DECAY HEAT UNCERTAINTY FOR BWR USED FUEL DUE TO MODELING AND NUCLEAR DATA UNCERTAINTIES[1]

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ABSTRACT

Characterization of the energy released from radionuclide decay in nuclear fuel discharged from reactors is essential for the design, safety, and licensing analyses of used nuclear fuel storage, transportation, and repository systems. There are a limited number of decay heat measurements available for commercial used fuel applications. Because decay heat measurements can be expensive or impractical for covering the multitude of existing fuel designs, operating conditions, and specific application purposes, decay heat estimation relies heavily on computer code prediction. Uncertainty evaluation for calculated decay heat is an important aspect when assessing code prediction and a key factor supporting decision making for used fuel applications. While previous studies have largely focused on uncertainties in code predictions due to nuclear data uncertainties, this study discusses uncertainties in calculated decay heat due to uncertainties in assembly modeling parameters as well as in nuclear data. Capabilities in the SCALE nuclear analysis code system were used to quantify the effect on calculated decay heat of uncertainties in nuclear data and selected manufacturing and operation parameters for a typical boiling water reactor (BWR) fuel assembly. The BWR fuel assembly used as the reference case for this study was selected from a set of assemblies for which high-quality decay heat measurements are available, to assess the significance of the results through comparison with calculated and measured decay heat data.

Keywords: decay heat, BWR, SCALE, Sampler, uncertainty, used nuclear fuel

1. Introduction

Characterization of energy released from radionuclide decay in nuclear fuel discharged from reactors (i.e., nuclear decay heat) is essential for the design, safety, and licensing analyses of used nuclear fuel storage in pools, transportation, interim dry storage, and repository systems. Because measurements of decay heat can be expensive or impractical for covering the multitude of existing fuel designs, operating conditions, and specific application purposes, decay heat estimation for commercial used fuel applications relies heavily on computer code predictions.

Decay heat generated in used nuclear fuel is determined by accounting for all contributions of recoverable energy released from the decay of radionuclides in fuel after its discharge from the reactor. Decay heat is driven by the isotopic composition in fuel at the end of irradiation and varies with the decay time after discharge (also known as cooling time). Calculation of decay heat can be performed with computational tools that simulate the nuclide transmutations and decay processes during fuel irradiation in the reactor, as well as the decay from discharge to a designated cooling time. The SCALE nuclear analysis code system (Bowman, 2011) is a computational system used internationally to support used nuclear fuel transportation and storage applications. The used fuel analysis capabilities in SCALE, particularly those in the ORIGEN isotopic depletion and decay code (Gauld et al., 2011), have been thoroughly validated against measurement data. These validation studies included analysis of nuclide inventories for over a hundred measured used fuel samples (Ilas et al., 2012) and of decay heat measurements (Ilas and Gauld, 2008; Ilas et al., 2014) performed for both pressurized water reactor (PWR) and boiling water reactor (BWR) used fuel assemblies.

Uncertainty in calculated decay heat is needed to assess the reliability in code predictions and to support decision making for used fuel applications for which decay heat has a significant impact on thermal performance. Bias and uncertainty in calculated metrics for a system of interest is generally estimated by direct comparison of calculated and experimental data, where available for the used fuel metric of interest. However, existing measurement data provide limited coverage of the parametric space (i.e., burnup, enrichment, cooling time) relevant to specific, current, or planned used fuel applications. The knowledge gap is greatly supplemented through computer simulations.

During the past decade, several institutions worldwide have developed computational approaches, complementing well-established methodologies that rely on direct or adjoint-based perturbation theory, to assess the effect of uncertainty in basic evaluated nuclear data on metrics of interest for used fuel applications. Many of these new uncertainty analysis approaches—known as stochastic sampling methods—include random sampling of nuclear data uncertainties, applying the perturbed nuclear data to the system of interest in repeated simulations, and processing the obtained response to determine its uncertainty due to the perturbed nuclear data uncertainties. The nuclear data uncertainty sampling can rely on covariance matrices (Klein et al., 2011) or nuclear reaction models (Rochman et al., 2016). The stochastic sampling methods are computationally intensive, requiring generally hundreds of repeated simulations for ensuring meaningful, adequately converged responses.

Stochastic sampling methods for applications involving isotopic depletion analysis have applied various random sampling approaches using existing cross section covariance files (Klein et al., 2011; Wieselquist et al., 2013a) and different depletion simulation systems such as CASMO (Leray et al., 2016), MCNP (García-Herranz et al., 2008), SCALE (Williams et al., 2013), or Serpent (Rochman et al., 2016). Most of the results published to date that are related to used fuel applications have focused more on propagating nuclear data uncertainties on uncertainty in isotopic compositions and less on uncertainty in integral responses such as decay heat (Williams et al., 2013; Fiorito et al., 2014).

While previous used fuel studies performed with the stochastic sampling capability in SCALE, which is named *Sampler*, were largely focused on response uncertainty due to nuclear data uncertainties (Williams et al., 2013; Wieselquist et al., 2013b), this study addresses uncertainties in calculated decay heat due to both nuclear data and assembly modeling parameters uncertainties. Sampler was used to quantify these uncertainties for a typical BWR fuel assembly configuration. The selected assembly modeling parameters include fuel material data (fuel density and enrichment, gadolinium content in gadolinia fuel rods), fuel rod geometry data (pellet radius, fuel rod radius), and operating data (coolant density, specific power, fuel temperature). The BWR fuel assembly used as the reference case for this study was selected from a set of previously analyzed assemblies (Ilas et al., 2014) for which high-quality decay heat measurements are available, to assess the significance of the results through comparison with calculated and measured decay heat data.

2. Assembly description and data

The reference BWR assembly has an 8 × 8 design, one of the most common fuel designs in the worldwide BWR fuel inventory. In the United States, ~45% of BWR assemblies discharged from reactors before 2013 (Hu et al., 2016) have an 8 × 8 lattice design. The selected assembly was measured at the Swedish Central Interim Storage Facility for Spent Nuclear Fuel, also called *Clab*. A comprehensive experimental program initiated and managed by Svensk Kärnbränslehantering AB (SKB), the Swedish Nuclear Fuel and Waste Management Company, is ongoing at Clab. Under this program, full-assembly decay heat measurements were performed for both PWR and BWR assemblies. In the past few years, SKB has closely collaborated with institutions in Europe and the United States under the Next Generation Safeguards Initiative – Spent Fuel (NGSI-SF) project, to develop new measurement technologies for verifying used nuclear fuel attributes (Humphrey et al., 2012). For testing of instruments and techniques developed under this project, 25 PWR and 25 BWR fuel assemblies stored at Clab were selected as a test bed, with 9 of the selected BWR assemblies having an 8 × 8 design (Vaccaro et al., 2016). Decay heat measurements are planned to be completed for each of these 50 assemblies.

