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Propagation of Isotopic Bias and Uncertainty to Criticality Safety Analyses of PWR Waste Packages

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PROPAGATION OF ISOTOPIC BIAS AND UNCERTAINTY TO CRITICALITY SAFETY ANALYSES OF PWR WASTE PACKAGES

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ACRONYMS

2-D	two-dimensional
B&W	Babcock and Wilcox
BPR	burnable poison rod
DTN	data tracking number
DVD	digital video disc
ENDF	evaluated nuclear data file
M/C	measured to calculated
MCNP	Monte Carlo N-Particle (transport code)
NEWT	New ESC-based Weighting Transport (code)
NRC	U.S. Nuclear Regulatory Commission
OCRWM	Office of Civilian Radioactive Waste Management
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor
QARD	quality assurance requirements and description
RCA	radiochemical assay (data)
S/U	sensitivity/uncertainty
SCALE	Standardized Computer Analysis for Licensing Evaluation
SNF	spent nuclear fuel
TAD	transport, aging, and disposal
TMI	Three Mile Island (Unit 1 reactor)
TRITON	Transport Rigor Implemented with Time-dependent Operation for Neutronic depletion (code)
YMP	Yucca Mountain Project

1. PURPOSE

Burnup credit methodology is economically advantageous because significantly higher loading capacity may be achieved for spent nuclear fuel (SNF) casks based on this methodology as compared to the loading capacity based on a fresh fuel assumption. However, the criticality safety analysis for establishing the loading curve based on burnup credit becomes increasingly complex as more parameters accounting for spent fuel isotopic compositions are introduced to the safety analysis. The safety analysis requires validation of both depletion and criticality calculation methods. Validation of a neutronic-depletion code consists of quantifying the bias and the uncertainty associated with the bias in predicted SNF compositions caused by cross-section data uncertainty and by approximations in the calculational method. The validation is based on comparison between radiochemical assay (RCA) data and calculated isotopic concentrations for fuel samples representative of SNF inventory. The criticality analysis methodology for commercial SNF disposal allows burnup credit for 14 actinides and 15 fission product isotopes in SNF compositions.[1] The neutronic-depletion method for disposal criticality analysis employing burnup credit is the two-dimensional (2-D) depletion sequence TRITON (Transport Rigor Implemented with Time-dependent Operation for Neutronic depletion)/NEWT (New ESC-based Weighting Transport code) and the 44GROUPNDF5 cross-section library in the Standardized Computer Analysis for Licensing Evaluation (SCALE 5.1) (Ref. 2) code system.[3] The SCALE 44GROUPNDF5 cross section library is based on the Evaluated Nuclear Data File/B Version V (ENDF/B-V) library. The criticality calculation code for disposal criticality analysis employing burnup credit is General Monte Carlo N-Particle (MCNP) Transport Code.[4]

The purpose of this calculation report is to determine the bias on the calculated effective neutron multiplication factor, k_{eff}, due to the bias and bias uncertainty associated with predicted spent fuel compositions (i.e., determine the penalty in reactivity due to isotopic composition bias and uncertainty) for use in disposal criticality analysis employing burnup credit. The method used in this calculation to propagate the isotopic bias and bias-uncertainty values to k_{eff} is the Monte Carlo uncertainty sampling method.[5]

The development of this report is consistent with *Test Plan for: Isotopic Validation for Postclosure Criticality of Commercial Spent Nuclear Fuel.*[6] This calculation report has been developed in support of burnup credit activities for the proposed repository at Yucca Mountain, Nevada, and provides a methodology that can be applied to other criticality safety applications employing burnup credit.

2. QUALITY ASSURANCE REQUIREMENTS

Development of this report has been determined to be subject to the Yucca Mountain Project (YMP) quality assurance requirements as described in *Test Plan for: Isotopic Validation for Postclosure Criticality of Commercial Spent Nuclear Fuel*.[6] The Test Plan identifies Oak Ridge National Laboratory (ORNL)–Office of Civilian Radioactive Waste Management (OCRWM) quality assurance procedures applicable to the development, documentation, and electronic management of the data for this report.

The development of the calculation and analysis documentation were performed in accordance with ORNL-OCRW-19.1, *Calculation Packages*.[7] The Test Plan for the development of the report was prepared in accordance with ORNL-OCRW-21.0, *Scientific Investigations*.[8] The control of electronic data was performed in accordance with ORNL-OCRW-23.0, *Control of the Electronic Management of Data*.[9] The computer codes used in this calculation have been qualified per ORNL-OCRW-19.0, *Software Control*.[10]

3. USE OF SOFTWARE

3.1 MCNP

The general-purpose Monte Carlo transport code MCNP was used to calculate the values of neutron multiplication factor, k_{eff}, for SNF waste packages. The MCNP 5.1.40 code[4] used herein has been qualified per ORNL-OCRW-19.0, *Software Control*.[10]

- Software Title: MCNP
- Version/Revision Number: Version 5/Revision 1.40
- Status/Operating System: Qualified/Linux 2.6.9-42.0.2 ELsmp #1, x86_64 GNU/Linux (Ref. 11)
- Computer Type: CPILE2 Linux cluster of the Nuclear Systems Analysis, Design, and Safety organization, Nuclear Science and Technology Division, ORNL

Rationale for Selection: The MCNP computer code employs the Monte Carlo method to perform radiation transport calculations. The Monte Carlo method stochastically simulates actual physical processes and determines a physical quantity as the expected value of a certain random variable (or combination of several variables). The primary reasons for using this computer code are the following: (1) it is accepted by the U.S. Nuclear Regulatory Commission (NRC) for criticality safety applications,[12] (2) it allows explicit geometrical modeling of material configurations, and (3) it uses continuous-energy cross sections.

The MCNP k_{eff} calculations documented in this report used sufficient inactive (300) and active (1000) cycles to obtain convergence of both the k_{eff} and the fission source distribution before starting active cycles for tallies. The value of estimated k_{eff} standard deviation for all MCNP calculations was 0.0003. The input and output files for the MCNP calculations are located on a DVD that accompanies this report (refer to Appendix C for the contents of the DVD), so that an independent repetition of the calculations may be performed.

3.2 SCALE

The SCALE code system was used to perform transport, depletion, and decay calculations. The SCALE 5.1 code system[2] used herein has been qualified per ORNL-OCRW-19.0, *Software Control*.[10]

- Software Title: SCALE
- Version/Revision Number: Version 5.1
- Status/Operating System: Qualified/Linux 2.6.9-42.0.2 ELsmp #1, x86_64 GNU/Linux (Ref. 13)
- Computer Type: CPILE2 Linux cluster of the Nuclear Systems Analysis, Design, and Safety organization, Nuclear Science and Technology Division, ORNL

Rationale for Selection: SCALE is accepted by the NRC for criticality safety applications.[12] This computer code system has multiple unique capabilities relevant to this work, including automated sequences to produce problem-dependent multigroup cross-section data and analysis sequences for transport, depletion, and decay calculations.

The input and output files for the SCALE depletion calculations are located on a DVD that accompanies this report (refer to Appendix C for the contents of the DVD), so that an independent repetition of the calculations may be performed.

3.3 EXCEL

The commercial off-the shelf software Microsoft Office Excel 2003 (copyright Microsoft Corporation) was used in calculations to manipulate the inputs and tabulate and chart results using standard mathematical expressions and operations. Excel was used only as a worksheet and not as a software routine. Therefore, Excel is exempt from the requirements of ORNL-OCRW-19.0, *Software Control*.[10] All necessary information for reproducing the operations performed is provided on the DVD that accompanies this report so that an independent repetition of the operations may be performed.

3.4 ORIGIN

The commercial off-the shelf software OriginPro 8.1 (copyright OriginLab Corporation) was used in calculations to manipulate the inputs and chart results using standard statistical methods and mathematical operations. Origin was used only as a worksheet and not as a software routine. Therefore, Origin is exempt from the requirements of ORNL-OCRW-19.0, *Software Control*.[10] All necessary information for reproducing the operations performed is provided on the DVD that accompanies this report so that an independent repetition of the operations may be performed.

4. INPUT DATA

Table 1 provides a summary of the data used as direct inputs to the calculations described in this document, the sources of input data, and a justification for use as direct inputs. Technical input data include YMP qualified data listed by data tracking number (DTN), technical products developed in accordance with Quality Assurance Requirements and Description (QARD),[14] and information accepted as established fact by the scientific and engineering community.

Table 1. Summary of direct inputs

Parameter	Value	Source	Justification
Principal isotopes for commercial SNF burnup credit	See Table 2	Ref. 1	Approved technical product developed in accordance with QARD requirements
Bounding assembly parameters for depletion calculations	See Table 3 and Fig. 1	Refs. 15 and 16	Approved technical product developed in accordance with QARD requirements
Zircaloy-4 and burnable poison material compositions and densities	See Table 5	Ref. 15	Approved technical product developed in accordance with QARD requirements
Additional bounding parameters for modeling depletion conditions	See Table 6	Ref. 15	Approved technical product developed in accordance with QARD requirements
Isotopic composition bias and bias uncertainty values for the burnup-credit isotopes	See Table 8	Ref. 3 and Ref. 17 (DTNs: MO1005PWRSNFIC.000 and MO1005RDMALIBU.000)	YMP qualified data (Ref. 17)
MCNP model for the pressurized water reactor (PWR) waste package with intact assemblies	See Sect. 7.3	Ref. 18 (DTN: MO0711LOADCURV.000)	Approved technical product developed in accordance with QARD requirements
Loading curve parameters	See Sect. 7.3.1	Ref. 18	Approved technical product developed in accordance with QARD requirements
Minimum cooling time for spent nuclear fuel	5 years	Ref. 19 (10 CFR 961.11)	Information accepted as established fact by scientific and engineering community
Tolerance-limit factors	See *DVD/xls/ validation.xls*	Refs. 20 and 21	Information accepted as established fact by scientific and engineering community

5.   ASSUMPTIONS

1. It is assumed that the isotopic validation data used in this calculation for each burnup credit isotope form a normal distribution. This assumption facilitates characterization of a probability frequency distribution by the sample mean and sample standard deviation. The rationale for this assumption is that the isotopic validation data are expected to approach the normal distribution as the sample size increases. Currently, a limited number of RCA data are available for use in isotopic validation studies. The statistical characteristics of the isotopic validation data used in this calculation were evaluated in Sect. 7.2.

2. It is assumed that correlations do not exist among the isotopic bias uncertainty values because the bias uncertainty captures the random effects of measurement errors and approximations used in determining modeling parameters that are not well defined, such as moderator density at sample location or effective temperature of the fuel sample. This assumption enables sampling the isotopic bias uncertainty intervals of the burnup credit isotopes independently. The use of tolerance intervals (rather than confidence intervals) to define the range of bias uncertainty is intended to compensate for the effect this assumption may have on the results of the calculations.

6.   METHODOLOGY

The biases and bias uncertainties in the SCALE 5.1 predictions for PWR SNF isotopic compositions have been evaluated in Ref. 3 by comparing isotopic concentration values obtained from measurement and calculation for 118 PWR fuel samples. The method employed in the current calculation to propagate the uncertainties in the calculated fuel isotopic composition to the k_{eff} values for PWR waste packages is the Monte Carlo uncertainty sampling method. This section describes the requirements of burnup credit methodology for disposal criticality analysis and the Monte Carlo uncertainty sampling method and provides an overview of other methods for determining the bias and uncertainty in k_{eff} due to uncertainty in predicted nuclide compositions.

6.1   BURNUP CREDIT METHODOLOGY FOR DISPOSAL CRITICALITY ANALYSIS

Waste package postclosure criticality analysis is based on burnup credit, as described in the *Disposal Criticality Analysis Methodology Topical Report*.[1] A set of 29 actinide and fission product isotopes established as being relevant to burnup credit is included in the spent fuel compositions for waste package criticality analyses. The 29 isotopes, which are referred to as principal isotopes for commercial SNF burnup credit in Ref. 1, are listed in Table 2.

Table 2. Principal isotopes for commercial SNF burnup credit

Actinide isotopes		Fission product isotopes	
^{233}U^a	^{239}Pu	^{95}Mo	^{149}Sm
^{234}U	^{240}Pu	^{99}Tc	^{150}Sm
^{235}U	^{241}Pu	^{101}Ru	^{151}Sm
^{236}U	^{242}Pu	^{103}Rh	^{152}Sm
^{238}U	^{241}Am	^{109}Ag	^{151}Eu
^{237}Np	^{242m}Am	^{143}Nd	^{153}Eu
^{238}Pu	^{243}Am	^{145}Nd	^{155}Gd
		^{147}Sm	

Source: Ref. 1.
  ^{a}Although present in negligible concentrations in the current commercial SNF, the ^{233}U
   isotope will build up from ^{237}Np (T$_{1/2}$ = 2.410E+06 years) (Ref. 22) to sufficient quantities
   over long disposal time periods to become a criticality concern.

The disposal criticality analysis methodology requires validation of the models and methods used to determine the k_{eff} values for waste packages and determination of a critical limit, *CL* [see Eq. (1)], at which waste package configurations are considered potentially critical. The criticality calculation method for disposal criticality analysis is MCNP (Ref. 23). The depletion calculation method for disposal criticality analysis is TRITON/NEWT (Refs. 24 and 25), which allows for a 2-D explicit representation of assembly heterogeneities, such as control rods, water holes, and burnable poison rods, and the 44GROUPNDF5 (Ref. 26) cross-section library in SCALE 5.1 (Ref. 2). The depletion sequence TRITON/NEWT is validated in this report (see Sect. 7.2) using the results of the isotopic evaluations documented in Ref. 3.

