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Range of Applicability and Bias Determination for Postclosure Criticality of Commercial Spent Nuclear Fuel

October 2007

Prepared by
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Nuclear Science and Technology Division

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ACRONYMS

ASM	American Society of Materials Engineers
ASME	American Society of Mechanical Engineers
ASTM	American Society of Testing and Materials
B&W	Babcock and Wilcox
BSS	borated stainless steel
BU	burnup
BWR	boiling water reactor
CFR	Code of Federal Regulations
CL	critical limit
CRC	commercial reactor critical
CSNF	commercial spent nuclear fuel
DFTL	distribution-free tolerance limit
DTN	data tracking number
DVD	digital video disc
EALF	energy of average lethargy of fission
EIA	Energy Information Administration
ENDF	Evaluated Nuclear Data File
FBT	fuel basket tube
GE	General Electric
HTC	Haut Taux de Combustion
IHECSBE	International Handbook of Evaluated Criticality Safety Benchmark Experiments
LBTL	lower bound tolerance limit
LCE	laboratory critical experiments
LEU	low enriched uranium (fuel)
LUTB	lower uniform tolerance band
MCNP	Monte Carlo N-Particle
MOX	mixed oxide (fuel)
NDTL	normal distribution tolerance limit
NEA	Nuclear Energy Agency
NRC	U.S. Nuclear Regulatory Commission
NSTD	Nuclear Science and Technology Division
OECD	Organization for Economic Co-Operation and Development
OCRW	Office of Civilian Radioactive Waste (Management)
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor
QARD	Quality Assurance Requirements and Description
S/U	sensitivity and uncertainty
SCALE	Standardized Computer Analysis for Licensing Evaluation
SDF	sensitivity data files
TAD	transportation, aging, and disposal (canister)
USL	upper subcritical limit
YMP	Yucca Mountain Project

1. PURPOSE

The purpose of this calculation report**,** *Range of Applicability and Bias Determination for Postclosure Criticality of Commercial Spent Nuclear Fuel*, is to validate the computational method used to perform postclosure criticality calculations. The validation process applies the criticality analysis methodology approach documented in Section 3.5 of the *Disposal Criticality Analysis Methodology Topical Report*.[1] The application systems for this validation consist of waste packages containing transport, aging, and disposal canisters (TAD) loaded with commercial spent nuclear fuel (CSNF) of varying assembly types, initial enrichments, and burnup values that are expected from the waste stream and of varying degree of internal component degradation that may occur over the 10,000-year regulatory time period.[2] The criticality computational tool being evaluated is the general-purpose Monte Carlo N-Particle (MCNP)[3] transport code. The nuclear cross-section data distributed with MCNP 5.1.40 and used to model the various physical processes are based primarily on the Evaluated Nuclear Data File/B Version VI (ENDF/B-VI) library. Criticality calculation bias and bias uncertainty and lower bound tolerance limit (LBTL) functions for CSNF waste packages are determined based on the guidance in ANSI/ANS 8.1-1998 (Ref. 4) and ANSI/ANS 8.17-2004 (Ref. 5), as described in Section 3.5.3 of Ref. 1.

The development of this report is consistent with *Test Plan for: Range of Applicability and Bias Determination for Postclosure Criticality*.[6] This calculation report has been developed in support of licensing activities for the proposed repository at Yucca Mountain, Nevada, and the results of the calculation may be used in the criticality evaluation for CSNF waste packages based on a conceptual TAD canister.

2. QUALITY ASSURANCE REQUIREMENTS

Development of this report has been determined to be subject to the Yucca Mountain Project quality assurance requirements as described in *Test Plan for: Range of Applicability and Bias Determination for Postclosure Criticality*.[6] The Test Plan identifies Oak Ridge National Laboratory (ORNL)–Office of Civilian Radioactive Waste (OCRW) 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](refer to Appendix F for the description of electronic management of data). The computer codes used in this calculation have been qualified per ORNL-OCRW-19.0, *Software Control*.[10]

3. USE OF SOFTWARE

3.1 GENERAL MONTE CARLO N-PARTICLE (MCNP) TRANSPORT CODE

The general-purpose Monte Carlo N-Particle (MCNP) transport code (MCNP 5.1.40.)[3] was used to calculate the neutron multiplication factors, k_{eff}, for the various cases. The MCNP code 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/Compaq Tru64 UNIX, Version 5.1 (Ref. 11) or Linux 2.6.9-42.0.2 ELsmp #1, x86_64 GNU/Linux (Ref. 12)
- Computer Type: DEC Alpha workstations or CPILE2 Linux cluster of the Nuclear Systems Analysis, Design, and Safety organization, Nuclear Science and Technology Division (NSTD), 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; (2) it allows explicit geometrical modeling of material configurations; and (3) it uses continuous-energy cross sections. Additional descriptions of MCNP features and capabilities are provided in Section 6.2.

The input and output files for the MCNP calculations are located in portable digital video discs (DVDs) that are attached to this document, so that an independent repetition of the calculations may be performed.

The MCNP calculations documented in this report had sufficient inactive and active cycles specified on the KCODE card to obtain convergence of both the k_{eff} and the fission source distribution before starting active cycles for tallies. The values of estimated k_{eff} standard deviation for all calculations were sufficiently small, that is, less than 0.0005. However, a few calculations did not pass some of the MCNP statistical checks, including the normality tests for the individual collision, absorption, and track-length k_{eff} cycle values at the 95% or 99% confidence interval. In addition, the MCNP calculations for models containing significantly large numbers of cells with fissionable material, such as the Grand Gulf and McGuire Commercial Reactor Critical (CRC) state-points, did not pass the MCNP test requiring that all cells with fissionable material be sampled and have fission neutron source points. In such cases the results were carefully reviewed, and in some cases additional calculations performed, to ensure that the final results used in this report are reliable. For example, the MCNP k_{eff} results for Grand Gulf and McGuire state-points are considered adequate for the purpose of this validation for the following reasons. As indicated in the MCNP output files, cells with fissionable material not being sampled may result in smaller k_{eff} values, which in turn result in lower, that is, conservative, LBTL values. A few calculations were repeated using an increased number of active cycles to obtain results with better statistical behavior. It was noticed that while the statistical behavior improved, the effect on the k_{eff} value was insignificant. For example, in the case of McGuire state-point 2, the k_{eff} results obtained with 500 and 2000 active cycles (each with 10,000 source neutrons) are 0.99172 ± 0.00030 and 0.99143 ± 0.00015, respectively, which shows that better spatial neutron source sampling has an insignificant effect on k_{eff} (refer to MCNP output files MG2o and MG2so in /DVD/exps/CRC/McGuire/mcnp), provided the statistical error is sufficiently small.

3.2 STANDARDIZED COMPUTER ANALYSIS FOR LICENSING EVALUATION (SCALE) CODE SYSTEM

The Standardized Computer Analysis for Licensing Evaluation (SCALE 5.1)[13] code system was used to perform various types of calculations by invoking the following code sequences: CSAS25,[14] TSUNAMI-3D,[15] and TSUNAMI-IP.[16] The SCALE code system 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/Compaq Tru64 UNIX, Version 5.1 (Ref. 17)
- Computer Type: DEC Alpha workstations or CPILE2 Linux cluster of the Nuclear Systems Analysis, Design, and Safety organization, NSTD, ORNL

Rationale for Selection: SCALE is accepted by the NRC for criticality safety applications. This computer code system has multiple unique capabilities relevant to this work including automated sequences to produce problem-dependent multigroup cross-section data, Monte Carlo radiation transport computer codes for criticality calculations (KENO V.a used in this calculation report), and three-dimensional cross-section sensitivity and uncertainty (S/U) analysis tools for criticality safety applications.

The input and output files for the CSAS25, TSUNAMI-3D, and TSUNAMI-IP calculations are located in portable DVDs that are attached to this document, so that an independent repetition of the calculations may be performed.

The convergence of each of the CSAS25/KENO V.a calculations was assessed for all cases by reviewing the plot of average k_{eff} by generation run and the plot of average k_{eff} by generation skipped. No trends were observed in these plots that would be indicative of improper convergence. In addition, the frequency distribution plots were examined. These frequency distribution plots show single k_{eff} peaks, which is also an indication of convergence. The k_{eff} results of KENO V.a forward and adjoint calculations, which are used in the S/U (TSUNAMI-3D) analysis, were adequately similar.

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. It was also used to implement the statistical methods for LBTL calculations that are described in References 18 (Appendix C), 19, and 20. Microsoft 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 in Section 6.5.1 and the spreadsheets (on the DVD attachment), as indicated in Section 6.5.2, so that an independent repetition of the operations can be performed.

3.4 MATHEMATICA

The commercial off-the shelf software Mathematica 5.2.0.0 (copyright Wolfgram Research, Inc.) was used to determine the *D* parameter in Eq. E-1 (see Appendix E). All necessary information for reproducing the operations performed is provided in the DVD attachment (/DVD/cl/D-search-numeric.nb) so that an independent repetition of the operations can be performed. Mathematica was used in its native form and therefore, it is exempt from the requirements of ORNL-OCRW-19.0, *Software Control*.[10]

4. INPUT DATA

4.1 DIRECT INPUTS

Direct inputs to the analysis include dimensional and material specifications for the waste package and the critical experiments, as detailed in the following sections.

4.1.1 Waste Package Data

The following data were used as direct inputs to the analyses described in Section 6. Table 1 lists direct inputs, their sources, and the justification for use as direct inputs. Technical input data includes Yucca Mountain Project (YMP) qualified data listed by data tracking number (DTN), American Society of Mechanical Engineers (ASME) specifications, American Society of Testing and Materials (ASTM) and American Society of Materials Engineers (ASM) consensus data, technical products developed in accordance with Quality Assurance Requirements and Description (QARD),[21] industry handbooks,[22, 23] and NRC- and industry-approved documents. The technical inputs were used to create MCNP and SCALE (CSAS25 and TSUNAMI-3D) input files for the waste packages containing TAD canisters loaded with either pressurized-water-reactor (PWR) or boiling-water-reactor (BWR) spent fuel assemblies.

Table 1. Direct inputs for waste package modeling

Parameter	Value	Source	Justification
Waste package and TAD canister specifications	See Table 2	Ref. 24, Section 4 and Appendix A.	Approved technical product developed in accordance with QARD requirements
TAD internal basket specifications	See Table 3	Ref. 25.	Approved NRC design for spent nuclear fuel storage
Minimum recommended absorber plate thickness	6 mm	Ref. 26.	Approved technical product developed in accordance with QARD requirements
PWR fuel assembly specifications	See Table 4 and Fig. 1	Ref. 27.	Approved technical product developed in accordance with QARD requirements
BWR fuel assembly specifications	See Table 5	Ref. 28.	Considered established fact data because they are from a report from the Electric Power Research Institute that is accepted by the scientific and engineering community
BWR fuel assembly channel dimensions	See Table 5	Ref. 29.	Approved technical product developed in accordance with QARD requirements
BWR TAD fuel basket tube (FBT) thickness	4.7625 mm (3/16 in.)	Ref. 30.	Representative of minimum thickness for BWR basket from approved technical product developed in accordance with QARD requirements
Composition of tuff	See Table 6	DTN: GS000308313211.001, Table S00224_001, mean values.[31]	YMP qualified data

Table 1. Direct inputs for waste package modeling (continued)

Density of tuff	Average of three hydrogeologic units; see Table 6	DTN: MO0109HYMXPROP.001, Table S01144_001 (rows 1333, 1345, and 1739 for samples tpt pmn, pll, and pln).[32]	YMP qualified data
Density for SA-240 S30464 neutron absorber plate	7.8 g/cm^3 (0.282 lb/in^3)	Ref. 24, Appendix A.	Approved technical product developed in accordance with QARD requirements
Material specifications for SB-575 N06022	See Table 7	DTN: MO0003RIB00071.001, Table S04196_001.[33]	YMP qualified data
Material specifications for SA-240 S31603	See Table 8	ASME 2001, Section II, SA-240, Table 1.[34]	Considered established fact data because this is code from a professional society (ASME)
Material density for SA-240 S31603	7.98 g/cm^3	ASTM G 1-90 1999, p. 7, Table X1.[35]	Considered established fact datum because this is a consensus standard from ASTM
Material specifications for Zircaloy-4	See Table 9	ASTM B 811-97 2000, p. 2, Table 2.[36]	Considered established fact data because this is a consensus standard from ASTM
Material density for Zircaloy-4	6.56 g/cm^3	ASM International 1990, p. 666, Table 6.[37]	Considered established fact datum because this is a consensus standard from ASM
Material specifications for Zircaloy-2	See Table 10	ASTM B 811-97 2000, Table 2.[36]	Considered established fact data because this is a consensus standard from ASTM
Material density for Zircaloy-2	6.55 g/cm^3	ASM International 1967.[38]	Considered established fact datum because this is a consensus standard from ASM
Material specifications for SA-240 S30464	See Table 11	ASTM A 887-89 2004, Table 1.[39]	Considered established fact data because this is a consensus standard from ASTM
PWR spent fuel isotopic compositions	Output, spreadsheet *LoadingCurve_v344.xls*, worksheet FuelIsotopics	Ref. 40.	Approved technical product developed in accordance with QARD requirements
BWR spent fuel isotopic compositions	Output, spreadsheet *LoadingCurve_v344.xls*, worksheet FuelIsotopics	Ref. 41.	Qualified supplier approved technical product developed in accordance with QARD requirements
Axial zone weighting factors	Output, spreadsheet *LoadingCurve_v344.xls*, worksheet FuelIsotopics	Ref. 42.	Approved technical product developed in accordance with QARD requirements