2.1. Assembly geometry and operating data

Previous analyses (Ilas et al., 2014) of decay heat measurements performed at Clab included one 8 × 8 BWR assembly for which 10 measurements were performed at different cooling times—the largest number of measurements for an assembly in that analyzed set. This assembly, identified as *6432R1*, is used for uncertainty analyses in this study. Detailed data for this assembly can be found in (SKB Report R-05-62, 2006). The assembly has an average enrichment of 2.9 wt% ^{235}U, an average burnup at discharge of 36.9 GWd/MTU, and an average (over all irradiation cycles and axial locations in the assembly) coolant density of 0.453 g/cm^3. The assembly includes 63 fuel rods — 59 regular fuel (UO_2) rods and 4 gadolinia (UO_2-Gd_2O_3) rods, and one water rod. The fuel rods located at the corners of the assembly (corner rods) have a diameter smaller than the remaining fuel rods in the assembly. The fuel enrichment map and assembly layout are illustrated in Fig. 1. The assembly has fuel rods with five enrichments: 1.38, 1.98, 2.49, 3.17, and 3.37 wt% ^{235}U. Unique rod colors in Fig. 1 indicate unique enrichment values, while the white rod indicates the water rod. The rods shown as containing multiple rings are the gadolinia rods. Fig. 2 shows the cumulative burnup of the assembly and the assembly-average specific power as a function of the irradiation cycle.

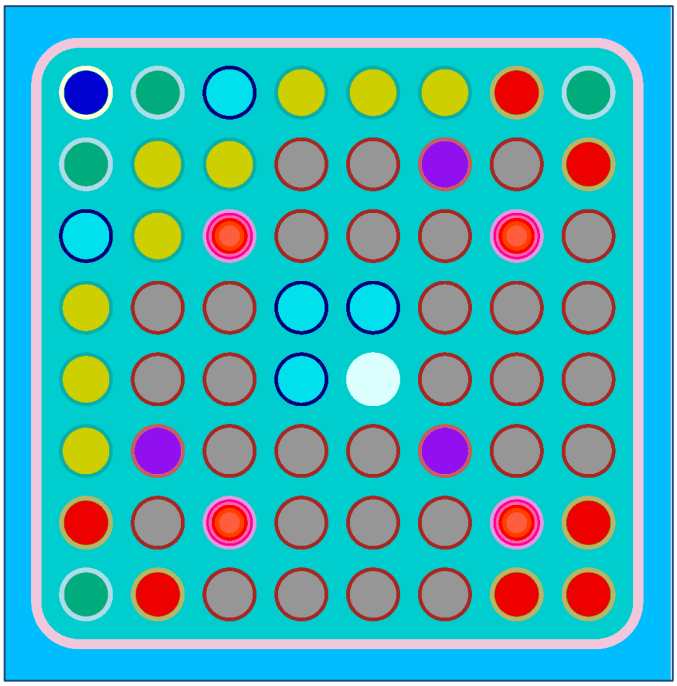

Fig. 1. Illustration of the 6432R1 BWR assembly configuration.

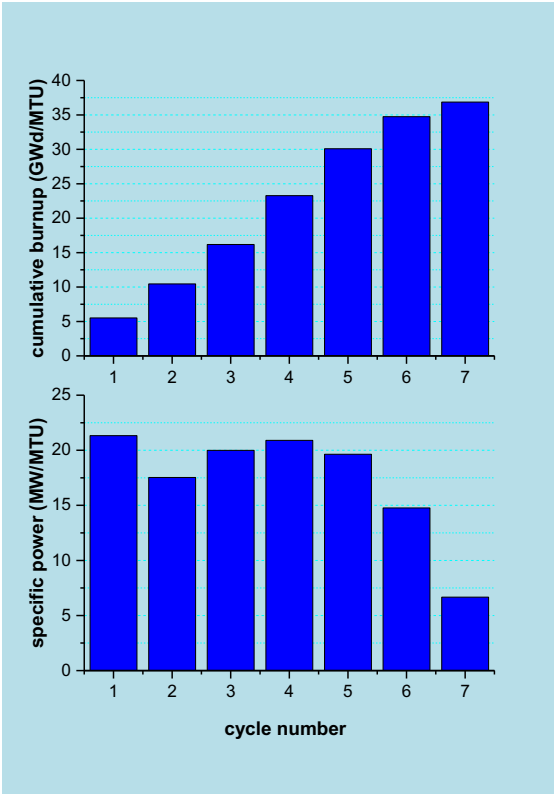

Fig. 2. Burnup and power for assembly 6432R1.

2.2. Assembly measurement data

Table 1 shows the experimental decay heat data obtained from 10 measurements (SKB Report R-05-62, 2006) performed over a period of almost 6 years that correspond to cooling times between 14.8 and 20.6 years. Five of these 10 measurements were completed within an 18-day period at ~15.6 years cooling time. At this cooling time, the change in decay heat over 18 days is less than 0.1% and these five measurements can be considered as repeat measurements of the same assembly at a specific cooling time. The measured decay heat used as the reference is 183.21 W (mean of the five measurements) at 5,681-day decay time, with a standard deviation (1σ) of 1.54 W or 0.8% of the mean measured value. This experiment-based, derived measurement uncertainty of 1.54 W is close to the measurement uncertainty reported for BWR assemblies. The reported measurement uncertainty (SKB Report R-05-62, 2006) at a 95% confidence level (2σ) was 4.2 W at 50W decay heat and 6.2 W at 350 W decay heat; if this uncertainty were assumed to vary linearly with the decay heat, the uncertainty (1σ) corresponding to 183.21 W decay heat would be ~2.5 W or 1.4%.