The critical limit for use in disposal criticality analyses is determined as follows:[1]

$$CL(x) = f(x) - \Delta k_{EROA} - \Delta k_{ISO} - \Delta k_m ,$$ (1)

where

x = a neutronic parameter used for trending analysis,

$f(x)$ = the lower bound tolerance limit function accounting for biases and uncertainties that cause the calculation results to deviate from the true value of k_{eff} for a critical experiment, as reflected over an appropriate set of critical experiments,

Δk_{EROA} = the penalty for extending the range of applicability,

Δk_{ISO} = the penalty for isotopic composition bias and uncertainty,

Δk_m = an arbitrary margin ensuring subcriticality for preclosure and turning the CL function into an upper subcritical limit function (it is not applicable for use in postclosure analyses because there is no risk associated with a subcritical event).

The term Δk_{ISO} in Eq. (1), which is referred to as the penalty for isotopic bias and uncertainty, is determined for PWR SNF waste packages in this calculation report, whereas the lower-bound tolerance limit function for commercial SNF waste packages has been determined in Ref. 23, *Range of Applicability and Bias Determination for Postclosure Criticality of Commercial Spent Nuclear Fuel*.

6.2 OVERVIEW OF METHODS FOR DETERMINING THE BIAS AND UNCERTAINTY IN k_{eff} DUE TO UNCERTAINTY IN THE CALCULATED NUCLIDE COMPOSITIONS

Methods previously used to determine the bias and uncertainty in k_{eff} due to uncertainty in the calculated nuclide compositions have included various bounding methods. For example, bounds of no credit to very limited credit for the reduced reactivity potential of irradiated commercial light-water reactor fuel assemblies have been made in criticality analyses and have provided a very conservative safety margin. Best-estimate methods provide for a mathematically derived and more realistic safety margin.[27] The best-estimate methods include Monte Carlo uncertainty sampling (see Sect. 6.3), direct difference, and cross-section sensitivity/uncertainty (S/U) analysis methods. The calculations and analysis described in Ref. 27 suggest that the three mentioned best-estimate methods produce similar results in terms of isotopic bias and uncertainty effects on k_{eff}.

As mentioned in Sect. 6.1, the disposal criticality analysis methodology specifies the use of 29 actinide and fission product isotopes (see Table 2) in spent fuel compositions. A bounding method for determining the bias and uncertainty in k_{eff} due to uncertainty in the calculated nuclide compositions consists of simultaneously correcting the concentrations of all isotopes relevant to burnup credit for bias and uncertainty in such a way that produces a maximum increase in system reactivity (see Sect. 6.4). In reality, isotopic composition uncertainties have a statistical behavior for most of the burnup-credit isotopes, with both increasing and decreasing effects on system reactivity relative to each other, and the probability for the most unfavorable situation that is specific to the bounding method is extremely small and would not be reproducible in a commercial nuclear power plant. Correlations are not expected to exist among the isotopic bias uncertainty values because the bias uncertainty captures the random effects of measurement errors and approximations used in determining modeling parameters that are not well defined, such as moderator density at sample location or effective temperature of the fuel sample. By averaging such random effects, a bias in calculated isotopic compositions can be obtained. Correlation is expected to exist between the bias of

an isotope that is almost entirely produced by decay and the bias of their precursors, such as the bias correlation between ^{241}Am ($T_{1/2}$ = 432.7 years) and ^{241}Pu ($T_{1/2}$ = 14.4 years) (Ref. 22). Best-estimate methods supplement the bounding method and provide a more realistic evaluation for the safety margin by crediting compensating effects of isotopic composition uncertainties on k_{eff}. An assumption associated with the best-estimate methods is that the bias uncertainties for the burnup-credit isotopes are independent variables.

The direct difference method consists of performing criticality calculations for the application system using the measured and calculated isotopic concentrations for the evaluated fuel samples and analyzing the k_{eff} results associated with the two isotopic composition sets to determine a lower tolerance limit for criticality. Application of this method is appropriate if a comprehensive database of measured fuel isotopic concentrations for all burnup-credit isotopes exists. The direct difference method was employed in Ref. 28 to determine the penalty in reactivity due to the bias and uncertainty associated with SNF isotopic compositions predicted by the one-dimensional depletion analysis code SAS2H in SCALE 4.4a. The direct difference method is not considered in the current calculation because this calculation is being developed to expand on that method by incorporating the individual nuclide uncertainty distributions into the overall bias and uncertainty term.

The cross-section S/U analysis method determines the response in k_{eff} caused by first-order linear perturbations in cross-section data. Since a relative change in the concentration of an isotope has the same effect on k_{eff} as the same relative change in the microscopic cross section of the isotope, sensitivity coefficients can be used to determine the system k_{eff} uncertainty caused by uncertainties in the concentrations of individual isotopes. TSUNAMI-3D (Ref. 29), the S/U analysis module in the SCALE code system, may be used to calculate the k_{eff} sensitivity profiles and coefficients for the burnup-credit isotopes. However, the S/U analysis method is not considered in the current calculation because the criticality method in the TSUNAMI-3D calculation sequence is KENO, whereas the criticality method used in waste package postclosure criticality calculations[23] is MCNP.

6.3   MONTE CARLO UNCERTAINTY SAMPLING METHOD

The current calculation uses the Monte Carlo uncertainty sampling method to propagate the values of bias and bias uncertainty associated with predicted fuel isotopic compositions to the k_{eff} values for waste packages. The characteristics of this method and its implementation are described in this section. Proper implementation of the Monte Carlo uncertainty sampling method is demonstrated in Appendix B.1.

6.3.1   Characterization of the Probability Frequency Distributions Obtained for the Ratio of Measured-to-Calculated Isotopic Concentrations

Many classical statistical methods rely on the assumption of normality of the data to make probabilistic inferences from samples to populations. The normal distribution is characterized by two parameters: the arithmetic mean (μ) and the standard deviation (σ). For datasets forming a normal distribution, the arithmetic mean and the standard deviation may be estimated by the sample mean ($\overline{X}$) and the sample standard deviation (s), respectively.

The isotopic composition bias and bias uncertainty values associated with the TRITON/NEWT depletion calculation method in SCALE 5.1 are determined in this calculation (see Sect. 7.2) using the isotopic validation data in Ref. 3, which consist of the values of the ratio of measured-to-calculated (M/C) fuel isotopic concentrations for the evaluated burnup credit isotopes. The random

variable X_i^j, defined as shown in Eq. (2), is used to characterize the probability frequency distributions of the isotopic validation data.

$$X_i^j = M_i^j / C_i^j , \qquad (2)$$

where

i = the index of an isotope in the series of 29 burnup-credit isotopes,

j = the index of a fuel sample in a series of N_S evaluated fuel samples,

M_i^j = the measured concentration for the isotope i in the evaluated fuel sample j,

C_i^j = the calculated concentration for the isotope i in the evaluated fuel sample j.

For large N_S, the X_i^j values are expected to form a normal distribution with sample mean $\overline{X}_i$ and sample standard deviation s_i given by Eqs. (3) and (4), respectively.

$$\overline{X}_i = \sum_{j=1}^{N_S} X_i^j / N_S . \qquad (3)$$

$$s_i = \sqrt{\frac{\sum_{j=1}^{N_S} (X_i^j - \overline{X}_i)^2}{N_S - 1}} . \qquad (4)$$

If the distribution parameters for a random variable were known exactly, the sample mean and standard deviation defined as shown in Eqs. (3) and (4) may be used to produce probability intervals. However, usually the distribution parameters are not known exactly, and tolerance intervals, rather than probability intervals, are used in statistical analyses. A tolerance interval is a statistical interval within which, with a specified certainty, a specified proportion p of a population falls. Tolerance intervals are defined by lower (L) and upper (U) tolerance limits. The one-sided tolerance interval above the lower tolerance limit ensures that p percentage of the population will not fall below the lower limit with a specified certainty, whereas the one-sided tolerance interval below the upper tolerance limit ensures that p percentage of the population will not exceed the upper limit with a specified certainty. A two-sided tolerance interval is delimited by the lower and upper tolerance limits. For the ratio of measured-to-calculated isotopic concentration, the two-sided interval is defined by Eq. (5), whereas the one-sided tolerance intervals are given by Eqs. (6) and (7).

$$X_{i,L} = \overline{X}_i - k_2 \cdot s_i; \quad X_{i,U} = \overline{X}_i + k_2 \cdot s_i . \qquad (5)$$

$$X_{i,L} = \overline{X}_i - k_1 \cdot s_i . \qquad (6)$$

$$X_{i,U} = \overline{X}_i + k_1 \cdot s_i , \qquad (7)$$

where

k_2 = two-sided tolerance-limit factor,
k_1 = one-sided tolerance-limit factor.

The k_1 and k_2 tolerance-limit factors depend on the type of the distribution, sample size, certainty, and percentage of the population. The values of the tolerance-limit factors used in this calculation were determined in the spreadsheet application available in *DVD/xls/validation.xls*, worksheet *tl-factors*, using the formulas provided in Appendix A.1.

6.3.2 Application of the Monte Carlo Uncertainty Sampling Method

A stochastic approach[5] for estimating the total uncertainty in k_{eff} resulting from uncertainties in calculated isotopic compositions is based on Monte Carlo sampling of probability distributions obtained for the isotopic bias. This method simulates the variation of bias within the range of bias uncertainty by randomly sampling the uncertainty values. It involves a large number of criticality calculations using spent fuel compositions obtained by correcting the predicted spent fuel compositions for the sampled bias.

The characteristics of the probability distributions of isotopic validation data are greatly affected by the various characteristics of the evaluated RCA data, such as measurement and modeling uncertainties and sample size (refer to Sect. 7.2 for the characteristics of the isotopic validation data used in the current calculation). An improvement of the quality of the validation data may be obtained if additional RCA data characterized by low measurement uncertainties and detailed descriptions of sample irradiation environment become available. This will allow omitting some of the RCA data characterized by high measurement and/or modeling uncertainties from the isotopic validation data sets. With the availability of quality RCA data, the probability distributions of the isotopic validation data are expected to be approximately normal and the mean and standard deviation of the isotopic data are expected to be mostly determined by the uncertainty of the depletion calculation method.

In this calculation, the sampling distributions established for the M/C isotopic concentration values are assumed to be normal with the expected mean and standard deviation given by Eqs. (3) and (4), respectively, and tolerance intervals (rather than confidence intervals) are used to define the range of bias uncertainty (see Sects. 6.3.1 and 7.2). The randomly sampled bias uncertainties for the burnup-credit isotopes in SNF compositions are applied to the predicted fuel concentrations as shown in Eq. (8) to determine new fuel isotopic concentrations for use in criticality calculations.

$$c_i^{'j} = c_i^j \times (\overline{X}_i + r_i^j \cdot k_2 \cdot s_i) \ , \tag{8}$$

where

i = the index of an isotope in the series of the 29 burnup-credit isotopes,
j = the index of a criticality calculation in a series of N_C criticality calculations,
$c_i^{'j}$ = isotopic concentration corrected for bias and uncertainty in the predicted isotopic composition,
c_i^j = predicted isotopic concentration,
$\overline{X}_i$ = the bias in the predicted fuel concentration for isotope i [see Eqs. (2) and (3)],
r_i^j = random number sampled from the standard normal distribution (i.e., the normal distribution with the distribution mean of zero and standard deviation of unity),

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k_2 = two-sided tolerance-limit factor for 95% certainty and 68.27% of the population,

s_i = uncertainty associated with the bias in predicted fuel concentration for isotope i [see Eq. (4)].

The sample mean and standard deviation of the k_{eff} values obtained using SNF compositions stochastically corrected for isotopic bias and uncertainty are determined as follows:

$$k_{eff-MC} = \sum_{j=1}^{N_C} k_{eff}^j / N_C \,.$$ (9)

$$\Delta k_{eff-MC} = \sqrt{\frac{\sum_{j=1}^{N_C} (k_{eff}^j - k_{eff-MC})^2}{N_C - 1}} \,,$$ (10)

where

N_C = the number of criticality calculations,

k_{eff}^j = the k_{eff} value for criticality calculation j in a series of N_C criticality calculations,

k_{eff-MC} = Monte Carlo estimate for k_{eff} showing the average effect on k_{eff} of isotopic composition correction for bias and bias uncertainty,

Δk_{eff-MC} = uncertainty in the Monte Carlo estimate for k_{eff}.

The Monte Carlo uncertainty sampling method requires a statistically significant number of criticality calculations to ensure that the sampled bias uncertainty values are representative of the underlying distribution of the isotopic bias. Non-normal distributions usually require sophisticated methods for calculating tolerance-limit factors. Their values are greater than those of the tolerance-limit factors for normal distributions for the same sample size, certainty, and percentage of the population. Deviation from normality can be accounted for by using tolerance-limit factors for normal distributions that correspond to smaller sample sizes. The tolerance-limit factor increases with decreasing sample size and the increase is significant for small sample sizes (<10).

6.3.3   Calculation of the Δk_{ISO} Term

The change in reactivity due to isotopic composition bias and uncertainty in the calculated nuclide composition is determined according to Eq. (11), where Δk_{eff-MC} is determined according to Eq. (10). The Δk_{ISO} value is based on the upper tolerance limit for 95% of the population and 95% certainty.

$$\Delta k_{ISO} = k_{eff-BE} - k_{eff} + k_1 \times \Delta k_{eff-MC} + 2u \,,$$ (11)

where

k_{eff} = neutron multiplication factor value based on the depletion code predictions,

k_{eff-BE} = neutron multiplication factor value based on the SNF composition corrected for isotopic bias (best-estimate value),

k_1 = 1.84, the value of the one-sided tolerance-limit factor for 200 statistical samples, 95% certainty, and 95% of the population (see spreadsheet *DVD/xls/validation.xls*),

u = uncertainty resulting from the propagation of the uncertainties of the MCNP k_{eff} values [see Eq. (12)].

The statistical uncertainty u associated with the Δk_{ISO} term is given by Eq. (12), which was obtained by propagating the statistical uncertainties of the MCNP k_{eff} values to the uncertainty of the k_{eff-MC} and Δk_{ISO} terms in accordance with Eq. (13). Its value is approximately 0.0004.

$$u = \sigma\sqrt{2 + \frac{k_1^2}{n-1}} \approx \sigma\sqrt{2} ,$$ (12)

where σ is the standard deviation of an MCNP k_{eff} value (0.0003).

