

COMPARISON OF BURNUP CREDIT UNCERTAINTY QUANTIFICATION METHODS

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ABSTRACT

The recent revision of Interim Staff Guidance (ISG-8 revision 3), issued by the US Nuclear Regulatory Commission, on burnup credit for criticality safety analysis of pressurized water reactor spent fuel in transportation and storage casks expands the nuclides that can be credited in the fuel composition to include minor actinides and fission products. The technical basis for development of the uncertainties associated with calculated nuclide concentrations in spent nuclear fuel that are recommended in ISG-8 was established through the use of measured isotopic data acquired from destructive radiochemical assay data for spent fuel samples. These data provide a direct experimental basis for determining uncertainties in the calculated nuclide concentrations. To provide additional insight into code uncertainties resulting from nuclear data and also the level of conservatism associated with using experimental assay benchmark data for uncertainty evaluation, a new uncertainty analysis tool in the SCALE code system that performs stochastic sampling of nuclear data has been applied to representative burnup credit calculations for spent fuel pool and dry cask storage applications methodology. The nuclear data uncertainty analysis capabilities in Sampler can account for uncertainty contributions from cross sections, fission yields, and decay data by using correlated sampling of covariance files developed for all nuclear data used by SCALE. These uncertainties associated with nuclear data evaluations are compared to corresponding values developed in ISG-8 that are based on destructive assay data, as well as to values obtained using an alternate methodology that was developed by the Electric Power Research Institute based on reactor core simulation data.

Key Words: ISG-8, burnup credit, stochastic sampling, SCALE, Sampler, uncertainty analysis

1 INTRODUCTION

The criteria for establishing subcriticality with burnup credit may be given in terms of bias and bias uncertainty terms [1] as

$$k_p(bu) + \Delta k_p(bu) + \beta + \Delta k_\beta + \Delta k_x + \Delta k_m + \beta_i(bu) + \Delta k_i(bu) \leq k_{limit}, \quad (1)$$

where k_p is the calculated multiplication factor for the system under consideration (e.g., spent fuel pool, storage, or transport cask) with Δk_p the associated uncertainty, which includes only statistical (convergence-related), material/fabrication, and geometric uncertainty; β is the bias

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resulting from the criticality calculation method (including nuclear data bias) with Δk_β the associated uncertainty; Δk_x is a supplement to the previous bias and uncertainty term; Δk_m is the administrative margin; $\beta_i(bu)$ is a depletion/decay code bias with $\Delta k_i(bu)$ the associated uncertainty in that bias; and k_{limit} is the declared upper limit on multiplication factor k_{eff} . Note that all Δk bias uncertainty terms are one-sided, 95%-coverage tolerance intervals with 95% certainty (95/95) [1].

The main focus of this paper is to discuss the calculation of the contribution of $\Delta k_i(bu)$ that is due solely to basic nuclear data uncertainty and discuss the result in the context of two recently reported approaches to calculate Δk_i and β_i from Eq. (1):

1. the recent revision of the Interim Staff Guidance (ISG-8 revision 3) [2] and
2. the Electric Power Research Institute's (EPRI) "Benchmarks for Quantifying Fuel Reactivity Depletion Uncertainty" [3].

The new Sampler uncertainty analysis tool in the SCALE code system [4] is used to predict the portion of Δk_i due to basic nuclear data uncertainty. Sampler can account for uncertainty contributions from cross sections, fission yields, and decay data by using correlated sampling of covariance files developed for all nuclear data used by SCALE.

1.1 Overview of ISG-8 Recommendations

The recent revision of ISG-8 (revision 3) on burnup credit for criticality safety analyses of pressurized water reactor (PWR) spent fuel in transportation and storage casks issued by the US Nuclear Regulatory Commission [2] expands the nuclides that can be credited in the fuel composition to include minor actinides and fission products. The total estimated uncertainty associated with the calculation of nuclide compositions, expressed as the net relative impact on the calculated multiplication factor value, is <1.6% (95% confidence level) for typical PWR fuel with a burnup less than about 40 GWd/MTU [1]. This uncertainty value is based on an analysis of radiochemical assay data (RCA) from destructive analysis measurements of the nuclide compositions for approximately 100 PWR spent fuel samples.

The ISG-8 discusses

1. limits for the licensing basis,
2. assessment of licensing basis model assumptions,
3. validation of depletion/decay codes,
4. validation of criticality codes, and
5. loading curve and burnup verification.

The recommendations in ISG-8 surrounding validation of depletion and decay codes and determination of Δk_i and β_i terms are largely based on the studies summarized in [1], using the SCALE 6.1 code system with ENDF/B-VII.0 data.

The ISG-8 recommends that available data only support allowance for burnup credit using major actinide compositions only (i.e., actinide-only burnup credit) or limited actinide and fission product compositions (Figure 1) associated with uranium dioxide (UO₂) fuel irradiated in a PWR up to an assembly-average burnup value of 60 gigawatt-days per metric ton uranium (GWd/MTU) and cooled out-of-reactor for a time period between 1 and 40 years. The range of available measured assay data for irradiated UO₂ fuel supports enrichment up to 5.0 wt % in ²³⁵U.

