heat that is shown in Fig. 3, with each data point corresponding to a particular measurement, shows a linear behavior. The data are presented separately for PWRs and BWRs, given the significant difference in the assembly fuel mass and consequently the assembly decay heat values for these two types of reactors. The modeling complexity for BWRs is increased compared with PWRs because of the increased heterogeneity of the fuel assembly design and operation (e.g., different fuel enrichments, presence of integral absorbers). Uncertainty in the modeling input data will manifest as uncertainty in the calculated decay heat [10]. A detailed analysis of the uncertainty sources and impact, for both calculation and experiment, is beyond the scope of this paper, though some aspects are briefly discussed. The primary focus herein is to present the comparison between calculated and measured decay heat values.

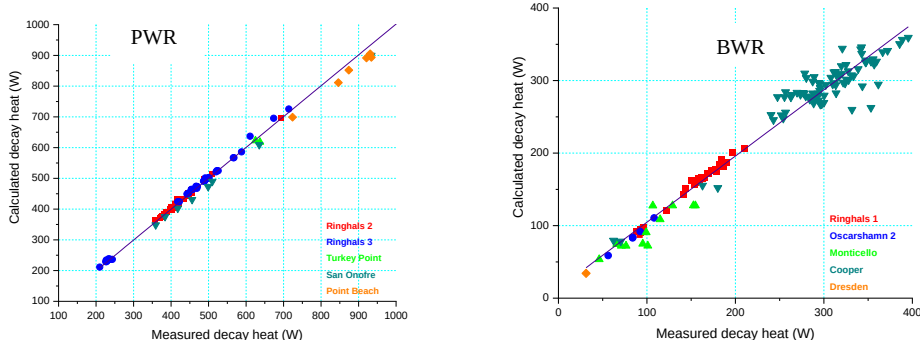


Fig 3. Calculated vs. Measured Decay Heat.

A summary of the calculated-to-experimental (C/E) ratios and the (C-E) differences is presented in Table II, grouped by reactor, as well as for the aggregate PWRs and BWRs. For each group of data, the mean C/E is reported, along with the corresponding standard deviation. For the PWR group, there is good agreement between the calculated and experimental data, with an average C/E of 1.006 and corresponding standard deviation of 1.6%. The comparison for each PWR sub-group is also good, with the decay heat predicted on average within the reported measurement uncertainty. The average C/E for the BWR group is 0.984, with a standard deviation of 7.7%. The large variation of the data around the mean is largely due to the variability of the C/E data for the Cooper assemblies, which with 81 measurements in the considered data set make a large contribution to the BWR average. However, the calculated decay heat is on average within the reported measurement uncertainty within the Cooper and the other BWR sub-groups. If the BWRs were grouped by the measurement laboratory in two sub-groups that correspond to measurements at GE-Morris (Cooper, Dresden, Monticello) and measurements at Clab (Oscarshamn 2 and Ringhals 1), the mean C/Es in this case would be: 0.971 ($\sigma=0.091$) for the former and 1.009 ($\sigma=0.024$) for the latter sub-group. A histogram of the C/E ratios is shown in Fig. 4, illustrating the greater spread around the mean value for the BWRs than for the PWRs.

Table II. Decay Heat Calculation-Experiment Comparison

Reactor name	Reactor type	No. of measurements	% relative exp. uncert. [2, 4] *	C/E		C-E (W)	
				mean	σ	mean	σ
Point Beach	PWR	6	4.7	0.966	0.007	-29.5	6.8
Ringhals 2	PWR	33	2.3 – 3.0	1.006	0.013	2.7	5.4
Ringhals 3	PWR	38	2.2 – 4.1	1.009	0.012	4.3	6.1
San Onofre	PWR	8	4.7	0.961	0.011	-20.8	8.7
Turkey Point	PWR	6	5.0 – 10.0	1.010	0.027	17.4	28.8
Cooper	BWR	81	5.9	0.970	0.078	-11.6	22.0
Dresden	BWR	1	5.9	1.095		3.0	na
Monticello	BWR	13	5.9	0.967	0.153	-5.8	15.6
Oskarshamn 2	BWR	5	4.2 – 7.5	1.010	0.024	0.7	1.7
Ringhals 1	BWR	45	2.5 – 5.1	1.009	0.025	1.5	3.6
PWR		91		1.006	0.016	2.8	5.5
BWR		145		0.984	0.077	-6.5	18.2
PWR+BWR		236		0.993	0.062	-2.9	15.3

* The experimental uncertainty for Clab measurements was taken from Ref. 4. Ref.2 shows for HEDL a reported measurement uncertainty of 5% at 1000W and 10% at 100W. For GE-Morris measurements, Ref.2 shows both a reported systematic error (2% at 700W and 4% at 200W) and a random error (4.3%). In the above table, the random and systematic errors were combined, with 2% systematic error considered for PWR and 4% for BWR measurements.