The uncertainty of a quantity y that has a functional dependence on independent quantities x_i, $i=1,...N$ may be determined by using Eq. (13) (Ref. 30).

$$\sigma_y^2 = \sum_{i=1}^{N}\left(\frac{\partial y}{\partial x_i}\right)^2 \sigma_{x_i}^2 ,$$ (13)

where σ_{x_i} is the standard uncertainty associated with the estimate x_i. The derivation of the uncertainty u was simplified based on the approximation shown in Eq. (14) so that the dependence between k_{eff-MC} and each k_{eff}^i could be removed:

$$k_{eff-MC} = \sum_{i=1}^{N_C} k_{eff}^i / N_C \approx (k_{eff}^1 + k_{eff}^2 + \cdots + k_{eff}^{i-1} + k_{eff}^{i+1} + \cdots + k_{eff}^{N_c}) / (N_c - 1) .$$ (14)

This approximation is valid for converged k_{eff-MC} values since omitting a single k_{eff} value from the series of N_c k_{eff} values has insignificant impact on the average value if the series is converged.

6.4 BOUNDING METHOD

The bounding method uses isotopic composition bias and bias uncertainty values in a way that maximizes the k_{eff} value. Specifically, the predicted concentration of a fissile (^{235}U, ^{239}Pu, and ^{241}Pu) isotope is replaced by its upper tolerance limit [see Eq. (7)], whereas the predicted concentration of a neutron absorbing isotope is replaced by its lower tolerance limit [see Eq. (6)] for one-sided tolerance intervals, as shown in Eq. (15). The tolerance-limit factor in Eq. (15) is a function of the number of evaluated fuel samples for the burnup-credit isotope and corresponds to specified certainty and percentage of the population (95/95 in this calculation).

$$c_i' = \begin{cases} c_i \times (\overline{X}_i + k_1 \cdot s_i) , & \text{for fissile isotopes} \\ c_i \times (\overline{X}_i - k_1 \cdot s_i) , & \text{for neutron absorbing isotopes} \end{cases} ,$$ (15)

where

i = the index of an isotope in the series of the 29 burnup-credit isotopes,

c_i' = isotopic concentration adjusted for bias and bias uncertainty to maximize positive reactivity,

c_i = predicted isotopic concentration,

$\overline{X}_i$ = the bias in the predicted fuel concentration for isotope i [see Eq. (3)],

k_1 = one-sided tolerance-limit factor,

s_i = uncertainty associated with the bias in predicted fuel concentration for isotope i [see Eq. (4)].

The bounding method requires a criticality calculation using adjusted SNF isotopic concentrations as shown in Eq. (15) and another criticality calculation using predicted SNF compositions. However, this method maximizes the effects of isotopic composition uncertainties on system reactivity in a nonphysical way when it is coupled with the use of conservative depletion parameters that maximize the spent fuel residual reactivity. Application of the bounding method can be justified if confidence in the RCA data available for validation is limited (i.e., in the case of large measurement uncertainties and inadequate availability of modeling data, if the range of parameters characteristic to the evaluated RCA data has limited applicability), or detailed assembly-specific operating history parameters are used in the depletion calculations.

7. CALCULATIONS

7.1 CALCULATION OF BOUNDING ISOTOPIC COMPOSITIONS FOR PWR WASTE PACKAGES

Considerable variation in design and irradiation history parameters exists among SNF assemblies. This section describes the assembly design and irradiation parameters established to be conservative with respect to waste package criticality (i.e., to increase residual reactivity at fuel discharge) and used in the development of loading curves for commercial SNF disposal.[18] Those modeling parameters were used in depletion calculations to determine bounding isotopic compositions for criticality calculations.

7.1.1 Bounding Assembly Parameters for Depletion Calculations

The PWR assembly type selected for depletion and criticality calculations is the Babcock and Wilcox (B&W) 15 × 15 assembly. The basis for this selection is that the B&W 15 × 15 assembly is one of the most reactive assembly designs in a waste package configuration, as established in a sensitivity study documented in Ref. 31, Attachment II. The sensitivity study compared the B&W 15 × 15 fuel assemblies with Westinghouse (15 × 15 and 17 × 17, OFA and STD) and Combustion Engineering (14 × 14, 15 × 15, and 16 × 16) assembly types using fresh fuel of 5 wt % ^{235}U enrichment. The MCNP k_{eff} values obtained for the B&W 15 × 15 and Westinghouse 17 × 17 OFA were statistically identical. Additional information supporting the selection of the B&W 15 × 15 design is provided in Ref. 15.

Fuel pin, guide tube, and instrument tube locations in the B&W 15 × 15 assembly are illustrated in Fig. 1; fuel assembly design parameters are presented in Table 3; selected assembly initial enrichment and burnup values for the PWR isotopic-composition database are shown in Table 4; material compositions for cladding and burnable poison rod (BPR) materials are presented in Table 5; and additional modeling parameters that are conservative with respect to waste package reactivity are presented in Table 6.
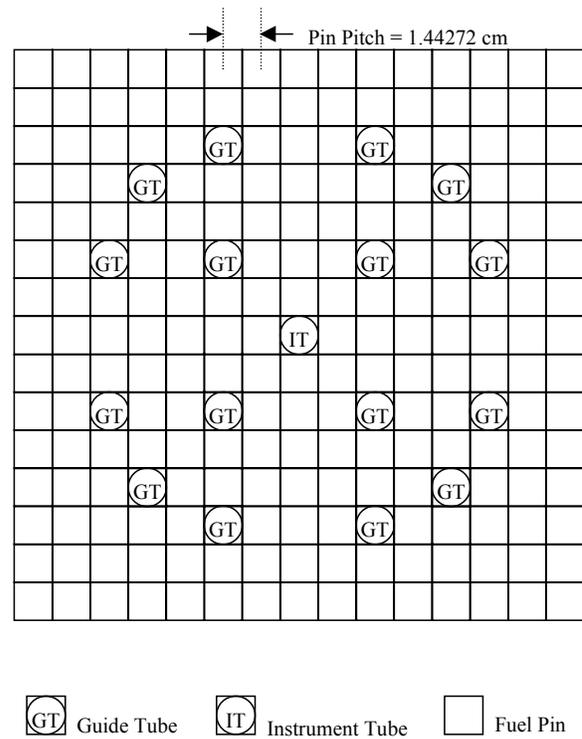
Fig. 1. Fuel pin, guide tube, and instrument tube locations in the B&W 15 × 15 PWR fuel assembly.

Table 3. PWR fuel assembly specifications for isotopic composition calculations

Design parameter	Parameter value
Lattice	15×15
Active fuel length	357.111 cm
Assembly pitch	21.811
Pin pitch	1.44272 cm
Fuel pellet outer diameter	0.9398 cm
Fuel rod cladding inner diameter	0.95758 cm
Fuel rod cladding outer diameter	1.0922 cm
Burnable poison rod (BPR) outer diameter	0.8636
BPR clad inner diameter	0.9144
BPR clad outer diameter	1.0922
Guide tube inner diameter	1.2649 cm
Guide tube outer diameter	1.3462 cm
Instrument tube inner diameter[a]	1.12014 cm
Instrument tube outer diameter[a]	1.38193 cm
Number of fuel cells in fuel assembly	208
Number of BPR cells in fuel assembly	16
Fuel density[b]	10.741 g/cm^3
Fuel initial enrichment and burnup values	See Table 4
Fuel clad, guide tube, and instrument tube material	Zircaloy-4 (See)
BPR material composition	3.5 wt % B_4C in Al_2O_3 (See)

Source: Ref. 15 unless otherwise noted.
[a]Ref. 16.
[b]Calculated based on 98% theoretical density value of 10.96 g/cm^3 for UO_2.

Table 4. Selected enrichment and burnup values for the PWR SNF isotopic database

Enrichment (^{235}U wt %)	Burnup (GWd/MTU)
1.5	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
2.0	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
2.5	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
3.0	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
3.5	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
4.0	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
4.5	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
5.0	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75
5.5	0.001, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, 20, 25, 30, 35, 40, 45, 50, 60, 65, 70, 75

Table 5. Chemical compositions and mass densities for Zircaloy-4 and burnable poison

Zircaloy-4		Burnable poison	
Element	**wt %**	**Element/isotope**	**wt %**
O	0.125	^{10}B	0.5023
Cr	0.100	^{11}Boron	2.2370
Fe	0.210	C	0.7608
Zr	98.115	Al	51.0727
Sn	1.450	O	45.4273
Density = 6.56 g/cm^3		Density = 3.7 g/cm^3	

Source: Ref. 15.

Table 6. Additional bounding modeling parameters

Modeling parameter	Parameter value	Justification/comments[a]
Fuel temperature	1144.1 K	The value was based on operating parameters for PWRs. A higher fuel temperature value results in more ^{239}Pu production.
Moderator temperature	588.7 K	The value was based on operating parameters for PWRs. The bounding temperature is approximately 20 degrees above the core average value.
Moderator density	0.6905 g/cm^3	Moderator density value was taken from steam tables and corresponds to the moderator temperature and pressure.
Soluble boron in moderator	1000 ppmB	Soluble boron value is constant throughout the irradiation time period. The value was based on operating parameters for the PWR Crystal River Unit 3. A larger soluble boron concentration results in more ^{239}Pu production.
BPR insertion	Maximum (16)	BPR insertion in every guide tube location throughout the irradiation time period maximizes the fissile isotope (primarily ^{235}U and ^{239}Pu) content
Specific power	29.74 MW/MTU	Specific power has a weak effect upon reactivity. Lower specific power values result in greater fuel reactivity.
Depletion time step interval	50 days	Provides adequate cross-section update frequency for BPR depletion calculations.

Source: Ref. 15.
[a]Parameter values are bounding with respect to criticality, as justified in Ref. 15.

7.1.2   TRITON/NEWT Modeling

TRITON/NEWT calculations were performed for all enrichment-burnup pair values listed in Table 4 to generate a PWR spent fuel composition database based on the assembly bounding parameters illustrated in Fig. 1 and tabulated in Table 3 and Table 6. Additional input data, such as minor actinide concentrations in fresh fuel and the time for the last depletion step, were taken directly from the similar depletion calculations using SAS2H documented in Ref. 15. One quarter of the B&W 15×15 assembly with reflective boundary conditions, as shown in Fig. 2, was modeled for TRITON/NEWT depletion calculations. The burnable poison ^{10}B was depleted throughout the entire irradiation time period. The burnable poison typically burns out after the first cycle, but the BPR was left inserted for its moderator displacement effects, which result in a harder spectrum and thus a higher residual reactivity at fuel discharge.
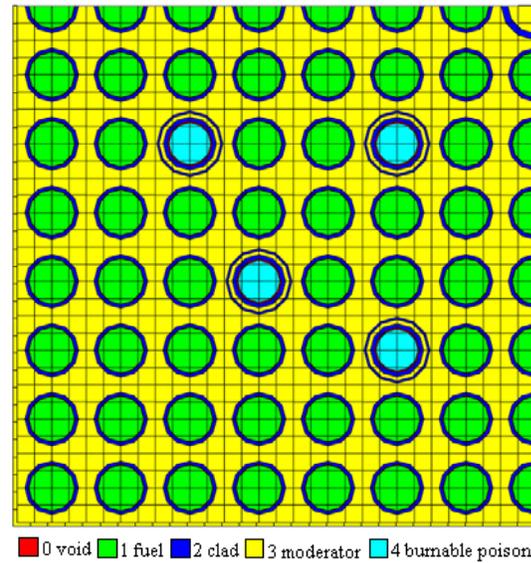
Fig. 2. TRITON/NEWT geometry representation of the B&W 15×15 assembly with BPRs fully inserted.

7.2   CHARACTERIZATION OF SCALE 5.1 ISOTOPIC VALIDATION DATA

Reference 3 provides a comprehensive evaluation of available PWR RCA data for use in depletion code validations and the comparison to measurement of the SCALE 5.1 isotopic concentration predictions. The evaluated RCA data comprise measured isotopic concentrations for 118 fuel samples obtained from low-, moderate-, and high-burnup fuel assemblies irradiated in the following nine PWRs: Trino Vercellese, Kernkraftwerk Obrigheim, Turkey Point Unit 3, H. B. Robinson Unit 2, Calvert Cliffs Unit 1, Three Mile Island (TMI) Unit 1, Takahama Unit 3, Gösgen, and GKN II. The initial enrichment and burnup of the evaluated fuel samples vary from 2.453 to 4.657 wt % ^{235}U and from 7.2 to 70.4 GWd/MTU, respectively. For illustrative purposes, a comparison of the enrichment and burnup values of the evaluated fuel samples to the actual and projected spent fuel assembly inventory and typical loading curve for PWR SNF assuming actinide and fission product burnup credit is shown in Fig. 3 (Ref. 3). Relevant parameters of the evaluated fuel samples are summarized in Table 7. For each individual RCA data set, the table presents the name of the reactor in which the measured fuel samples were irradiated, the name of the experimental program, fuel assembly design and initial enrichment, the range of the burnup for the evaluated fuel samples, the number of measured samples/rods, and the number of burnup credit isotopes evaluated. The number of the isotopes with measured concentrations varies depending on the experimental program. The earlier experimental programs generally provided measurement data for the uranium and plutonium isotopes, whereas the more recent experimental programs provided measurement data for up to 50 isotopes, including actinide and fission product isotopes relevant to burnup credit. The computer code and the cross-section library used in Ref. 3 to perform depletion calculations for the 118 evaluated fuel samples is the two-dimensional transport and depletion module, TRITON/NEWT, and the 44GROUPNDF5 cross-section library, respectively, in the SCALE 5.1 code system.[3]

Fig. 3. Enrichment and burnup values of the evaluated spent fuel samples compared to the actual and projected spent fuel assembly inventory and typical loading curve for PWR SNF assuming actinide and fission product burnup credit. (Note: Each point for the existing inventory represents multiple assemblies.)