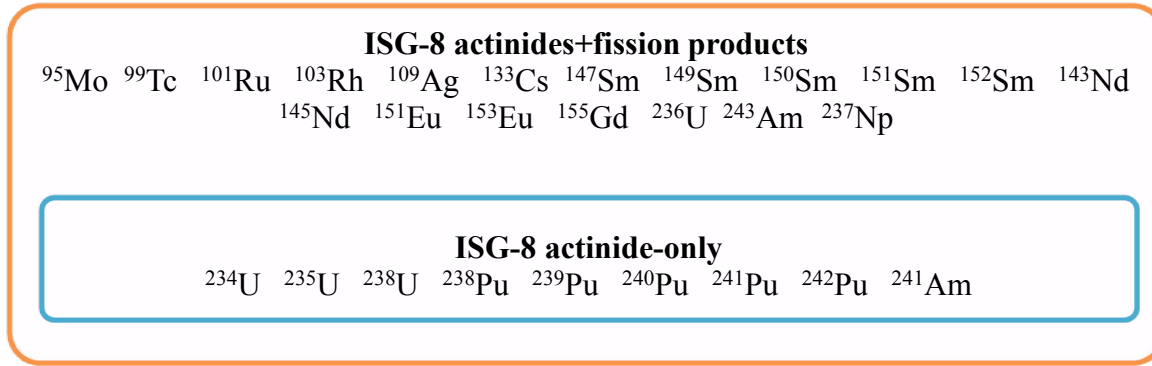


Figure 1. ISG-8 recommended nuclide sets for burnup credit

1.1.1 ISG-8 isotopic validation

The depletion/decay code validation recommended by the ISG-8 requires assessment of the distribution of isotopic concentration biases, in terms of the mean isotopic bias (\bar{X}_n) and isotopic bias uncertainty (σ_n), for each burnup credit nuclide n using RCA data. The RCA data used should include detailed information about the samples, including the pin location in the assembly, axial location of the sample in the pin, any exposure to strong absorbers, boron letdown, moderator temperature, specific power, and any other cycle-specific data for the cycles in which the samples were irradiated.

To determine the k_{eff} bias (β_i) and uncertainty in that bias (Δk_i) as needed by Eq. (1), a Monte Carlo sampling procedure has been developed with SCALE 6.1 and ENDF/B-VII.0 nuclear data [1], which effectively "transforms" the distribution of isotopic concentration biases determined from the analysis of spent fuel assay measurements to a distribution of k_{eff} biases for a particular configuration (e.g., transport cask or spent fuel pool). This Monte Carlo procedure is a robust extension of the "direct difference" method, where criticality calculations are performed directly using measured RCA isotopics, without the need to assess the bias and uncertainty distributions of each burnup credit nuclide, and the resulting impact on k_{eff} is assessed. A shortcoming of the direct difference method is that not all RCA data sets have the same isotopes; therefore, to ensure a consistent comparison, for each calculation it becomes necessary to fill in gaps with surrogate data for the isotopes that were not measured in a particular sample. On the other hand, the Monte Carlo procedure considers each isotope individually and uses the available data across all measurements to develop a bias distribution for each isotope, taking into account the additional uncertainty implied by finite sample sizes (i.e., isotopes with fewer measurements will have an additional uncertainty contribution). The Monte Carlo, direct difference, and the older, more conservative "isotopic correction factor" methods used to transform isotopic bias and uncertainty to k_{eff} bias and uncertainty are reviewed in ISG-8 [2] and discussed in detail in Ref. [1].

1.1.2 ISG-8 results

Table I shows k_{eff} bias results for the representative PWR Spent Fuel Pool (SFP) model described in Section 5.2 (results shown in Table 7.1) of Ref. [1].

Table I. Summary of isotopic bias and uncertainty (pcm) from [1] for actinides and fission products using TRITON in SCALE 6.1

Burnup (GWd/MTU)	10	25	30	40
β_i	340	340	280	340
Δk_i	1500	1540	1480	1680

The ISG-8 recommendation in Table II is based on the above data but simplified to have zero bias and to be used for both SFP and transport cask models (see Table 3 in Ref [2]). Note that beyond 40 GWd/MTU the bias uncertainty increases due to the limited quantity and quality of RCA data for the high-burnup range.

Table II. Summary of ISG-8 recommended isotopic bias and uncertainty (pcm) from [2] for actinides and fission products using TRITON in SCALE 6.1 (pcm)

Burnup (GWd/MTU)	5-10	18-25	25-30	30-40	45-50	50-60
β_i	0	0	0	0	0	0
Δk_i	1480	1540	1610	1630	2190	3000

1.2 Overview of EPRI Methodology

The EPRI methodology [3] uses experimental data from another source to determine the “reactivity decrement uncertainty”: standard flux trace measurements during PWR operation. The final expression for the EPRI method bias uncertainty (2-sigma) due to depletion effects is given as

$$\Delta k_i(bu) = 2\sqrt{\left(s_{k_\infty}^{HFP,base}\right)^2 + \left(s_{k_\infty}^{T_{fuel}}\right)^2 + \left(s_{k_\infty}^{*data}(bu)\right)^2}, \quad (2)$$

consisting of three independent terms. These terms are given as standard deviations, s , with

1. a conservative (burnup-independent) hot full power (HFP) base term, $s_{k_\infty}^{HFP,base}$;
2. a conservative fuel (burnup-independent) temperature uncertainty term, $s_{k_\infty}^{T_{fuel}}$; and
3. a burnup-dependent HFP-to-cold condition plus nuclear data uncertainty term, $s_{k_\infty}^{*data}(bu)$.

The total bias and bias uncertainty (i.e., including all nuclides) according to the EPRI method is shown in Table III, directly extracted from [3], where components uncertainties were always presented as 2-sigma uncertainties. However, the formulas in this section [Eqs. (2)–(11)] are *not* explicitly shown in [3] and represent the authors’ interpretation of the text and tables.

Table III. Summary of EPRI isotopic bias and uncertainty (pcm) from [3] for all nuclides using CASMO-4/CASMO-5 and SIMULATE-3

Burnup (GWd/MTU)	10	20	30	40	50	60
β_i (CASMO-4)	81	140	178	196	192	167
β_i (CASMO-5)	19	46	81	125	177	238
$\Delta k_i(bu)$	521	576	571	560	544	534
$2 s_{k_{\infty}}^{HFP,base}$	250	250	250	250	250	250
$2 s_{k_{\infty}}^{T_{fuel}}$	255	255	255	255	255	255
$2 s_{k_{\infty}}^{*data}$	380	452	446	430	410	398

