TECHNICAL BASIS FOR PEAK REACTIVITY BURNUP CREDIT FOR BWR SPENT NUCLEAR FUEL IN STORAGE AND TRANSPORTATION SYSTEMS

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ABSTRACT

Oak Ridge National Laboratory and the United States Nuclear Regulatory Commission have initiated a multiyear project to investigate application of burnup credit for boiling-water reactor (BWR) fuel in storage and transportation casks. This project includes two phases. The first phase (1) investigates applicability of peak reactivity methods currently used in spent fuel pools (SFPs) to storage and transportation systems and (2) evaluates validation of both reactivity (k_{eff}) calculations and burnup credit nuclide concentrations within these methods. The second phase will focus on extending burnup credit beyond peak reactivity. This paper documents the first phase, including an analysis of lattice design parameters and depletion effects, as well as both validation components. Initial efforts related to extended burnup credit are discussed in a companion paper.

Peak reactivity analyses have been used in criticality analyses for licensing of BWR fuel in SFPs over the last 20 years. These analyses typically combine credit for the gadolinium burnable absorber present in the fuel with a modest amount of burnup credit. Gadolinium burnable absorbers are used in BWR assemblies to control core reactivity. The burnable absorber significantly reduces assembly reactivity at beginning of life, potentially leading to significant increases in assembly reactivity for burnups less than 15–20 GWd/MTU. The reactivity of each fuel lattice is dependent on gadolinium loading. The number of gadolinium-bearing fuel pins lowers initial lattice reactivity, but it has a small impact on the burnup and reactivity of the peak. The gadolinium concentration in each pin has a small impact on initial lattice reactivity but a significant effect on the reactivity of the peak and the burnup at which the peak occurs. The importance of the lattice parameters and depletion conditions are primarily determined by their impact on the gadolinium depletion.

Criticality code validation for BWR burnup credit at peak reactivity requires a different set of experiments than for pressurized-water reactor burnup credit analysis because of differences in actinide

compositions, presence of residual gadolinium absorber, and lower fission product concentrations. A survey of available critical experiments is presented along with a sample criticality code validation and determination of undercoverage penalties for some nuclides.

The validation of depleted fuel compositions at peak reactivity presents many challenges which largely result from a lack of radiochemical assay data applicable to BWR fuel in this burnup range. In addition, none of the existing low burnup measurement data include residual gadolinium measurements. An example bias and uncertainty associated with validation of actinide-only fuel compositions is presented.

KEYWORDS
BWR burnup credit, peak reactivity, storage, transportation, spent nuclear fuel

1. INTRODUCTION

Oak Ridge National Laboratory (ORNL) and the United States Nuclear Regulatory Commission (NRC) have initiated a multiyear project to investigate application of burnup credit for boiling-water reactor (BWR) fuel in storage and transportation systems (often referred to as casks) and spent fuel pools (SFPs). This work is divided into two main phases. The first phase investigates the applicability of peak reactivity methods currently used in SFPs to casks and examines the validation of reactivity calculations and depleted number densities within these methods. The second phase will focus on extending burnup credit beyond peak reactivity. This paper documents work performed in the first phase relating to peak reactivity methods. A companion paper being presented at this conference describes work performed to date on the second phase of the project to extend burnup credit beyond peak reactivity [1].

Peak reactivity analyses have been performed for licensing of BWR fuel in SFPs over the last 20 years. These analyses combine credit for the gadolinium burnable absorber present in the fuel assemblies with a modest amount of burnup credit. Gadolinium burnable absorbers are used in BWR assemblies to control core reactivity in the first portion of the fuel cycle. The burnable absorber significantly reduces assembly reactivity at beginning of life but depletes more quickly than ^{235}U, leading to potential increases in assembly reactivity for burnups less than 15–20 GWd/MTU of depletion. The reactivity variation for a number of fuel lattices is shown in Fig. 1, demonstrating peak behavior and its dependence on gadolinium loading. Higher loadings of gadolinium tend to shift the reactivity peak to higher burnup and thus to a lower absolute reactivity. The reduction of the reactivity value at its peak is caused by additional fuel depletion that occurs before the reactivity peak is reached. The objective of the work presented here is to evaluate the application of peak reactivity methods for BWR spent fuel to transportation and storage casks.

Sections 1.1 and 1.2 provide a brief description of the codes and methods, and section 2 describes a series of sensitivity studies performed to examine the effects of depletion and lattice design parameters on peak reactivity of BWR fuel in casks. Section 3 addresses k_{eff} calculation validation efforts associated with peak reactivity analyses. Section 4 discusses depleted composition validation. All work presented in this paper has been published by the NRC [2].

1.1 Code Descriptions

The SCALE code system [3], version 6.1.2, was used for all calculations performed in these studies. The TRITON two-dimensional (2D) lattice physics sequence was used for depletion calculations, and

KENO V.a was used for reactivity calculations in cask geometries. These codes are part of the SCALE code package.