Table 1. Decay heat measurement data for assembly 6432R1

Measurement number	Cooling time (days)	Decay heat (W)
1	5,422	185.48
2	5,424	189.55
3	**5,670**	**184.44**
4	**5,680**	**182.79**
5	**5,681**	**185.17**
6	**5,687**	**181.63**
7	**5,688**	**181.99**
8	6,425	175.92
9	7,521	161.72
10	7,526	161.72

2.3. Assembly uncertainty data

The assembly modeling parameters investigated in this study are selected fuel design and operating history parameters. Generally, fuel design data are proprietary to the fuel vendors and information on uncertainties and manufacturing tolerances may not be available. The design parameters' uncertainties used in this study are not directly known for the considered assembly, but rather are estimated based on prior experience and uncertainties commonly applied in criticality safety evaluations. The considered fuel design parameters are initial fuel enrichment, UO_2 density, Gd_2O_3 content in UO_2-Gd_2O_3, fuel pellet radius, and clad outer radius, as listed in Table 2 along with commonly used tolerance intervals for these parameters. It was assumed that the uncertainties in these parameters are normally distributed and that three standard deviations (3σ) correspond to the tolerance interval. Values for individual pins were considered correlated – identical values were used for all pins for a given perturbation of a parameter.

For the operating history data, three parameters were considered: specific power, coolant density, and effective fuel temperature (Table 3). Uncertainties in these parameters are usually provided by plant operators based on their core simulator and fuel performance tools. They can be estimated based on available benchmark data (Grandi and Borkowski, 2003; Kruners et al., 2010; Hu and Gauld, 2014). The values used in this study are based on previous reports (Grandi and Borkowski, 2003; Kruners et al., 2010) stating that coolant density and fuel temperature are "within 10%," and specific power is "within 5%" on a node level, where the node refers to a specific axial location along the assembly's height. The analyzed assembly had no known control rod presence. For assessments discussing the effect of control rod usage on isotopic composition in used BWR fuel, see (Hu and Gauld, 2014) and (Ade et al., 2016). In

this study, the uncertainty in the three considered operating parameters were treated as uncorrelated and normally distributed. No spatial or time dependence was considered for the coolant density and fuel temperature – the analysis model considered that the nominal values are assembly and irradiation history average values. For these two parameters, the standard deviation (1σ) corresponding to the normal distribution assumed for uncertainty was estimated by considering that 3σ correspond to 10% of the nominal value; therefore, 1σ is 30K for fuel temperature and 0.015 g/cm^3 for coolant density. The assembly average specific power was available for each of the irradiation cycles. It was assumed that the uncertainty in the specific power for each cycle is normally distributed and that 3σ correspond to 5% of the specific power for that cycle.

Table 2. Uncertainty in fuel design parameters

Parameter	Units	Tolerance	1σ
Enrichment	wt% ^{235}U	0.05	0.0167
UO_2 density	g/cm^3	0.125	0.0417
Gd_2O_3 content	wt% Gd_2O_3	0.10	0.0333
Pellet radius	mm	0.075	0.025
Clad outer radius	mm	0.25	0.083

Table 3. Uncertainty in operating history parameters

Parameter	1σ (%)
Specific power	1.67
Coolant density	3.33
Fuel temperature	3.33

3. Computational methods and data

All analyses in this study were performed using the computational capabilities and nuclear data available in the most recent version of SCALE, 6.2.1 (Rearden and Jessee, 2016). The SCALE codes and sequences used are briefly discussed in this section, along with a description of the assembly computational models.

3.1. Computational tools and data

3.1.1 TRITON and ORIGEN

The assembly irradiation and decay simulations were based on the two-dimensional (2D) TRITON depletion sequence (DeHart and Bowman, 2011) and the ORIGEN point depletion and decay code (Gauld et al., 2011) in SCALE 6.2.1. TRITON was used to simulate the assembly irradiation history, while ORIGEN standalone was employed for decay simulations of the irradiated fuel. The 2D TRITON depletion involves three main steps used in an iterative process to simulate the assembly irradiation history: resonance cross section processing, deterministic multigroup neutron transport with the NEWT code, and transmutation and decay with ORIGEN. Enhanced capabilities relevant for TRITON in SCALE 6.2.1 (Rearden and Jessee, 2016) compared to previous releases include improved integrated cross section processing with XSPROC, accelerated calculations with NEWT, and a new solver (Isotalo and Wieselquist, 2015) and modernized input with ORIGEN. The assembly depletion simulation in this study used 252-group ENDF/B-VII.1 cross sections with the transport solver; the libraries used with ORIGEN include decay data based on ENDF/B-VII.1 and fission yields based on ENDF/B-VII.0.

3.1.2 Sampler

Although in development and internal use since 2011 as an uncertainty analysis tool in SCALE (Williams et al., 2013), Sampler was not officially released with SCALE until 2016. Sampler is an overarching

sequence that propagates uncertainties in nuclear data and input parameters to estimate the resulting uncertainty in virtually any SCALE calculated response. The uncertainties are propagated through all computational steps in the simulation, providing a fully coupled uncertainty analysis that accounts for all correlations inherent to the calculation. The treated nuclear data uncertainties can include uncertainties in multigroup cross section data used in neutron transport calculations, as well as uncertainties in fission product yield and decay constants used in depletion simulations. The applied perturbed nuclear data are precalculated based on covariance data files by using a stochastic sampling approach (Williams et al., 2013). A set of 1,000 perturbed nuclear data libraries are included in the SCALE 6.2.1 release. The covariance data for neutron cross sections are based on ENDF/B-VII.1 evaluated data and supplemented with data calculated at Oak Ridge National Laboratory (ORNL) (Rearden and Jessee, 2016). The fission product yield perturbed data available in SCALE 6.2.1 were obtained by sampling of the independent fission yield uncertainties in ENDF/B-VII.0. Fission product yield covariance data that were not available in the ENDF/B data were generated using a Bayesian method (Pigni et al., 2015). The effect of decay data uncertainty, which is expected to be very small (Wieselquist et al., 2013), was not considered in this study.

Sampler can also be used to determine uncertainties and correlations in calculated responses resulting from uncertainties in user-provided modeling data in a SCALE input file. Examples of these modeling input data can include geometry (i.e., dimensions), temperature, material density and composition, etc. Perturbed values are obtained by random sampling of user-provided distribution functions and uncertainty data for any modeling parameters of interest.

Previous analyses with Sampler have focused on nuclear data uncertainty for various PWR used fuel applications, including nuclide inventories and decay heat (Williams et al., 2013), burnup credit (Wieselquist et al., 2013), criticality safety (Williams et al., 2014), or radiation sources (Hu and Gauld, 2014). These studies were performed with cross section covariance data as available at the time in SCALE, based primarily on ENDF/B-V, ENDF/B-VI, and JENDL data. Earlier application of Sampler for assessing the effect of uncertainty in modeling data (that are not related to nuclear data) have focused on criticality safety analyses (Rearden et al., 2013; Marshall and Rearden, 2015), with limited use for used fuel applications (Bratton et al., 2014). The current study involves a BWR fuel assembly, uses extended covariance data in SCALE 6.2.1 that includes ENDF/B-VII.1 data for 187 nuclides, and addresses uncertainty in both nuclear data and assembly modeling data.