1.2.1 HFP reactivity decrement bias and uncertainty

Based on CASMO-4 or CASMO-5 data, the nodal simulator SIMULATE-3 [3] can simulate the fission chamber detector response, expressed as a core-normalized, detector reaction rate shape. Flux maps from 44 cycles of Catawba Units 1 and 2 and McGuire Units 1 and 2 were used to determine burnup corrections, Δx_m , for each group of assemblies m , according to

$$\min_{\Delta x_m} \sum_{n \in m} (C_{rr}^n(bu_n + \Delta x_m) - M_{rr}^n)^2, \quad (3)$$

where n is a measurement index (many assemblies are measured and many times per cycle), and bu_n is the calculated assembly burnup, C_{rr}^n is the calculated assembly-average reaction rate (changing with search parameter Δx_m), and M_{rr}^n is the measured reaction rate. The burnup corrections imply a reactivity correction (error)

$$\Delta k_{\infty}^{HFP,m}(bu_n) = k_{\infty}^{HFP}(bu_n + \Delta x_m) - k_{\infty}^{HFP}(bu_n). \quad (4)$$

Linear or quadratic regression analysis is performed on the reactivity error data,

$$\beta_i(bu) = regress(\Delta k_{\infty}^{HFP,m}(bu_n)), \quad (5)$$

in order to determine the mean bias as a function of burnup, $\beta_i(bu)$. The uncertainty in the bias is calculated using a second set of reactivity decrement data in which the lumped fission product (LFP) cross-section data in the CASMO-4 library was set to zero,

$$s_{\Delta k_{\infty}}^{HFP,base} = \max_{bu} |\beta_i(bu) - \beta_i^{no LFP}(bu)|. \quad (6)$$

The maximum error between the “no LFP” library and the nominal library was found to be $s_{\Delta k_{\infty}}^{HFP,base} = 125$ pcm.

1.2.2 Fuel temperature uncertainty

Using the maximum and minimum fuel temperatures given by the fuel performance modeling code INTERPIN [3], $T_{\max} = 946\text{K}$ and $T_{\min} = 897\text{K}$ over the 60 GWd/MTU burnup range, the maximum differences between multiplication factors at HFP conditions,

$$s_{\Delta k_{\infty}}^{HFP, T_{fuel}} = \max_{bu} |k_{\infty}^{HFP}(T_{\max}, bu) - k_{\infty}^{HFP}(T_{\min}, bu)|, \quad (7)$$

and cold conditions (293K),

$$s_{\Delta k_{\infty}}^{cold, T_{fuel}} = \max_{bu} |k_{\infty}^{cold}(T_{\max}, bu) - k_{\infty}^{cold}(T_{\min}, bu)|, \quad (8)$$

were calculated. The maximum differences were -150 pcm at HFP conditions and +206 pcm at cold conditions. These were statistically combined into a **2-sigma** burnup decrement uncertainty,

$$\left(2 s_{\Delta k_{\infty}}^{T_{fuel}}\right)^2 = \left(s_{\Delta k_{\infty}}^{HFP, T_{fuel}}\right)^2 + \left(s_{\Delta k_{\infty}}^{cold, T_{fuel}}\right)^2, \quad (9)$$

yielding a total uncertainty of 255 pcm due to fuel temperature.

1.2.3 HFP-to-cold condition uncertainty including nuclear data

In order to determine the HFP-to-cold condition uncertainty, including nuclear data, SCALE/TSUNAMI is used to estimate the correlation of uncertainties in the HFP and the SFP systems, and the following formula is applied [3]:

$$\left(s_{\Delta k_{\infty}}^{data}\right)^2 = \left(s_{\Delta k_{\infty}}^{HFP, data}\right)^2 + \left(s_{\Delta k_{\infty}}^{cold, data}\right)^2 - 2\rho s_{\Delta k_{\infty}}^{HFP, data} s_{\Delta k_{\infty}}^{cold, data}, \quad (10)$$

where ρ is the correlation coefficient calculated by TSUNAMI for the HFP and cold (SFP) systems. This formula implies no nuclear data uncertainty at HFP conditions, and a portion of the nuclear data uncertainty at other conditions is based solely on the nuclear data correlation coefficient between the two systems. All terms in the above formula are burnup dependent, with correlations greater than 0.98 in many cases. The maximum (2-sigma) nuclear data uncertainty is estimated to be 555 pcm and occurred at 20 GWd/MTU. Although the nuclear data uncertainties calculated for both HFP and SFP conditions are monotonically increasing, the correlation coefficient has a minimum value at 20 GWd/MTU, which creates the maximum uncertainty with respect to burnup.

A final correction to the nuclear data uncertainty term is applied to reduce the uncertainty for fresh fuel. The minimum uncertainty at zero burnup in a matrix of test cases is statistically subtracted from the nominal data set,

$$\left(s_{\Delta k_{\infty}}^{*data}(bu)\right)^2 = \left(s_{\Delta k_{\infty}}^{data}(bu)\right)^2 - \left(s_{\Delta k_{\infty}}^{min, data}(0)\right)^2, \quad (11)$$

in order to arrive at the final nuclear data uncertainty. In the EPRI report, a small-radius fuel rod case had the minimum uncertainty at zero burnup, $2 s_{\Delta k_{\infty}}^{min, data}(0) = 322$ pcm.

2 SCALE NUCLEAR DATA UQ METHODOLOGY AND MODEL DESCRIPTION

Sampler is a new super sequence to be released in SCALE 6.2, currently in pending beta release, for general stochastic sampling-based uncertainty quantification (UQ). The general procedure is simple.

1. Develop uncertainties and correlations for nuclear data.
2. Create N samples for each nuclear data parameter according to the distributions, respecting correlations if present.
3. Perform a calculation for each set of N sets of samples.
4. Statistically analyze the distribution of outputs (e.g., with sample mean and sample standard deviation formulas, histograms, quantiles).

Although Sampler has the capability to include uncertainty in any input file parameter (e.g., clad thickness or fuel temperature), it is only used here to analyze uncertainty due to nuclear data.

2.1 Nuclear Data Uncertainties in SCALE 6.2

SCALE 6.2 contains a new ENDF/B-VII based nuclear data library [5] with three types of nuclear data uncertainty that may be included in calculations:

1. nuclear cross-section data uncertainty (e.g., ^{238}U capture or ^{239}Pu fission);
2. fission product yields uncertainties (e.g., xenon yield of ^{235}U); and
3. decay constants uncertainties (e.g., half-life of ^{135}I).