Table 7. Relevant parameters of the evaluated RCA data

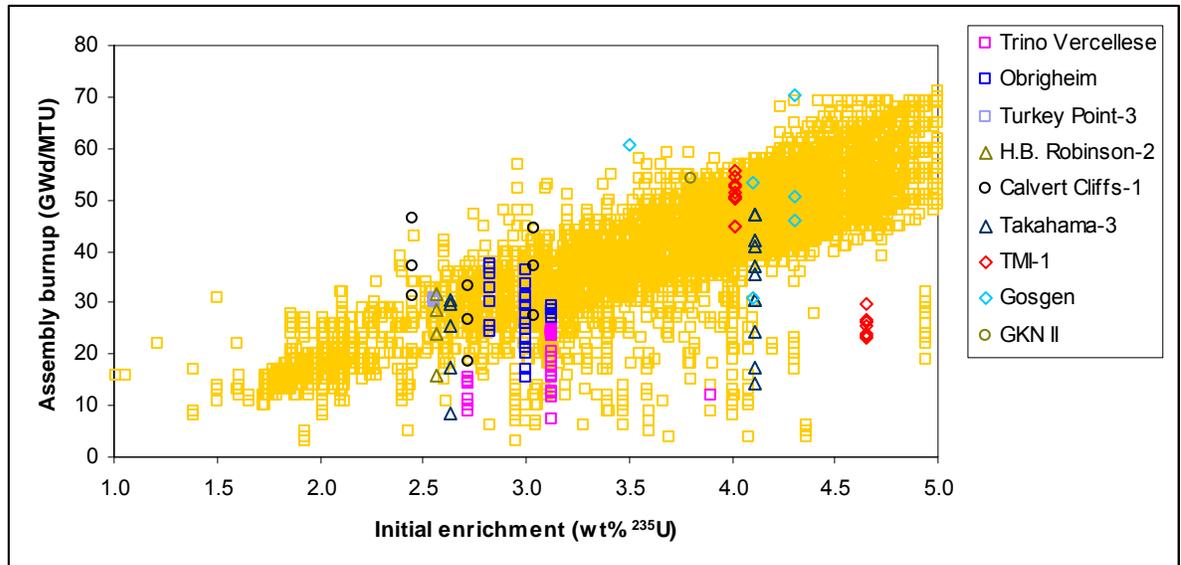| Reactor	Experimental program name	Assembly design	Initial enrichment (wt % ^{235}U)	No. of samples/ fuel rods	Burnup (GWd/MTU)	No. of measured burnup credit isotope[a]
Trino	EURATOM	15 × 15	2.719, 3.13, 3.897	15/5	7.2–17.5	8
Vercellese	EURATOM	15 × 15	3.13	16/5	12.8–25.3	10
Obrigheim	EURATOM	14 × 14	2.83, 3.00	22/6	15.6–37.5	8
	ICE[b]	14 × 14	3.13	5/5	27.0–29.4	8
Turkey Point-3	C-SFT[c]	15 × 15	2.556	5/2	30.5–31.6	9
H. B. Robinson-2	ATM-101[d]	15 × 15[e]	2.561	4/1	16.0–31.7	13
Calvert Cliffs-1	ATM-104	14 × 14	3.038	3/1	27.4–44.3	20
	ATM-103	14 × 14	2.72	3/1	18.7–33.2	12
	ATM-106	14 × 14	2.453	3/1	31.4–46.5	21
Takahama-3	JAERI[f]	17 × 17[g]	2.63, 4.11	16/3	7.8–47.3	20
TMI-1	DOE YMP[h]	15 × 15[e]	4.013	11/1	44.8–55.7	28
	DOE YMP	15 × 15[e,g]	4.657	8/3	22.8–29.9	23
Gösgen	ARIANE[i]	15 × 15	3.5, 4.1	3/2	29.1–59.7	28
	MALIBU[i]	15 × 15	4.3	3/1	47.2–70.4	28
GKN II	REBUS[i]	18 × 18	3.8	1/1	54.1	27

Source: Ref. 3.

[a]Maximum number of burnup credit isotopes in a sample measured/evaluated for each experimental program. The evaluated isotopes are tabulated in the tables included in Sect. 10.1 of Ref. 3. Note that measurement data for ^{233}U is not available because ^{233}U concentrations in the current commercial SNF are negligible.

[b]Isotopic Correlation Experiment.

[c]CLIMAX – Spent Fuel Test.

[d]Approved Testing Material.

[e]Assembly with burnable poison rods.

[f]Japan Atomic Energy Research Institute (now Japan Atomic Energy Agency)

[g]Assembly with Gd$_2$O$_3$ rods.

[h]U.S. Department of Energy Yucca Mountain Project.

[i]International Experimental Programs coordinated by Belgonucleaire, Belgium – currently managed by Studiecentrum voor Kernenergie – Centre d'étude de l'Energie Nucléaire (SCK·CEN) Laboratory (Ref. 32).

The measured-to-calculated (M/C) isotopic concentration values provided in Ref. 3, Tables 97 through 106, for the measured isotopes in the 118 PWR fuel samples comprise the isotopic validation data for disposal criticality analysis of PWR waste packages and are used in this calculation to determine the penalty in waste package reactivity due to isotopic composition bias and uncertainty in calculated SNF isotopic compositions. The characteristics of the frequency distributions of the validation data, including sample mean and standard deviation [see Eqs. (3) and (4), respectively], the results of a normality test, and the results of hypothesis testing for identifying statistically significant trending of the M/C isotopic concentration values with sample burnup are presented in Table 8. The M/C isotopic concentration values are not correlated with sample initial enrichment (see spreadsheet *DVD/xls/isotopics_for_criticality.xls*, worksheet *MoC stats*).

Table 8. Characteristics of the frequency distributions of the M/C isotopic concentration values

Isotope	$\overline{X}_i$ [a]	s_i [a]	No. of samples	Enrichment range (wt % ^{235}U)	Burnup range (GWd/MTU)	Normal distribution[b]	Correlation with burnup[c]
^{234}U	0.9348	0.1254	70	2.453–4.657	7.2–70.4	No	No
^{235}U	0.9934	0.0517	118	2.453–4.657	7.2–70.4	No	No
^{236}U	1.0069	0.0373	118	2.453–4.657	7.2–70.4	Yes	Yes
^{238}U	1.0014	0.0035	118	2.453–4.657	7.2–70.4	No	Yes
^{237}Np	0.9485	0.1340	49	2.453–4.657	8.6–70.4	No	No
^{238}Pu	1.0758	0.1091	103	2.453–4.657	8.6–70.4	No	No
^{239}Pu	0.9526	0.0528	118	2.453–4.657	7.2–70.4	No	Yes
^{240}Pu	0.9668	0.0488	118	2.453–4.657	7.2–70.4	No	Yes
^{241}Pu	1.0065	0.0643	118	2.453–4.657	7.2–70.4	No	No
^{242}Pu	1.0071	0.0763	117	2.453–4.657	7.2–70.4	No	No
^{241}Am	0.9795	0.2143	59	2.453–4.657	8.6–70.4	Yes	No
^{242m}Am	0.9320	0.2173	44	2.63–4.657	8.6–70.4	Yes	Yes
^{243}Am	0.8745	0.1654	52	2.63–4.657	8.6–70.4	No	No
^{95}Mo	0.9935	0.0610	18	3.5–4.3	31.1–70.4	Yes	No
^{99}Tc	0.9203	0.1306	31	2.453–4.3	16.0–70.4	No	No
^{101}Ru	0.9452	0.0798	18	3.5–4.3	31.1–70.4	Yes	No
^{103}Rh	0.9240	0.1084	19	2.453–4.3	31.1–70.4	No	No
^{109}Ag	0.5507	0.2009	17	3.5–4.3	44.8–70.4	No	No
^{143}Nd	0.9742	0.0439	50	2.453–4.657	8.6–70.4	No	Yes
^{145}Nd	0.9812	0.0275	50	2.453–4.657	8.6–70.4	No	No
^{147}Sm	0.9890	0.0759	36	2.453–4.657	17.4–70.4	No	No
^{149}Sm	0.8885	0.0694	32	3.5–4.657	17.4–70.4	Yes	No
^{150}Sm	0.9442	0.0534	36	2.453–4.657	17.4–70.4	No	No
^{151}Sm	0.7486	0.0560	36	2.453–4.657	17.4–70.4	Yes	No
^{152}Sm	0.7888	0.0612	36	2.453–4.657	17.4–70.4	Yes	Yes
^{151}Eu	1.0688	0.3831	23	3.5–4.657	23.7–70.4	No	No
^{153}Eu	0.9735	0.0727	30	2.453–4.657	23.7–70.4	No	Yes
^{155}Gd	1.7161	0.3452	30	2.453–4.657	23.7–70.4	No	No

Source: Ref. 3.

[a]Sample mean ($\overline{X}_i$) and standard deviation (s_i) of the M/C isotopic concentration values derived in *DVD/xls/isotopics_for_criticality.xls,* worksheet *bias* (see Appendix C). The M/C isotopic concentration values in file *isotopics_for_criticality.xls* were obtained from Ref. 3, Appendix B.1, *DVD/xls.zip/all_results.xls*.

[b]The *r*esults of Shapiro-Wilk normality test at the 0.05 significance level performed using Origin are available in *DVD/opj/bias.opj* (see Appendix C).

[c]Statistical significance of trending with burnup was determined in spreadsheet *DVD/xls/isotopics_for_criticality.xls*, worksheet *MoC stats* (see Appendix C) using the hypothesis test for slope of regression line described in Appendix A.2 and the upper critical values of Student's distribution corresponding to a significance level of 0.05, which are provided in Ref. 20, Sect. 1.3.6.7.2.

Many classical statistical methods, including the Monte Carlo uncertainty sampling method described in Sect. 6.3, rely on the assumption of normality of data to make probabilistic inferences from samples to populations. As indicated in Table 8, the M/C isotopic concentration values obtained for the majority of the burnup-credit isotopes do not approach the normal distribution. However, the frequency distributions of the M/C isotopic concentration values appear to be unimodal and symmetrical about a central value with varying degrees of kurtosis (see the histogram plots for the frequency distributions of the M/C isotopic concentration values for each burnup-credit isotope in *DVD/opj/bias.opj)*. Positive kurtosis indicates that a larger fraction of the M/C isotopic concentration values are concentrated symmetrically about a central value than that observed in the case of the normal distribution. The frequency distributions of the M/C isotopic concentration values for fission products with a small number of evaluated samples, such as ^{109}Ag and ^{151}Eu, appear to be unimodal and skewed. As shown in Table 9, the frequencies with which the M/C isotopic concentration values fall within ± 1, ± 2, and ± 3 standard deviations of the distribution's mean vary from 60 to 88 %, from 92 to 100 %, and from 95 to 100%, respectively. For the normal distribution of mean μ and standard deviation σ, 68.27 % of the population fall between $\mu \pm 1\sigma$, 95.45% of the population falls between $\mu \pm 2\sigma$, and 99.73% of the population fall between $\mu \pm 3\sigma$ (Ref. 20, Sect. 6.5.1).

Statistical hypothesis testing (see Appendix A.2) was used to determine whether an observed correlation between the M/C isotopic concentration and burnup values had occurred by chance or was statistically significant. Linear relationships between the M/C isotopic concentration and burnup values were determined for the eight isotopes identified in Table 8. By removing the M/C isotopic concentration values obtained for the TMI-1 assembly NJ05YU, a dependence on burnup was indicated by the hypothesis test only for the ^{238}U and ^{240}Pu isotopes. As indicated in Ref. 3, the TMI-1 assembly NJ05YU was burnt to approximately 50 GWd/MTU in atypical irradiation conditions and the M/C isotopic concentration values obtained for the TMI samples are likely affected by large experimental and modeling uncertainties; therefore, the isotopic validation results for this assembly also appear to be atypical. The M/C isotopic concentration values for the other measured fuel samples with burnup greater than 45 GWd/MTU (i.e., Gösgen, Takahama, Calvert Cliffs, and GKN samples) are well within the range of the M/C isotopic concentration values obtained for the lower-burnup fuel samples. Therefore, a real variation of the M/C isotopic concentration values with burnup appears to be unlikely; rather, the M/C isotopic concentration values for the samples from the TMI-1 assembly NJ05YU are likely affected by measurement and/or computational modeling bias. No correlation between the M/C isotopic concentration values and sample initial enrichment was identified for any of the burnup-credit isotopes.

Bias and uncertainty associated with measurement and calculation modeling, as well as the bias and uncertainty associated with the depletion code, are intrinsic components of isotopic validation data. The reported measurement uncertainties vary considerably, depending on the experimental program. For instance, the measurement uncertainties for the uranium and plutonium isotopes in the Takahama fuel samples and in the TMI-1 fuel samples (from assembly NJ05YU) measured at Argonne National Laboratory vary from 0.1 to 2% and from 3.7 to 7.9%, respectively.[3] Sources of potential modeling uncertainties have been identified for some of the evaluated fuel samples (e.g., the measured samples in the Obrigheim assemblies BE124 and BE210) (Ref. 3). However, a quantification of the potential effects that modeling uncertainties may have on the isotopic bias and bias uncertainty is not possible since the required data for more detailed modeling is not available for some of the evaluated fuel samples. The variations in the magnitude of measurement and modeling uncertainties across the evaluated fuel samples affect the calculated M/C isotopic concentration values in a nonuniform manner, thus producing anomalies in the frequency distributions of the isotopic validation data. The intent of this brief analysis was only to emphasize the complexity of the isotopic validation data. No attempt was made to remove atypical data from the isotopic validation data set.