Table 2. Waste package and TAD canister specifications

Component	Material	Parameter	Dimension (mm)
Waste Package Outer Barrier	SB-575 N06022 (Alloy 22)	Outer diameter	1,881.60 (74.08 in.)
		Thickness	25.40 (1.00 in.)
		Inner diameter	1,830.80 (calculated)
		Total length	5,691.38 (224.07 in.)
		Thickness of bottom	25.40 (1.00 in.)
Waste Package Inner Vessel	SA-240 S31600[a] (Stainless Steel Type 316)	Outer diameter	1,821.20 (71.70 in.)
		Thickness	50.80
		Inner diameter	1,719.6 (calculated)
		Total length	5,499.1
		Thickness of bottom	50.8 (2 in.)
TAD Canister	SA-240 S31603 (Stainless Steel Type 316L)	Outer diameter	1,689.1 (66.5 in.)
		Thickness	25.4 (1.00 in.)
		Inner diameter	1,638.3 (calculated)
		Total length	5,384.8 (212.0 in.)
		Thickness of bottom	88.9 (3.5 in.)
TAD Canister Shield Plug	SA-240 S31603 (Stainless Steel Type 316L)	Thickness	381 (15.0 in.)

Source: Ref. 24, Section 4 and Appendix A.
[a]Represented as SA-240 S31603 in MCNP representations. This is considered to have a negligible impact (change in k_{eff} is within the statistical uncertainty) on the results since the waste package inner vessel acts as a secondary reflector.

Table 3. Internal basket specifications

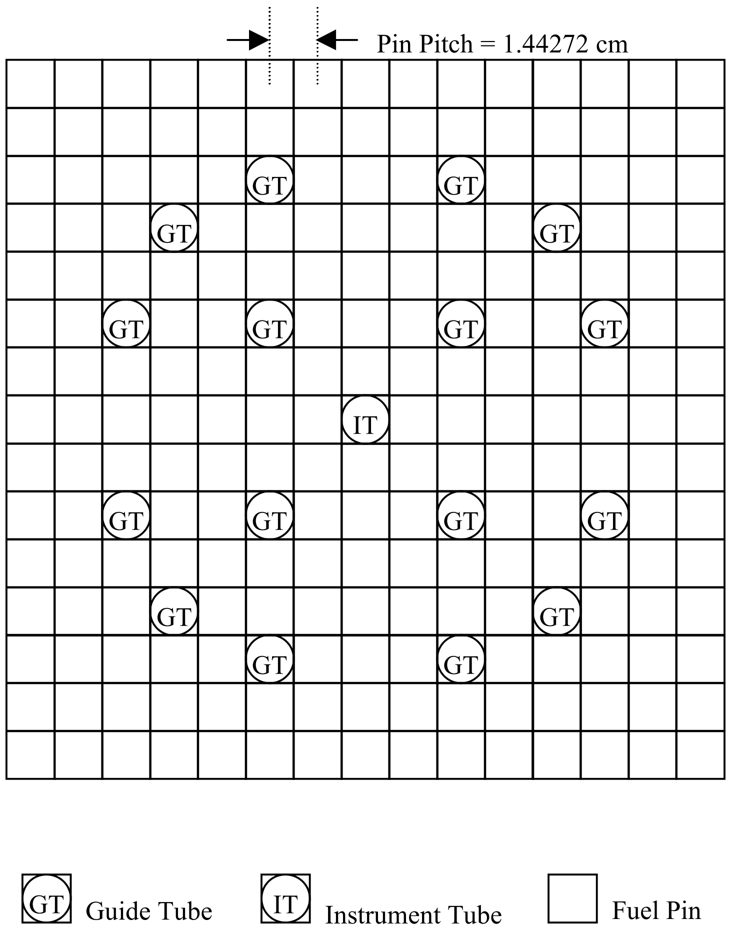
Component	Material	Parameter	Dimension (mm)
PWR Fuel Basket Tube	SA-240 S31603 (Stainless Steel 316L)	Internal distance across flats	220.726 (8.69 in.)[a]
		Thickness	7.9375 (5/16 in.)
		Length	4889.5 (192.5 in.)[b]
PWR-Fuel Neutron Absorber Plate	SA-240 S30464 (Borated Stainless Steel)	Thickness	11.1125 (nominal)
		Width	190.5 (7.50 in.)[a]
		Length	4889.5[c]
BWR Fuel Basket Tube	SA-240 S31603 (Stainless Steel 316L)	Internal distance across flats	152.2222 (5.993 in.)[a]
		Thickness	4.7625 (3/16 in.)[c]
		Length	4889.5 (192.5 in.)[b]
BWR-fuel Neutron Absorber Plate	SA-240 S30464 (Borated Stainless Steel)	Thickness	11.1125 (nominal)
		Width	120.65 (4.75 in.)[a]
		Length	4889.5[d]

[a]Ref. 25, Figures 6.3.2 and 6.3.3.
[b]Derived based on total TAD canister length and having 1-in. clearance between top of basket and lid to allow for thermal expansion.
[c]Value taken from Ref. 30, Table 21.
[d]Same length as FBT.

Table 4. Pressurized-water-reactor fuel assembly specifications

Assembly component	Specification
Lattice	15 × 15
Fuel pellet (outer diameter)	0.93980 cm
Fuel rod cladding (inner diameter)	0.95758 cm
Fuel rod cladding (outer diameter)	1.09220 cm
Active fuel length	360.172 cm
Pin pitch	1.44272 cm
Guide tube (inner diameter)	1.26492 cm
Guide tube (outer diameter)	1.34620 cm
Instrument tube (inner diameter)	1.12014 cm
Instrument tube (outer diameter)	1.38193 cm
Fuel clad, guide tube, and instrument tube material	Zircaloy-4
Fuel density[a]	10.741 g/cm^3

Source: Ref. 27, pp. 2–5.
[a]Calculated based on 98% theoretical density value of 10.96 g/cm^3 for UO_2 (Ref. 43).



This sketch is not to scale.

Fig. 1. Fuel pin, guide tube, and instrument tube locations in PWR fuel assembly.

Table 5. Boiling-water-reactor fuel assembly specifications

Assembly component	Specification[a]
Lattice	7 × 7
Fuel pellet (outer diameter)[b]	1.23952 cm (0.488 in.)
Fuel rod cladding (thickness)	0.08128 cm (0.032 in.)
Fuel rod cladding (inner diameter)	1.26746 cm
Fuel rod cladding (outer diameter)	1.43002 cm (0.563 in.)
Active fuel (length)	365.76 cm (144 in.)
Clad material	Zircaloy-2
Channel material	Zircaloy-4
Pin pitch	1.87452 cm (0.738 in.)
Channel (inner width)[c]	13.246 cm
Channel (thickness)[c]	0.3048 cm
Fuel density[d]	10.741 g/cm^3

Source: Ref. 28, pp. A-1 to A-3.
[a]Values in parentheses are from the source reference.
[b]The representations use a smeared pellet density over the inner clad diameter.
[c]Channel dimensions were taken from Ref. 29, Table 2-1.
[d]Calculated based on 98% theoretical density value of 10.96 g/cm^3 for UO_2 (Ref. 44).

Table 6. Material specifications for tuff

Mineral	wt %[a]	Mineral	wt %[a]
SiO_2	76.29	Na_2O	3.52
Al_2O_3	12.55	K_2O	4.83
FeO	0.14	TiO_2	0.11
Fe_2O_3	0.97	P_2O_5	0.05
MgO	0.13	MnO	0.07
CaO	0.5	Density[b] = 2.54 g/cm^3	

Source: Refs. 31 and 32.
[a] DTN: GS000308313211.001, Table S00224_001, mean values.
[b]Average of three hydrogeologic units for tptpmn, tptpll, and tptpln (rows 1333, 1345, and 1739) of DTN: MO0109HYMXPROP.001, Table S01144_001.
Note: The iron elemental weight percents were expanded into their constituent natural isotopic weights percents for use in MCNP and SCALE calculations (refer to Section 6.2 for the set of MCNP data tables being validated).

Table 7. Material specifications for SB-575 N06022

Element/ isotope	ZAID[a]	wt %	Element/ isotope	ZAID[a]	wt %
C-nat	6000.66c	0.0150	^{59}Co	27059.66c	2.5000
^{55}Mn	25055.62c	0.5000	^{182}W [b]	74182.62c	0.7877
Si-nat	14000.60c	0.0800	^{183}W [b]	74183.62c	0.4278
^{50}Cr	24050.62c	0.8879	^{184}W [b]	74184.62c	0.9209
^{52}Cr	24052.62c	17.7863	^{186}W [b]	74186.62c	0.8636
^{53}Cr	24053.62c	2.0554	V	23000.62c	0.3500
^{54}Cr	24054.62c	0.5202	^{54}Fe	26054.62c	0.2260
^{58}Ni	28058.62c	36.8024	^{56}Fe	26056.62c	3.6759
^{60}Ni	28060.62c	14.6621	^{57}Fe	26057.62c	0.0865
^{61}Ni	28061.62c	0.6481	^{58}Fe	26058.62c	0.0116
^{62}Ni	28062.62c	2.0975	^{32}S	16032.62c	0.0200
^{64}Ni	28064.62c	0.5547	^{31}P	15031.66c	0.0200
Mo-nat	42000.66c	13.5000	Density = 8.69 g/cm^3		

Source: Ref. 33, DTN: MO0003RIB00071.000, Table S04196_001.
[a]ZAID = MCNP data table identifier (refer to Section 6.2).
[b]W-180 cross-sectional libraries are not available, so the atom percents of the remaining W isotopes were used to renormalize the elemental weight and derive isotopic weight percents, excluding the negligible 0.120 atom percent of W-180 in natural W.

Table 8. Material specifications for SA-240 S31603

Element/ isotope	ZAID[a]	wt %	Element/ isotope	ZAID[a]	wt %
C-nat	6000.66c	0.0300	^{54}Fe	26054.62c	3.7036
^{14}N	7014.62c	0.1000	^{56}Fe	26056.62c	60.2343
Si-nat	14000.60c	0.7500	^{57}Fe	26057.62c	1.4167
^{31}P	15031.66c	0.0450	^{58}Fe	26058.62c	0.1904
^{32}S	16032.62c	0.0300	^{58}Ni	28058.62c	8.0641
^{50}Cr	24050.62c	0.7103	^{60}Ni	28060.62c	3.2127
^{52}Cr	24052.62c	14.2291	^{61}Ni	28061.62c	0.1420
^{53}Cr	24053.62c	1.6443	^{62}Ni	28062.62c	0.4596
^{54}Cr	24054.62c	0.4162	^{64}Ni	28064.62c	0.1216
Mn-55	25055.62c	2.0000	Mo-nat	42000.66c	2.5000
Density = 7.98 g/cm^3					

Source: Refs. 34 and 35.
[a]ZAID = MCNP data table identifier (refer to Section 6.2).

Table 9. Material specifications for Zircaloy-4

Element/ isotope	ZAID[a]	wt %	Element/ isotope	ZAID[a]	wt %
^{50}Cr	24050.62c	0.0042	^{57}Fe	26057.62c	0.0045
^{52}Cr	24052.62c	0.0837	^{58}Fe	26058.62c	0.0006
^{53}Cr	24053.62c	0.0097	^{16}O	8016.62c	0.1250
^{54}Cr	24054.62c	0.0024	Zr-nat	40000.66c	98.1150
^{54}Fe	26054.62c	0.0119	Sn-nat	50000.42c	1.4500
^{56}Fe	26056.62c	0.1930	Density = 6.56 g/cm^3		

Source: Refs. 36 and 37.
[a]ZAID = MCNP data table identifier (refer to Section 6.2).