Nuclear data uncertainty is fully propagated through all SCALE modules [e.g., CENTRM (resonance self-shielding), NEWT (lattice physics), ORIGEN (depletion and decay), and KENO (criticality) modules typically used in burnup credit analysis]. Sampler also allows input file parameters (e.g., clad thickness) to have distributions as well. Sampler methodology is fully described in a companion paper [4]. In the current preliminary implementation of the fission product yield covariance data, complete correlations have been developed only for ^{235}U . Other fissionable nuclides are analyzed using fission yield uncertainties without full correlations [7]. The uncertainty in the multiplication factor is evaluated using the sample standard deviation

$$(s_k^{data})^2 = \frac{1}{N-1} \sum_{i=1}^N (k_{eff}^{(n)} - \bar{k}_{eff})^2, \quad (12)$$

with sample mean calculated as

$$\bar{k}_{eff} = \frac{1}{N} \sum_{i=1}^N k_{eff}^{(n)}, \quad (13)$$

where multiplication factor for sample n is denoted $k_{eff}^{(n)}$.

2.2 Models

The SCALE/Sampler stochastic sampling methodology was applied to obtain the uncertainty in the multiplication factors due to nuclear data uncertainty for a simulation of a 17×17 PWR assembly in a spent fuel storage pool, consisting of two calculations:

1. TRITON fuel assembly calculation using NEWT (2-D transport) and ORIGEN (depletion) and
2. KENO-V.a spent fuel storage pool criticality simulation of the depleted assembly in an infinite array (no radial leakage) at cold, borated conditions.

In order to speed up calculations, the modeling procedure has been slightly modified in obtaining depleted isotopic concentrations by using single-pin TRITON simulations. The pin pitch has been adjusted such that the total water moderator in the fuel assembly is evenly distributed for each fuel pin. The comparison of the assembly model and the single pin model for the nominal (unperturbed) calculation showed differences between these two models of less than 50 pcm in eigenvalue and less than 1% for concentrations of important nuclides over the considered burnup range. For investigatory UQ studies in this paper, the adjusted single-pin model is considered an adequate substitute for a full fuel assembly model.

In the TRITON depletion and KENO-V.a criticality calculations, the ENDF/B-VII.1 based 238-group AMPX library was utilized and self-shielded cross sections were obtained by using BONAMI and CENTRM. The same cross-section library (with uncertainties) was used for both the depletion and the criticality calculation. Therefore, the uncertainty results include the contributions from both calculations and also account for any correlations in nuclear data uncertainties in the calculations. *All* available uncertainty data were used (~300 isotopes), and thus uncertainty in *all* isotopics was considered in the criticality calculation (i.e., well beyond the sets shown in Figure 1). The number of perturbed data libraries (samples) was $N=300$. The KENO-V.a model includes 100 and 1100 inactive and active neutron generations, respectively, and 25000 particles per generation, which results in <0.00013 standard deviation in the multiplication factor.

The matrix of modeling cases studied is shown in Table IV. The enrichment (2.5, 4.0, and 5.0 wt % ^{235}U) and discharge burnups (10, 30, 50 GWd/MTU) were chosen to roughly match the loading curve from [1]. Decay times after discharge were 5 days, 30 days, and 5 years.

Table IV. Modeling cases for 17×17 PWR assembly

Case	^{235}U enrichment (wt %)	Discharge burnup (GWd/MTU)	Decay time (days)		
			5	30	1825
A	2.5	10.0	5	30	1825
B	4.0	30.0	5	30	1825
C	5.0	50.0	5	30	1825

Previously, a similar analysis was performed to obtain uncertainty in spent fuel nuclide concentrations due only to nuclear *cross-section* data uncertainty [6]. In this study perturbed data for decay and fission product yields have been considered, and additionally, the analysis has been extended to include the criticality calculations.

3 RESULTS

Table V shows the uncertainty results for the multiplication factor, due to nuclear data uncertainty for the spent 17×17 PWR fuel assembly in the spent fuel storage pool (i.e., at cold conditions). The sample mean and sample standard deviation have been calculated from $N=300$

samples according to Eq. (12) and (13), respectively. Uncertainties shown in units of pcm (1 pcm = 10⁻⁵) are simply the standard deviations.

Table V. Sample mean and standard deviation in spent fuel pool multiplication factor due to nuclear data uncertainty

Case	²³⁵ U wt %	Burnup (GWd/MTU)	Decay time (days)	\bar{k}_{eff}^*	S_k^{data} (pcm)
A	2.5	10.0	5	0.94614	459
			30	0.94537	463
			1825	0.94017	464
B	4.0	30.0	5	0.92380	519
			30	0.92289	523
			1825	0.90680	536
C	5.0	50.0	5	0.86345	559
			30	0.86250	563
			1825	0.83748	588

*Maximum standard deviation of KENO-5: 0.00013.

The distribution of k_{eff} for the spent fuel storage pool is shown in Figures 2, 3, and 4, for each case A, B, and C, respectively, in bins of width 0.002.