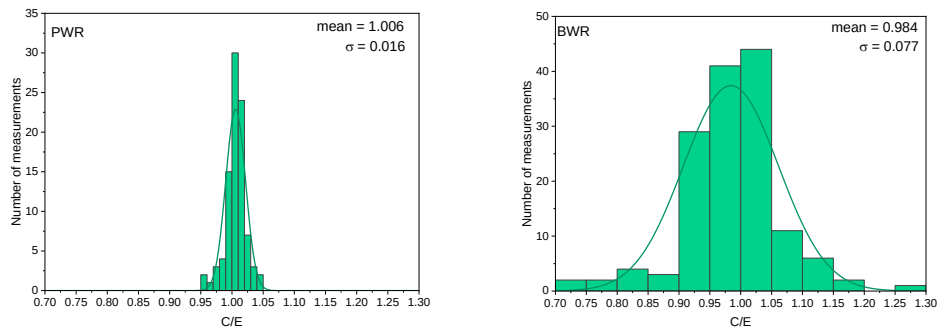


Fig 4. Histogram of Decay Heat C/E Ratios.

Decay heat is primarily driven by the nuclide inventory in the fuel assembly at discharge and the cooling time from discharge to a reference date of interest (measurement date in this analysis). The nuclide inventory (actinides and fission products) at discharge depends on the assembly burnup, which is a measure of the integral number of fissions (primarily from ^{235}U and ^{239}Pu) in the fuel during irradiation. The C/E and (C-E) variation as a function of burnup is illustrated in Figs. 5 and 6, respectively. The C/E variation as a function of cooling time is presented in Fig. 7. No significant trending is observed as a function of burnup or cooling time.

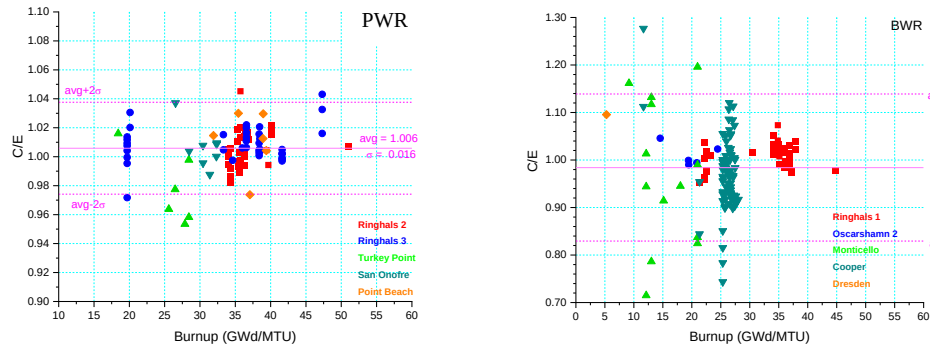


Fig 5. Decay Heat C/E vs. Burnup.

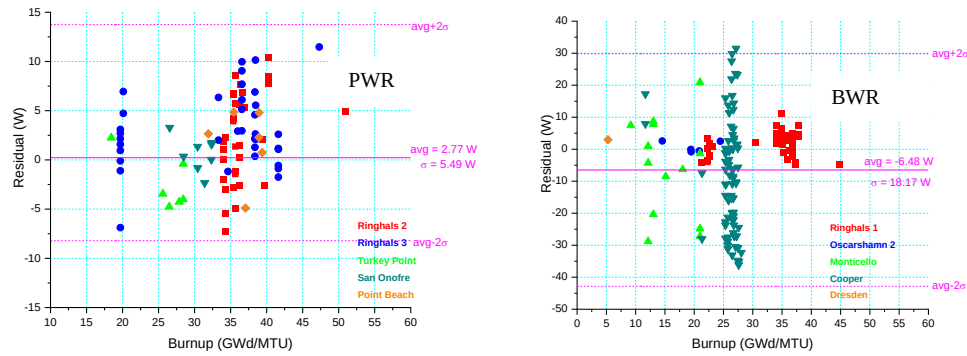


Fig 6. Decay Heat (C-E) vs. Burnup.