7.2.1 Area of Applicability

The initial enrichment and burnup for the spent fuel in the application model range from 2.5 to 5 wt % ^{235}U and from 5 to 45 GWd/MTU, respectively.[18] The ranges of initial enrichment and burnup for each burnup-credit isotope in the evaluated spent fuel samples vary depending on the isotope, as shown in Table 8. In this calculation, the range of applicability of the isotopic composition validation data is expanded upward to higher initial enrichment values and downward to lower burnup values. The enrichment applicability was extended from either 4.657 or 4.3 wt % ^{235}U to 5 wt % ^{235}U. The burnup applicability was slightly expanded downward for actinide isotopes from either 7.2 or 8.6 GWd/MTU to 5 GWd/MTU and was significantly expanded for most of the fission product isotopes.

A conservative approach was used to compensate for the effects of unknown uncertainties associated with the extension of the area of applicability of the validation data. The extension of the area of applicability was performed simultaneously with augmentation of the bias uncertainty values by using two-sided tolerance-limit factors as multiplication factors (see Sect. 6.3.1 and Appendix A.1), thereby increasing the uncertainty in k_{eff} due to depletion uncertainty. Statistical tolerance limits are values such that the probability is equal to γ that the limits include at least a proportion p of the population. Tolerance-limit factors depend on the type of the distribution and on the sample size. The value of the tolerance-limit factor increases as the sample size decreases. The values applied to the calculated sample standard deviation correspond to 95% certainty and 68.27% of the population and vary from 1.126 (118 samples) to 1.459 (17 samples) (see Appendix A.1). Therefore, a larger augmentation was applied to the uncertainties in the calculated fission product concentrations than the augmentation applied to the uncertainties in the calculated actinide concentrations. However, the effect on k_{eff} of additional uncertainties introduced by extending of the area of applicability of the validation data for fission product isotopes diminishes with decreasing burnup because k_{eff} sensitivity to fission product cross section decreases with decreasing burnup (see Ref. 33, Table 4.1).

The use of two-sided tolerance-limit factors as augmentation factors for the calculated standard deviation of the M/C isotopic concentration values is also intended to account for potential uncertainties associated with the identified non-normality of frequency distributions and dependence on burnup for some burnup credit isotopes. This approach appears to adequately account for the various additional uncertainty sources associated with the isotopic validation process. For illustrative purposes, the validation data for ^{235}U and ^{240}Pu are discussed further. The frequency distribution of the M/C isotopic concentration values for ^{235}U is highly peaked since 81% of the M/C isotopic concentration values fall within one standard deviation. However, as illustrated in Fig. 4, the 3σ sampling interval contains 98% of the values, which is adequately close to the ideal 99.73% expected for the normal distribution. A linear dependency of the M/C isotopic concentration values on burnup was identified for eight burnup-credit isotopes, including ^{240}Pu. The downward trend in the M/C isotopic concentration values as a function of burnup is clearly noticeable for ^{240}Pu on the graph shown in Fig. 5 (a). The 3σ sampling interval used in this calculation for ^{240}Pu is illustrated in Fig. 5 (a) and contains 100% of the M/C isotopic concentration values. Fig. 5 (b) shows that the sampling interval would be smaller (i.e., less conservative for criticality) if the M/C isotopic concentration values for the evaluated samples in the TMI-1 assembly NJ05YU were excluded from the validation data set on the basis of their atypical characteristics. The error bars in Fig. 4 and Fig. 5 indicate the reported measurement (one sigma) uncertainty.

Table 9. Isotopic bias and bias uncertainty values

Isotope	$\bar{X}_i{}^a$	s_i	Frequency within $\bar{X}_i \pm s_i$ (%)	Frequency within $\bar{X}_i \pm 2s_i$ (%)	Frequency within $\bar{X}_i \pm 3s_i$ (%)	$\sigma_i{}^{a,\,b}$
^{234}U	0.9348	0.1254	70	93	100	0.1470
^{235}U	0.9934	0.0517	81	94	98	0.0582
^{236}U	1.0069	0.0373	70	94	99	0.0420
^{238}U	1.0014	0.0035	88	93	95	0.0040
^{237}Np	0.9485	0.1340	76	92	98	0.1631
^{238}Pu	1.0758	0.1091	77	95	98	0.1241
^{239}Pu	0.9526	0.0528	75	95	99	0.0595
^{240}Pu	0.9668	0.0488	78	94	98	0.0550
^{241}Pu	1.0065	0.0643	71	95	98	0.0724
^{242}Pu	1.0071	0.0763	75	94	98	0.0859
^{241}Am	0.9795	0.2143	69	98	98	0.2555
^{242m}Am	0.9320	0.2173	75	93	100	0.2678
^{243}Am	0.8745	0.1654	73	98	98	0.1999
^{95}Mo	0.9935	0.0610	61	94	100	0.0878
^{99}Tc	0.9203	0.1306	77	97	97	0.1690
^{101}Ru	0.9452	0.0798	72	89	100	0.1147
^{103}Rh	0.9240	0.1084	68	95	95	0.1540
^{109}Ag	0.5507	0.2009	71	94	100	0.2931
^{143}Nd	0.9742	0.0439	72	94	100	0.0533
^{145}Nd	0.9812	0.0275	78	94	100	0.0333
^{147}Sm	0.9890	0.0759	75	94	100	0.0961
^{149}Sm	0.8885	0.0694	66	94	100	0.0893
^{150}Sm	0.9442	0.0534	78	94	100	0.0676
^{151}Sm	0.7486	0.0560	72	97	100	0.0709
^{152}Sm	0.7888	0.0612	67	97	100	0.0775
^{151}Eu	1.0688	0.3831	78	96	100	0.5225
^{153}Eu	0.9735	0.0727	60	100	100	0.0945
^{155}Gd	1.7161	0.3452	77	97	97	0.4491

[a]Isotopic bias and the uncertainty associated with the bias used in the Monte Carlo uncertainty sampling calculations.
[b]The product of sample standard deviation and the two-sided tolerance limit factor for 95% certainty and 68.27 % of the population. The values for tolerance-limit factors were calculated in spreadsheet *DVD/xls/validation.xls*, worksheet *tl-factors*.

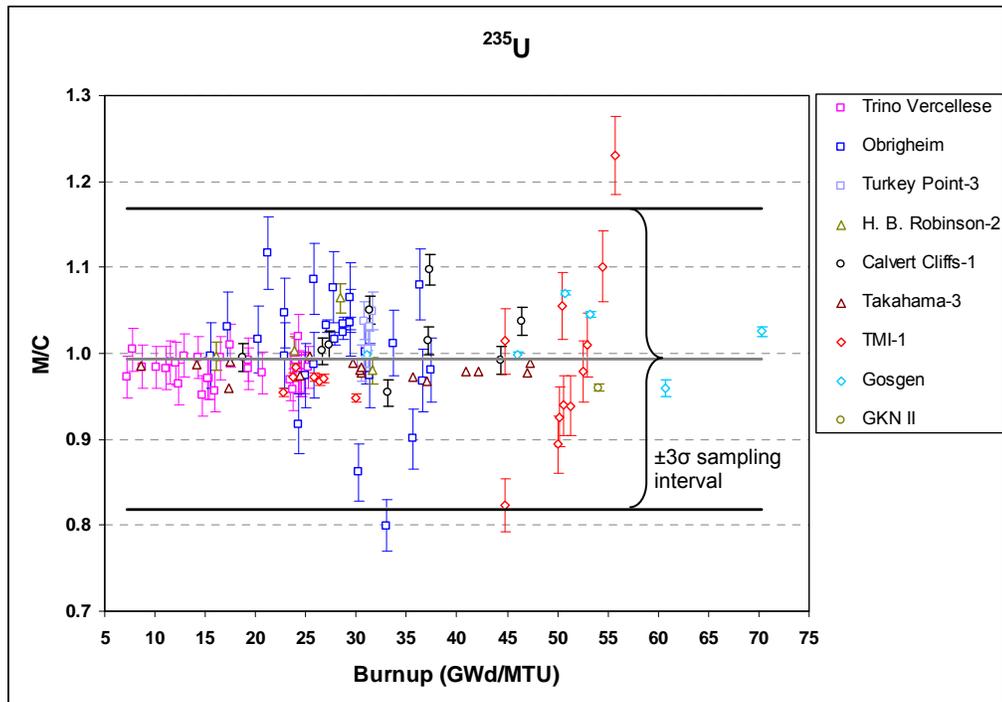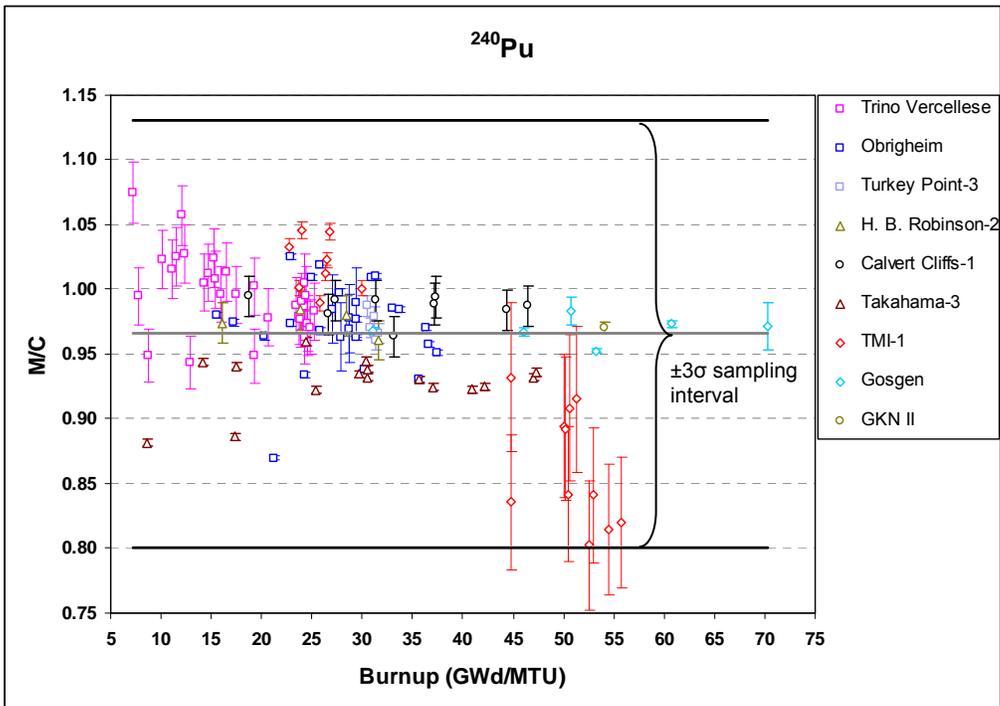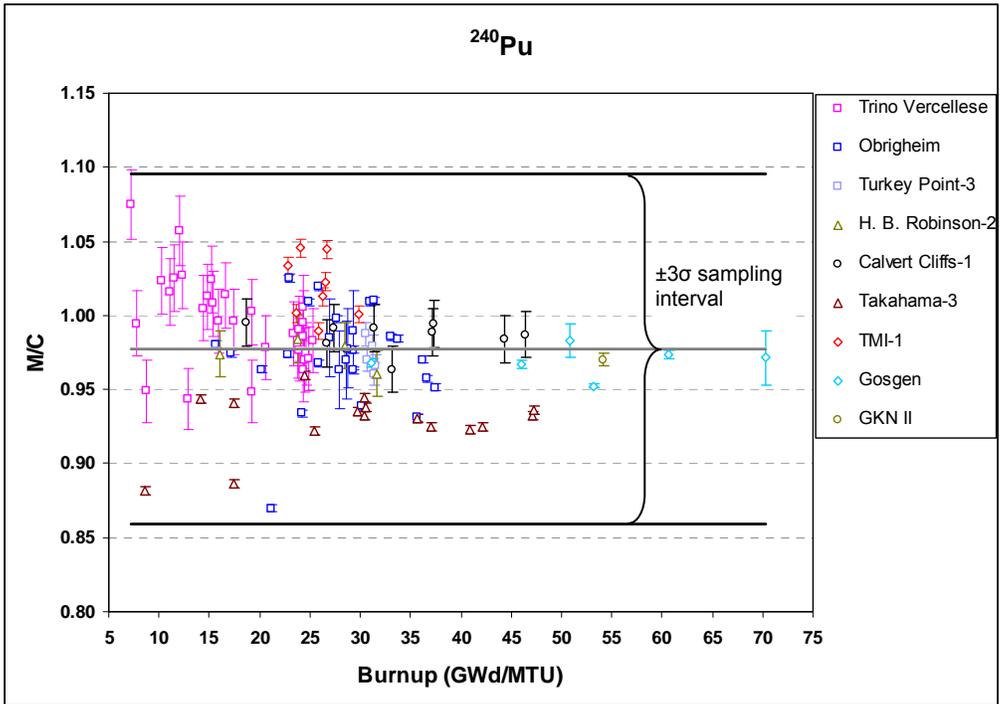**Fig. 4. M/C isotopic concentration ratio as a function of burnup and the sampling interval for ^{235}U.**

Fig. 5. M/C isotopic concentration ratio as a function of burnup and the sampling interval for ^{240}Pu based on (a) entire set of evaluated spent fuel samples and (b) the set of evaluated spent fuel samples without the samples from TMI-1 assembly NJ05YU.

7.3 DESCRIPTION OF THE MCNP MODEL FOR WASTE PACKAGES

The PWR waste package configuration consists of 21 fully-flooded, intact B&W 15 × 15 fuel assemblies, intact fuel tubes, and borated stainless steel plates placed inside a conceptual transport/aging/disposal (TAD) canister waste package configuration and reflected by tuff, simulating the repository environment. A horizontal cross section of the MCNP model for the PWR waste package is shown in Fig. 6. The thickness of the absorber plate in the model is 6 mm, as compared to 11 mm for intact absorber plates, to account for possible absorber plate corrosion over 10,000 years.