3.2. Computational model

The assembly model illustrated in Fig. 1 corresponds to a 2D cross section at the assembly midplane. Individual depletion mixtures shown in different colors in Fig. 1 were modeled based on a half assembly diagonal symmetry. The gadolinia rods were represented with five concentric equal-area fuel zones. For each fuel rod, Dancoff factors calculated separately with the SCALE/McDancoff code were applied in the TRITON model; these factors were assumed constant for the cases with perturbed values in pellet and cladding radii. The isotopic compositions of individual fuel pins were tracked independently in the depletion simulation using the ASSIGN approximation (DeHart and Bowman, 2011) in TRITON; fuel pins with the same initial enrichment were grouped together to use a common set of microscopic cross section in the depletion calculation, with the purpose of reducing the runtime spent in the resonance cross section processing. An assembly-average value of 0.453 g/cm^3 was used for coolant density over all irradiation cycles. A nominal fuel temperature value of 900 K was considered for each fuel rod in the assembly during irradiation.

Sampler simulations were performed to assess the separate effects of the uncertainties in both assembly modeling parameters and nuclear data used in depletion simulations on the assembly calculated decay

heat. The simulations correspond to perturbation of the following four modeling data groups: (1) operating history data, (2) fuel design data, (3) nuclear cross section data, and (4) fission yield data. For each of these Sampler simulations, 500 perturbed calculations were performed. For each category of data, all data in that category were perturbed at the same time. A reference case used nominal values for all input parameters and unperturbed nuclear data.

For each Sampler calculation, a depletion simulation with TRITON was performed for the considered assembly to simulate its irradiation in the reactor for a total cumulative burnup of 36.9 GWd/MTU. A nuclide concentration data file produced by TRITON was saved for later use with ORIGEN for standalone decay calculations. This data file includes the isotopic concentrations for each of the depleted mixtures in the problem, as well as the assembly-average isotopic composition at each depletion step.

ORIGEN decay calculations were performed over a cooling time range of 0–100 years using the isotopic compositions at the end of each of the assembly's irradiation cycles (for burnups of 5.5, 10.4, 16.2, 23.3, 29.8, 30.4, and 36.9 GWD/MTU). The calculated responses consisted of the total decay heat and the isotopic contents of nuclides of importance to decay heat.

Activation of the fuel assembly hardware was not included in the model. The contribution of activation to decay heat, dominated by ^{60}Co, is primarily dependent on the amount of cobalt present in the assembly hardware material before assembly's irradiation in the reactor. Since all modern fuel designs use zirconium alloys in the active region of the fuel, the amount of cobalt is very low (<20 ppm), and the contribution to the total decay heat is negligible. For fuel assemblies made before 1990, Inconel with high amounts of cobalt was used in spacer grids. However, because the half-life of ^{60}Co is ~5.3 years, the impact is only of interest for short cooling times (Ilas and Gauld, 2008).

4. Results and discussion

The calculated results provide a basis for investigating the effect of the uncertainty in modeling parameters and nuclear data on the calculated decay heat as function of burnup and cooling time, for a burnup range of 5.4–36.9 GWd/MTU and cooling times up to 100 years. Second, they enable an assessment of the calculated uncertainties by direct comparison with measurement data and measurement uncertainty for a specific burnup (36.9 GWd/MTU) and cooling time (5,681 days) for assembly 6432R1.

4.1. Decay heat of assembly 6432R1

The calculated decay heat for the reference assembly at a cooling time of 5,681 days (~15.6 years), using nominal values for all modeling parameters and unperturbed nuclear data, was 183.20 W, in very good agreement with the measurement value of 183.21 W. At this cooling time, ~99% of the total decay heat practically comes from only 11 isotopes, as illustrated in Fig. 3. Almost 70% of this decay heat is due to ^{137m}Ba, ^{137}Cs, ^{90}Y, and ^{90}Sr. These are parent-daughter nuclides: ^{137}Cs β-decays to ^{137m}Ba with $T_{1/2}$ = 30.2 years, and ^{90}Sr β-decays to ^{90}Y with $T_{1/2}$ = 28.8 years.

The isotopes that are the major contributors to assembly 6432R1 decay heat vary with cooling time. The most important contributors are illustrated in Fig. 4 as a function of the cooling time from one year after the assembly's discharge (at burnup 36.9 GWd/MTU) to 100 years. As the results show, at cooling times shorter than ~15 years, there are more contributors than those identified in Fig. 3, including fission products ^{144}Pr, ^{106}Rh, and ^{154}Eu. At longer cooling times, these fission products decay out, and at 100 years cooling almost 60% of the decay heat is due to actinides ^{241}Am (daughter of ^{241}Pu) and ^{238}Pu.

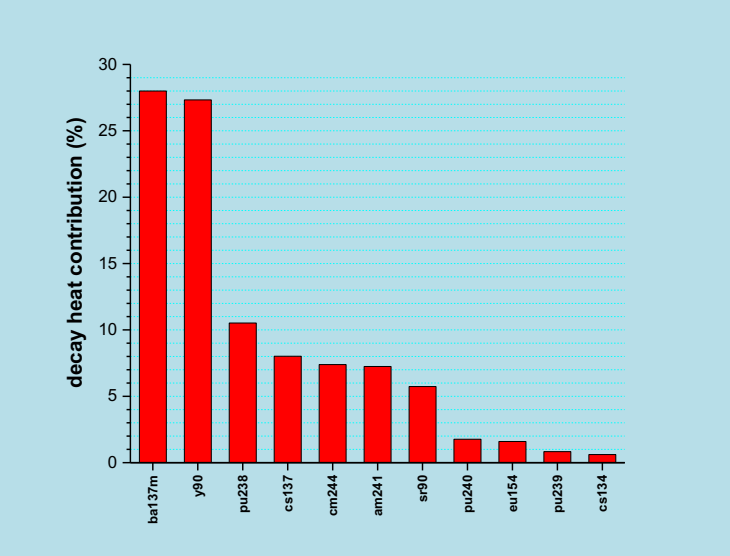

Fig. 3. Nuclide contribution to 6432R1 assembly decay heat at 15.6-year cooling time.