TRITON was used to perform resonance self-shielding, 2D neutron transport, and fuel depletion calculations for each time step of the depletion calculations. Many steps are simulated in sequence in order to perform full depletion calculations simulating exposure in the reactor. The selection of an adequate depletion step size is governed by the depletion of the gadolinium burnable absorber. Steps of approximately 0.5 GWd/MTU were used in the low burnup range before peak reactivity, and ranged up to 3 GWd/MTU after.

The KENO V.a Monte Carlo code was used to perform k_{eff} eigenvalue calculations of the BWR fuel in the GBC-68 computational benchmark model cask [4] using depleted fuel compositions determined with TRITON. The KENO calculations used reflective axial boundary conditions to create an effectively 2D model, as commonly used in the SFP peak reactivity methods. All calculations were performed using the SCALE 238-group ENDF/B-VII.0 neutron cross section library.

Actinide-only (AO) and actinide and fission product (AFP) compositions were used in all studies to determine appropriate modeling approaches for both sets of burnup credit isotopes. The AFP set included gadolinium present as residual burnable absorber material and as a fission product. The AO set did not consider any gadolinium.

1.2 Model Descriptions

The GE14 10 × 10 fuel design type was considered in this work. This selection is based on the design's prevalence in currently operating US BWR plants. While the magnitudes of the effects observed in these studies may differ from those for other fuel design types, the general trends should be consistent across designs. Thus, modeling and design parameters determined to be conservative for the GE14 assembly design should also be conservative for other fuel design types, although additional calculations may be necessary to confirm this premise.

The cask used for storage and transportation configuration calculations is the GBC-68 computational benchmark developed at ORNL as a generic BWR fuel cask [4]. In many ways the GBC-68 is analogous to the GBC-32 cask developed for use in pressurized-water reactor (PWR) burnup credit analyses [5]. The cask design includes 68 fuel storage cells with a B_4C/Al neutron absorber panel inserted between the faces of adjacent storage cells. The absorber panels and basket are assumed to have the same height as the active fuel stack in the fuel assemblies, but these axial details are not included in this work, as only 2D slices of the fuel and cask were modeled. The cask body and basket are stainless steel.

2. SENSITIVITY STUDIES

An acceptable approach was identified for modeling the complex initial and depleted distributions of fissile and absorbing nuclides with the fuel assembly. Detailed models were constructed for baseline calculations to investigate the conservatism of simplified models that can be generated and executed more quickly. Results from this study provided a basic modeling approach used for the remaining sensitivity studies.

Additional studies focused on the impact of lattice design and operational parameters on fuel assembly reactivity. The effects of gadolinium loading (varying both the number of gadolinium-bearing pins and the gadolinium content of these pins), gadolinium pin pattern, void fraction, control blade insertion, and core operating parameters were investigated. Depletion calculations were performed with the same

nuclide set for each set of parameters/conditions being modeled. The depleted isotopic number densities were then decayed for 5 years to represent an approximate minimum post-irradiation cooling time prior to cask loading. The AO and AFP isotope sets were then modeled in the storage/transportation configuration. The reactivity effect of each parameter was established for both isotope sets.

2.1 Results

The isotopic modeling studies examined the representation of fresh fuel and burnable absorber compositions as well as the tracking of compositions during depletion. The two options for modeling initial distributions are pin-specific enrichment (PE) or assembly average enrichment (AE), and the depletion can also be tracked on a pin-specific isotopics (PI) or assembly average isotopics (AI) basis. The most accurate model includes pin-wise initial distributions and depletion tracking (PEPI), though this involves building and executing more complicated models. The simplest approximation is the average enrichment and average depletion (AEAI) approach; in this case, the gadolinium burnable absorber pins are modeled and tracked separately from the non-gadolinium pins. Results for AO and AFP isotopes sets indicated that the AEAI approach yields conservative estimates of cask reactivity by approximately 0.3%–0.5% Δk. All further studies were conducted with this average initial loading and average tracking approach.

The gadolinium loading study consisted of calculations that varied the number of gadolinium pins from 0 to 8 and the gadolinium loading per pin from 0 to 10 wt% Gd_2O_3. The changes in peak reactivity and its burnup were generally as expected: heavier gadolinium loadings had lower reactivity peaks at higher burnups than lighter gadolinium loadings. This effect is shown in Fig. 1. In general, the number of gadolinium pins affects the beginning of life reactivity, while the loading per pin impacts the burnup at which peak reactivity occurs. This is a result of a larger absorber surface area at fresh conditions for a greater number of pins, and greater self-shielding delaying depletion for a higher loading per pin. The results of all the sensitivity studies, which are summarized in Table I, indicate that the gadolinium loading has the greatest impact on peak reactivity of any of the parameters studied.