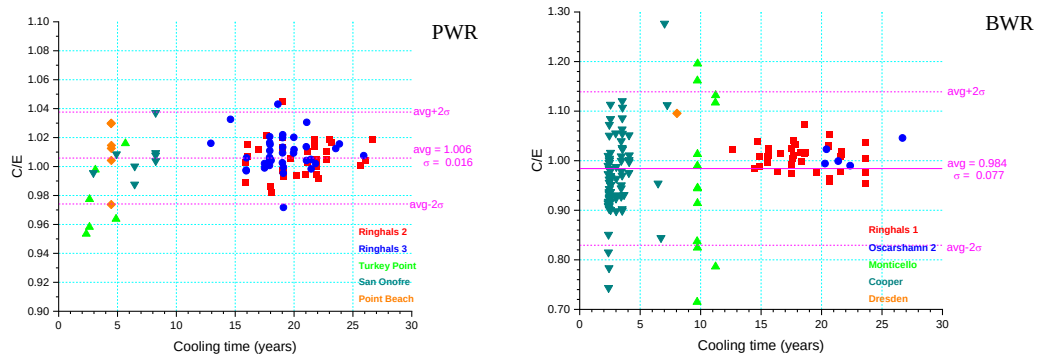


Fig 7. Decay Heat C/E vs. Cooling Time.

A linear fit of the data in Figs. 5-7 that was performed with the Origin graphing and data analysis software [13] indicated that the slope is not significantly different from zero with 95% confidence level. The data points variability at cooling times of less than ~15-year is greater than at longer cooling times. In case of the PWR data (Fig.7, left plot) all C/E points are within the reported experimental uncertainty. That's not the

case for the BWR data (Fig.7, right plot) at cooling times smaller than 15-year. For the latter case though, there are multiple potential sources of uncertainties that might have caused the observed differences, from either the experiment or the simulation data. For example, some modeling data (coolant density, channel water density, fuel and coolant temperature, presence of burnable absorber rods) were missing for the Cooper assemblies, for which assumptions were made based on typical BWR plant data. A detailed discussion of these modeling assumptions is available in [2], which served as the source of the modeling data that was used in the current study for the Cooper and Monticello assemblies. Evaluating the quality and applicability of the decay heat experimental data is beyond the scope of the current paper. Readers who would be interested in such topics are referred to references [2,8].

In assessing the relevance of the C/E data for different end-user applications, it is important to note some important aspects of decay heat change with cooling time and burnup and the primary nuclides driving decay heat. Decay heat varies significantly, by orders of magnitude, over a time interval from discharge to 100-year cooling time. An example illustrated in Fig. 8 (left) shows the variation of decay heat as function of cooling time for typical LWR fuel and selected burnups up to 37 GWd/MTU. It shows that decay heat decreases from $\sim 10^4$ to 10^6 W/MTU at discharge, to hundreds of W/MTU at 100-year after discharge. Even though a relative bias in the decay heat calculation (as measured by C/E) would be large, the absolute bias value would be on the order of a few watts at long times after discharge.

Another important aspect to bear in mind when assessing the bias and uncertainty in decay heat calculations is that only a handful of nuclides are contributing to the total decay heat, and their relative contribution varies with the cooling time. For example, 99% of the decay heat for a 37 GWd/MTU assembly at 15-year cooling comes from

only 11 nuclides [10]. For a typical LWR fuel with 50 GWd/MTU burnup, the percentage contribution of the nuclides that are the main contributors to decay heat up to 1000 years after discharge [14] is illustrated in Fig. 8 (right). Though the relative contribution may change as a function of burnup, it is well known that, at short cooling times, fission products are the major contributors [10,11,14]; and while these fission products decay out in time, the actinides become the major contributors at long cooling times. The better the code capabilities and associated nuclear data that are available for simulating the nuclear transmutation and decay processes in fuel during irradiation, the better the estimate for these nuclide inventories and consequently decay heat will be.

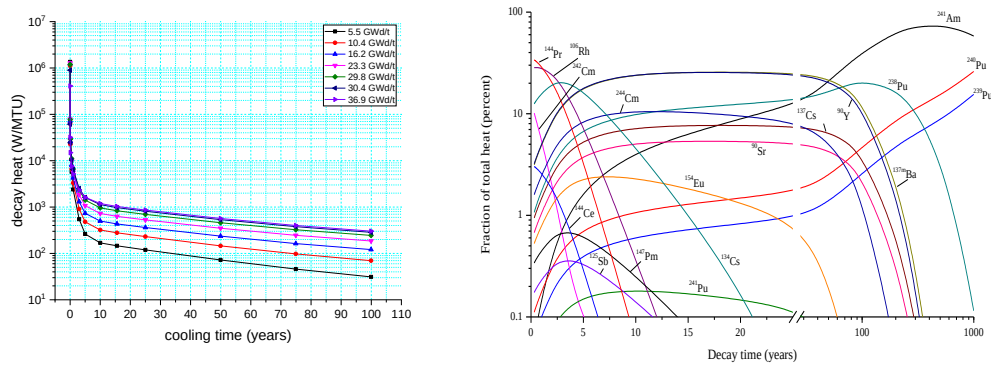


Fig 8. Decay Heat Variation and Main Contributing Nuclides vs. Cooling Time [11,13].