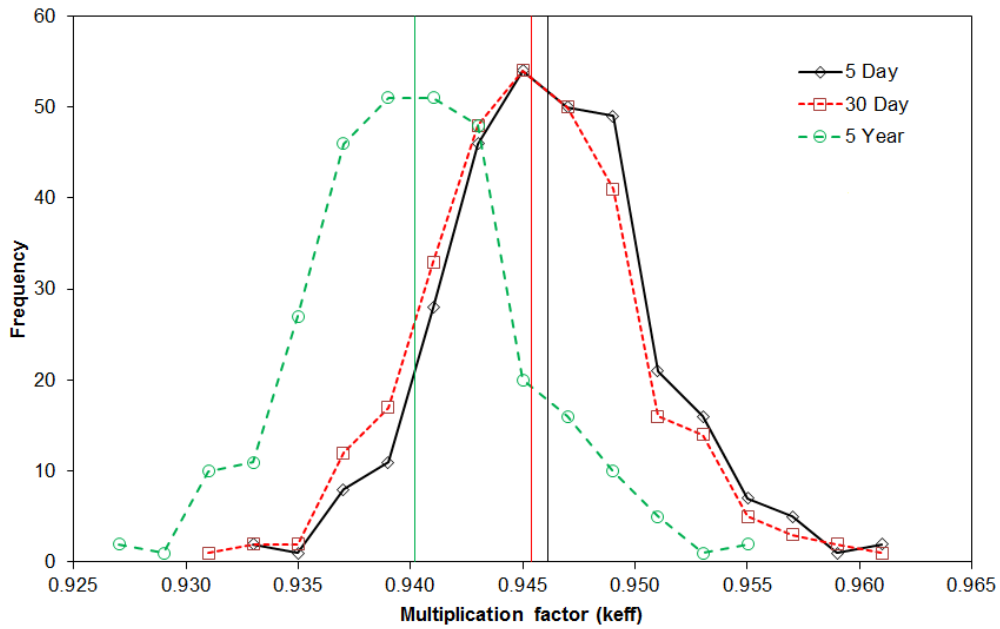


Figure 2. Distribution of k_{eff} in spent fuel pool for Case A

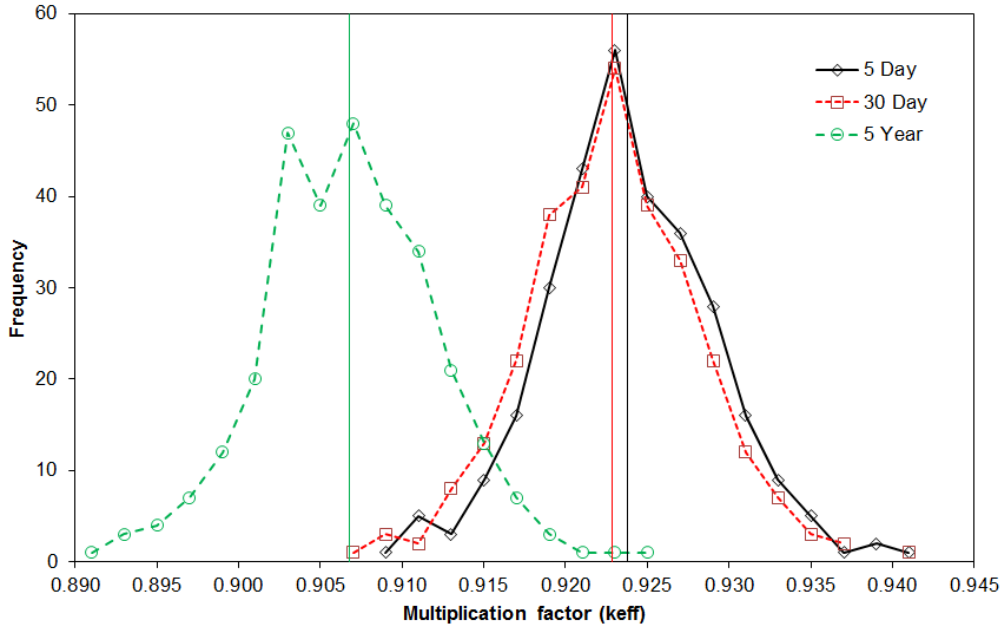


Figure 3. Distribution of k_{eff} in spent fuel pool for Case B

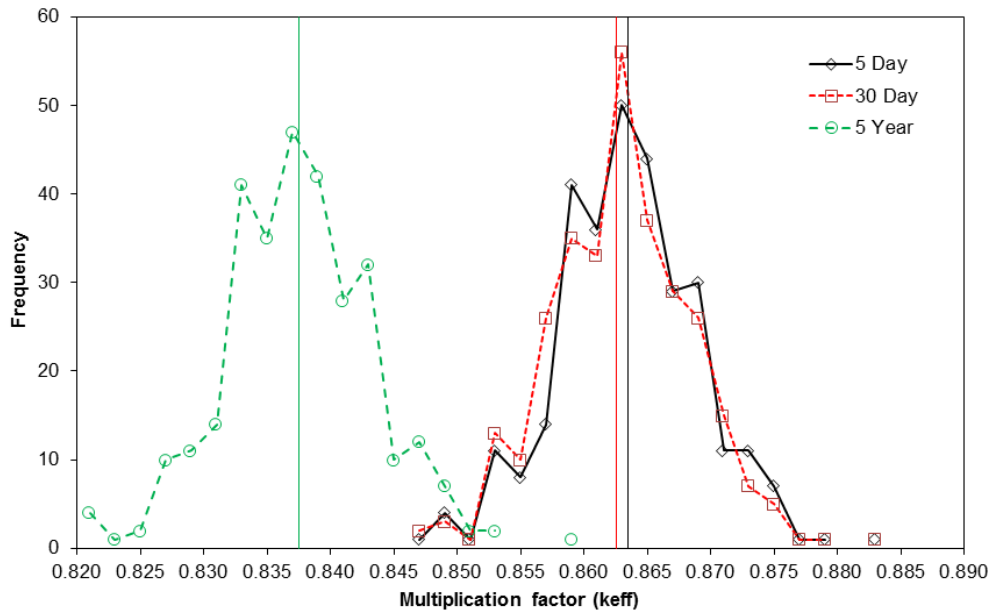
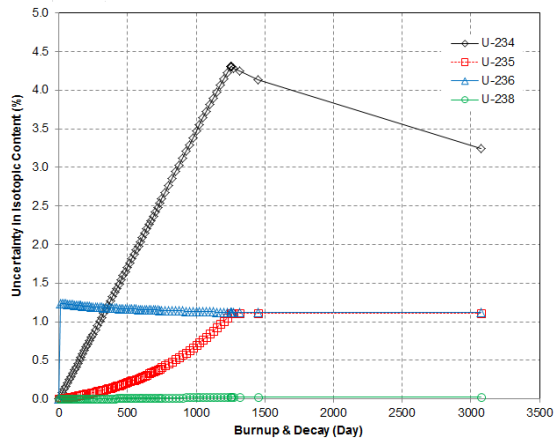