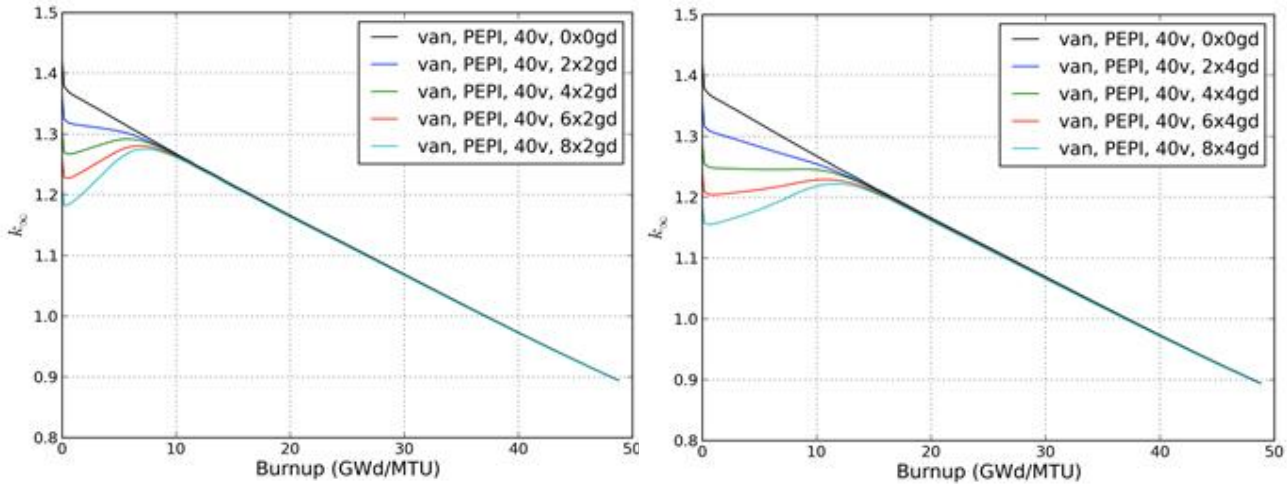
The base case lattice is derived from a realistic set of lattice designs in Ref. [6]. The enrichment zoning is used without alteration, but the gadolinium pin pattern is simplified to a single loading of 2 wt% Gd_2O_3 in six pins. This selection of six pins with a 2 wt% loading is arbitrary, but is selected as it leads to a clear reactivity peak below 10 GWd/MTU that is near a k_{eff} of 0.9. This is the desired burnup range for the reactivity peak since it is representative of design basis lattice designs in current license applications in SFPs. A range of 14 additional gadolinium patterns other than the base case was considered in the gadolinium pattern study. The patterns were constrained such that only pins with fuel in both lattices (vanished and full) and 4.9 wt% ^{235}U enrichment are considered as potential gadolinium pins. Virtually all Gd rods in a vanished lattice also contain Gd in the full lattice. The pattern constraints prevent other changes, like variations in fuel loading, from affecting the results. The gadolinium pattern has a very small impact on results for the AO isotope set and a fairly modest impact on results for the AFP set. Patterns with gadolinium pins grouped together caused lower reactivity peaks at higher burnups because the flux near the pins is suppressed, resulting in slower gadolinium depletion. Patterns with gadolinium pins largely dispersed across the assembly, and especially those with pins near large thermal flux regions, lead to earlier, higher reactivity peaks due to faster gadolinium depletion.

The moderator void fraction was varied over a range from 0% to 80% void, causing a significant change in reactivity for the AO isotope set but a more modest one for the AFP set. High void fractions cause increases in reactivity for the AO set because of spectral hardening and increased plutonium production. Conversely, lower void fractions cause increased reactivity for the AFP isotope set because the lower void fractions cause a more thermalized spectrum, resulting in faster gadolinium depletion. The impact of the

spectrum changes on the gadolinium depletion is the primary factor causing the sensitivity difference between the two isotope sets. The magnitude of the effect is also smaller for the AFP set than for the AO set. It is important to note that the conservative values for analysis are at opposite ends of the range for the two isotope sets for this parameter.

Control blade insertion caused a reactivity increase in both the AO and AFP isotope sets. The control blade contains B_4C as the absorber, so its presence during depletion hardens the neutron spectrum. This causes an increase in plutonium production which leads to higher reactivity in the AO case. The harder spectrum reduces gadolinium depletion, which would be expected to cause a lower reactivity peak at higher burnup. In this case, however, the control blade presence causes a radial shift in the power distribution that increases gadolinium depletion compared to the unrodded depletion. This is a result of the base case pattern having four pins in the quadrant opposite the control blade and only two in the quadrant nearest the blade. This indicates that the effect of control blade insertion is dependent on the gadolinium pattern used in the design basis lattice. It is possible that the sensitivity of reactivity to the gadolinium pattern in rodded conditions is significantly larger than it is in unrodded conditions, but more study is needed to reach a definitive conclusion.