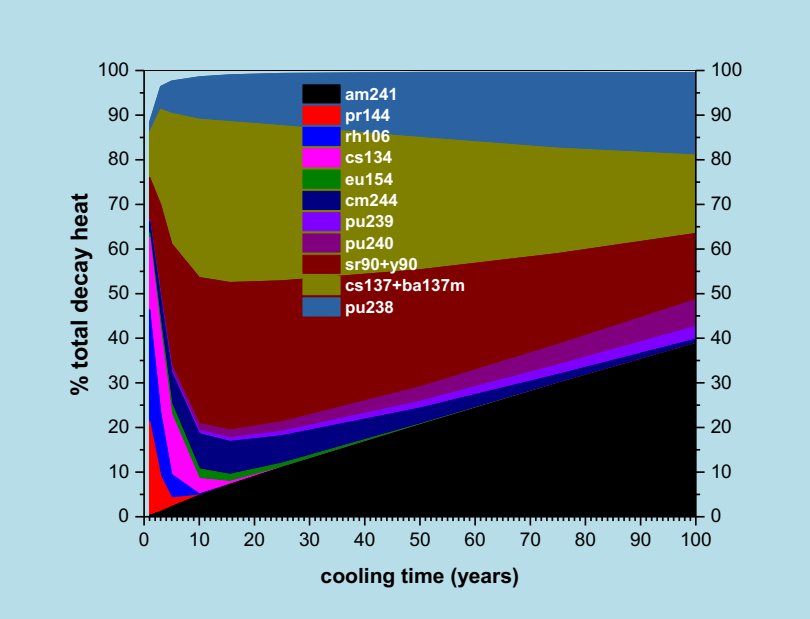

Fig. 4. Nuclide contribution to 6432R1 assembly decay heat vs. cooling time.

4.2. Assembly decay heat sensitivity study

A preliminary assessment was performed to determine the sensitivity of the assembly's calculated decay heat to each of the modeling parameters (Tables 2–3) considered. Each parameter was varied individually within its range of variation. Depletion simulations and decay heat calculations were made for a few values within the range of variation for the perturbed parameter, including its nominal value and the minimum and maximum values. The sensitivity of the decay heat calculated for assembly 6432R1 at the measurement time is presented in Table 4; the relative sensitivity is calculated as percent change in decay heat value for a 1σ increase of the parameter relative to its nominal value, and the sensitivity coefficient is calculated as percent change in decay heat for one percent change in parameter.

Table 4. Assembly decay heat sensitivity

Data set	Parameter	Relative Sensitivity[a]	Sensitivity Coefficient[b]
Fuel design	Enrichment	-0.03	-0.05
	UO_2 density	0.07	0.17
	Gd_2O_3 content	<0.01	<0.01
	Pellet radius	0.16	0.03
	Clad outer radius	0.18	0.01
Operating data	Specific power	1.99	1.19
	Coolant density	-0.31	-0.09
	Fuel temperature	0.03	0.01

[a] % change in decay heat due to 1σ change in parameter from its nominal value;
[b] % change in decay heat due to 1% change in parameter.

The largest effect comes from uncertainty in the specific power, whereas initial enrichment, Gd_2O_3 content, fuel temperature, and UO_2 density have a much smaller or insignificant effect on the total assembly decay heat at the time of measurement. However, these parameters, especially enrichment, are likely to have a larger impact on the isotopic composition at the fuel rod level.

4.3. Uncertainty from fuel design and operating data

Using Sampler, the effect of uncertainty in fuel data or operating data was analyzed by simultaneously perturbing all parameters in each set. A total of 500 perturbed calculations were performed for each set. Results obtained were used to study the decay heat variation as a function of burnup and cooling time.

For the fuel design data group, the average value for the assembly decay heat at 15.6 years cooling was 182.83 W, with a standard deviation of 0.37 W (0.20%). The average decay heat for the operating data group was 183.35 W, and the corresponding standard deviation was 1.56 W (0.85%). The average and nominal decay heat values differ by 0.08% for the operating data set and 0.20% for the fuel design data set. These mean values are expected to be the same as the nominal value; if different, that may indicate that the assumed uncertainty distributions would not be completely adequate. However, because the effect of the fuel design data here is relatively small, no further refinement was pursued in testing other types of distribution for fuel design data uncertainties.

Uncertainties for the fuel and operator data variation are less than the measurement uncertainty of 1.4% discussed in Section 2.2. The decay heat distributions for each of the two perturbed data groups are shown in Fig. 5. The size of the histogram bin is equal to one standard deviation in each of the two plots. The same scale was used for the histograms for comparisons of various effects.

When the uncertainties were examined at the fuel rod level, it was observed that the decay heat uncertainty was larger for fuel rods closer to the edge of the assembly. For fuel rods located at the edges and corners of the assembly, changes in the coolant density have a higher impact on the neutron spectrum than for non-edge fuel rods. (Note that the coolant density within the assembly can is different from the density of the water moderator outside the assembly can.)

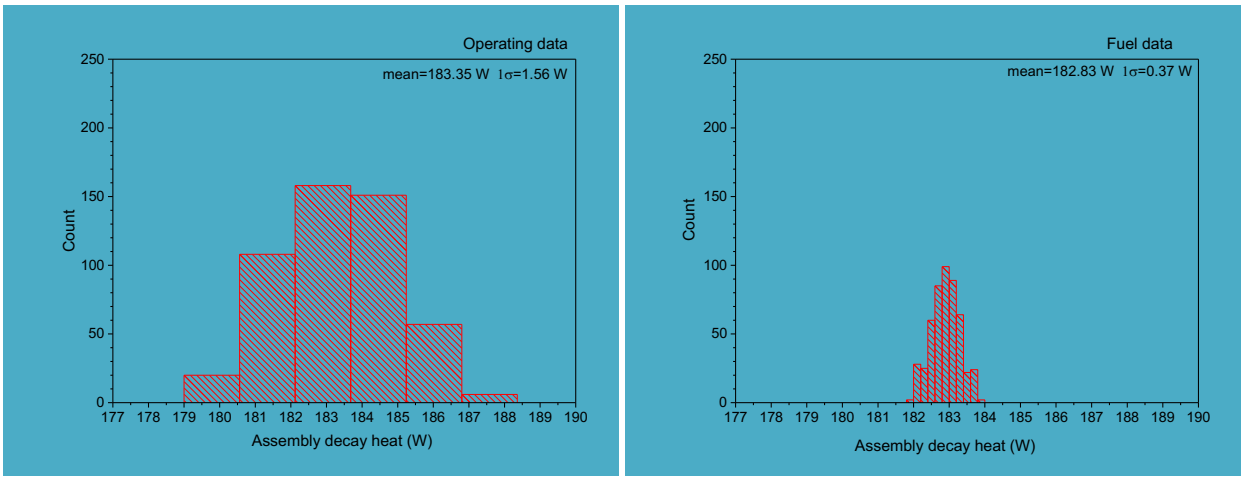

Fig. 5. Histograms of the decay heat variation for assembly 6432R1 due to uncertainties in fuel and operating data.