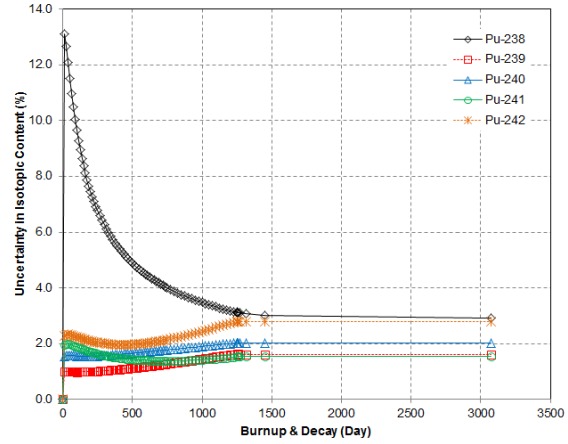
Figure 4. Distribution of k_{eff} in spent fuel pool for Case C

The uncertainty in the calculated isotopics for the 28 nuclides in the actinide and fission product burnup credit set recommended in ISG-8 (Figure 1) is illustrated in Figure 5 for Case C (5 wt % ^{235}U enrichment, 50 GWd/MTU burnup, 5-year cooling time). Figure 6 compares the relative uncertainties in ^{235}U and ^{239}Pu , the main contributors to bias uncertainty according to the ISG-8 [2], as a function of initial ^{235}U enrichment, for cases A, B, and C.

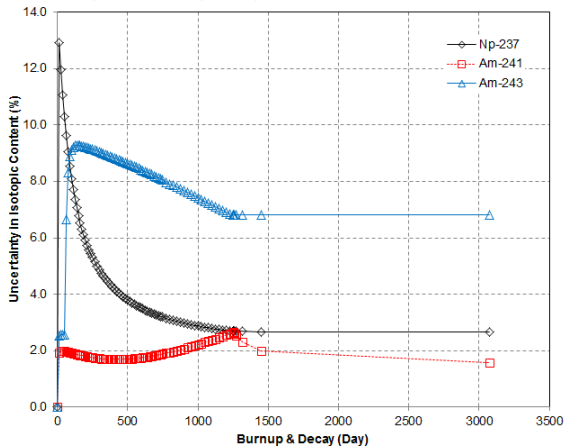
Comparison of Burnup Credit Uncertainty Quantification Methods



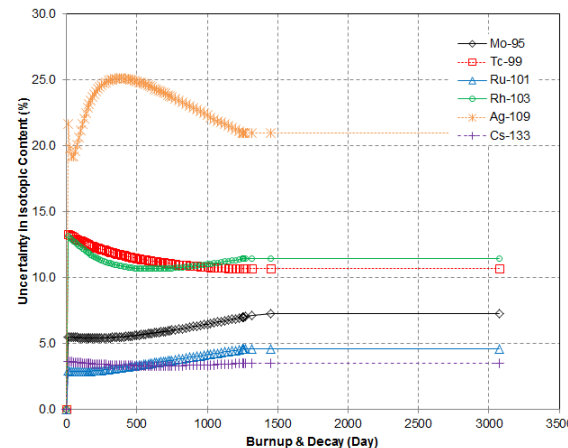
(a) U



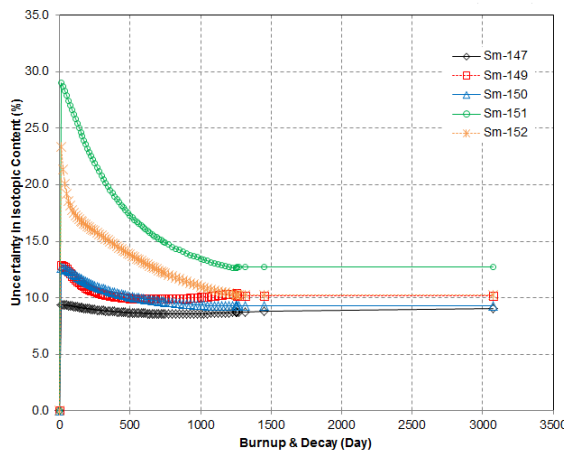
(b) Pu



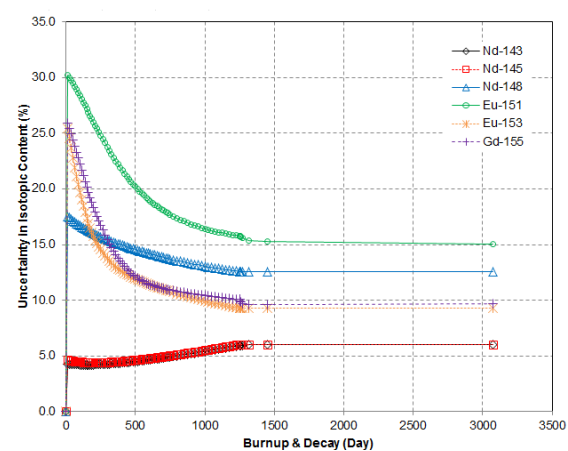
(c) Np and Am



(d) Mo, Tc, Ru, Rh, Ag and Cs



(e) Sm



(f) Nd, Eu and Gd

Figure 5. Relative uncertainty (1-sigma) in calculated isotopic inventories due to nuclear data for Case C with 5 years of decay