IV.A. Effect of Using Axially Varying vs. Assembly-Average Modeling Data

Generally, the use of assembly-average burnups and water moderator densities is adequate for assembly decay heat calculations, in particular for PWR assemblies, for which there is no significant axial variation of the moderator density. As shown elsewhere [3,4], the use of axially varying burnup and moderator density in the assembly decay heat simulation does not have a major impact on the assembly calculated decay heat; the resulting change in the assembly calculated decay heat is of the order of 1–2%, varies slightly with burnup and cooling time, and is typically within the measurement uncertainty for assembly decay heat measurements.

To compare with previous findings obtained with other codes and nuclear data versions, simulations were performed in this study to quantify the effect of using axially varying moderator density and burnup in PWR assembly decay heat calculations for which axial modeling data were available from core simulators. Single-zone and multi-zone simulations were performed for the Ringhals PWR fuel assemblies listed in Table I. In the single-zone models, the moderator densities and burnups used in the simulations were assembly-average values. In the multi-zone models, the simulations were performed over 24 axial nodes for which axial burnup and moderator density data were available; the assembly decay heat was calculated as a sum of the decay heat values for all nodes. The results, summarized in Table III, show that, on average, the effect on assembly decay heat C/E is less than 1% for the considered assemblies. The C/E differences for these specific assemblies were between 0.2% and 0.9%. The axial variations of the decay heat for all cases listed in Table III indicated that the decay heat axial profiles for the considered assemblies generally follow the burnup axial profiles.

Table III. Effect of Using Axially-Varying Data on Assembly Decay Heat C/E

Assembly lattice	No. of measurements	Burnup (GWd/MTU)	Cooling time (year)	C/E impact (%)	
				mean	σ
15×15	33	34.0 – 51.0	15.9 – 26.7	0.5	0.1
17×17	38	19.7 – 47.3	12.9 – 25.9	0.6	0.2
All	71	19.7 – 51.0	12.9 – 26.7	0.5	0.2

IV.B. Effect of Nuclear Data on Calculated Decay Heat

Changes in the nuclear data used in simulations have impact on the calculated assembly nuclide inventory at discharge and consequently on the assembly decay heat. The discussion herein addresses the effect of the changes in the SCALE version and the associated nuclear data libraries used for simulations. A detailed analysis of the uncertainties in the calculated decay heat due to uncertainties in the nuclear data (cross

sections and fission yields) or uncertainties in the modeling parameters (e.g., geometry or operation history parameters) can be found in other publications [10,11,15].

Table IV presents the decay heat comparison for a subset of the decay heat validation cases listed in Table I. Calculations performed with SCALE 6.2.4 and ENDF/B-VII.1 nuclear data are compared with those previously performed [4] with SCALE 6.1 and ENDF/B-VII.0 nuclear data. Given that the basic methods for nuclear transmutations and decay have not changed significantly between SCALE 6.1 and SCALE 6.2 implementations, any difference in results would be primarily due to changes in nuclear data from ENDF/B-VII.0 to ENDF/B-VII.1. Past validation studies performed with SCALE 5.1 and ENDF/B-V nuclear data are not considered in the comparison here, given that the codes involved have changed significantly from SCALE 5.1 to SCALE 6.2 and differences in results would be less relevant to the effects of nuclear data only.

Table IV. Effect of Nuclear Data on Decay Heat C/E

Reactor name	Reactor type	No. of measurements	Cooling time (year)	C/E SCALE 6.2.4 ENDF/B-VII.1		C/E SCALE 6.1 ENDF/B-VII.0		C/E (VII.1) – C/E (VII.0)	
				mean	σ	mean	σ	mean	σ
Ringhals 2	PWR	33	15.9 – 26.7	1.006	0.013	0.998	0.012	0.008	0.003
Ringhals 3	PWR	38	12.9 – 25.9	1.009	0.012	1.005	0.011	0.004	0.006
Ringhals 1	BWR	45	12.6 – 23.6	1.009	0.025	0.999	0.024	0.010	0.002
Oskarshamn 2	BWR	5	20.3 – 26.7	1.010	0.024	0.975	0.020	0.036	0.007
PWR		71	15.9 – 25.9	1.008	0.012	1.013	0.013	0.006	0.005
BWR		50	12.6 – 26.7	1.009	0.024	1.002	0.012	0.012	0.008
PWR+BWR		121	12.6 – 26.7	1.008	0.018	1.000	0.017	0.009	0.007