The reactor operating condition studies considered a matrix of fuel temperatures, specific powers, and operating histories. Fuel temperatures of 850K, 950K, and 1100K were considered; the base case was 950K. The specific powers used were 25 W/g, 35 W/g, and 45 W/g, with the base case at 25 W/g. A range of operating histories from the full power base case to half power was considered. Each set of conditions was analyzed, and the effect of each individual parameter was examined. The results were consistent and indicate that each operational parameter has little to no impact on cask reactivity for both the AO and AFP isotope sets at the burnups considered. The primary noteworthy result is that constant, low specific power operation bounds other results for the AFP isotope set.



(a) 2 wt% Gd_2O_3 **(b) 10 wt% Gd_2O_3**

Figure 1. BWR fuel reactivity variation as a function of burnup for different gadolinium loadings, 40% void fraction during depletion.

Table I. Summary of sensitivity study results

Parameter	Range studied	Reactivity impact, AO (%Δk)	Reactivity impact, AFP (%Δk)
Fuel composition modeling	AEAI, PEAI, PEPI	0.3 (AEAI)	0.5 (AEAI)
Number of gadolinium pins	0 to 8 pins (0 pins base case)	~0 (≤0.06 at 7 GWd/MTU)	+1.3 to -0.2 (2 pins to 8 pins)
Loading of gadolinium pins	0 to 10 wt%	0 to 0.5 (9 – 25 GWd/MTU)	-3 to -11 (4 wt% to 10 wt%)
Gadolinium pattern	15 patterns	~0 (±0.03 at 7 GWd/MTU)	±0.25 at peak reactivity (~7.5 GWd/MTU)
Moderator void fraction, unrodded	0 to 80% (40% base case)	-0.4 to +0.7 (0% void to 80% void)	+0.2 to -0.2 (0% void to 80% void)
Moderator void fraction, rodded	0 to 80% (40% base case)	-0.6 to +1.1 (0% void to 80% void)	+0.1 to -0.2 (0% void to 80% void)
Control blade insertion	unrodded vs. rodded (full depletion)	≤ 1 (rodded)	~1.0 (rodded)
Fuel temperature	850 to 1100 K (950 K base case)	~20 pcm / 100 K	0
Specific power	25 to 45 W/g (25 W/g base case)	0.1 (35 and 45 W/g)	-0.1 (peak reactivity)
Operating history	4 histories (FP base case)	-0.1	0.1 (HP case)

3. CRITICALITY CALCULATION VALIDATION

The primary purpose of the work documented in this section is to identify a suitable set of critical experiments to validate criticality (k_{eff}) calculations for casks containing BWR fuel at peak reactivity. This could be challenging given the relatively low burnup at which peak reactivity occurs. The fuel compositions in this burnup range have sufficient burnup to contain noticeable quantities of plutonium yet a low enough burnup that the uranium enrichment is still significantly above natural. Most mixed-oxide critical experiments use natural or depleted uranium, so the presence of enriched uranium with plutonium is problematic. The plutonium isotopic distribution is also very different from higher burnup discharged assembly compositions that have a significantly larger fraction of ^{240}Pu; at peak reactivity nearly 90% of the plutonium is ^{239}Pu. Also, few experiments are available for validation of gadolinium or fission products. Past studies have identified only a limited number of experiments that may be applicable to validation of BWR fuel in storage configurations at peak reactivity [7].

3.1 Methodology

The reactivity calculation validation was performed using the SCALE [3] code system's Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) suite [8]. TSUNAMI uses forward and adjoint KENO Monte Carlo calculations to generate sensitivity data files (SDFs) for each benchmark experiment or application. TSUNAMI is also capable of performing similarity assessments that quantify the similarity of the sensitivity data between SDFs of the application and experiment.

The metric used to assess similarity is the c_k value, which is a correlation coefficient. The c_k value is determined by dividing the covariance between the experiment and application by the product of the uncertainties in the experiment and the application, as shown in Equation 1,

$$c_k = \frac{\sigma^2_{AppExp}}{\sigma_{App}\sigma_{Exp}}, \quad (1)$$

where:

c_k is the similarity between an application and an experiment,
σ^2_{AppExp} is the covariance between the application and the experiment,
σ_{App} is the uncertainty in the application k_{eff} based on cross-section covariances, and
σ_{Exp} is the uncertainty in the experiment k_{eff} based on cross-section covariances.

The determination of similarity was made by comparing GBC-68 [4] cask model applications to a variety of critical experiments. Each application was compared to each experiment using sensitivity data generated for both systems. While a c_k of 1 represents identical systems, a c_k value of 0.8 or higher is viewed as acceptable similarity for validation [8].