4.4. Uncertainty from cross-section and fission yield data

Using Sampler, 500 calculations were performed for each of the two considered perturbed data sets: cross-section data and fission yield data. All data in each set were perturbed simultaneously. Currently, Sampler cannot perturb cross sections for individual nuclides to assess individual nuclide effects.

The average assembly decay heat for the cross section data perturbation was 183.28 W, with a standard deviation of 1.62 W (0.88%). The average decay heat for the fission yield data perturbation was 183.08 W, and the corresponding standard deviation was 0.47 W (0.26%). The decay heat distributions for each of the two groups are shown in Fig. 6. The effect of fission yield uncertainty is much smaller than that of uncertainties in cross section data.

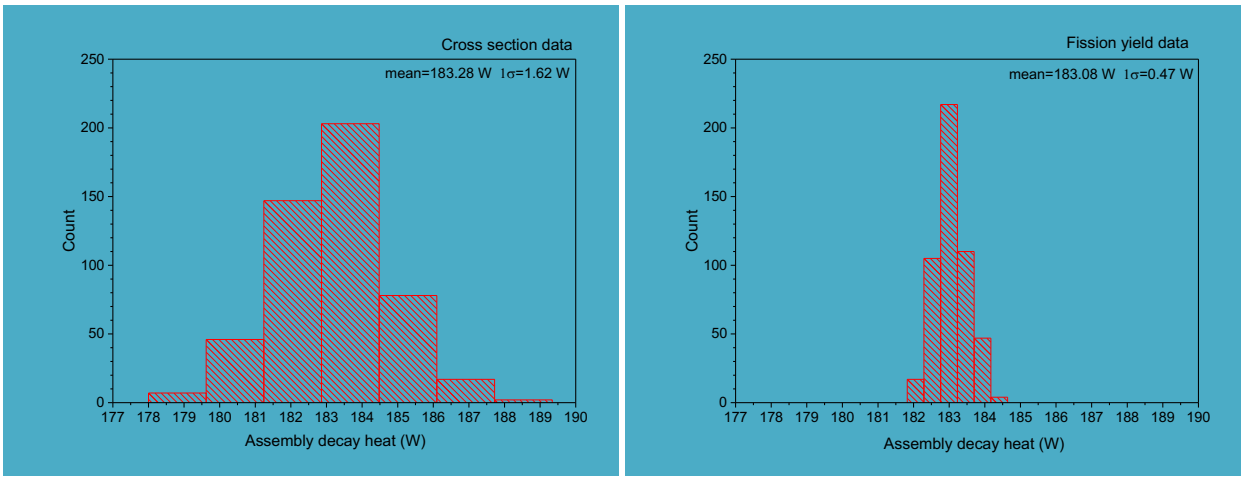

Fig. 6. Histograms of decay heat variation for assembly 6432R1 due to uncertainties in cross sections and fission yields.

The uncertainties in the calculated decay heat at 15.6 years cooling time are summarized in Table 5. The combined decay heat uncertainty due to modeling data uncertainty is 0.87%; whereas, the combined uncertainty due to nuclear data uncertainty is 0.92%. The overall decay heat uncertainty due to both modeling and nuclear data uncertainties, assuming that these uncertainties are uncorrelated, is 1.27%.

Table 5. Decay heat uncertainty summary

Data set	Data set	Uncertainty (1σ) (%)
Modeling data	Fuel design	0.20
	Operating data	0.85
	Total	0.87
Nuclear data	Cross sections	0.88
	Fission yields	0.26
	Total	0.92
Overall effect	Total	1.27

Decay heat uncertainties at the time of measurement for assembly 6432R1 are driven in large part by uncertainty in isotopic concentrations of the important decay heat contributors, as illustrated in Fig. 3. The uncertainty in calculated mass for ^{137}Cs, ^{90}Sr, ^{238}Pu, ^{244}Cm, and ^{241}Am that arise from uncertainty in each of the considered perturbed data groups is illustrated in Fig. 7. Uncertainties of ^{137m}Ba and ^{90}Y, daughter isotopes of ^{137}Cs and ^{90}Sr, are similar to those of the parent isotopes. Only the uncertainties of the parents are included in Fig. 7. At this large cooling time, uncertainty in ^{241}Am is primarily driven by uncertainty of the ^{241}Pu parent nuclide ($T_{1/2}$ = 14.4 years). Though the impact on uncertainty in the ^{238}Pu and ^{244}Cm content of cross section data uncertainties may seem large (4.0–4.5%), the compounded effect on decay heat is small because the contribution to decay heat of these two nuclides is only ~17% (see Fig. 3).

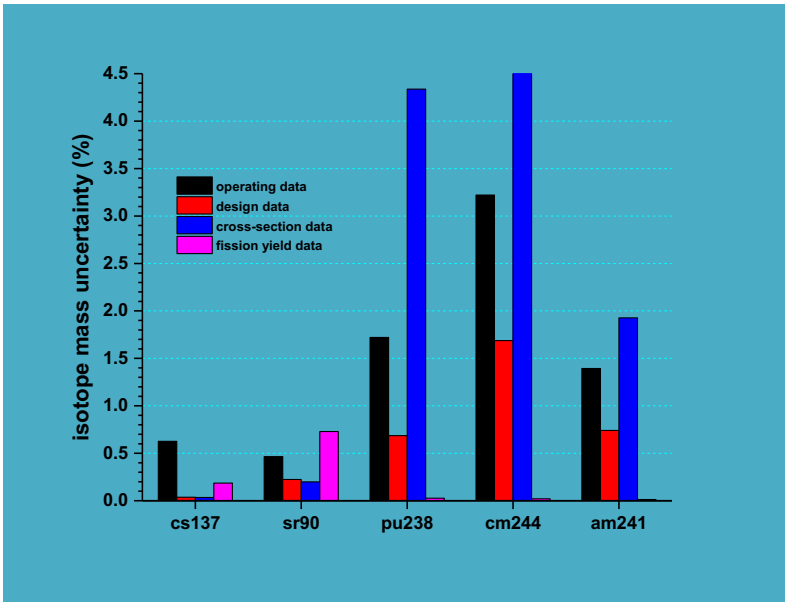

Fig. 7. Uncertainty in calculated mass of major contributors to assembly decay heat at measurement time.