Table 10. Material specifications for Zircaloy-2

Element/ isotope	ZAID[a]	wt %	Element/ isotope	ZAID[a]	wt %
^{50}Cr	24050.62c	0.0042	^{58}Ni	28058.62c	0.0370
^{52}Cr	24052.62c	0.0837	^{60}Ni	28060.62c	0.0147
^{53}Cr	24053.62c	0.0097	^{61}Ni	28061.62c	0.0007
^{54}Cr	24054.62c	0.0024	^{62}Ni	28062.62c	0.0021
^{54}Fe	26054.62c	0.0076	^{64}Ni	28064.62c	0.0006
^{56}Fe	26056.62c	0.1241	^{16}O	8016.62c	0.1250
^{57}Fe	26057.62c	0.0029	Zr-nat	40000.66c	98.1350
^{58}Fe	26058.62c	0.0004	Sn-nat	50000.42c	1.4500
Density = 6.55 g/cm^3					

Source: Refs. 36 and 38.
[a]ZAID = MCNP data table identifier (refer to Section 6.2).

Table 11. Material specifications for SA-240 S30464

Element/ isotope	ZAID[a]	wt %	Element/ isotope	ZAID[a]	wt %
C-nat	6000.66c	0.0800	^{55}Mn	25055.62c	2.0000
^{14}N	7014.62c	0.1000	^{54}Fe	26054.62c	3.5855
^{10}B	5010.66c	0.1548	^{56}Fe	26056.62c	58.3137
^{11}B	5011.66c	0.6852	^{57}Fe	26057.62c	1.3715
Si-nat	14000.60c	0.7500	^{58}Fe	26058.62c	0.1843
^{31}P	15031.66c	0.0450	^{58}Ni	28058.62c	9.0721
S-nat	16032.62c	0.0300	^{60}Ni	28060.62c	3.6143
^{50}Cr	24050.62c	0.7939	^{61}Ni	28061.62c	0.1598
^{52}Cr	24052.62c	15.9031	^{62}Ni	28062.62c	0.5171
^{53}Cr	24053.62c	1.8378	^{64}Ni	28064.62c	0.1367
^{54}Cr	24054.62c	0.4652	^{59}Co	27059.66c	0.2000
Density = 7.8 g/cm^3 (0.282 lb/in^3)					

Source: Refs. 39 and 24.
[a]ZAID = MCNP data table identifier (refer to Section 6.2).

4.1.2 Critical Experiment Data

The following subsections describe critical experiment data that are used as input to this analysis. The critical experiments include public and proprietary Laboratory Critical Experiments (LCEs) and CRCs. Table 12 summarizes the input data used in MCNP and SCALE modeling, their sources, and the justification for use as direct inputs.

Table 12. Critical experiment input data

Critical experiment set	Input description	Source	Justification
Public Laboratory Critical Experiments	Experimental configurations, material compositions, experimental k_{eff} value, benchmark model uncertainty	Ref. 45.	Established fact
Proprietary Haut Taux de Combustion LCEs	Experimental configurations, material compositions, experimental k_{eff} value, benchmark model uncertainty	Refs. 46, 47, 48, 49, 50.	YMP qualified data (Ref. 51)
Crystal River Unit 3 CRCs	Calculation descriptions and MCNP input files	Refs. 52 and 53.	Approved technical products developed in accordance with QARD requirements
McGuire Unit 1 CRCs	Calculation descriptions and MCNP input files	Refs. 54 and 55.	Approved technical products developed in accordance with QARD requirements
Sequoyah Unit 2 CRCs	Calculation descriptions and MCNP input files	Refs. 56 and 57.	Approved technical products developed in accordance with QARD requirements
Three Mile Island Unit 1 CRCs	Calculation descriptions and MCNP input files	Refs. 58 and 59.	Approved technical products developed in accordance with QARD requirements
Grand Gulf Unit 1 CRCs	Calculation descriptions and MCNP input files	Ref. 60.	Approved technical product developed in accordance with QARD requirements

4.1.2.1 Public Laboratory Critical Experiment Data

The data source of publicly available LCEs included as a component of validation methodology is found in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE)[45] from the Nuclear Energy Agency of the Organization for Economic Co-Operation and Development (OECD-NEA). The IHECSBE contains evaluations of criticality benchmark experiments that have been peer reviewed and have a detailed description of relevant experimental conditions. MCNP and CSAS25/KENO V.a modeling directly uses the critical experiment descriptions available in the IHECSBE. Another input to the validation methodology obtained from the IHECSBE is experimental k_{eff} value.

4.1.2.2 Proprietary LCE Data—Haut Taux de Combustion Critical Experiments

Haut Taux de Combustion (HTC) (French for "high burnup") LCE descriptions are data qualified per YMP applicable procedures.[46, 51] The HTC data are acceptable for the intended use since these experiments were performed to support criticality validation, were evaluated and documented to be consistent with the IHECSBE guidelines, and were performed by the same facility and organization that has produced many data reports already accepted as qualified for the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, the internationally recognized and accepted source for LCE data.

4.1.2.3 Commercial Reactor Criticals

The CRC data considered in this validation consist of 45 state-points from five PWRs: Crystal River Unit 3 (33 configurations), McGuire Unit 1 (six configurations), Sequoyah Unit 2 (three configurations), and Three Mile Island (TMI) Unit 1 (three configurations), and 16 state-points from BWR Grand Gulf Unit 1. CRC state-point configuration descriptions are documented in approved YMP reports.[52, 54, 56, 58, 60] The MCNP calculations documented in this report for Crystal River Unit 3, McGuire Unit 1, Sequoyah Unit 2, TMI Unit 1, and Grand Gulf Unit 1 state-points used the MCNP input files from Refs. 53, 55, 57, 59, and 60, respectively, as direct input. Those files were modified as described in Section 6.3.3.

General information for the selected CRC state-points, including core average burnup, cycle length to state-point, and cycle downtime, is presented in Table 13. Core average burnup was used as a direct technical input to this calculation.

Table 13. General information for selected CRC state-points

State-point	Cycle	Cycle length to state-point (EFPD)[a]	Enrichments (wt % ^{235}U in U of UO_2)[b]	Cycle downtime (days)	Core average burnup (GWd/MTU)
Crystal River Unit 3					
1	1A	0.0	(1.93, 2.54, 2.83)	0.0	0.00
2	1B	268.8	1.93, 2.00, 2.54, 2.83	195.3	8.09
3	1B	411.0	1.93, 2.00, 2.54, 2.83	14.8	12.34
4	2	0.0	2.54, (2.64), 2.83	97.0	8.67
5	3	0.0	2.54, (2.62), 2.64, 2.83	164.0	7.50
6	3	168.5	2.54, 2.62, 2.64, 2.83	16.8	12.54
7	3	250.0	2.54, 2.62, 2.64, 2.83	12.3	14.98
8	4	0.0	2.62, (2.62), 2.64, (2.95)	73.0	6.92
9	4	228.1	2.62, 2.64, 2.95	15.2	14.00
10	4	253.0	2.62, 2.64, 2.95	24.0	14.77
11	5	0.0	2.62, 2.64, 2.95, (2.95, 3.29)	127.0	7.08
12	5	388.5	2.62, 2.64, 2.95, 2.95, 3.29	5.0	19.12
13	6	0.0	2.62, 2.64, 2.95, 3.29, (3.49)	163.0	12.01
14	6	96.0	2.62, 2.64, 2.95, 3.29, 3.49	168.9	14.99
15	6	400.0	2.62, 2.64, 2.95, 3.29, 3.49	10.4	24.41
16	7	0.0	2.54, 2.62, 2.64, 3.29, 3.49, (3.84)	113.0	10.02
17	7	260.3	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	18.9	18.09
18	7	291.0	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	39.5	19.04
19	7	319.0	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	109.5	19.91
20	7	462.3	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	2.2	24.35
21	7	479.0	2.54, 2.62, 2.64, 3.29, 3.49, 3.84	7.2	24.87
22	8	0.0	1.93, 2.62, 3.29, 3.49, 3.84, (3.94)	99.0	12.26
23	8	97.6	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	15.5	15.27
24	8	139.8	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	6.2	16.58
25	8	404.0	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	44.4	24.74
26	8	409.6	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	4.9	24.91
27	8	515.5	1.93, 2.62, 3.29, 3.49, 3.84, 3.94	7.6	28.19
28	9	0.0	1.93, 3.84, (3.90), 3.94	75.0	14.18
29	9	158.8	1.93, 3.84, 3.90, 3.94	2.1	19.10
30	9	219.0	1.93, 3.84, 3.90, 3.94	53.1	20.96
31	9	363.1	1.93, 3.84, 3.90, 3.94	1.6	25.42
32	10	0.0	3.84, 3.90, 3.94, (4.167)	55.0	15.24
33	10	573.7	3.84, 3.90, 3.94, 4.167	16.4	33.00

Table 13. General information for selected CRC state-points (continued)

State-point	Cycle	Cycle length to state-point (EFPD)[a]	Enrichments (wt % ^{235}U in U of UO_2)[b]	Cycle downtime (days)	Core average burnup (GWd/MTU)
Three Mile Island Unit 1					
1	1	0	(2.06, 2.75, 3.05)	0	0.00
2	5	0	2.64, 2.85, (2.85)	2,420	10.33
3	5	114.4	2.64, 2.85	32.2	13.87
McGuire Unit 1					
1	1	0.0	(2.108, 2.601, 3.106)	0.0	0.00
2	6	0.0	2.92, 3.204, 3.40, (3.60)	78.0	11.67
3	6	62.4	2.92, 3.204, 3.40, 3.60	62.7	14.34
4	7	0.0	2.92, 3.204, 3.40, 3.60, (3.75)	130.0	10.76
5	7	129.0	2.92, 3.204, 3.40, 3.60, 3.75	29.6	16.14
6	7	282.3	2.92, 3.204, 3.40, 3.60, 3.75	18.8	22.54
Sequoyah Unit 2					
1	1	0.0	(2.10, 2.60, 3.10)	0.0	0.00
2	3	0.0	2.60, 3.10, 3.50, (3.60, 3.80)	81.0	11.11
3	3	210.9	2.60, 3.10, 3.50, 3.60, 3.80	995.7	19.20
Grand Gulf					
5	4	0.00	2.81, 3.01, (3.25, 3.37)	41.4	11.00
6	4	4.01	2.81, 3.01, 3.25, 3.37	17.7	11.00
7	4	73.49	2.81, 3.01, 3.25, 3.37	8.5	13.00
10	5	0.00	3.01, 3.25, 3.37, (3.42)	55.8	13.00
11	5	16.54	3.01, 3.25, 3.37, 3.42	11.4	13.00
12	5	148.27	3.01, 3.25, 3.37, 3.42	4.8	17.00
13	5	165.29	3.01, 3.25, 3.37, 3.42	3.5	17.00
14	5	203.58	3.01, 3.25, 3.37, 3.42	7.7	18.00
15	5	340.41	3.01, 3.25, 3.37, 3.42	10.3	22.00
16	6	0.00	3.25, 3.37, 3.42, (2.94, 3.38)	48.3	13.00
18	7	0.00	2.94, 3.38, 3.42, (3.20, 3.42)	60.0	14.00
19	7	108.81	2.94, 3.38, 3.42, 3.20, 3.42	5.8	17.00
20	7	245.05	2.94, 3.38, 3.42, 3.20, 3.42	3.9	20.00
21	8	0.00	2.94, 3.20, 3.38, 3.42, (3.07, 3.56)	56.2	13.00
22	8	0.00	2.94, 3.20, 3.38, 3.42, (3.07, 3.56)	3.8	13.00
23	8	17.59	2.94, 3.20, 3.38, 3.42, 3.07, 3.56	4.4	14.00

Source: Ref. 61.
[a]Effective full-power days.
[b]Fresh fuel enrichment at the beginning of a cycle is shown in parentheses.

4.2 CRITERIA

The safety criteria for postclosure criticality are best described in *Criticality Input to Canister Based System Performance Specification for Disposal* (Ref. 62) as follows:

There are no specific design criteria for postclosure criticality control in 10 CFR Part 63 but requirements are consistent with a risk-informed, performance-based regulation, which treats criticality in 10 CFR Part 63 as one of the features, events, processes that must be considered for the overall system performance assessment, i.e.:

…The features, events, and processes considered in the performance assessment should represent a wide range of both beneficial and potentially adverse effects on performance (e.g., beneficial effects of radionuclide sorption; potentially adverse effects of fracture flow or a criticality event)…. [§ 63.102(j)]

Various measures are implemented to satisfy the 10 CFR Part 63 acceptance criteria applicable to the postclosure performance assessment for the Yucca Mountain site; these include examining the significant factors contributing to the probability of criticality in the repository and possibly implementing additional analyses or design enhancements to reduce the overall probability of criticality if the respective criteria are exceeded. Such measures are addressed in 10 CFR Part 63, which, in discussing "concepts" of the performance assessment regulations, states in part:

…Those features, events, and processes expected to materially affect compliance with § 63.113(b) or be potentially adverse to performance are included, while events (event classes or scenario classes) that are very unlikely (less than one chance in 10,000 over 10,000 years) can be excluded from the analysis… [§ 63.102(j)]

4.3 INDUSTRY STANDARDS AND FEDERAL REGULATIONS

Applicable Code of Federal Regulations is

- 10 CFR 63 Parts: 113(b), 113(c), 114(d) through 114(f).