3.2 Sources of Sensitivity Data

SDFs are required for each application and each experiment for which a similarity assessment is desired. These data were collected for experiments from three sources: the VALID library maintained at ORNL [9], SDFs generated by the Nuclear Energy Agency (NEA) [10], and sensitivity data used in NUREG/CR-7109 [7]. The NEA data contain SDFs for more than 1000 low-enriched uranium (LEU) experiments and 225 mixed uranium and plutonium (MIX) systems. A total of 123 LEU-COMP-THERM (LCT) and 49 MIX-COMP-THERM cases are included from the VALID library. Almost 200 SDFs involving MIX systems, including the Haut Taux de Combustion (HTC) experiments, were drawn from the collection of data used in NUREG/CR-7109. Pooled together, these three sources provided SDFs for 1643 unique critical experiments with a thermal neutron energy spectrum (THERM).

3.3 Potentially Applicable Experiments

The critical experiments were compared with three GBC-68 application models: a GE14 vanished lattice (i.e., use of part-length rods in lower sections of the assembly leave empty lattice positions) with AO fuel compositions, a GE14 vanished lattice with AFP fuel compositions, and a GE14 full lattice with AFP fuel compositions. All three models included fuel at a peak reactivity burnup of approximately 7.5 GWd/MTU. The number of applicable experiments with a c_k no less than 0.8 for each case was 71 for the AO vanished lattice, 62 for the AFP vanished lattice, and 51 for the AFP full lattice. These cases are listed in Table II. Distribution of c_k values for the AFP vanished lattice is shown in Fig. 2, and a plot including only cases with c_k values of 0.8 or greater is shown in Fig. 3.

The experiments with the highest c_k values are all taken from experiments performed with the same fuel at the Babcock and Wilcox Lynchburg Research Center and currently comprise LCT-008, LCT-011, and LCT-051 in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [11]. The 44 highest c_k values for the AO and AFP vanished lattice cases come from these experiment series. Ideally, a range of experiments from different facilities involving different fuel, experimental facilities, and experimenters would provide a broader range of similar experiments to consider. The potential for correlation among the experiments might need to be considered when a large number of experiments are used incorporating many similar features. Although the impact of experiment correlation has been

investigated [12], it is as yet unclear whether the impact would be significant in this case. At this time, the applicable consensus standard on validation [13] requires validation with experiments that are as similar as possible to the safety application and does not address the potential impact of experimental correlations. It is also possible that using a large number of experiments from the same set or facility will include a systematic bias that results from the material, machine, measurements, or techniques used in the experiment. Such a bias, if it exists, would be impossible to detect without additional experiments from different facilities, and could reduce or eliminate a bias within the computational method being validated.

A data assimilation tool such as TSURFER could be used to incorporate potentially useful experiments that have low similarity to the GBC-68 application. Data assimilation techniques can use data from dissimilar experiments to determine potential adjustments to cross sections in these situations and then determine the effect of those adjustments on the application case. These techniques have not been applied previously in licensing a criticality safety analysis in the US and are therefore not considered in this work.

Table II. Critical experiments with c_k values of 0.8 or greater

AO Vanished Lattice		AFP Vanished Lattice		AFP Full Lattice	
Evaluation	***Cases***	***Evaluation***	***Cases***	***Evaluation***	***Cases***
LCT-005	10–11	**LCT-005**	10	**LCT-008**	1–17
LCT-008	1–17	**LCT-008**	1–17	**LCT-011**	2–11
LCT-011	2–15	**LCT-011**	2–15	**LCT-014**	5
LCT-014	5	**LCT-014**	1	**LCT-047**	1
LCT-015	26, 129, 146, 151, 158	**LCT-015**	151	**LCT-051**	2–12, 15–18
LCT-036	25–26	**LCT-017**	26–27	**LCT-076**	1–7
LCT-047	1, 3	**LCT-047**	1		
LCT-051	1–12, 15–19	**LCT-051**	1–12, 15–19		
LCT-052	3, 6	**LCT-055**	1		
LCT-055	1–2	**LCT-076**	1–7		
LCT-076	1–7				

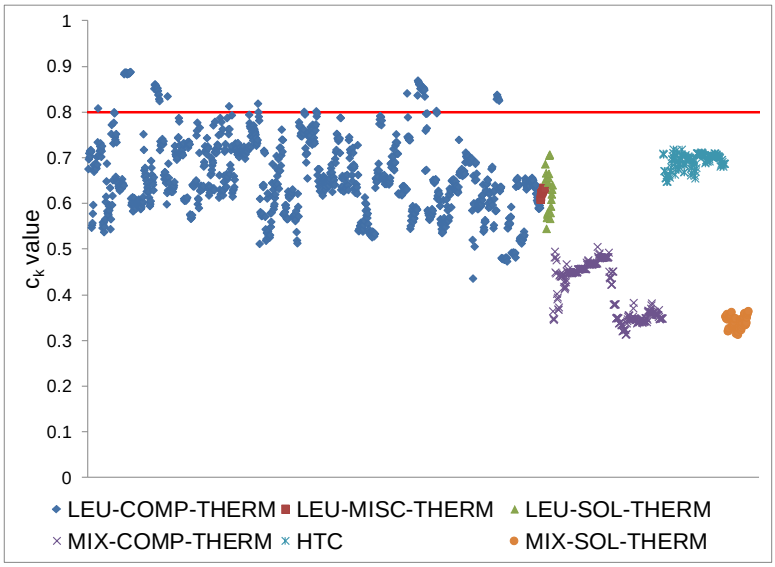


Figure 2. c_k values for critical experiments compared with GBC-68 with vanished lattice and AFP isotopics.