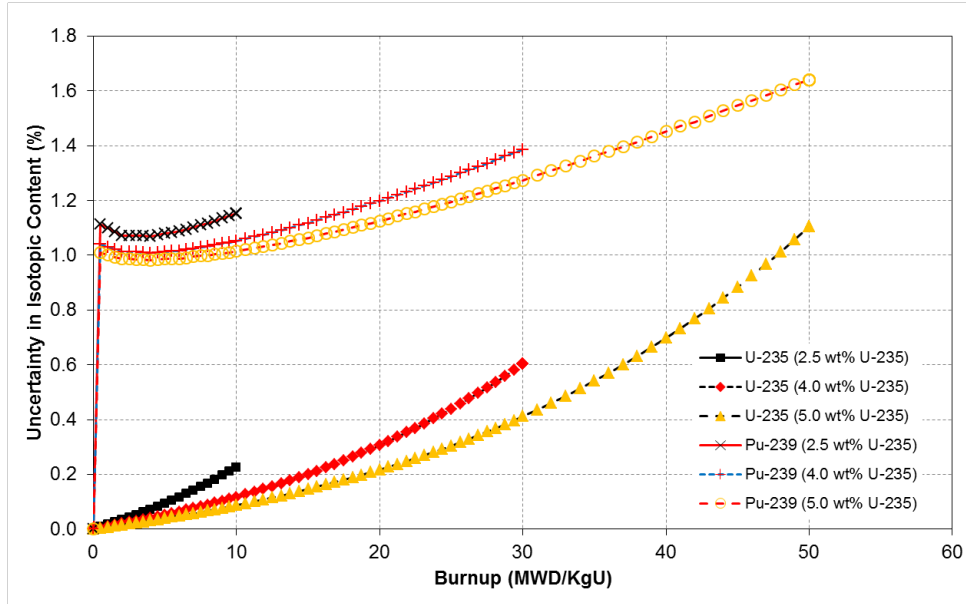


Figure 6. ²³⁵U and ²³⁹Pu relative isotopic uncertainty (1-sigma) due to nuclear data

Table VI shows the contributions of nuclear data uncertainty from each component of the nuclear data, for Case B with 5 days of decay time.

Table VI. Uncertainty in k_{eff} due to nuclear data uncertainty for Case B with 5-day decay time

Perturbed Data Sets	S_k^{data} (pcm)
Cross section + Decay + F.P. yield	519
Cross section	476
Cross section + Decay	479
Cross section + F.P. yield	518

F.P = fission product.

4 DISCUSSION

There are numerous interesting features to examine from the preceding section. First, in Table V, one sees that the eigenvalue uncertainty due to nuclear data uncertainty increases with increasing burnup [e.g., at 5 years of decay from 460 to 540 to 590 pcm (1-sigma) for 10, 30, and 50 Gwd/MTU]. However, each of these burnups corresponded to different enrichments, as noted in Table V. Examining the first 10 Gwd/MTU of Figure 6 indicates that the uncertainty in ²³⁵U and ²³⁹Pu, the major players in k_{eff} uncertainty according to Ref. [1], increases faster if enrichment is lower. This makes sense as the lower enrichment systems have higher plutonium production and thus will be driven more by plutonium isotopes with larger nuclear data uncertainty. Therefore, because of the enrichment and burnup combinations considered (values approximately on a loading curve), a smaller net burnup effect is observed.

The histograms of k_{eff} (Figures 2–4) show slight differences in shape, attributed to the limited number of random samples evaluated and choice of bins, but the same basic trends are observed across the three considered cases. The variance of the k_{eff} distribution due to nuclear data uncertainty changes very little with decay time up to 5 years. Table VI indicates that the decay component of the nuclear data uncertainty does not play a large role in the uncertainty of k_{eff} for the short decay times considered in this study, but could play a larger role at longer storage times.

The relative uncertainty (1-sigma) in the ^{235}U isotopic content increases to slightly more than 1% with increasing burnup, whereas the ^{238}U relative uncertainty due to nuclear data is $\ll 1\%$ in relative terms. Most of the plutonium isotopes exhibit a relative uncertainty of about 2%. It may seem intuitive that isotopes would generally show increasing uncertainty with increasing burnup; however, Figure 5 shows that for many isotopes this is not the case. For example, ^{243}Am has a maximum of 9% (1-sigma) uncertainty before decreasing to 7%. Neptunium-237 decreases rapidly from 13% to 3%. Europium-151 uncertainty halves from 30% initially to 15%. Silver-109, which has a large isotopic bias and uncertainty in RCA comparisons, has a predicted uncertainty of about 20 to 25% (1-sigma) due to nuclear data alone. The isotopic concentrations of ^{149}Sm and ^{151}Sm reach an equilibrium condition at the burnup of 20 and 200 days, respectively, but the uncertainty values decrease during irradiation. These changes in the uncertainty are driven largely by variations in the nuclide production routes that occur during irradiation. Similar changes can occur during decay cooling, with ^{241}Am being one of the notable isotopes with a decreasing uncertainty. Since ^{241}Pu is converted into ^{241}Am by a β^- decay, the isotopic concentration of ^{241}Am is increasing and the isotopic concentration of ^{241}Pu is decreasing. Therefore, as the majority of ^{241}Am originates from ^{241}Pu decay, the uncertainty in ^{241}Am becomes the same as the uncertainty in ^{241}Pu . Therefore, this is not an effect of the ^{241}Am decay constant uncertainty.

It is shown in Table VI that the uncertainty in the multiplication factor, at short times, is not significantly sensitive to the uncertainty in decay and fission product yield data. The decay data uncertainty, in particular, does not make any impact on the uncertainty in the multiplication factor, at short times, increasing from 518 pcm to 519 pcm with inclusion of the decay uncertainty data. This result is intuitive since most burnup credit nuclides are either stable or long lived, and this study did not consider very long cooling times.

Finally, the multiplication factor uncertainty due to nuclear data uncertainty is shown in Table VII, compared to other measurement-based estimates of bias uncertainty given in ISG-8 [2] and the EPRI report [3]. The total nuclear data uncertainty estimate (depletion plus criticality) is converted to approximate 95/95 tolerance intervals by multiplying the standard deviation by two (i.e., $2 s_k^{data}$). An additional isotopics-only uncertainty result is shown in the last column as $2 s_k^{iso}$. This result was obtained by perturbing nuclear data only in the depletion calculation, and the criticality calculation used the resultant perturbed isotopics with the nominal nuclear data library. Only results for Case B with 5-year decay are shown in the table.