The following standards are used as the bases of validation methodology presented in this report:

- ANSI/ANS-8.1-1998. *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*.

- ANSI/ANS-8.17-2004. *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors.*

The following codes and standards are used as direct input to material composition calculations:

- *2001 ASME Boiler and Pressure Vessel Code (includes 2002 addenda).*

- ASTM G 1-90 (Reapproved 1999). *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens*.

- ASTM B 811-97. *Standard Specification for Wrought Zirconium Alloy Seamless Tubes for Nuclear Reactor Fuel Cladding.*

- ASTM A 887-89 (Reapproved 2004). *Standard Specification for Borated Stainless Steel Plate, Sheet, and Strip for Nuclear Application*.

5. ASSUMPTIONS

1. It is assumed that the CRC k_{eff} values have an uncertainty of 1% (one standard deviation) due to uncertainties in various CRC model components (e.g., isotopic compositions of burned fuel, operation history, physical and material specifications data). The rationale for this assumption is provided in Section 6.3.3. The assumption is used in the calculations and analyses described in Section 6.5.2.

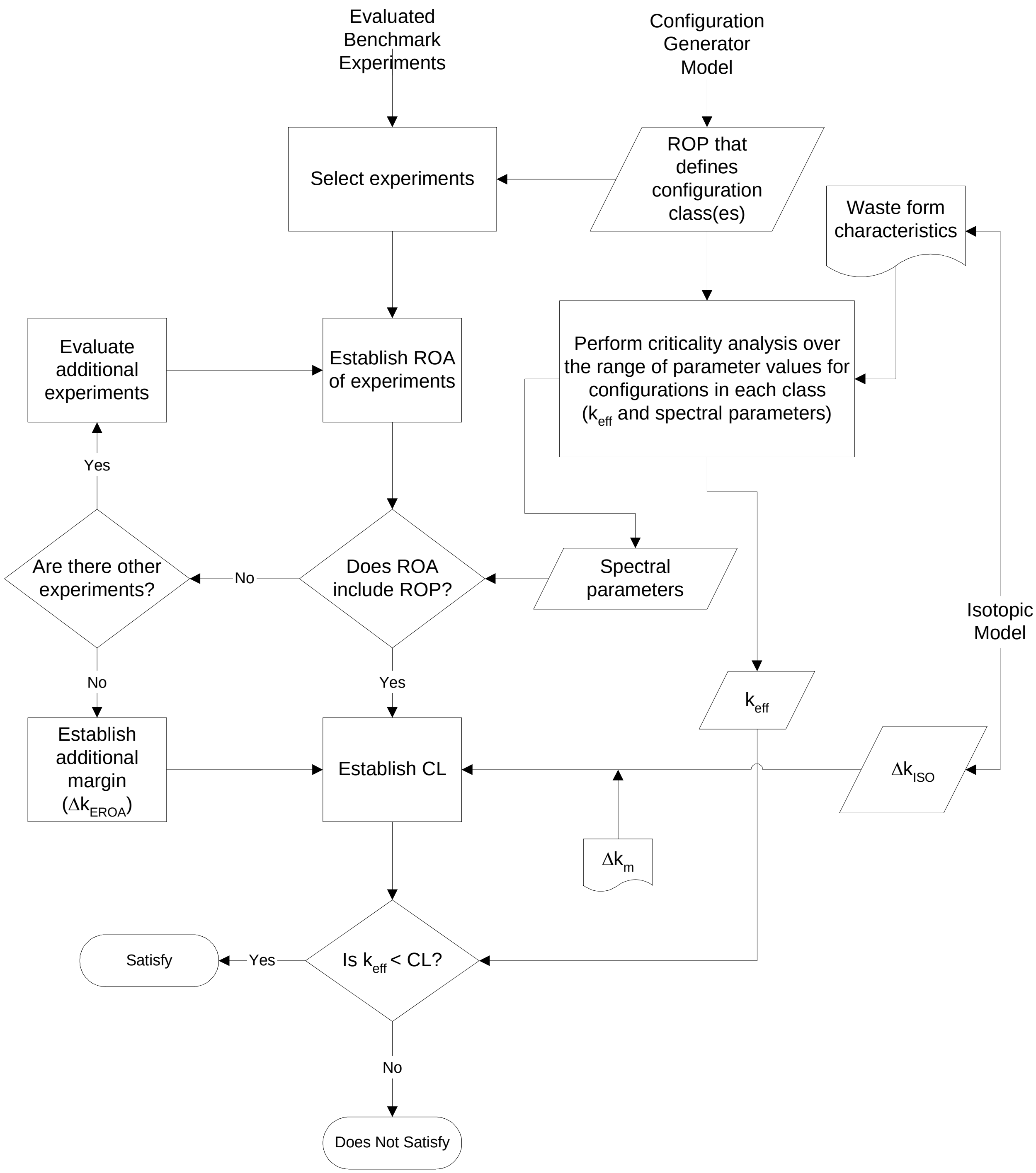
2. It is assumed that the CRCs considered in this validation, other than the Crystal River CRCs, have similar integral c_k values to the c_k values determined for the Crystal River CRCs. The rationale for this assumption is that the CRCs are reactor critical configurations with similar material compositions and geometry. The assumption is used in the calculations and analyses described in Section 6.5.2.

6. VALIDATION METHODOLOGY

The process used to validate the computational method for postclosure criticality of CSNF waste packages applies the disposal criticality analysis methodology approach documented in Section 3.5.1 of the *Disposal Criticality Analysis Methodology Topical Report,*[1] which is illustrated in Figure 2. The methodology is based on the guidance in ANSI/ANS 8.1-1998 and ANSI/ANS 8.17-2004.

The validation is comprised of the following steps:

- Identify the application systems and the range of parameters and conditions for which the validation will apply (see Section 6.1).
- Identify the computer code implementing the physics and numerical techniques and the cross sections to be used in all calculations (see Section 6.2).
- Select critical experiments for consideration based on similarities in physical characteristics between the application systems and critical experiments (see Section 6.3).
- Identify applicable critical experiments based on neutronic similarity between the application systems and the selected critical experiments, as determined by the sensitivity/uncertainty (TSUNAMI) computational tools. Use the published (Refs. 63 and 64) guidance for similarity criteria based on experience at ORNL to identify applicable critical experiments (see Section 6.4).
- Determine bias and bias uncertainty over the area of applicability using industry and NRC accepted tools and procedures (Ref. 18). Only critical experiments that have neutronic similarities, that is, similar material compositions, neutron spectra, and leakage, with the application systems are used in the determination of bias and uncertainty associated with the bias (see Section 6.5).



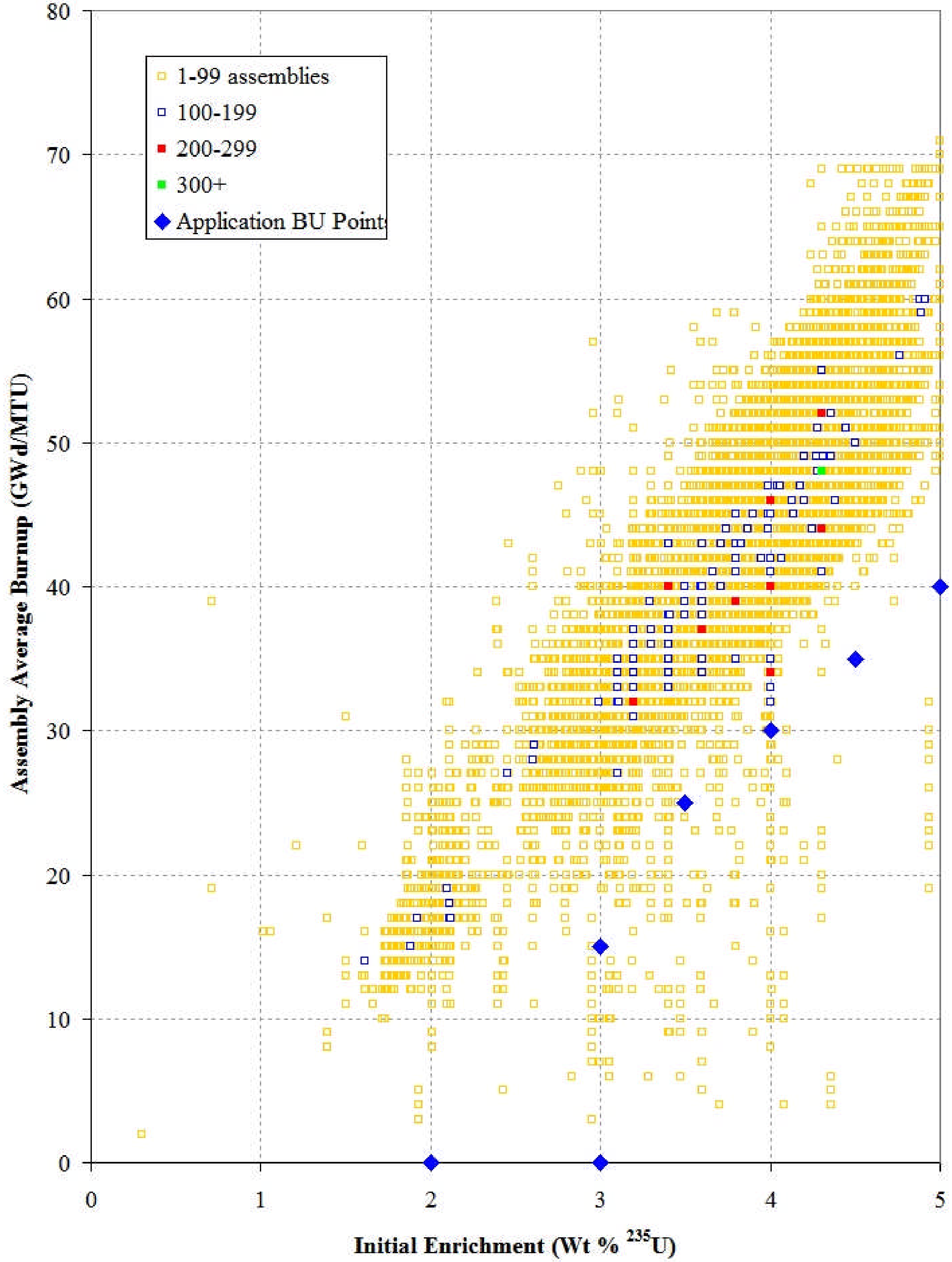
Note: ROA = range of applicability
ROP = range of parameters
CL = critical limit (refer to Section 6.5.1 for the definition of various CL components)

Fig. 2. Criticality model overview.