4.5. Uncertainty as function of burnup and cooling time

The nuclide concentration data files available from the TRITON simulations were used to extract the nuclide data corresponding to different burnups and use them as input in ORIGEN decay-only simulations to investigate behaviors as function of both burnup and cooling time. The variation of the nominal (unperturbed) decay heat values as a function of burnup (5.5 to 36.9 GWd/MTU) and cooling time from discharge to 100 years is illustrated in Fig. 8. The decay heat decreases significantly from discharge time (10^5-10^6 W/MTU) to 100 years, when it becomes orders of magnitudes smaller (< 300

W/MTU). Consequently, even though the relative uncertainty in decay heat might be large at a longer cooling time, the absolute uncertainty would be small (on the order of a few W).

Uncertainty in decay heat as a function of burnup and cooling time is illustrated in the surface plots presented in Fig. 9 for each of the perturbed data sets. These plots use the same scale to facilitate comparisons.

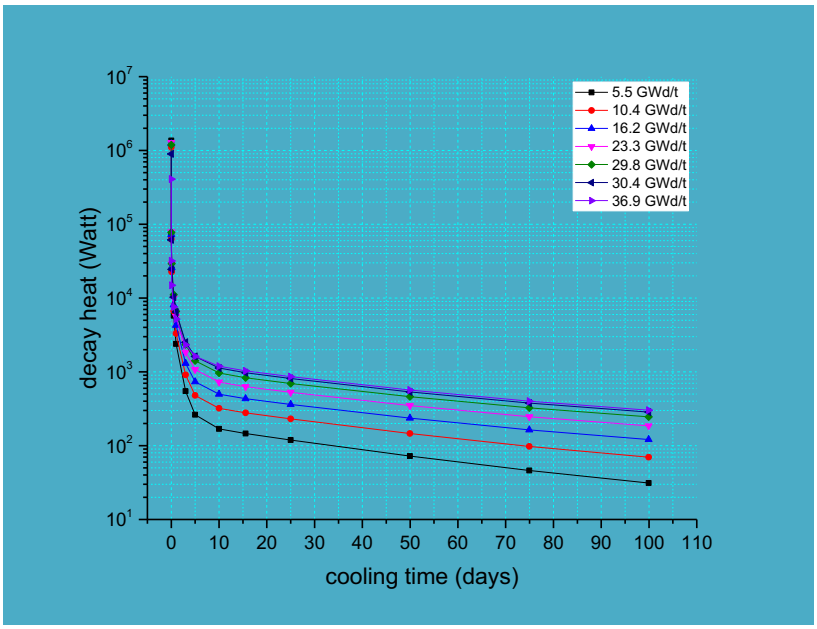

Fig. 8. Decay heat as function of burnup and cooling time.

Uncertainty in decay heat due to fission yield uncertainty is less then ~0.4% over the considered burnup and cooling time range. Its variation is driven by variation in isotopic uncertainty of those fission products that are significant contributors to decay heat. For example, for a 5.5 GWd/MTU burnup, more than 70% of the total decay heat for cooling times between 10 and 75 years is due to decay of a few fission products (^{137}Cs, ^{137m}Ba, ^{90}Sr, ^{90}Y), with a maximum contribution of these isotopes of ~90% at 15–25 years of cooling. The effect of the fission product uncertainty decreases with increasing burnup as the relative contribution to decay heat of the fission products decreases and the actinides become major contributors.

Uncertainty in decay heat due to cross section data uncertainties increases with burnup due to increasing actinide relative contribution to decay heat. Its variation with cooling time reflects the relative contribution to decay heat of actinides and fission products, along with the corresponding uncertainties in these isotopes. For those actinides that contribute significantly to decay heat, the uncertainties in their content increase with increasing burnup, and the trends are like those observed for the PWR used fuel (Williams et al., 2013). The maximum relative decay heat uncertainty for the considered burnups and cooling times was ~1.25%.

Uncertainty in decay heat due to fuel design data is less than ~0.5% over the considered burnup and cooling time ranges. It increases with increasing cooling time for a given burnup because of the impact of fuel data uncertainties on the isotopic content of actinides that contribute significantly to decay heat.

Uncertainty in decay heat due to uncertainties in operating data has in general different trends as a function of burnup and cooling time than those observed for the other three categories of perturbed data. The magnitude of this uncertainty varies in the approximate range 0.8–2.2%. The uncertainty variation is driven by variation in nuclide uncertainties for nuclides that are important decay heat contributors. The