Table VII. Comparison of the total uncertainties (pcm) from ISG-8[2] and EPRI[3] to SCALE/Sampler nuclear data only uncertainty prediction with 5-year decay

Burnup (GWd/MTU)	Burnup credit terms $\beta_i \pm \Delta k_i$		Predicted uncertainty	
	ISG-8	EPRI	total nuclear data $2 s_k^{data}$	isotopics-only $2 s_k^{iso}$
10	0±1480	19±590	928	414
30	0±1610	81±639	1072	644
50	0±2190	177±614	1176	826

It is important to note a fundamental difference between the bias and bias uncertainty estimates based on comparison to measurement (ISG-8 and EPRI methods) and uncertainty propagation methods (e.g., Sampler). Uncertainty propagation provides only a prediction, or *forecast*, of the expected distribution of the bias, or uncertainty range of the bias, while the evaluation of bias from comparison to measurement provides a *true* measure of bias. By comparing the forecast bias uncertainty due to a particular source (e.g., nuclear data) to a true measure of bias uncertainty, information is gained about the portion of the true measure that could be due to that particular source.

The EPRI 95/95 uncertainty (~640 pcm) is much lower than both the ISG-8 uncertainty (~1600 pcm), and the 2-sigma uncertainty due to nuclear data predicted by Sampler (~1000 pcm). However, the total nuclear data uncertainty, $2 s_k^{data}$, includes nuclear data uncertainty in the criticality calculation, captured in another term of Eq. (1), Δk_β . Therefore, the isotopics-only uncertainty, $2 s_k^{iso}$, is a better estimate of Δk_i and can be interpreted as the portion due explicitly to nuclear data uncertainty. The ISG-8 result is much larger than $2 s_k^{iso}$, by a factor of approximately three, implying other non-nuclear data sources of error are significant (e.g., errors in the measurements and errors in modeling local operating conditions at the location of the measurements). Note that in the ISG-8 method, the nuclear data uncertainty is present but purely implicit, as a component in each bias calculated from comparison to RCA data. The EPRI result is much closer in magnitude to the isotopics-only uncertainty predicted by Sampler, although $2 s_k^{iso}$ has a clear increase with burnup, whereas the EPRI result does not. For the high-burnup case with 50 GWd/MTU, the EPRI method yields an uncertainty 200 pcm lower than Sampler predicts due to nuclear data alone. Note that in the EPRI method, nuclear data uncertainty is included implicitly in Eqs. (3)–(6) and explicitly in the additional uncertainty at cold conditions in Eq. (10).

5 CONCLUSIONS

The ISG-8 recommendations for burnup-credit bias and bias uncertainty were investigated using the SCALE stochastic sampling tool, Sampler, which will be released in SCALE 6.2. Sampler can account for uncertainty contributions from cross sections, fission yields, and decay data by using correlated sampling of covariance files developed for all nuclear data used by the SCALE codes. The fission yield and decay covariance data are recent developments to be released initially in SCALE 6.2.

Using a simple model of a 17×17 PWR assembly with UO₂ fuel, three cases with varying enrichment and discharge burnup were analyzed for spent fuel pool configurations for decay times of 5 days, 30 days, and 5 years after fuel discharge. The decay time does not appear to have a large impact on the spent fuel pool multiplication factor uncertainty due to nuclear data. After 5 years of decay, the 2-sigma uncertainties in multiplication factor from assuming uncertainty in nuclear data in both the depletion and criticality calculation were 928, 1072, and 1176 pcm for 10, 30, and 50 GWd/MTU burnups, respectively. Including the fission product yield uncertainty data was observed to only introduce a small additional uncertainty (~50 pcm) in the multiplication factor. The decay data uncertainty was observed to introduce almost no uncertainty (<3 pcm). The uncertainty in multiplication factor due only to uncertainty in isotopics was estimated by performing the criticality calculation with the nominal nuclear data and perturbed isotopics. This “isotopics-only” uncertainty was 414, 644, and 826 pcm for 10, 30, and 50, GWd/MTU burnups, respectively, and may be interpreted as the nuclear data component of the burnup credit bias uncertainty term, Δk_i . The ISG-8 Δk_i values, based on comparison to measured RCA data, were 1480, 1610, and 2190 pcm for 10, 30, and 50 GWd/MTU burnups, respectively. The larger depletion uncertainty values presented in ISG-8 derive directly from the decision to use experimental RCA data as the technical basis for the analysis of depletion model uncertainties.

Comparisons were also made to an alternative methodology developed by EPRI, based on reactor core simulation and measurement data, that gives a total bias uncertainty (Δk_i) of 600 pcm (2-sigma) in the cold condition multiplication factor. The total bias uncertainty includes three components: (1) 250 pcm in the hot full power nuclear data and modeling error, (2) 255 pcm in fuel temperature error, and (3) approximately 400 pcm *extra* nuclear data uncertainty at cold conditions for nonzero burnups.

It is important to note here that the Sampler code and the nuclear data covariance data required for uncertainty analysis represent an emerging capability that is currently under development. Therefore, the results presented here are preliminary and subject to change as the covariance data are updated and refined. Although the methods are based on rigorous propagation of experimental uncertainties in the measured nuclear data, the methods and data have not been extensively validated or independently benchmarked. The results are therefore intended to provide an initial assessment and demonstration of the approximate importance of nuclear data uncertainties in criticality calculations involving spent nuclear fuel.

Sampler provides an extremely powerful uncertainty analysis tool that can be applied to any calculation that can be performed using SCALE. This capability is able to assess application regimes where direct experimental validation data are not available (e.g., very short cooling times, long-term storage and used fuel repository studies, and nuclides that have few or no measurements). Future work will further investigate the differences in the burnup credit uncertainty quantification methodologies as well as the impact of the new decay and fission product yield uncertainties available in Sampler for other problems. Additional validation work is necessary to migrate the Sampler code from a research and development tool to a production code that can be used to support safety and licensing evaluations.

6 ACKNOWLEDGMENTS

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