6.1 RANGE OF PARAMETERS TO BE VALIDATED

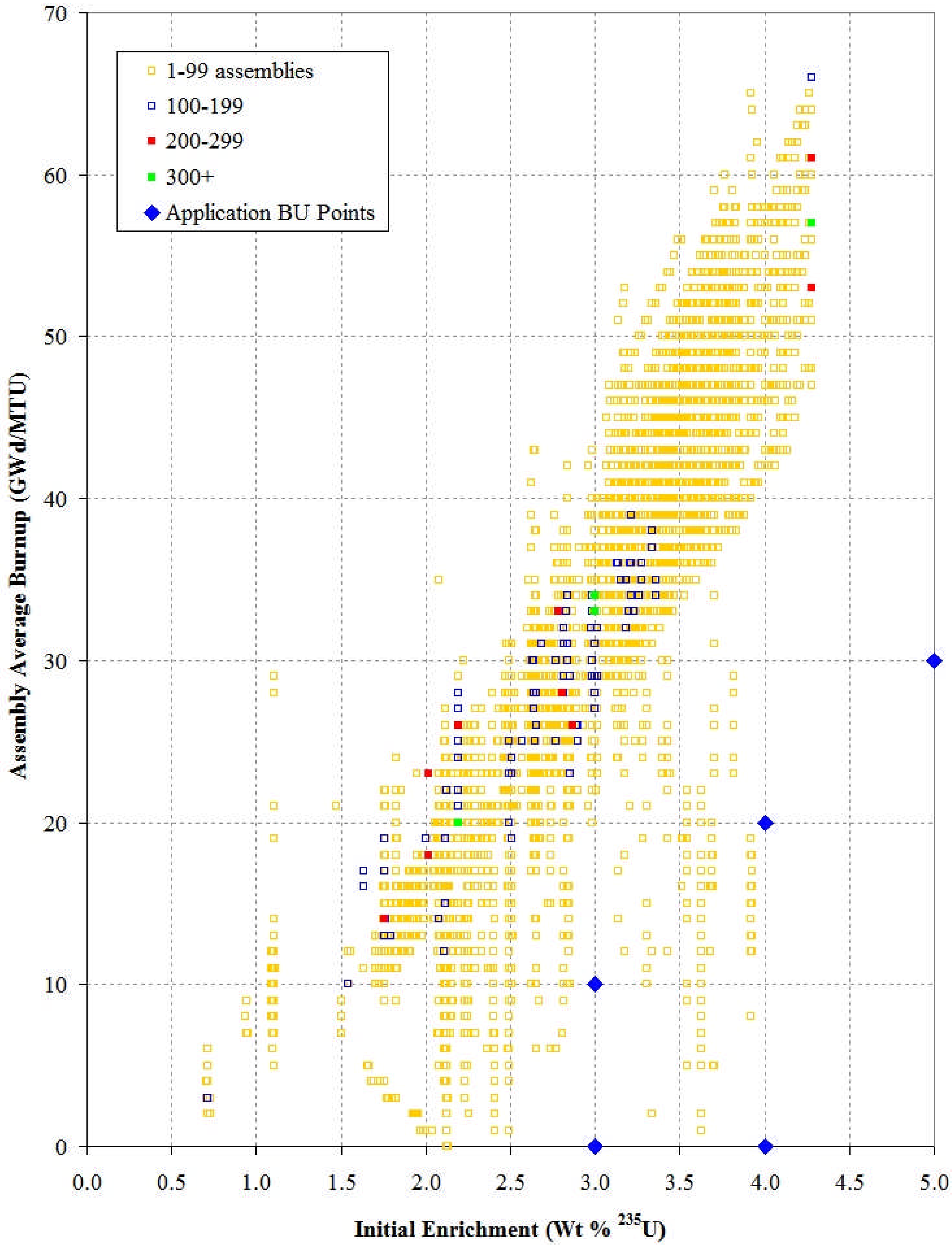
The application systems for this validation consist of waste packages containing TAD canisters loaded with CSNF of varying assembly types, initial enrichments, and burnups that are expected from the waste stream. The evaluated systems will have varying degrees of waste package internal component degradation that may occur over the 10,000-year regulatory time period.

The PWR and BWR assembly types selected for the various calculations and analyses presented in this report are Babcock and Wilcox (B&W) 15 × 15 and General Electric (GE) 7 × 7, respectively. The basis for the selection is that the B&W 15 × 15 and the GE 7 × 7 assemblies are more reactive in a waste package configuration than other PWR and BWR assembly types, respectively, as documented in Ref. 43, Attachment II, and Ref. 44, Attachment I , respectively. For each type of assembly, several initial enrichment-burnup (initial enrichment in wt% ^{235}U and burnup in GWd/MTU) pairs were selected. For the B&W 15 × 15 assemblies, these pairs are: 2%-0 GWd/MTU, 3%-0 GWd/MTU, 3%-15 GWd/MTU, 3.5%-25 GWd/MTU, 4%-30 GWd/MTU, 4.5%-35 GWd/MTU, and 5%-40 GWd/MTU, whereas for the GE 7 × 7 assemblies, the pairs are: 3%-0 GWd/MTU, 3%-10 GWd/MTU, 4%-0 GWd/MTU, 4%-20 GWd/MTU, and 5%-30 GWd/MTU. The selected CSNF assembly types with the selected maximum initial enrichment-minimum burnup combinations are more reactive than the majority of the waste stream assemblies, as can be seen from Figs. 2 and 3, which illustrate the selected initial enrichment-burnup pairs relative to the PWR and BWR waste stream inventories, respectively. The waste stream, as illustrated in Figs. 3 and 4, is represented by 1999 discharge data (Refs. 65 and 66) that correspond to CSNF assemblies discharged from U.S. PWRs through the end of 1999.



Note: BU = burnup

Fig. 3. PWR inventory and application burnup points.



Note: BU = burnup

Fig. 4. BWR inventory and application burnup points.

During the postclosure time period, processes and events may occur that degrade the contents of the waste package after the package has been breached and the inert environment lost. Two waste package configurations for each CSNF type are investigated: a waste package configuration consisting of intact CSNF assemblies and intact fuel basket, which will be referred to as "nominal configuration" throughout this report, and a waste package configuration consisting of intact assemblies and degraded waste package basket plates, which will be referred to as "design-basis configuration" throughout this report. For the design-basis configuration, the thickness of the borated stainless steel plates was reduced from 1.1112 cm (nominal thickness) to 0.6 cm to account for corrosion degradation over the 10,000-year time period from emplacement (Ref. 26). For both nominal and design-basis configurations, the modeled borated stainless steel chemical composition contains only 75% of the actual ^{10}B weight fraction for conservatism in the k_{eff} estimations. The PWR assemblies contain a seven-zone axial burnup profile, whereas the BWR assemblies have a uniform axial burnup profile. To ensure conservatism throughout the 10,000-year regulatory time frame, all computational models use spent fuel compositions at 5-year cooling time (Ref. 67). The selected application systems and modeling parameters for these systems are considered adequate for the purpose of this calculation since they are used only to identify applicable critical experiments to the validation of criticality calculations for CSNF waste packages and not directly used in determining the LBTL.

Consistent with the *Disposal Criticality Analysis Methodology Topical Report* (Ref. 1), the criticality analysis model uses a subset of the isotopes present in the CSNF that consists of 14 actinides and 15 fission products, referred to as "Principal Isotopes." The principal isotopes are presented in Table 14.

Table 14. Principal isotopes for CSNF burnup credit

Actinide isotopes		Fission product isotopes	
^{233}U	^{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[a]	^{143}Nd	^{153}Eu
^{238}Pu	^{243}Am	^{145}Nd	^{155}Gd
		^{147}Sm	

[a]The *m* refers to a long-lived metastable state of ^{242}Am.
Note: Isotopes with very low atom densities were omitted from the MCNP and SCALE compositions (e.g., ^{233}U atom densities below 5.0E-11 atoms/barn-cm).

6.2 COMPUTATIONAL TOOLS AND NUCLEAR CROSS-SECTION DATA FOR CRITICALITY CALCULATIONS

The computational tool and nuclear data to be validated are MCNP and the nuclear data identified in Table 15. MCNP is a general-purpose Monte Carlo computer code that is routinely used for criticality safety applications and has been accepted by the NRC for applications involving CSNF (e.g., Ref. 25). A Monte Carlo calculation is a numerical simulation of the actual physical process (e.g., neutron transport and interactions with matter) that determines the value of a physical quantity as the expected value of a certain random variable (or combination of several variables). The method of source iteration or successive generations serves as the basis of a Monte Carlo simulation for the statistical estimation of the effective multiplication factor, k_{eff}, for a nuclear system. In this method, k_{eff} is computed as the mean number of fission neutrons produced in one generation per fission neutron started. MCNP allows for an accurate material and geometry representation of the application configurations. Thus, the method statistically evaluates the system with few approximations. However, the MCNP results represent statistical estimates with associated uncertainties. In criticality calculations, collision, absorption, and track-length k_{eff} estimators are computed and the recommended (Ref. 3) k_{eff} and confidence interval are based on a combination of the three estimators. All MCNP calculated k_{eff} values cited in this report correspond to this recommended k_{eff} estimator. The quality of a calculated k_{eff} value and confidence interval depends on a series of factors, including material and geometric model representation and whether the fission-source distribution has converged.

The MCNP continuous-energy data identifiers for the various nuclides used in the waste package models are listed in Table 15. The selected MCNP ZAIDs for waste package/TAD material compositions were used consistently throughout the MCNP calculations for application and experiment systems. A data table identifier in MCNP is called a ZAID and contains the atomic number Z, mass number A, and a library specifier ID. The library specifiers related to the ENDF/B-VI library are 49c, 60c, 62c, or 66c. MCNP data tables based on the ENDF/B-VI library were used where available. For the few nuclides that ENDF/B-VI data are not available with MCNP, data tables based on either the ENDF/B-V library (ID=50c) or LLNL ENDL92FP library (ID=42c)[3] were used, as shown in Table 15.

Table 15. Selected MCNP ZAIDs for waste package/TAD material compositions

Element	Isotope	Neutron cross-section library ZAID[a]	Element	Isotope	Neutron cross-section library ZAID
Hydrogen	^{1}H	1001.62c	Technetium	^{99}Tc	43099.66c
Boron	^{10}B	5010.66c	Ruthenium	^{101}Ru	44101.50c
	^{11}B	5011.66c	Rhodium	^{103}Rh	45103.66c
Carbon	C (natural)	6000.66c	Silver	^{109}Ag	47109.66c
Nitrogen	^{14}N	7014.62c	Tin	Sn (natural)	50000.42c
Oxygen	^{16}O	8016.62c	Neodymium	^{143}Nd	60143.50c
Sodium	^{23}Na	11023.62c		^{145}Nd	60145.50c
Magnesium	Mg (natural)	12000.62c	Samarium	^{147}Sm	62147.66c
Aluminum	^{27}Al	13027.62c		^{149}Sm	62149.66c
Silicon	Si (natural)	14000.60c		^{150}Sm	62150.49c
Phosphorus	^{31}P	15031.66c		^{151}Sm	62151.50c
Sulfur	^{32}S	16032.62c		^{152}Sm	62152.49c
Potassium	K (natural)	19000.62c	Europium	^{151}Eu	63151.66c
Calcium	Ca (natural)	20000.62c		^{153}Eu	63153.66c
Titanium	Ti (natural)	22000.62c	Gadolinium	^{155}Gd	64155.66c
Vanadium	V (natural)	23000.62c	Tungsten	^{182}W	74182.62c
Chromium	^{50}Cr	24050.62c		^{183}W	74183.62c
	^{52}Cr	24052.62c		^{184}W	74184.62c
	^{53}Cr	24053.62c		^{186}W	74186.62c
	^{54}Cr	24054.62c	Uranium	^{233}U	92233.66c
Manganese	^{55}Mn	25055.62c		^{234}U	92234.66c
Iron	^{54}Fe	26054.62c		^{235}U	92235.66c
	^{56}Fe	26056.62c		^{236}U	92236.66c
	^{57}Fe	26057.62c		^{238}U	92238.66c
	^{58}Fe	26058.62c	Neptunium	^{237}Np	93237.66c
Cobalt	^{59}Co	27059.66c	Plutonium	^{238}Pu	94238.66c
Nickel	^{58}Ni	28058.62c		^{239}Pu	94239.66c
	^{60}Ni	28060.62c		^{240}Pu	94240.66c
	^{61}Ni	28061.62c		^{241}Pu	94241.66c
	^{62}Ni	28062.62c		^{242}Pu	94242.66c
	^{64}Ni	28064.62c	Americium	^{241}Am	95241.66c
Zirconium	Zr (natural)	40000.66c		^{242m}Am	95242.66c
Molybdenum	Mo (natural)	42000.66c		^{243}Am	95243.66c
	^{95}Mo	42095.50c			

[a]ZAID = MCNP data table identifier.

The CSAS25 sequence of SCALE, which is also routinely used for criticality safety applications and accepted by the NRC for such purposes, was used to perform extensive independent verification calculations. These independent calculations provide considerable additional confidence in the MCNP modeling and results. CSAS25/KENO V.a was also used as a component of TSUNAMI-3D S/U analysis. The comparisons of MCNP and CSAS25/KENO results provide confidence in the modeling consistency, which is important to obtaining appropriate sensitivity coefficients that are used to assess the applicability of experiments to validation of the applications (PWR and BWR waste packages). The CSAS25 sequence calls functional modules BONAMI, CENTRM/PMC, and KENO V.a to automate cross-section processing and criticality calculations. BONAMI performs resonance self-shielding of the cross sections in the unresolved energy range for nuclides that have Bondarenko factors. CENTRM calculates fluxes using point-wise cross sections in the one-dimensional transport equation, and PMC generates flux-weighted multi-group cross sections for use in the KENO V.a calculation. Effective multiplication factors (k_{eff}) of the configurations are then calculated by using the three-dimensional, multi-group Monte Carlo code KENO V.a. All calculations supporting the validation in this report used the 238-energy-group library that is based on ENDF/B-VI data, except for the Crystal River CRC calculations that used the SCALE 238-energy-group library based on ENDF/B-V data (see Section 6.4.2). The 238-group library has 148 fast and 90 thermal groups below 3 eV. The MCNP and SCALE5.1/CSAS25 k_{eff} results and the energy of average lethargy of fission (EALF) values for the application systems considered in the validation are presented in Table 16. The SCALE5.1/CSAS25 and MCNP k_{eff} results are in very good agreement (all values within 0.3%), which demonstrates consistency for material composition specification and geometry modeling between MCNP and CSAS25/KENO V.a calculation inputs as well as consistency in the underlying physics modeling and data. Figures 5 and 6 present a horizontal cross section of the MCNP models for the 21-PWR and 44-BWR waste packages, respectively.