The [10]B weight fraction in the models is 75% of the actual fraction for consistency with the guidance in NUREG-1536 (Ref. 34). The conservative PWR waste package model with respect to criticality was used in the development of loading curves for commercial SNF TAD canisters (Ref. 18). The MCNP input files for the current criticality calculations are based on the MCNP input file *d0a00* for a PWR waste package (DTN: MO0711LOADCURV.000, Ref. 18). In the MCNP model, the fuel is represented as a single axial zone with uniform isotopic compositions. The one-axial-zone fuel representation appears to be slightly more conservative than the seven-axial-zone representation for the majority of PWR SNF with potential for waste package criticality based on a comparison study considering the two fuel axial representations (see Ref. 18, Fig. 6–9).
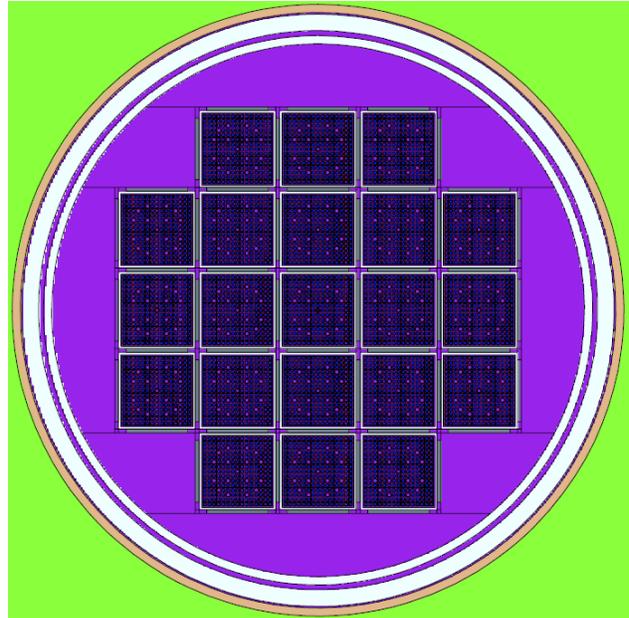
Fig. 6. Horizontal cross section of the MCNP model for the PWR waste package.

7.3.1 Selected Fuel Initial Enrichment, Burnup, and Decay Time for Criticality Calculations

The fuel isotopic compositions selected for criticality calculations correspond to the following combinations of fuel initial enrichment, in wt % [235]U, and burnup, in GWd/MTU: 2.5/10, 3/15, 3.5/25, 4/30, 4.5/35, and 5/40, for SNF cooling times of 5, 100, and 10,000 years. The initial enrichment and burnup combinations characterize data points in the proximity of the loading curve established for PWR waste packages in Ref. 18, Table 6–26 and Figure 6–24. The burnup values for the six initial enrichment-burnup combinations represent the nearest integers obtained by either rounding up or rounding down the burnup values in Ref. 18, Table 6-26. The critical limit used in the loading curve analysis in Ref. 18 is based on the isotopic bias in predicted nuclide composition using the one-dimensional depletion analysis code SAS2H in SCALE 4.4a (Ref. 28). For the 5-year cooling time only, the burnup was also varied by ± 5 GWd/MTU to observe the sensitivity of the k_{eff} uncertainty values to data points in the proximity of the established loading curve. The SCALE ft71f001 binary files are available in the DVD/TRITON.zip archive (refer to the *.den files) to facilitate ORIGEN decay calculations for other decay time values.

8. RESULTS

The results obtained for Δk_{ISO}, the penalty in waste package reactivity due to bias and uncertainty in calculated SNF isotopic compositions (see Sect. 6.1), are summarized in Table 10, Table 11, and Table 12 for PWR SNF at 5-, 100-, and 10,000-year cooling times, respectively, and for six combinations of initial enrichment and burnup characterizing data points in the proximity of the loading curve established for disposal of PWR SNF (see Sect. 7.3.1). Additional combinations of initial enrichment and burnup were considered for the SNF at 5-year cooling time, as shown in Table 10, to determine the sensitivity of Δk_{ISO} to the burnup values in the proximity of the loading curve. The 100-, and 10,000-year cooling time compositions were analyzed to determine whether the Δk_{ISO} values increase with increasing cooling time and whether the increase in the Δk_{ISO} values is sufficient to offset the decrease in k_{eff} values that occurs with increasing cooling time.

The Monte Carlo uncertainty sampling method (see Sect. 6.3) allows compensating effects of positive and negative changes in system reactivity due to statistical corrections for isotopic bias and bias uncertainty. The Δk_{ISO} results are based on a minimum of 200 MCNP calculations for each combination of fuel initial enrichment, burnup, and cooling time, using fuel isotopic compositions stochastically corrected for bias uncertainty according to the established frequency distributions of the isotopic validation data (see Sect. 7.2). The Δk_{ISO} values determined in this calculation are based on the upper tolerance limit for 95% of the k_{eff} population and 95% certainty [see Eq. (11)].

Tables 10 through 12 provide the calculation results for the following:

- the effective neutron multiplication factor k_{eff} based on unadjusted predicted isotopic compositions;
- the effective neutron multiplication factor based on predicted isotopic compositions corrected for isotopic bias, k_{eff-BE};
- the statistical uncertainty in k_{eff-BE} due to isotopic bias uncertainty, Δk_{eff-MC} [see Eq. (10)];
- the penalty in reactivity due to isotopic composition bias and uncertainty in calculated nuclide compositions, Δk_{ISO} [see Eq. (11)]; and
- the bounding effective neutron multiplication factor based on the most unfavorable combination of isotopic bias uncertainty, $k_{eff-bounding}$ [see Eq. (15)].

The $k_{eff-BE} - k_{eff}$ component of Eq. 11 represents the effect on k_{eff} of the corrections for isotopic bias. The results summarized in Tables 10 through 12 show that Δk_{ISO} values vary to a small degree with fuel enrichment, burnup, and cooling time since fuel isotopic composition depends on these parameters. The variation of fuel isotopic concentration with time is illustrated in Fig. 7 for PWR SNF of 5.0-wt % ^{235}U initial enrichment and 40-GWd/MTU burnup.

For the selected SNF compositions with potential for criticality corresponding to the 5-year cooling time, the values obtained for $k_{eff-BE} - k_{eff}$ were almost negligible as compared to the k_{eff} values (less than 0.4%); the Δk_{eff-MC} values varied from 0.0114 to 0.0134; and the Δk_{ISO} values varied from 0.0188 to 0.0244. The average Δk_{ISO} value was 0.0215. The Δk_{ISO} values represent 1.97 to 2.45% of the corresponding k_{eff} values based on predicted spent fuel compositions, with an average value of 2.26%. The largest Δk_{ISO} value was obtained for the SNF composition corresponding to 2.5-wt %

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[235]U initial enrichment and 5-GWd/MTU burnup. However, the isotopic bias and uncertainty in predicted fuel compositions for very low burnup are expected to be fairly small since these compositions are mainly dominated by the uranium isotopes. In the case of this calculation, the extension of the applicability of the isotopic validation data based on fuel samples with a broad range of burnup values (up to 70 GWd/MTU) to very low burnup values (e.g., 5 GWd/MTU) is considered to have an unrealistically penalizing effect. Therefore, the Δk_{ISO} value of 0.0229 obtained for the SNF composition corresponding to 3.5-wt % [235]U initial enrichment and 25-GWd/MTU burnup is considered to be a more realistic bounding value. For very low burnup (e.g., < 10 GWd/MTU), criticality safety analyses based on the fresh fuel assumption are justified because (1) very few RCA data for low burnup fuel are available for use in isotopic validation studies and (2) the impact of assembly design and operation variability on SNF compositions for low burnup is more significant than on the SNF compositions for higher burnup.

For the 100-year cooling time isotopic compositions, the values of $k_{eff-BE} - k_{eff}$ varied from -0.0033 to -0.0065; the Δk_{eff-MC} values varied from 0.0138 to 0.0175; and the Δk_{ISO} values varied from 0.0224 to 0.0281. Although the Δk_{ISO} values for 100-year cooling time are higher than those obtained for the 5-year cooling time, the increase is insufficient to offset the decrease in k_{eff} that occurs with increasing cooling time. For the 10,000-year cooling time isotopic compositions, the values of $k_{eff-BE} - k_{eff}$ varied from -0.0037 to -0.0070; the Δk_{eff-MC} values varied from 0.0124 to 0.0146; and the Δk_{ISO} values varied from 0.0200 to 0.0217.

For comparison purposes only, the values of the penalty in reactivity due to isotopic composition bias and uncertainty based on the bounding method (see Sect. 6.4) are also provided in Table 10 through Table 12. As expected, the bounding method produces significantly larger bias values than the Monte Carlo uncertainty sampling method (e.g., 0.0557 versus 0.0221 for the SNF composition corresponding to the 5-wt % [235]U initial enrichment, 45-GWd/MTU burnup, and 5-year cooling time) because this method maximizes the effects of isotopic composition bias uncertainties on system reactivity. The significant conservatism of the bounding method is not justified when this method is coupled with the use of conservative depletion parameters that maximize the spent fuel residual reactivity, which is the case of the disposal criticality analysis methodology.

The results of the Monte Carlo uncertainty sampling method are not always intuitive due to the nature of the method itself, which allows for compensating positive and negative reactivity effects produced by varying isotopic uncertainties. The compensating effects appear to be more effective in the case of SNF compositions for which the reactivity worth of the fission product isotopes becomes significant (e.g., SNF compositions for 5-year cooling time and higher burnup) as compared to the case of SNF compositions dominated by main actinide isotopes (e.g., SNF compositions for very low burnup or for larger cooling times).

Table 10. Δk_{ISO} **for waste packages containing PWR SNF at 5 years after discharge**

Enrichment (wt % ^{235}U)/burnup (GWd/MTU)	2.5/10	3.0/15	3.5/25	4.0/30	4.5/35	5.0/40
$k_{eff}^{\ a, b}$	0.9588	0.9674	0.9381	0.9416	0.9437	0.9440
$k_{eff-BE}^{\ a, c}$	0.9577	0.9660	0.9373	0.9411	0.9423	0.9435
$k_{eff-BE} - k_{eff}^{\ d}$	-0.0011	-0.0014	-0.0008	-0.0005	-0.0014	-0.0005
$\Delta k_{eff-MC}^{\ e}$	0.0118	0.0122	0.0124	0.0114	0.0118	0.0119
$\Delta k_{eff-MC} \times k_1^{\ f}$	0.0217	0.0224	0.0228	0.0210	0.0217	0.0219
$k_{eff-BE} + \Delta k_{eff-MC} \times k_1$	0.9794	0.9884	0.9601	0.9621	0.9640	0.9654
$\Delta k_{ISO}^{\ g}$	0.0215	0.0219	0.0229	0.0213	0.0212	0.0222
$\Delta k_{ISO} / k_{eff}$ (%)	2.24	2.26	2.44	2.26	2.24	2.36
$k_{eff-bounding}^{\ a, h}$	0.9966	1.0085	0.9857	0.9919	0.9950	0.9979
$k_{eff-bounding} - k_{eff}$	0.0378	0.0411	0.0476	0.0503	0.0513	0.0539
Enrichment (wt % ^{235}U)/burnup (GWd/MTU)	2.5/5	3.0/10	3.5/20	4.0/25	4.5/30	5.0/35
$k_{eff}^{\ a, b}$	0.9958	1.0040	0.9710	0.9734	0.9731	0.9726
$k_{eff-BE}^{\ a, c}$	0.9947	1.0016	0.9704	0.9724	0.9726	0.9727
$k_{eff-BE} - k_{eff}^{\ d}$	-0.0011	-0.0024	-0.0006	-0.0010	-0.0005	0.0001
$\Delta k_{eff-MC}^{\ e}$	0.0134	0.0116	0.0113	0.0123	0.0116	0.0111
$\Delta k_{eff-MC} \times k_1^{\ f}$	0.0247	0.0213	0.0208	0.0226	0.0213	0.0204
$k_{eff-BE} + \Delta k_{eff-MC} \times k_1$	1.0194	1.0229	0.9912	0.9950	0.9939	0.9931
$\Delta k_{ISO}^{\ g}$	0.0244	0.0198	0.0210	0.0225	0.0217	0.0214
$\Delta k_{ISO} / k_{eff}$ (%)	2.45	1.97	2.17	2.31	2.23	2.20
$k_{eff-bounding}^{\ a, h}$	1.0296	1.0401	1.0145	1.0188	1.0215	1.0229
$k_{eff-bounding} - k_{eff}$	0.0338	0.0361	0.0435	0.0454	0.0484	0.0503

Table 10 (continued)

Enrichment (wt % ^{235}U)/burnup (GWd/MTU)	2.5/15	3.0/20	3.5/30	4.0/35	4.5/40	5.0/45
k_{eff} [a, b]	0.9234	0.9323	0.9067	0.9124	0.9141	0.9162
k_{eff-BE} [a, c]	0.9202	0.9311	0.9051	0.9103	0.9136	0.9156
$k_{eff-BE} - k_{eff}$ [d]	-0.0032	-0.0012	-0.0016	-0.0021	-0.0005	-0.0006
Δk_{eff-MC} [e]	0.0116	0.0118	0.0128	0.0109	0.0112	0.0119
$\Delta k_{eff-MC} \times k_1$ [f]	0.0213	0.0217	0.0236	0.0201	0.0206	0.0219
$k_{eff-BE} + \Delta k_{eff-MC} \times k_1$	0.9415	0.9528	0.9287	0.9304	0.9342	0.9375
Δk_{ISO} [g]	0.0190	0.0214	0.0222	0.0188	0.0210	0.0221
$\Delta k_{ISO} / k_{eff}$ (%)	2.06	2.29	2.45	2.06	2.29	2.42
$k_{eff-bounding}$ [a, h]	0.9651	0.9774	0.9586	0.9647	0.9703	0.9739
$k_{eff-bounding} - k_{eff}$	0.0417	0.0451	0.0519	0.0523	0.0562	0.0577

[a]The standard deviation for an MCNP k_{eff} value is 0.0003.