The results in Table IV indicate that the calculated decay heat changes on average by 0.6% ($\sigma=0.5\%$) for the considered PWR assemblies and by 1.2% ($\sigma=0.8\%$) for the BWR assemblies when changing the nuclear data. Though this relative change in

decay heat is small compared with the reported measurement uncertainties or with the impacts of other modeling parameters [10], preliminary investigations were performed to identify any major change in the nuclear data that might have caused the observed change in decay heat. The largest difference of 1.6% in calculated decay heat for the PWR assemblies included in Table IV, when the different ENDF/B libraries were used, was noticed for the highest-burnup PWR assembly (51 GWd/MTU, 16-year cooling time). A detailed analysis of the decay heat variation and primary nuclides contributing to decay heat for this assembly, and for another assembly with similar cooling time but smaller burnup (19 GWd/MTU), led to the identification of the primary source of the observed difference as the change in the capture cross-section of ^{238}Pu between ENDF/B-VII.0 and ENDF/B-VII.1 (see Fig. 9). The calculated concentration in fuel at discharge of this nuclide is greater when using ENDF/B-VII.1 than when using ENDF/B-VII.0. In the considered cooling time range listed in Table IV, the typical ^{238}Pu contribution to assembly decay heat is around 10% (see Fig. 8). For the mentioned 51 GWd/assembly that was analyzed in detail, the total contribution to decay heat of ^{238}Pu increased from 13% when ENDF/B-VII.0 was used to 15% when ENDF/B-VII.1 was used. The ^{238}Pu nuclide was also identified as the primary contributor to the decay heat change for others assemblies that were analyzed here.

It is worth mentioning that a different validation study focused on nuclide inventory prediction for PWR used fuel [16] has shown a significant improvement in predicting the concentration of ^{238}Pu with SCALE 6.2.4 and ENDF/B-VII.1 libraries. The study, which compared calculated nuclide concentrations with corresponding experimental radiochemical assay data for 77 PWR samples, showed for ^{238}Pu an average C/E concentration ratio of 0.959 ($\sigma=0.074$) when using SCALE 6.2.4 with ENDF/B-VII.1 data and of 0.883 ($\sigma=0.059$) when using SCALE 6.1 with ENDF/B-

VII.0 data. The significant change in ^{238}Pu prediction has been attributed to the change in its (n, γ) cross section between ENDF-B/VII.0 and ENDF-B/VII.1. The impact on decay heat is generally small, as the contribution of this nuclide to decay heat for typical LWR fuel is less than $\sim 10\%$ (see Fig. 8).

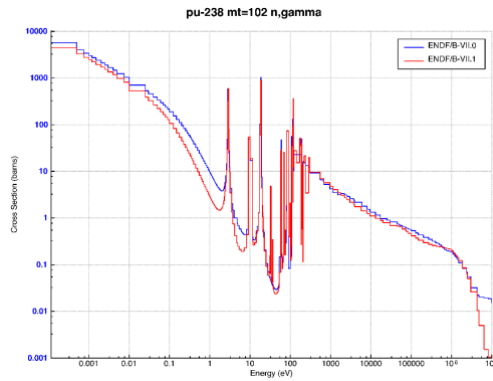


Fig 9. ^{238}Pu (n,gamma) Cross-Section.

V. CONCLUSIONS

Validation of the SCALE nuclear analysis code system version 6.2.4 for LWR used fuel decay heat analysis was performed based on more than 200 full-assembly decay heat experimental data that cover assembly burnups of 5–51 GWd/MTU and cooling times after discharge in the 2–27 year range. The comparison between calculated and experimental decay heat showed good agreement, with a relative difference of less than 2% averaged over all considered assemblies. The effect of using assembly-average versus axially varying modeling data on the calculated decay heat, of consequence to thermal analyses for used fuel transportation and storage systems, was studied for PWR assemblies. This study showed that on average the calculated decay heat change was less than 1% and varied slightly as a function of burnup and cooling time. The nuclear data libraries change from ENDF/B-VII.0 to ENDF/B-VII.1 resulted in a change of calculated decay heat that was on average less than 1% for the considered assemblies. The difference between calculated and experimental decay heat was on

average less than the reported experimental uncertainty. The validation database used herein, though it covers a large range of burnups, assembly designs, and cooling times, needs to be expanded with new measurements to fill the existing gap of measurement data for shorter cooling times (<5 years), modern assembly designs, and higher burnups.

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