Table 16. Criticality calculation results for 21-PWR and 44-BWR waste packages

Application system		**MCNP[a]**				**SCALE5.1/ CSAS25[b]**			
Waste package	**Enrichment (wt% ^{235}U)/ burnup (GWd/MTU)**	**Output file**	k_{eff}	σ	***EALF[c]* (eV)**	**Output file**	k_{eff}	σ	***EALF[c]* (eV)**
21 PWR nominal configuration	2.0/ 0	omb2-0	0.94348	0.00012	2.00E-01	sb2-0	0.94093	0.00016	1.97E-01
	3.0/ 0	omb3-0	1.05473	0.00013	2.34E-01	sb3-0	1.05179	0.00018	2.31E-01
	3.0/ 15	omb15	0.94523	0.00012	3.21E-01	sb15	0.94328	0.00016	3.16E-01
	3.5/ 25	omb25	0.92654	0.00013	3.62E-01	sb25	0.92425	0.00018	3.57E-01
	4.0/ 30	omb30	0.93117	0.00013	3.89E-01	sb30	0.92884	0.00017	3.84E-01
	4.5/ 35	omb35	0.93142	0.00013	4.19E-01	sb35	0.92898	0.00016	4.13E-01
	5.0/ 40	omb40	0.93700	0.00013	4.42E-01	sb40	0.93504	0.00018	4.36E-01
21 PWR design-basis configuration	2.0/ 0	omt2-0	0.97026	0.00011	1.96E-01	st2-0	0.96752	0.00015	1.94E-01
	3.0/ 0	omt3-0	1.08432	0.00013	2.30E-01	st3-0	1.08172	0.00017	2.27E-01
	3.0/ 15	omt15	0.97166	0.00012	3.16E-01	st15	0.96919	0.00018	3.11E-01
	3.5/ 25	omt25	0.95197	0.00013	3.56E-01	st25	0.94972	0.00017	3.51E-01
	4.0/ 30	omt30	0.95662	0.00013	3.82E-01	st30	0.95407	0.00018	3.77E-01
	4.5/ 35	omt35	0.95717	0.00012	4.10E-01	st35	0.95467	0.00018	4.05E-01
	5.0/ 40	omt40	0.96247	0.00013	4.35E-01	st40	0.96027	0.00020	4.29E-01
44 BWR nominal configuration	3.0/ 0	omb3-0	0.84621	0.00013	2.91E-01	sb3-0	0.84568	0.00017	2.89E-01
	3.0/ 10	omb3-10	0.83446	0.00013	4.86E-01	sb3-10	0.83327	0.00018	4.81E-01
	4.0/ 0	omb4-0	0.90764	0.00014	3.42E-01	sb4-0	0.90685	0.00020	3.39E-01
	4.0/ 20	omb4-20	0.84049	0.00013	6.22E-01	sb4-20	0.83913	0.00015	6.14E-01
	5.0/ 30	omb5-30	0.83283	0.00013	7.17E-01	sb5-30	0.83215	0.00016	7.07E-01
44 BWR design-basis configuration	3.0/ 0	omt3-0	0.88991	0.00013	2.77E-01	st3-0	0.88934	0.00018	2.75E-01
	3.0/ 10	omt3-10	0.87683	0.00013	4.60E-01	st3-10	0.87549	0.00015	4.54E-01
	4.0/ 0	omt4-0	0.95391	0.00014	3.25E-01	st4-0	0.95379	0.00018	3.22E-01
	4.0/ 20	omt4-20	0.88261	0.00013	5.88E-01	st4-20	0.88099	0.00018	5.81E-01
	5.0/ 30	omt5-30	0.87476	0.00013	6.75E-01	st5-30	0.87313	0.00017	6.68E-01

[a]MCNP input and output files are included in the DVD attachment, paths: /DVD/apps/21pwr/mcnp and /DVD/apps/44bwr/mcnp. The name of an output file was obtained by adding the character "o" in front of an input file name (e.g., mb15 is an input file and omb15 is its corresponding output file).
[b]SCALE/CSAS25 input and output files are included in the DVD attachment, paths /DVD/apps/21pwr/scale and /DVD/apps/44bwr/scale. The CSAS25 input and output files have the extension inp and output, respectively (e.g., sb25.inp is an input file and sb25.output is its corresponding output file).
[c]energy of average lethargy of fission.

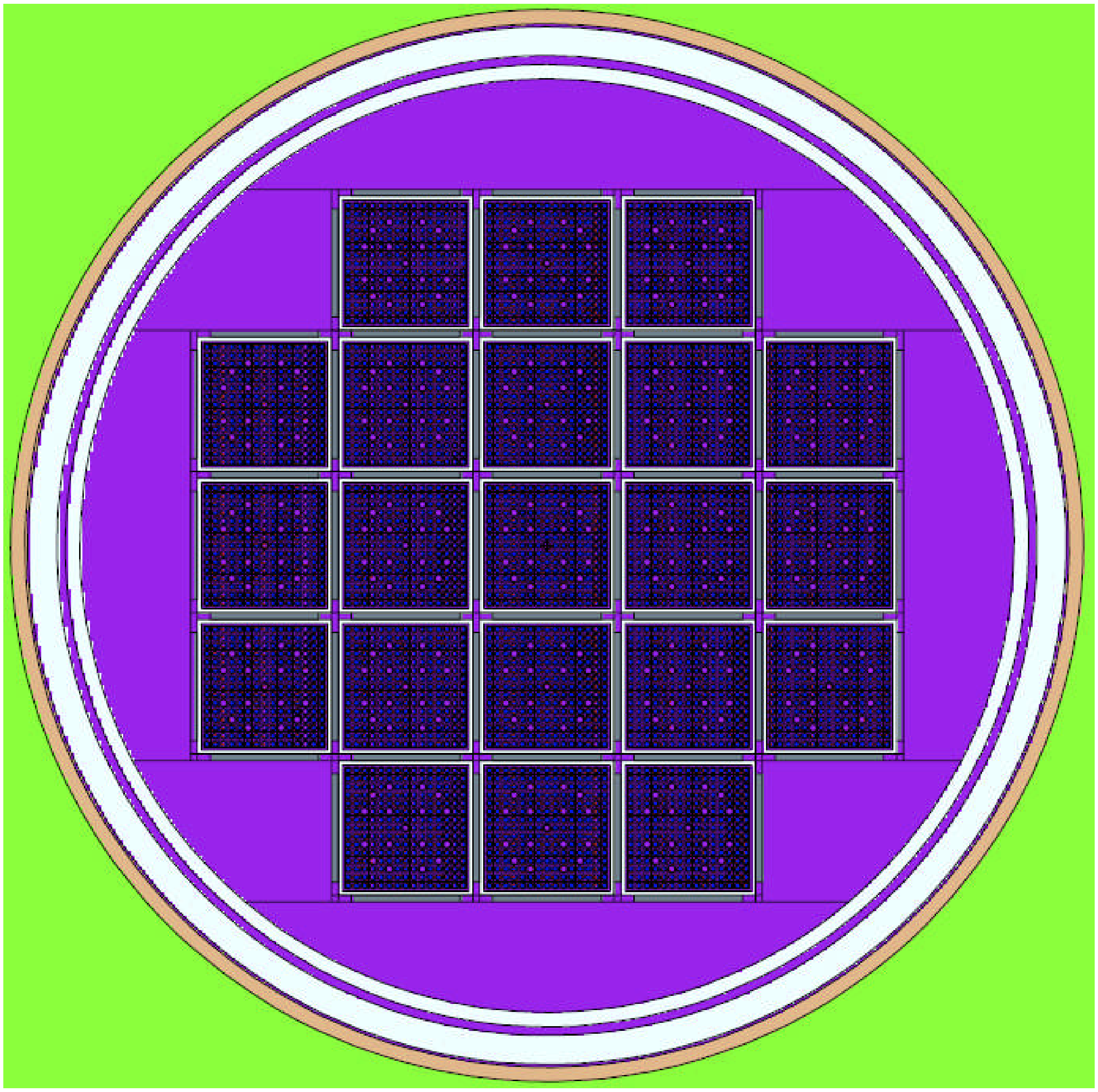


Fig. 5. Horizontal cross section of the MCNP model for the 21-PWR waste package.

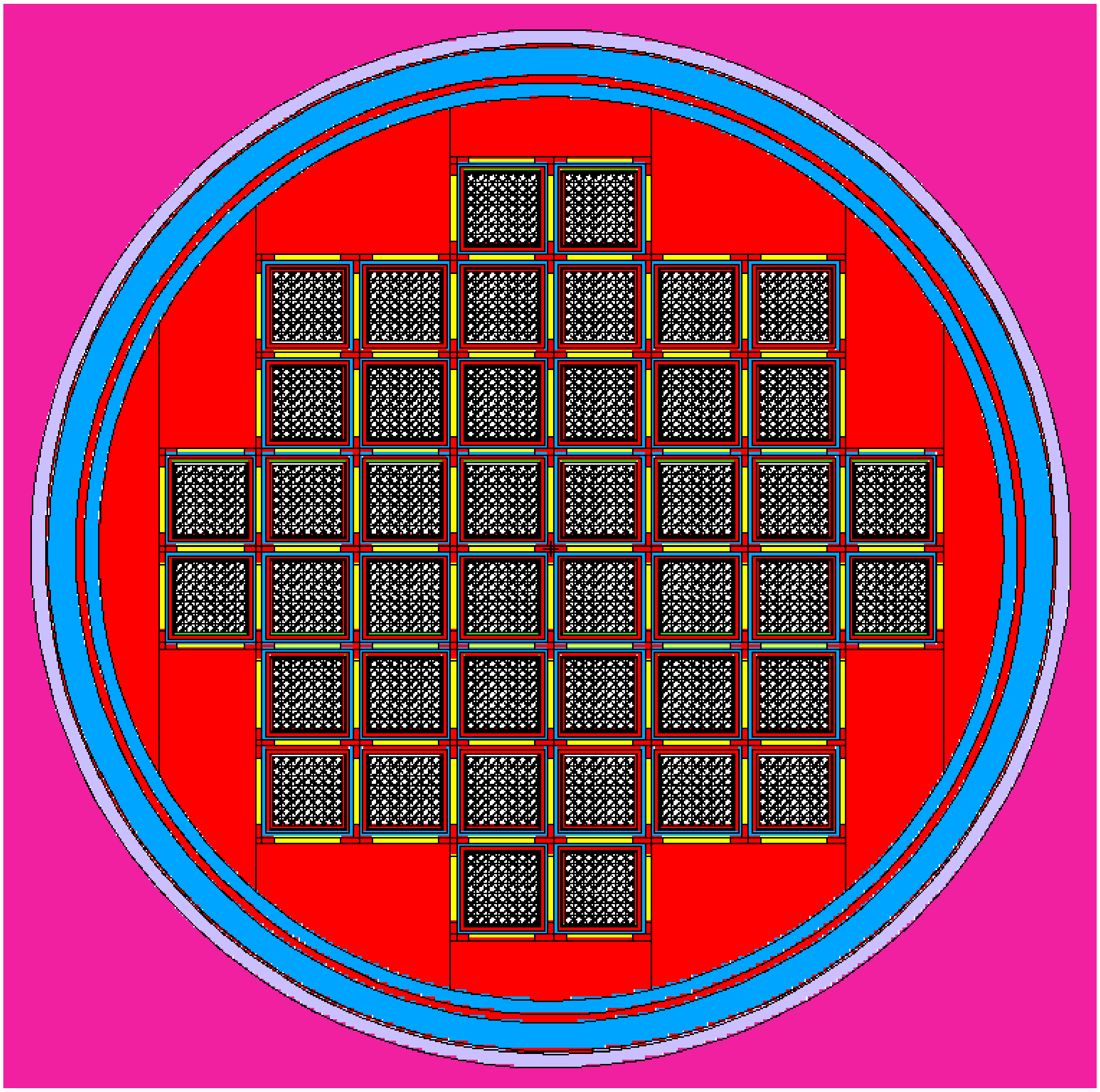


Fig. 6. Horizontal cross section of the MCNP model for the 44-BWR waste package.

6.3 SELECTION OF CRITICAL EXPERIMENTS FOR CONSIDERATION

The accuracy of the computational method and cross-section data is established by evaluating critical experiments. The critical benchmarks selected as a component of this criticality validation consist of four different sets of critical experiments: public mixed-oxide (PuO_2 and UO_2) (MOX) and low-enriched uranium (LEU) LCE data from the IHECSBE, proprietary HTC MOX LCE data, and CRCs (refer to Table 12 for the sources of critical experiment data). Selection of the critical experiments for consideration is based on similarities of physical characteristics between the application and experiment systems. A description of the selected critical experiments is provided in the following subsections. The selected critical experiments will be analyzed in Section 6.4 using the TSUNAMI methodology to identify the applicable critical experiments to criticality validation based on indices that quantify neutronic similarities between application and experiment systems.