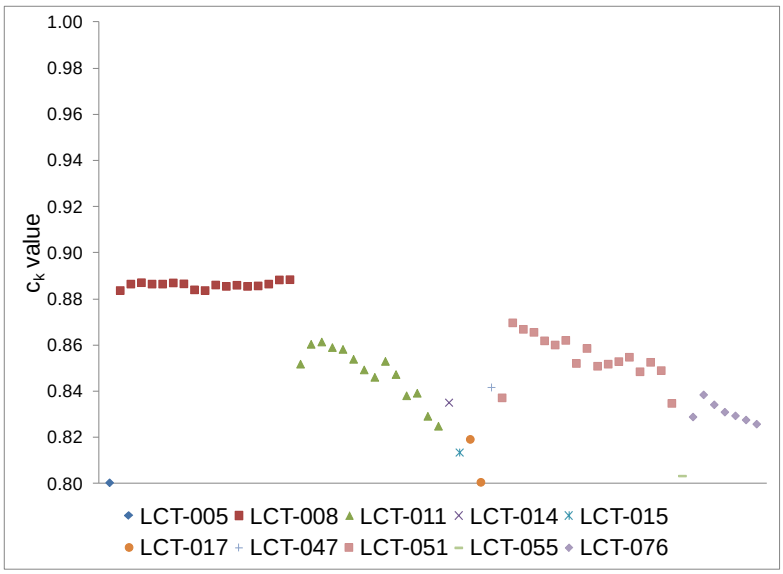


Figure 3. c_k values in excess of 0.8 for critical experiments compared with GBC-68 with vanished lattice and AFP isotopics.

3.4 Determination of Bias and Uncertainty

The potential bias and bias uncertainty that could result from a validation for a peak reactivity analysis of BWR fuel in a storage and transportation cask was examined briefly. The analysis was not intended to be a rigorous and complete validation and should not be viewed as a complete example validation. Results were determined only for the vanished lattice with AFP fuel compositions and are presented for a non-trending method, a traditional trending analysis considering enrichment, and a TSUNAMI-based trend of c_k values.

The bias and bias uncertainty results are similar among all three methods. The reported uncertainties for all methods represent a 95% probability and a 95% confidence level, and all values are reported in Δk units. The non-trending method results in a bias of -0.00354 with an associated uncertainty of 0.00526. The bias and bias uncertainty from the enrichment trend, for the 3.51 wt% ^{235}U enrichment of the fuel at peak reactivity, are -0.00136 and 0.00604, respectively. The c_k trend results in a bias of -0.00275 with an uncertainty of 0.00695. The total of the bias and bias uncertainty for these three methods ranges from -0.00740 to -0.00970, indicating generally good agreement among the methods.

3.5 Validation Gap Analysis

All potentially useful experiments identified in this work are LCT experiments involving arrays of LEU fuel pins moderated with light water. This presents validation gaps for plutonium, gadolinium, and other actinides and fission products. These gaps, caused by insufficient representation of these isotopes in the critical experiments similar enough to the application model to be useful for validation, can be accounted for with a reactivity penalty derived from uncertainty analysis. TSUNAMI calculates the uncertainty in system k_{eff} caused by cross section uncertainties by combining the nuclear data covariances with the calculated sensitivities. These k_{eff} uncertainties, representative of the 1 standard deviation level, provide a quantitative estimate of the bias expected to result from potential nuclear data errors because the error in the cross section is expected to be bounded by its uncertainty [8]. The use of this sensitivity/uncertainty analysis has been used previously in NUREG/CR-7109 [7]. The penalty factors are doubled to provide

additional conservatism leading to penalty factors for lack of validation that are approximately 0.3% Δk for plutonium and americium, 0.05% Δk for residual gadolinium, and 0.06% Δk for major fission products and minor actinides. The plutonium penalty is the largest because the system sensitivity to plutonium is significantly higher than it is to the other nuclides. The major fission product and minor actinide penalty is small enough that the penalty factor recommended in NUREG/CR-7109, 1.5% of the worth of the fission products and minor actinides, could conservatively be applied instead. Additional critical experiments utilizing a mixed uranium/plutonium oxide fissile material representative of the low burnup fuel compositions in an appropriately moderated system could significantly improve the suite of available experiments for validating BWR peak reactivity applications.