[b]k_{eff} values obtained by using predicted isotopic compositions.

[c]Best estimate k_{eff} values obtained by using predicted isotopic compositions corrected for isotopic bias (predicted isotopic concentrations multiplied by the isotopic bias values).

[d]The standard uncertainty associated with the $k_{eff-BE} - k_{eff}$ values is approximately 0.0004.

[e]Bias uncertainty determined by using the Monte Carlo uncertainty sampling method [see Eq. (10)].

[f]k_1 is the tolerance-limit factor for the one-sided tolerance interval, assuming 200 samples, 95% of the population, and 95% certainty, whose value is 1.84.

[g]Values calculated using Eq. (11).

[h]Bounding k_{eff} limit based on the most unfavorable combination of isotopic uncertainty [see Eq. (15)].

Table 11. Δk_{ISO} for waste packages containing PWR SNF at 100 years after discharge

Enrichment (wt % ^{235}U)/burnup (GWd/MTU)	2.5/10	3.0/15	3.5/25	4.0/30	4.5/35	5.0/40
k_{eff} [a, b]	0.9403	0.9392	0.8902	0.8878	0.8853	0.8833
k_{eff-BE} [a, c]	0.9370	0.9355	0.8853	0.8833	0.8804	0.8768
$k_{eff-BE} - k_{eff}$ [d]	-0.0033	-0.0037	-0.0049	-0.0045	-0.0049	-0.0065
Δk_{eff-MC} [e]	0.0138	0.0137	0.0145	0.0163	0.0175	0.0166
$\Delta k_{eff-MC} \times k_1$ [f]	0.0254	0.0252	0.0267	0.0300	0.0322	0.0305
$k_{eff-BE} + \Delta k_{eff-MC} \times k_1$	0.9624	0.9607	0.9120	0.9133	0.9126	0.9073
Δk_{ISO} [g]	0.0229	0.0224	0.0226	0.0263	0.0281	0.0249
$k_{eff-bounding}$ [a, h]	0.9828	0.9869	0.9473	0.9488	0.9489	0.9498
$k_{eff-bounding} - k_{eff}$	0.0425	0.0477	0.0571	0.0610	0.0636	0.0665

[a]The standard deviation for an MCNP k_{eff} value is 0.0003.

[b]k_{eff} values obtained by using predicted isotopic compositions.

[c]Best estimate k_{eff} values obtained by using predicted isotopic compositions corrected for isotopic bias (predicted isotopic concentrations multiplied by the isotopic bias values).

[d]The standard uncertainty associated with the $k_{eff-BE} - k_{eff}$ values is approximately 0.0004.

[e]Bias uncertainty determined by using the Monte Carlo uncertainty sampling method [see Eq. (10)].

[f]k_I is the tolerance-limit factor for the one-sided tolerance interval, assuming 200 samples, 95% of the population, and 95% certainty, whose value is 1.84.

[g]Values calculated using Eq. (11).

[h]Bounding k_{eff} limit based on the most unfavorable combination of isotopic uncertainty [see Eq. (15)].

Table 12. Δk_{ISO} for waste packages containing PWR SNF at 10,000 years after discharge

Enrichment (wt % ^{235}U)/burnup (GWd/MTU)	2.5/10	3.0/15	3.5/25	4.0/30	4.5/35	5.0/40
k_{eff} [a, b]	0.9540	0.9601	0.9203	0.9225	0.9232	0.9231
k_{eff-BE} [a, c]	0.9503	0.9557	0.9146	0.9165	0.9172	0.9161
$k_{eff-BE} - k_{eff}$ [d]	-0.0037	-0.0044	-0.0057	-0.0060	-0.0060	-0.0070
Δk_{eff-MC} [e]	0.0124	0.0137	0.0141	0.0137	0.0146	0.0144
$\Delta k_{eff-MC} \times k_1$ [f]	0.0228	0.0252	0.0259	0.0252	0.0269	0.0265
$k_{eff-BE} + \Delta k_{eff-MC} \times k_1$	0.9731	0.9809	0.9405	0.9417	0.9441	0.9426
Δk_{ISO} [g]	0.0200	0.0217	0.0211	0.0201	0.0217	0.0203
$k_{eff-bounding}$ [a, h]	0.9943	1.0026	0.9712	0.9751	0.9776	0.9800
$k_{eff-bounding} - k_{eff}$	0.0403	0.0425	0.0509	0.0526	0.0544	0.0569

[a] The standard deviation for an MCNP k_{eff} value is 0.0003.

[b] k_{eff} values obtained by using predicted isotopic compositions.

[c] Best estimate k_{eff} values obtained by using predicted isotopic compositions corrected for isotopic bias (predicted isotopic concentrations multiplied by the isotopic bias values).

[d] The standard uncertainty associated with the $k_{eff-BE} - k_{eff}$ values is approximately 0.0004.

[e] Bias uncertainty determined by using the Monte Carlo uncertainty sampling method [see Eq. (10)].

[f] k_1 is the tolerance-limit factor for the one-sided tolerance interval, assuming 200 samples, 95 percentage of the population, and 95% certainty, whose values is 1.84.

[g] Values calculated using Eq. (11).

[h] Bounding k_{eff} limit based on the most unfavorable combination of isotopic uncertainty [see Eq. (15)].
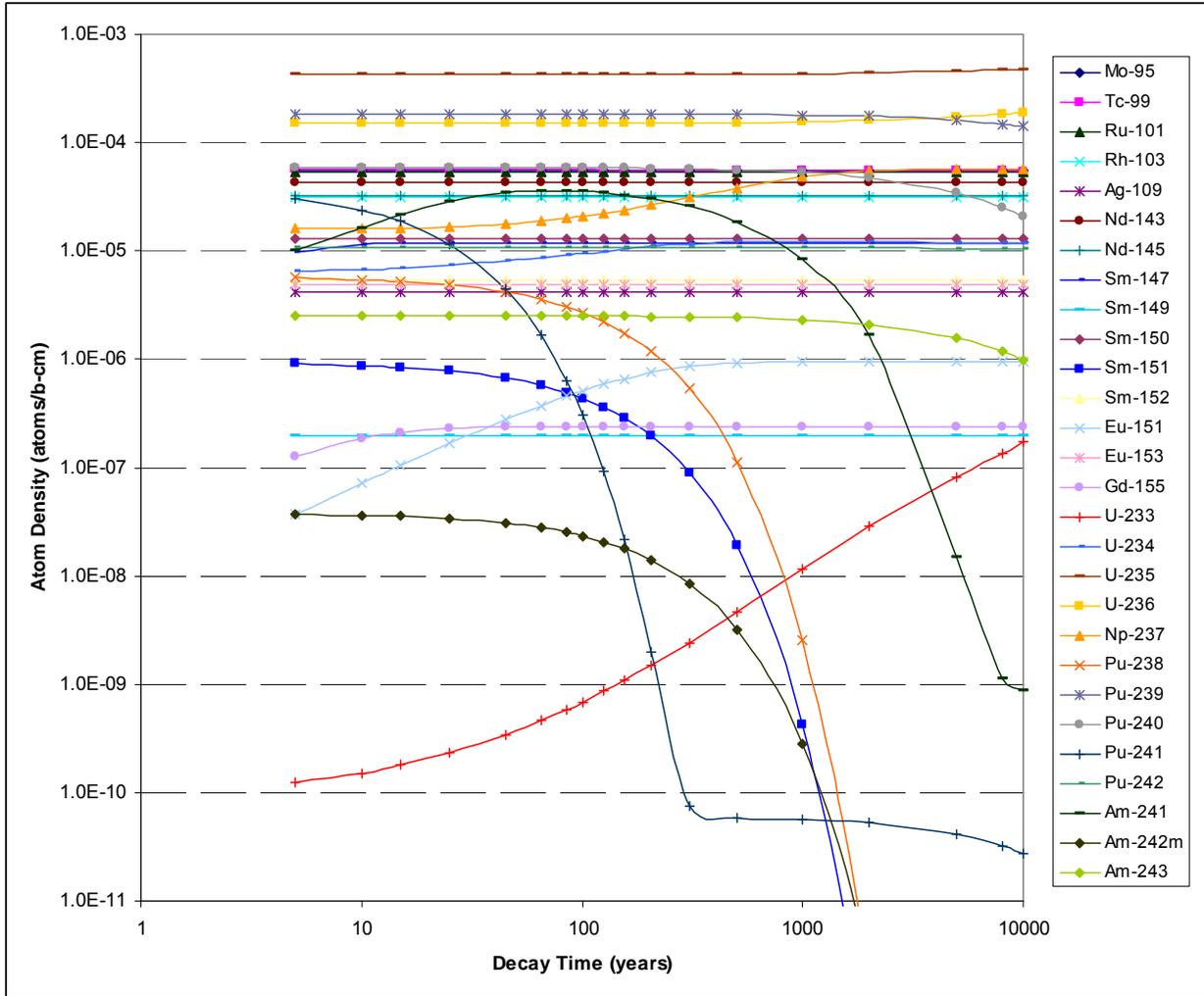
Fig. 7. Isotopic concentration versus time after discharge for PWR SNF of 5.0-wt % ^{235}U initial enrichment and 40-GWd/MTU burnup.

9. SUMMARY

The disposal criticality analysis methodology is based on burnup credit.[1] The burnup-credit methodology requires validation of both the depletion method (SCALE 5.1) used to calculate the concentrations of the credited actinide and fission product isotopes in SNF compositions and the criticality method (MCNP 5.1.40) used to calculate the k_{eff} values for waste packages. The results of the validation studies are used to establish a critical limit at which waste packages are considered potentially critical. The validation of the criticality method has been documented in Ref. 23. The accuracy of the depletion calculation method and the effect of depletion uncertainty on k_{eff} were evaluated in the current calculation report.

Specifically, this calculation provides the value for the penalty in waste package reactivity due to the bias and uncertainty associated with predicted SNF isotopic compositions for use in the development of loading curves for disposal of PWR SNF. For consistency with the previous loading curve analyses,[18] this calculation used a PWR waste package model that is conservative with respect to criticality (see Sect. 7.3 and Sect. 7.1.1). The results were determined for PWR SNF assemblies with six combinations of initial enrichment and burnup characterizing data points in the proximity of the established loading curve for PWR SNF (see Sect. 7.3.1). Additional data points located slightly above and below the established loading curve were considered to evaluate the sensitivity of the results to burnup variation. The variation with time of the effect of depletion uncertainty on k_{eff} and its impact on criticality safety were also evaluated.

The isotopic validation data for SCALE 5.1 consists of the M/C isotopic concentration values determined in Ref. 3 for 118 PWR fuel samples with initial enrichment ranging from 2.453 to 4.657 wt % ^{235}U and burnup ranging from 7.2 to 70.4 GWd/MTU. The isotopic bias and bias uncertainty for each burnup-credit isotope were determined in this calculation as the sample mean and the sample standard deviation, respectively, of the M/C isotopic concentration values (see Sect. 6.3.1). The bias uncertainty was conservatively adjusted to account for uncertainties related to non-normality, dependence on burnup, and extension of the area of applicability of the validation data (see Sect. 7.2.1). The method used to propagate the isotopic composition bias and bias uncertainty to the k_{eff} values for waste packages was Monte Carlo uncertainty sampling (see Sect. 6.3.2). This method provides a more realistic evaluation for the safety margin than the bounding method by crediting compensating reactivity effects of isotopic composition uncertainties on k_{eff}.

The current calculation determined that the penalty in waste package reactivity due to the bias and uncertainty associated with predicted SNF isotopic compositions is 0.0229 (see Sect. 8). This value is intended to be used in the development of loading curves for disposal of PWR SNF and should not be generalized to other applications because it is dependent upon the specific application system. The work described in this calculation report was performed under the ORNL Quality Assurance Plan for the OCRWM and OCRWM Lead Laboratory Program, ORNL-OCRW-QAP-001 (Ref. 35).

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APPENDIX A.

STATISTICAL CONCEPTS AND METHODS USED

IN VARIOUS ANALYSES

A.1 TOLERANCE-LIMIT FACTORS FOR ONE- AND TWO-SIDED INTERVALS

Statistical tolerance limits are values such that the probability is equal to γ that the limits include at least a proportion *p* of the population. Tolerance-limit factors depend on the type of the distribution and on the sample size. The one-sided tolerance-limit factors, k_1, for normal distributions can be determined as shown in Eq. (A-1) (Ref. A-1, Sect. 7.2.6.3).

$$k_1 = \frac{z_{1-p} + \sqrt{z_{1-p}^2 - a \cdot b}}{a} ,$$

$$a = 1 - \frac{z_{1-\gamma}^2}{1(N_S - 1)}; b = z_{1-p}^2 - \frac{z_{1-\gamma}^2}{N_S} ,$$

(A-1)

where

$z_{(1-p)}$ = the critical value of the normal distribution that is exceeded with probability $(1-p)$,

$z_{(1-\gamma)}$ = the critical value of the normal distribution that is exceeded with probability $(1-\gamma)$.

The two-sided tolerance-limit factors, k_2, for normal distributions can be determined as shown in Eq. (A-2) (Ref. A-1, Sect. 7.2.6.3).

$$k_2 = \sqrt{\frac{(N_S - 1)(1 + \frac{1}{N_S})z_{(1-p)/2}^2}{\chi_{\gamma, N_S - 1}^2}} .$$

(A-2)

In Eq. (A-2), $\chi_{\gamma, N-1}^2$ is the critical value of the chi-square distribution, with degrees of freedom $N_S - 1$, that is exceeded with probability γ, and $z_{(1-p)/2}$ is the critical value of the normal distribution that is exceeded with probability $(1-p)/2$.