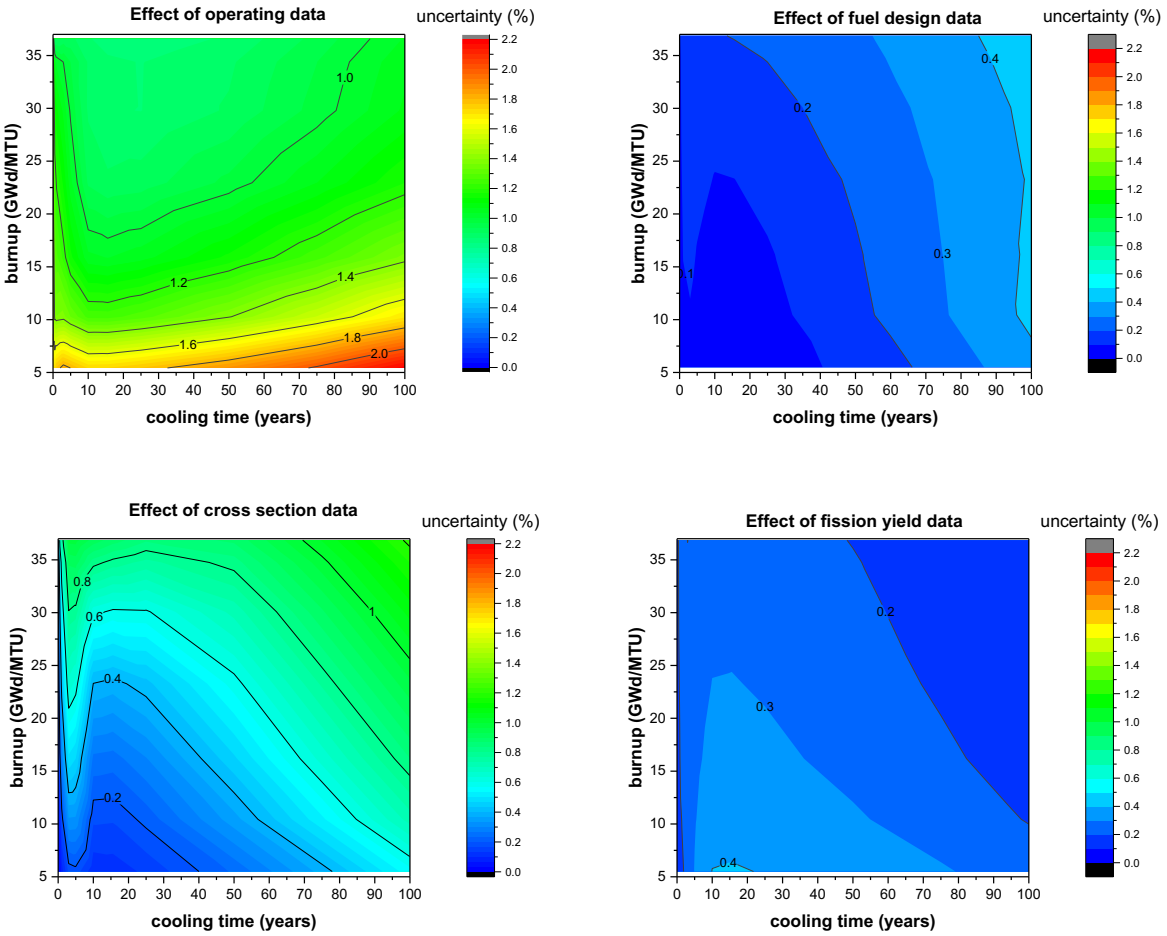

Fig. 9. Decay heat uncertainty as a function of burnup and cooling time.

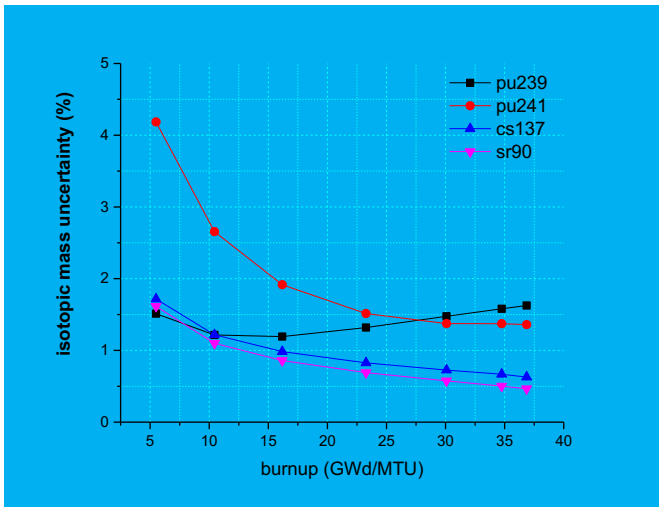

Fig. 10. Uncertainty in selected isotopes' contents vs. burnup.

maximum decay heat uncertainty is observed for low burnup and long cooling time. However, at typical BWR discharge burnups, this uncertainty is less than 1%. Fig. 10 illustrates the uncertainty variation for selected isotopes relevant for decay heat as a function of burnup. For a 5.5 GWD/MTU burnup and 100 years of cooling time, 92% of the total decay heat comes from ^{90}Sr+^{90}Y (31%), ^{137}Cs+^{137m}Ba (28%), ^{241}Am (20%), and ^{239}Pu (14%). At this very low burnup, uncertainties in these isotope contents are greater than 1.5%, with that of ^{241}Am reaching almost 4.5%. The uncertainty in ^{241}Pu, which practically drives the uncertainty in its daughter nuclide ^{241}Am, is greater at low burnups and decreases with increasing burnup.

6. Conclusion

This study evaluates the effect on the calculated decay heat for a typical BWR fuel assembly of uncertainties in nuclear data (cross sections and fission yields) and selected manufacturing and operation parameters. The analysis considered as reference an assembly for which multiple decay heat measurements are available to provide a reference measured decay heat with an accurate estimate of measurement uncertainty. Depletion and decay simulations, along with uncertainty estimations, were performed using computational capabilities and nuclear data in SCALE 6.2.1.

The effect of the perturbed parameters and nuclear data on the calculated decay heat was estimated as a function of burnup and cooling time, for burnups up to 36.9 GWd/MTU and cooling times up to 100 years. Decay heat is an integral metric, and its behavior is driven by variations in the concentrations of those isotopes that are the most important contributors to decay heat. At shorter cooling times, decay heat values and corresponding uncertainties are dominated by fission products. With increasing cooling time, the contribution of the fission products decreases and actinides become dominant players.

The calculated assembly decay heat uncertainty at 15.9 years cooling, which corresponds to the time of measurement for the considered assembly, is not significantly affected by uncertainties in fission product data (0.3%) or fuel design parameters (0.2%). The effect of cross section data uncertainties is similar to the effect of the operating data uncertainties (each ~0.9%). The total uncertainty on the calculated decay heat due to both modeling data and nuclear data uncertainties is ~1.3%. This total modeling uncertainty is comparable with the measurement uncertainty.

The trend of the decay heat uncertainty with burnup and cooling time due to cross section data uncertainties has a similar behavior for the analyzed BWR assembly as previously estimated for PWR used fuel (Williams et al., 2013). The maximum decay heat uncertainty due to uncertainties in either fission yield data or fuel design parameter data is less than 0.45% for the considered burnup and cooling time ranges. The effect of the operating data uncertainty is less than 1% for typical discharge burnups and cooling times less than 100 years.

This study demonstrates a practical approach for evaluating uncertainties in calculated decay heat due to both modeling and nuclear data uncertainties. Though the magnitude of the decay heat uncertainty for the considered assembly is not large, it may vary for other parameter ranges. Quantifying this type of uncertainty can provide useful information and inform decisions on design and operation of used fuel storage facilities, particularly in regimes where measurement data are not available or are not practical to obtain.

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