4. VALIDATION OF SPENT FUEL NUCLIDE COMPOSITIONS

This section provides a review of studies performed to validate the spent fuel nuclide concentrations in BWR spent fuel at peak reactivity, and the bias and uncertainty in the cask reactivity calculations associated with uncertainties in the spent fuel composition. Validation of calculated spent fuel compositions is performed by comparison of calculated and measured isotopic concentrations in spent fuel samples from BWR assemblies obtained by destructive radiochemical analysis. This approach to validating the spent fuel calculations for use in criticality analyses is broadly accepted and applied by the international nuclear criticality safety community [14].

4.1 Applicable Experimental Data

Validation of calculated spent fuel compositions for BWR fuel is challenging due to a limited number of measured samples that are publicly available for code benchmarking. Experimental data for burnups near peak reactivity are further limited since these burnups are generally lower than typical burnup values of measured BWR fuel samples from discharged fuel assemblies. In addition, much of the applicable validation data identified in this study are available from experimental programs performed in the 1970s and 1980s. These studies involved older assembly designs, and the measurements did not include many of the fission products currently considered in burnup credit. The availability of applicable experimental data for validation has a direct impact on the ability to validate the nuclides considered in a criticality safety analysis, and it also influences the burnup credit approach (e.g., AO, AFP, or a reduced set of nuclides).

The main characteristics of the spent fuel samples identified in this study as applicable to depletion code validation are summarized in Table III. The burnup range of the 16 BWR fuel samples is between 2.77 and 27.18 GWd/MTU, which encompasses the assembly peak reactivity burnup values (i.e., less than ~20 GWd/MTU) associated with different gadolinium concentrations and configurations analyzed in this work (see Fig. 1). The three PWR samples are included because they are the only measurements of gadolinium isotopes in a gadolinium burnable absorber rod with a burnup below 30 GWd/MTU. These data include samples with burnups exceeding the region of peak reactivity and were included to evaluate potential trends in the data in the low burnup regime.

The available measurement data for the actinide nuclides ^{234}U, ^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu in BWR fuel samples within the burnup range associated with peak reactivity provide the technical basis for the depletion code validation in terms of k_{eff} uncertainty presented here. Only the GBC-68 application model with GE14 vanished lattice and AO fuel compositions is included in this section. A model with AFP fuel compositions would require applicable fission product validation data from radiochemical assay measurements of BWR fuel near peak reactivity, which is not publicly available at this time.

Table III. Evaluated experimental spent fuel nuclide data

Reactor name	Reactor type	Lattice type	Measured fuel rod type	Number of samples	Enrichment (wt % ^{235}U)	Burnup (GWd/MTU)	Gadolinium isotope measurements
Gundremmingen-A	BWR	6 × 6	UO_2	8	2.53	14.39	No
						15.84	No
						17.49	No
						21.24	No
						22.25	No
						22.97	No
						23.51	No
						25.19	No
JPDR	BWR	6 × 6	UO_2	4	2.597	2.77	No
						3.38	No
						4.13	No
						4.35	No
Fukushima-Daini-2	BWR	8 × 8-2[b]	UO_2–Gd_2O_3	4	3.41	16.65	No
						21.83	No
						22.63	No
			UO_2	1	3.91	27.18	No
Ohi-2 [a]	PWR	17 × 17	UO_2–Gd_2O_3	3	3.20	21.92	Yes
						29.45	Yes
						25.73	Yes

[a] PWR fuel samples analyzed to obtain data on residual ^{155}Gd in gadolinium-bearing fuel rods.
[b] An 8 × 8 lattice design with two water rods.

4.2 Bias and Uncertainty Determination

The bias and bias uncertainty values associated with BWR nuclide compositions within the burnup range characteristic to a BWR assembly reactivity peak are presented in this section. The nuclides with available validation data considered in this study include ^{234}U, ^{235}U, ^{238}U, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, and ^{155}Gd (residual and fission product). The analysis does not include ^{241}Am due to large measurement uncertainties. In addition, fission products are not included due to the lack of adequate measurement data. The bias and uncertainty in the calculated nuclide compositions are derived directly from comparisons of the calculated and measured nuclide concentrations. The nuclide bias, X_i^j, is calculated as the ratio of the measured concentration to the calculated concentration. The average ($\overline{X}_i$) and standard deviation (s_i) for each isotope, i, is then calculated over all samples, j, using standard statistical formulae. Further modifications are made to the average ($\overline{X}_i$) to ensure conservative analysis results, including no reduction of the predicted concentration of fissile species and no increase in the predicted concentration of absorbing species. After adjustment, the average prediction of the nuclide concentration is converted into the "nuclide bias," $\overline{X}_i'$. A one-sided 95/95 tolerance factor is also determined for each isotope based on the number of samples in the population. The results of the determinations are shown in Table IV.