6.3.1 Public Laboratory Critical Experiments

The source of LCEs is found in *International Handbook of Evaluated Criticality Safety Benchmark Experiments*[45] from the OECD-NEA. The LCEs included in the validation methodology consist of moderated lattice configurations containing either mixed oxide fuel or low-enriched uranium dioxide fuel and MOX solutions. The selected MOX (52 cases) and LEU (37 cases) LCEs are listed in Sections 6.3.1.1 and 6.3.1.2, respectively. MCNP and CSAS25/KENO V.a modeling for the LCEs uses critical experiment descriptions available in the IHECSBE and produces results consistent with those reported in the handbook.

6.3.1.1 MOX LCEs

The selection of MOX LCEs is based on physical characteristic similarities between CSNF waste packages and experiment systems. The 52 selected MOX critical experiments are water-moderated thermal systems containing either MOX in a lattice configuration or MOX solution. The MOX compound contains the isotopes ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{238}Pu through ^{242}Pu, and ^{241}Am.

MIX-COMP-THERM-002 Rectangular Arrays of Water-Moderated UO_2 – 2 Wt.% PuO_2 (8% ^{240}Pu) Fuel Rods. Cases 1 through 6.

MIX-COMP-THERM-003 Rectangular Arrays of Water-Moderated UO_2 – 6.6 Wt.% PuO_2 Fuel Rods. Cases 1 through 6.

MIX-COMP-THERM-004 Critical Arrays of Mixed Plutonium-Uranium Fuel Rods with Water-to-Fuel Volume Ratios Ranging from 2.4 to 5.6. Case 1.

MIX-COMP-THERM-006 Water-Moderated Mixed Oxide Hexagonal Lattices – 2.0 Wt.% PuO_2, 8% ^{240}Pu, Natural Uranium. Case 1.

MIX-COMP-THERM-007 Hexagonal Lattices of Mixed Oxide Fuel Pins UO_2 – 2 Wt.% PuO_2 (16% ^{240}Pu), Natural Uranium. Case 2.

MIX-COMP-THERM-008 Hexagonal Lattices of Mixed Oxide Fuel Pins UO_2 – 2 Wt.% PuO_2 (24% ^{240}Pu), Natural Uranium. Cases 1 through 6.

MIX-SOL-THERM-001 Criticality Experiments with Mixed Plutonium and Uranium Nitrate Solution at a Plutonium Fraction of 0.2 and 1.0 in Annular Cylindrical Geometry. Cases 1 through 6 and 8 through 13.

MIX-SOL-THERM-002 Criticality Experiments with Mixed Plutonium and Uranium Nitrate Solution at a Plutonium Fraction of 0.2 and 0.5 in Large Cylindrical Geometry. Cases 1 through 3.

MIX-SOL-THERM-004 Criticality Experiments with Mixed Plutonium and Uranium Nitrate Solution at a Plutonium Fraction of 0.4 in Small Cylindrical Geometry. Cases 1 through 9.

MIX-SOL-THERM-005 Criticality Experiments with Mixed Plutonium and Uranium Nitrate Solution at a Plutonium Fraction of 0.4 in Slab Geometry. Cases 1 through 7.

6.3.1.2 LEU LCEs

The selection of LEU LCEs is based on physical characteristic similarities between fresh fuel waste packages and experiment systems. The 37 selected LEU critical experiments are water-moderated thermal systems containing LEU in a lattice configuration, where the LEU compound contains the isotopes ^{234}U, ^{235}U, ^{236}U, ^{238}U.

LEU-COMP-THERM-010 Critical Arrays of Water-Moderated $U(4.31)O_2$ Fuel Rods Reflected by Two Lead, Uranium, or Steel Walls. Cases 5 and 16 through 19.

LEU-COMP-THERM-017 Critical Arrays of Water-Moderated $U(2.35)O_2$ Fuel Rods Reflected by Two Lead, Uranium, or Steel Walls. Cases 3 through 17, 19 through 25, 28, and 29.

LEU-COMP-THERM-026 Water-Moderated $U(4.92)O_2$ Fuel Rods in 1.29, 1.09, and 1.01 cm Pitch Hexagonal Lattices at Different Temperatures. Case 3.

LEU-COMP-THERM-042 Water-Moderated Rectangular Clusters Of $U(2.35)O_2$ Fuel Rods (1.684 cm Pitch) Separated By Steel, Boral, Boroflex, Cadmium, Or Copper Plates With Steel Reflecting Walls. Cases 1 through 7.

6.3.2 Proprietary LCE Data—Haut Taux de Combustion Laboratory Critical Experiments

In the late 1980s, a series of critical experiments referred to as the HTC experiments were conducted at the experimental criticality facility in Valduc, France. These experiments were designed to provide a basis for validation of actinide-only burnup credit calculations. The simulated fuel rods used in these experiments contained a mixture of uranium and plutonium oxides. The plutonium-to-uranium ratio and the isotopic compositions of both the uranium and plutonium were designed to be similar to what would be found in a typical PWR fuel assembly that initially had an enrichment of 4.5 wt % ^{235}U and was burned to 37,500 MWd/MTU. The fuel material includes ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{238}Pu through ^{242}Pu, and ^{241}Am, which is present due to the decay of ^{241}Pu.

The 156 critical configurations were designed to approximate fuel handling, fuel storage rack, and spent fuel shipping cask conditions and were categorized into four phases.[46] The first phase[47] included 18 configurations, each involving a single square-pitched array of rods with rod pitch varying from 1.3 to 2.3 cm. The arrays were flooded and reflected with clean water. The second phase[48] included 41 configurations that were similar to the first group except that the water used as moderator and reflector included either boron or gadolinium in solution. The third phase[49] simulated fuel-assembly storage rack conditions included 26 configurations with the rods arranged into four assemblies in a 2 × 2 array. The spacing between assemblies was varied, and some of the assemblies had borated stainless steel (which is used in the waste package), Boral®, or cadmium plates attached to the sides of the four assemblies. The fourth phase[50] simulated cask conditions and included 71 configurations similar to the Phase 3 configurations except thick steel or lead shields were placed around the outside of the 2 × 2 array of fuel assemblies. A total of 156 configurations are documented in the final reports, and a total of 145 configurations are used in this validation. The following HTC LCE cases are not well defined in the documented reports and therefore were not used in this validation: HTC Phase 3, cases 2, 6, and 8; HTC Phase 4, lead shield, cases 1, 12, 13, 14, and 17; and HTC Phase 4, steel shield, cases 1, 12, and 14. The results of the criticality calculations are presented in Appendix A, Table A-1. These data were selected because they were specifically developed for this use, that is, validation of criticality methods for burnup credit, and have been shown in previous studies (Ref. 68) to have excellent applicability to CSNF applications.

6.3.3 Commercial Reactor Criticals

The CRCs are the only critical experiments that include actual spent nuclear fuel representative of the waste stream assemblies. In fact, the assemblies in the CRCs are part of the waste stream. The CRCs included as a component of the validation methodology are comprised of 45 critical state-points from five PWRs: Crystal River Unit 3 (33 configurations), McGuire Unit 1 (six configurations), Sequoyah Unit 2 (three configurations), and Three Mile Island (TMI) Unit 1 (three configurations), and 16 state-points from BWR Grand Gulf Unit 1. The CRC state-points used in this validation are reactor hot zero-power critical conditions attained after sufficient down time to allow the fission product xenon inventory to decay. The selection of the CRCs was based on the similar nuclear and physical characteristics between the application systems and the CRC state-points, including similar actinide and fission-product compositions. A number of studies have been previously carried out to demonstrate the suitability of CRCs as spent-fuel benchmark experiments and their applicability for criticality calculation validation.[69, 70, 71] These studies focused on general characteristic comparisons between the CRCs and waste packages and showed that, although a neutron spectral shift exists between the two systems due to various effects (e.g., moderator temperature differences and material differences), the CRCs closely represent the reaction rates in a waste package configuration.

The CRC state-point configurations were modeled in MCNP with fine details. Changes were made to the original MCNP input files to create new input files for MCNP 5.1.40 calculations with ENDF/B-VI data. The original input files used MCNP data tables based on the ENDF/B-V library (refer to Section 4.1.2.3 for the sources of the MCNP input files for the CRCs). Therefore, the MCNP input files were modified to replace data tables based on the ENDF/B-V library with data tables presented in Table 15 and additional ENDF/B-VI library data tables available in MCNP 5.1.40. An additional change made to the original MCNP files for the MCNP 4B version (Ref. 53) for one-eighth symmetry CRC models was replacement of the geometry cutting plane that defines a one-eighth symmetry core model with a cutting plane that defines a one-fourth symmetry core model. Note that the modeling for a one-fourth symmetry core was already implemented in the original MCNP input files for these cases. The k_{eff} results for one-fourth symmetry geometry and the k_{eff} results for the one-eight symmetry geometry provided in Ref. 52 are almost identical, as shown in Table D-1, Appendix D, which indicate that the two MCNP core models are identical.

Consistent with the MCNP modeling, CSAS25/KENO V.a modeling was performed for Crystal River Unit 3 CRC state-points for use in TSUNAMI-3D calculations. The input data for these models were extracted from the MCNP 4B input files (Ref. 53) and reactor core descriptions available in Ref. 52, and the CSAS25/KENO V.a models have the same geometry and material description details as the MCNP models. Spent fuel zone compositions contain oxygen and up to 85 actinide and fission-product isotopes (Ref. 52), since short-lived fission products have relevant reactivity worth in the CRCs. A horizontal and a partial vertical cross section of the KENO V.a geometry for a Crystal River state-point is illustrated in Fig. 7. The verification of the CSAS25/KENO V.a models was made though comparison between the MCNP 4B k_{eff} results (Ref. 52) and CSAS25 k_{eff} results, which are presented in Table D-2, Appendix D. Generally, the CSAS25 k_{eff} results are in good agreement with the results described in the referenced document (±0.3%), indicating that the mixture compositions and geometry models are consistent between the CSAS25 and MCNP calculations. Only the results for the last two Crystal River state-points are significantly lower than the corresponding MCNP calculation results. However, the impact on sensitivity coefficients is expected to be less important because these coefficients are defined in terms of relative values (see Appendix B).

The results of the MCNP calculations with ENDF/B-VI data for the 61 CRC state-points are presented in Appendix A, Table A-4. As was observed in the previous analysis (Ref. 60) of the Grand Gulf state-points, a significant deviation from unity was obtained for CRC Grand Gulf state-point 20 (k_{eff} = 0.9681). This value is also significantly different from the k_{eff} results for Grand Gulf state-points with similar average core burnup, such as state-points 15 (k_{eff} = 0.9816) and 19 (k_{eff} = 0.9803) (see Appendix A, Table A-4). Therefore, the Grand Gulf state-point 20 was not used in bias and bias uncertainty determination.

All critical experiment configurations have some quantity of uncertainty. For this reason, evaluations of critical experiments included in the IHECSBE include an assessment of the experimental uncertainties, which for LCE are typically quite small, for example, less than ~0.3% in k_{eff}. For CRC state-points, which are large and complex systems, it is recognized that larger uncertainties are expected to exist, as compared to LCEs. Although a detailed assessment of the uncertainties in these configurations has not been performed to accurately quantify the uncertainty in these configurations, a qualitative assessment has been performed to assign a justifiable upper bound (conservative) uncertainty value to be used in this analysis. An uncertainty of 2% (two standard deviations at 95% confidence level) for CRC k_{eff} values is used in statistical analyses for bias and bias uncertainty determination presented in Section 6.5.2. The rationale for selecting this uncertainty value is as follows:

- A statistically significant number of CRC state-points (61) were selected as a component of this validation methodology. The MCNP 5.1.40 k_{eff} values for all selected CRCs but one (Grand Gulf state-point 20) (see Appendix A, Table A-4) are contained within unity ± 2%. The statistical distributions of the k_{eff} values for the PWR and BWR CRCs pass a normality test. Figure D-1, Appendix D, shows a distribution histogram plot for PWR and BWR (Grand Gulf) CRC k_{eff} values. The sample standard deviation for the applicable PWR CRC and BWR (Grand Gulf) k_{eff} values is approximately 0.005, which is smaller than the assumed 1% one standard deviation in calculated k_{eff} values due to modeling uncertainties.

- CRC k_{eff} values exhibit an increasing or decreasing trend as a function of parameters burnup, *EALF*, and integral index c_k (refer to Appendix B for the definition and meaning of the integral index c_k) that can be distinguished from random behavior.

- The statistical method used to determine bias and bias uncertainty[18] also quantifies uncertainties associated with any modeling approximations and uncertainties in the experimental conditions as reflected in the random scatter of the data points about the bias, since the CRC k_{eff} values satisfy the required statistical behavior.