Tolerance-limit factors for two-sided intervals (95% certainty/68.27% of the population) and one-sided intervals (95% certainty/95% of the population; N > 50) were calculated in a Microsoft Office Excel application (see *DVD/xls/validation.xls*) using standard Excel statistical functions NORMSINV and CHIINV and the formulas shown by Eqs. (A-2) and (A-1), respectively, based on the procedure described in *NIST/SEMATECH e-Handbook of Statistical Methods*, Sect. 7.2.6.4 (Ref. A-2); whereas the tolerance-limit factors for one-sided intervals (95% certainty/95% of the population; N ≤ 50) were taken from Ref. A-2.

A.2 STATISTICAL SIGNIFICANCE OF TRENDING

The hypothesis test presented in this section was used to identify the sets of M/C isotopic concentration values that show significant dependence on sample burnup. In this hypothesis test, the normal distribution assumption is used to find significance levels. For the linear regression models, statistical significance of trending is determined by the test of hypothesis that the slope differs from zero, as described in Ref. A-3.

The statistical model is a linear relationship between an independent variable predictor variable, x (e.g., fuel burnup or initial enrichment) and the dependent variable, $y(x)$ (e.g., M/C isotopic concentration ratio):

$$y(x) = \beta_0 + \beta_1 x + \varepsilon \quad,$$

where ε is a random variable possessing a specified probability distribution with mean zero so that the expected value for y(x) is $E(Y) = \beta_0 + \beta_1 x$. Inferences concerning the parameter β_1 can be obtained using the test statistic shown in Eq. (A-3) that possesses a Student's distribution with n-2 degrees of freedom, where n is the sample size:

$$T = \frac{\hat{\beta}_1 - \beta_{10}}{S\sqrt{c_{11}}}, \qquad\qquad\qquad (A-3)$$

where

$\hat{\beta}_1 = \dfrac{S_{xy}}{S_{xx}}$ is an unbiased, normally distributed estimator of β_1,

β_{10} is a specified value of β_1, which is zero in the case of null hypothesis testing,

$S^2 = SSE / (n - 2)$,

$SSE = S_{yy} - \hat{\beta}_1 S_{xy}$,

$c_{11} = \dfrac{1}{S_{xx}}$,

$S_{xx} = \displaystyle\sum_{i=1}^{n}(x_i - \bar{x})^2$,

$S_{xy} = \displaystyle\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$,

$\bar{x} = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n}x_i$.

The Test of Hypothesis for β_1 is

H_0:	$\beta_1 = 0$
H_a:	$\beta_1 \neq 0$ (two-tailed rejection region)
Test Statistic:	$T = \dfrac{\hat{\beta}_1 - \beta_{10}}{S\sqrt{c_{11}}}$
Rejection Region:	$|t| > t_{\alpha/2}$ (two-tailed alternative), where α is the level of significance.

A.1 REFERENCES

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APPENDIX B.

VALIDATION OF THE MONTE CARLO UNCERTAINTY

SAMPLING METHOD

The purpose of Appendix B is to document the validation of the automated processes employed in this calculation, thereby demonstrating correct implementation of the Monte Carlo uncertainty sampling method (refer to Sect. 6.3 for method description). The application case used in support of the validation study is the PWR waste package containing SNF of 3.5 wt % ^{235}U initial enrichment, 25 GWd/MTU burnup, and 5-year cooling time. The validation study addresses the following requirements for the successful implementation of the Monte Carlo uncertainty sampling method:

(1) generation of random numbers from the standard normal distribution;
(2) proper use of the generated random numbers to correct the predicted isotopic compositions for bias and bias uncertainty; and
(3) convergence of the k_{eff-MC} and Δk_{eff-MC} values [see Eqs. (9) and (10), respectively, in Sect. 6.3].

An automated procedure named "kronossm" was executed within the SCALE code system to generate random numbers from the standard normal distribution and to adjust the predicted spent fuel compositions in accordance with Eq. (8). The kronossm executable compiled with INTEL FORTRAN 11.1.064 is provided in *DVD/kronossm*. A kronossm input file must contain the path of the kronossm executable, such as the following for a Linux system (see the *.inp files in *DVD/MC.zip*):

```
=shell
 ln -s /scale/scale6.dev/Linux_x86_64/kronossm/kronossm
end
=kronossm
```

The results presented in this calculation report are not dependent upon the automated procedure that performed implementation of the Monte Carlo uncertainty sampling method. Other means that may be used to generate random numbers from the standard normal distribution include Excel and ORIGIN applications.

B.1 GENERATION OF RANDOM NUMBERS FROM A STANDARD NORMAL DISTRIBUTION

The procedure used to automatically generate random numbers from the standard normal distribution is described in Ref. B-1. It is based on the ziggurat method, the name being suggested by the shape of a single, convenient density that provides for both the fast and the slow parts of the generating process. The method leads to exceptionally fast algorithms for generating variates with decreasing or unimodal, symmetric density functions. The generated random numbers generally pass a normality test. For each MCNP calculation, 28 sets of 500 random numbers were generated. As demonstrated in *DVD/opj/validation.opj*, of the 28 sets of 500 random numbers, only one set of random numbers did not pass the Shapiro-Wilk normality test at the 0.05 significance level. Similarly, only 1 in 28 sets of 200 random numbers did not pass the Shapiro-Wilk normality test. The random numbers generated for use in each Monte Carlo simulation are available in the files *.output (see *DVD/MC.zip*).

B.2 ADJUSTMENT OF THE PREDICTED SPENT FUEL ISOTOPIC COMPOSITIONS

Five hundred MCNP input files specifying spent fuel compositions stochastically corrected for bias and bias uncertainty were created based on Eq. (8) (see Sect. 6.3.2) and the 28 sets of 500 random numbers generated. Correct implementation of Eq. (8) is demonstrated in *DVD/xls/validation.xls*, worksheet *input-ver*, for several MCNP cases. The spreadsheet application used a set of 28 numbers randomly sampled from the standard normal distribution as described above and the bias and bias uncertainty values established for the SCALE 5.1 predictions for each burnup credit isotope (see Sect. 6.3.1) to determine new isotopic compositions in accordance with Eq. (8). The results of the spreadsheet application were

then compared with the fuel isotopic concentrations existing in the corresponding MCNP input file. The comparison shows no difference between the isotopic concentration values determined by using the automated procedure employed and the Excel application. Similarly, correct implementation of Eq. 15 applicable to the bounding uncertainty method (see Sect. 6.4) is demonstrated in *DVD/xls/validation.xls*, worksheet *input-ver*.

B.3 CONVERGENCE OF THE EXPECTED VALUES FOR k_{eff-MC} AND Δk_{eff-MC}

The Monte Carlo uncertainty sampling method is computationally intensive because of the large number of criticality calculations required. k_{eff} bias uncertainty determined in this calculation report is based on a minimum of 200 MCNP calculations using isotopic concentrations randomly sampled from the normal distributions characterized by the mean and standard deviation values tabulated in Sect. 7.2.1, Table 9. A comparison between the statistical behavior of the quantities of interest k_{eff-MC} and Δk_{eff-MC} [see Eqs. (9) and (10), respectively] for 200 and 500 random cases is illustrated in Fig. B-1. As seen in the figure, approximately 200 random cases adequately ensure the convergence of both k_{eff-MC} and Δk_{eff-MC}. Figure B-2(a) and (b) illustrate the histogram diagrams obtained for the k_{eff} values based on 200 and 500 random cases, respectively. The k_{eff-MC} values based on 200 and 500 random cases were 0.9381 and 0.9368, respectively, as compared to 0.9373 (best estimate k_{eff} value) obtained by correcting the predicted isotopic composition for bias only. The Δk_{eff-MC} values based on 200 and 500 random cases were 0.0118 and 0.0124, respectively. The standard deviation of a MCNP k_{eff} value was 0.0003.
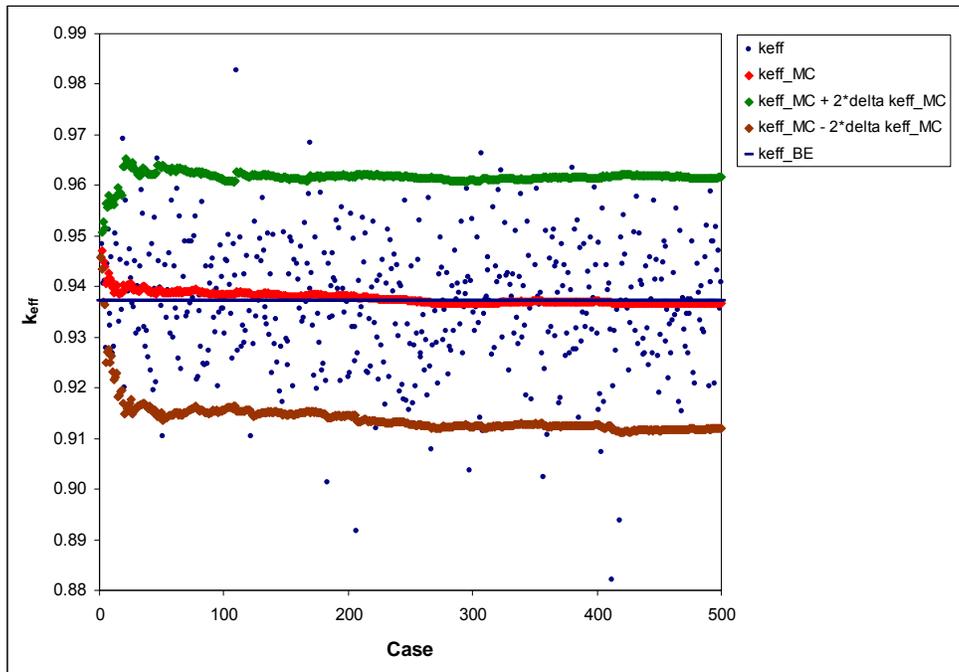
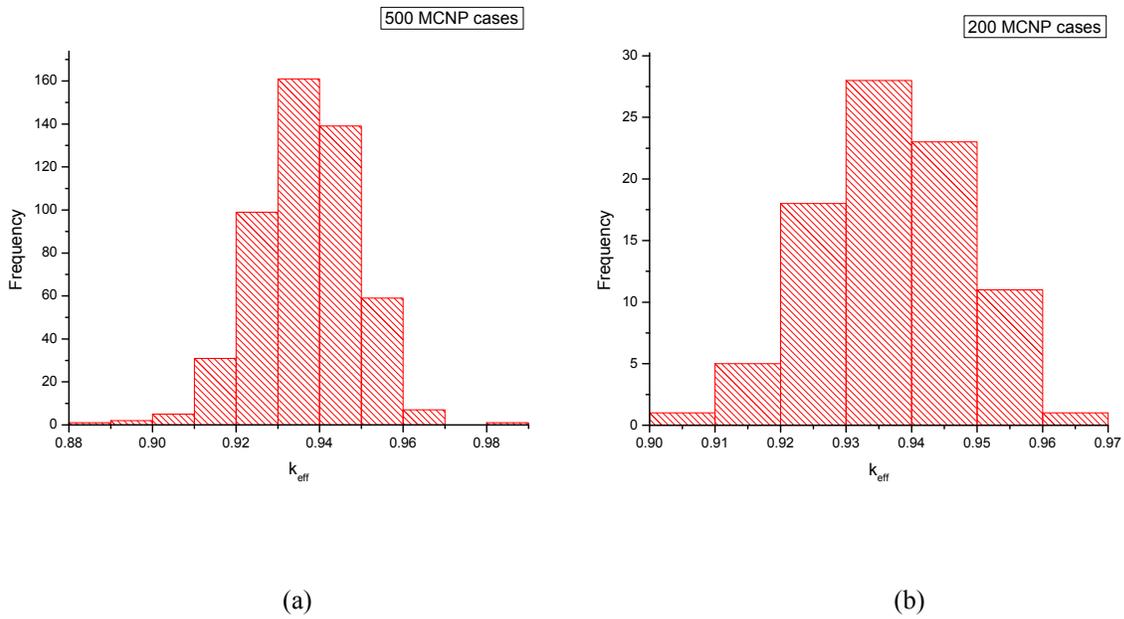Fig. B-1. k_{eff-MC} and Δk_{eff-MC} convergence.

(a)

(b)

Fig. B-2. k_{eff} frequency histograms from (a) 500 MCNP cases and (b) from 200 MCNP cases.

B.4 REFERENCES

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APPENDIX C.

ELECTRONIC DATA SPECIFICATIONS

This appendix contains a listing and description of the files contained in the Digital Versatile/Video Discs (DVD-R format) that are attached to the calculation report *Propagation of Isotopic Bias and Uncertainty to Criticality Safety Analyses of PWR Waste Packages*. The operating system used to create the electronic data on the DVDs was Microsoft Windows XP Professional, Version 2002. The zip archives were created using standard Windows XP compress capabilities. The following process controls for storage and protection of electronic data apply.

Medium: DVD
Conditions: Fireproof cabinet kept at ambient temperature
Location: OCRWM QA Records, currently stored in Building 5700, Room H330
Retention Time: Lifetime
Security: Fireproof cabinet is locked
Access: Project manager and records custodian only

The attributes of the electronic files are as follows:

File/folder name	Size (bytes) (on disk)	Number of files	File date	File time	Description
DVD 1 of 2 [a]					
kronossm	1,468,416	1	06/22/2010	1:38:47 pm	FORTRAN executable for kronossm
MC.zip	526,270,464	14,126	06/22/2010	1:27:21 pm	Archive containing all kronossm and MCNP input and output files for criticality calculations
DVD 2 of 2 [a]					
TRITON.zip	276,850,688	900	06/22/2010	2:06:27 pm	Archive containing SCALE/TRITON input and output files for depletion calculations
ORIGEN.zip	5,496,832	36	06/22/2010	2:05:16 pm	Archive containing SCALE/ORIGEN input and output files for decay calculations
xls	9,668,608	3	06/22/2010	2:11:24 pm	Folder containing all Excel files used in this calculation
opj	4,102,144	2	06/22/2010	2:11:24 pm	Folder containing all ORIGIN files used in this calculation

[a]The DVDs were created on June 22, 2010, by G. Radulescu.