A number of methods for calculating k_{eff} uncertainty associated with uncertainties in calculated nuclide concentrations in spent fuel have previously been explored. The methods investigated in NUREG/CR-6811 [15] include both conservative bounding and best estimate approaches to uncertainty estimation. The bounding method applies bias and uncertainty associated with calculated isotopic concentrations in a way that maximizes the k_{eff} uncertainty value. This method increases the concentrations of the fissile nuclides based on their individual nuclide uncertainties estimated from validation studies, and it decreases the concentrations of the neutron absorbing nuclides.

The bounding method for uncertainty determination was applied for BWR fuel near peak reactivity in this study. Specifically, the predicted concentrations of the fissile nuclides in Table IV (i.e., ^{235}U, ^{239}Pu, and ^{241}Pu) are adjusted to their upper one-sided 95%/95% tolerance limit values [16] to account for the uncertainty in the calculations as determined from the experimental data. The concentrations of all neutron-absorbing nuclides (i.e., ^{234}U, ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{155}Gd) are adjusted to their lower one-sided tolerance limit values.

This approach requires two criticality calculations to be performed for the application model. The first calculation applies the nuclide concentrations as calculated directly by the depletion code without any corrections. The second calculation applies nuclide concentrations adjusted for estimated bias and uncertainty. The difference in the system eigenvalues between these calculations provides a direct and bounding estimate of the bias and uncertainty associated with the calculated nuclide compositions.

The uncertainty in k_{eff} associated with nuclide biases and bias uncertainties was determined for the GBC-68 cask application model. The k_{eff} margin for uncertainty was calculated as the difference between the k_{eff} value using nuclide concentrations adjusted for bias and uncertainty and the k_{eff} value using calculated nuclide concentrations (i.e., base case). The bias and uncertainty values used and the one-sided tolerance limit factors for 95% probability and 95% confidence level are listed in Table IV. The calculated k_{eff} margin for uncertainty due to the calculated nuclide concentrations is 0.0165 (1.65% Δk).

Table IV. Isotopic bias and bias uncertainty values associated with calculated BWR isotopic concentrations

Isotope	No. of samples	Burnup range (GWd/MTU)	Mean $\overline{X}_i$	Nuclide bias ($\overline{X}_i'$)	Standard Deviation (s_i)	One-sided tolerance limit factor [c] (k_1)
^{234}U	8	2.77–27.18	0.969	0.969	0.040	3.187
^{235}U	16	2.77–27.18	0.985	1.000	0.023	2.524
^{238}U	16	2.77–27.18	1.000	1.000	0.002 [b]	2.524
^{238}Pu	16	2.77–27.18	1.039	1.000	0.098	2.524
^{239}Pu	16	2.77–27.18	0.950	1.000	0.039	2.524
^{240}Pu	16	2.77–27.18	0.967	0.967	0.048	2.524
^{241}Pu	16	2.77–27.18	1.059	1.059	0.129	2.524
^{242}Pu	16	2.77–27.18	1.012	1.000	0.121	2.524
^{155}Gd [a]	3	21.47–29.45	2.440	1.000	1.719	7.656

[a] Surrogate isotopic validation data from gadolinium-bearing PWR UO_2 fuel samples.
[b] Standard deviation for ^{238}U values was doubled to account for the non-normality of the distribution.
[c] One-sided 95%/95% tolerance limit factors.

5. CONCLUSIONS

The physics of BWR fuel depletion are well understood, reliable, and predictable in their calculated effects on discharged fuel reactivity near peak reactivity. A conservative set of analysis conditions can be identified and implemented to allow criticality safety analysis of BWR spent fuel at peak reactivity in storage and transportation systems. The conservative set of parameters used in any analysis will be dependent on the methodology developed and implemented by an applicant, including the specific set of isotopes credited in the analysis. A summary of the results of the sensitivity studies performed is provided in Table I. This work has not identified any apparent technical reasons to preclude implementation of peak reactivity methods in BWR fuel storage and transportation casks.

Validation of criticality calculations can be performed in compliance with the consensus standard [13] and prior NUREG/CR recommendations [17, 18]. The bias determined for SCALE 6.1 for these systems ranges from -0.00140 to -0.00350 Δk and the bias uncertainty ranges from approximately 0.00525 to 0.00700 Δk with the three validation techniques used. Example penalty factors have been determined that would allow extension of the validation area of applicability to account for isotopes that cannot be validated with critical experiments at this time. The penalty factors, which are not generically applicable to other casks, are 0.3% Δk for plutonium and americium, 0.05% Δk for residual gadolinium, and 0.06% Δk for fission products. Overall, the validation of cask reactivity calculations does not present a technical barrier that would prevent implementation of peak reactivity methods for demonstrating the criticality safety of BWR fuel in storage and transportation canisters.

A method for determining the uncertainty in k_{eff} calculations associated with the BWR spent fuel nuclide concentrations near peak reactivity has been demonstrated for the GBC-68 cask model. This method is based on the direct application of measured BWR spent fuel composition data to estimate the uncertainties associated with the calculated nuclide composition used in burnup credit application models. The resulting k_{eff} margin is 1.65% Δk.

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