- Bias (and bias uncertainty) associated with the isotopic compositions are evaluated separately (Ref. 72) , as described in Section 3.5.3.1 of the *Disposal Criticality Analysis Methodology Topical Report*,[1] and combined with the bias determined for the criticality computational method (determined in this report) as if they were independent variables (Ref. 1, Section 3.5.3.2.5). In reality, these two bias components are not independent since any isotopic composition bias will propagate to the criticality calculation results. Therefore, this approach determines conservative bias and uncertainty associated with the bias.

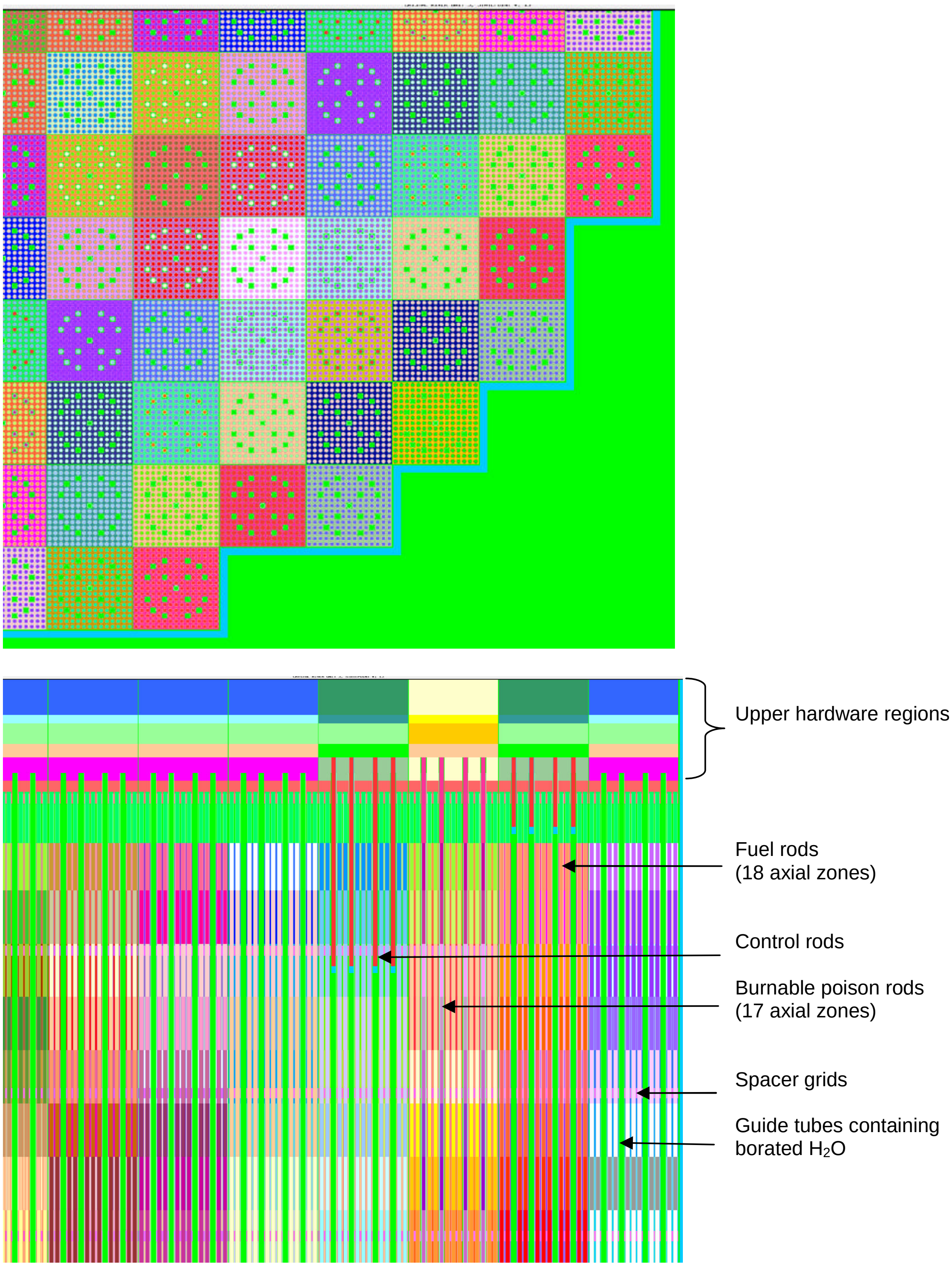


Fig. 7. Horizontal and partial vertical cross sections of KENO V.a geometry for a Crystal River Unit 3 state-point.

6.4 DETERMINATION OF APPLICABILITY OF CRITICAL EXPERIMENTS

Sensitivity/uncertainty analysis methods can be used to demonstrate that nuclear systems with similar physical characteristics, including material compositions, geometry, and neutron flux spectra, exhibit similar sensitivities of the effective neutron multiplication factor, k_{eff}, to perturbations in the neutron cross-section data on an energy-dependent, nuclide-reaction specific level. The assessment of system similarities and shared variance, due to cross-section uncertainties, in the computed values of k_{eff} is particularly useful in determining applicability of critical experiments to be used to determine bias and bias uncertainty of criticality safety calculations. Scientists at ORNL have formulated the theoretical bases for use of S/U analysis methods in criticality safety validation and developed the software tools needed to implement the methodology in the SCALE code system.[15, 16] A set of indices has been defined for use in S/U analyses that provides a measure of the neutronic similarity between a design system and a critical experiment. Integral index c_k is the correlation coefficient between sensitivity-weighted uncertainties in the application system and an experiment system. A c_k value of 0.0 represents no correlation between the systems, a value of 1.0 represents full correlation between the systems, that is, indicates identical systems, and a value of -1.0 represents a full anticorrelation. The definition of integral index c_k, the parameter used in this methodology to identify applicable critical experiments for use in bias and bias uncertainty determination, is provided in Appendix B. Reference 63 demonstrates that c_k values of 0.80 or higher constitute systems that are similar to the extent that they are useful in the determination of bias and associated uncertainty. Further, Ref. 63 recommends that the validation methodology should include about 15 to 20 very correlated systems (c_k of 0.90 or higher) or 25 to 40 moderately correlated systems (c_k of 0.80 or higher). This validation uses this published guidance; that is, a critical configuration is applicable to an evaluation case if the c_k value is ≥ 0.9, a critical configuration is considered marginally applicable if c_k is ≥ 0.8 and <0.9, and a critical configuration is considered not applicable if c_k <0.8.

6.4.1 Methods

Although the objective of this work is validating MCNP, MCNP does not have an S/U capability. Hence, the sensitivity/uncertainty analysis was performed with the TSUNAMI-3D sequence and the TSUNAMI-IP module distributed as part of the SCALE 5.1 package, and was used to quantify the applicability of the experiments for the determination of the LBTL. TSUNAMI-3D is a Monte Carlo – based eigenvalue sensitivity analysis sequence. This software tool calculates energy-, mixture-, nuclide-, and region-dependent sensitivity of the system k_{eff} to variations in nuclear data of modeled materials. TSUNAMI-3D uses first-order linear-perturbation theory to calculate sensitivity coefficients (refer to Appendix B for the definition of sensitivity coefficients). The functional modules executed by the TSUNAMI-3D sequence for the calculations presented in this report are BONAMIST, CENTRMST/PMCST/WORKER or NITAWLST, KENO V.a, and SAMS. The functional modules BONAMIST, NITAWLST, and CENTRMST/PMCST/WORKER perform resonance processing of the cross sections. KENO V.a performs forward and adjoint Monte Carlo calculations using the resonance-processed cross sections, and SAMS uses the forward and adjoint solutions in a standard linear perturbation theory method to calculate neutron energy-dependent sensitivity profiles. The profiles for each modeled system are saved in a sensitivity data file (SDF). CENTRMST/PMCST/WORKER and the SCALE ENDF/B-VI 238-group cross-section library were used in cross-section resonance processing for all cases except for the CRC calculations, which used NITAWLST and the SCALE ENDF/B-V 238-group cross-section library (see Section 6.4.2). To increase confidence that the sensitivity profiles are accurate, selected direct perturbation calculations were performed. Appendix C describes the direct perturbation method used to verify that the TSUNAMI-3D calculated sensitivity coefficient values are consistent with the sensitivity coefficients that MCNP would estimate. As implemented in the TSUNAMI tools, sensitivity is the fractional change in the k_{eff} value resulting from a fractional change in the nuclear data parameter of interest. For example, if the capture sensitivity for ^{10}B in a model is -0.1, then a 1% increase in the capture cross sections would result in a 0.1% reduction in the system k_{eff} value.

TSUNAMI-IP, also a part of the SCALE 5.1 computer software package, is used to compare the sensitivity data for two systems. It generates a variety of total and partial relational parameters that quantify the similarity between two systems. The integral index c_k (refer to Appendix B for the definition of c_k) is a single-valued parameter used to assess similarity of nuclear data uncertainty-weighted sensitivity profiles for all nuclide-reactions between a design system and a criticality experiment. A c_k value of 0.0 represents no correlation between the systems, a value of 1.0 represents full correlation between the systems, that is, indicates identical systems, and a value of -1.0 represents a full anticorrelation. The premise behind the c_k parameter is that calculation biases are due primarily to errors in cross-section data with larger uncertainties. Systems that demonstrate similarly high sensitivities to highly uncertain cross-section data will have similar computational biases. The similarity work presented in this report utilizes the c_k parameter.

6.4.2 TSUNAMI-3D and TSUNAMI-IP Calculations

The results of the TSUNAMI-IP calculations are presented in Appendix B. Tables B-1 through B-12 show the c_k values for each of the 24 application systems (refer to Table 16) and each set of critical experiments. All critical experiments with $c_k \geq 0.8$ are considered marginally applicable. Table 17 provides the number of applicable critical experiments to bias and bias determination, that is, critical experiments with $c_k \geq 0.8$, for each of the 24 application systems. Cell shading was used in Tables B-1 through B-12 to identify these applicable critical experiments. More than 40 marginally applicable critical experiments that also include at least 15 to 20 very correlated systems (c_k of 0.90 or higher), as recommended in Ref. 63, are available for bias and bias uncertainty determination for all application systems except for the fresh fuel waste packages. For these systems, only the LEU LCEs and fresh fuel CRCs are at least marginally applicable among the selected critical experiments. Between 41 and 43 LCEs and fresh-fuel CRCs are at least marginally applicable to the fresh fuel PWR and BWR applications due to similar sensitivities to ^{1}H, ^{235}U, and ^{238}U, which are the predominant contributors to c_k for the fresh fuel systems. The HTC and MOX LCEs and CRCs with burned fuel were not applicable to these systems due primarily to the presence of plutonium.

The LEU LCEs and the fresh fuel CRCs are most neutronically similar to fresh fuel waste packages because their k_{eff} values exhibit significant sensitivities only to ^{1}H, ^{235}U, and ^{238}U, that is, these experiments and the fresh fuel waste packages have common components of uncertainty in k_{eff} due to cross-section uncertainties for those nuclides.

Only sensitivity data files for the Crystal River state-points are available for assessing similarity between a CRC state-point and the application systems. These Crystal River CRC sensitivity files were obtained with a non-qualified version of SCALE 5.1 and the 238-group ENDF/B-V SCALE library and NITAWL for resonance-cross section processing, as described in Refs. 73 and 74. To reduce the computer time of a TSUNAMI-3D calculation for a Crystal River state-point, the total number of nuclides in KENO V.a fuel mixtures was reduced from more than 40,000 to approximately 20,000 by including in fuel compositions only the actinides and the major fission products that have been identified as being important to burnup credit criticality calculations (see Sect. 6.1). While this approach significantly reduced the required computer time, it had minimal effects on the accuracy of the sensitivity coefficients because these coefficients are defined in terms of relative values. Note that sensitivity data for Crystal River state-points is used only to determine the applicability of the CRCs considered in this validation and is not directly used in bias and bias uncertainty determination; therefore, use of the non-qualified Crystal River sensitivity files is adequate for this calculation. As shown in Tables B-10 through B-12, Appendix B, all Crystal River state-points, except for the beginning-of-life state-point, exhibit at least marginal similarity with the 21-PWR waste packages containing CSNF with burnup (that is, cases not based on fresh fuel) and the 44-BWR waste packages containing CSNF of 3-wt% ^{235}U initial enrichment and 10 GWd/MTU burnup, whereas 27 Crystal River state-points (out of 33 state-points) exhibit at least marginal similarity with the other 44-BWR waste packages containing CSNF with burnup. Based on this observation, the state-points other than beginning of life state-points for the other CRCs considered in this validation are considered applicable to bias and bias uncertainty determination for the CSNF waste packages (that is, expected to have c_k values > 0.8).

Table 17. Summary of applicable critical experiments to bias and bias uncertainty determination

Application system		Number of applicable critical experiments					
Waste package	**Enrichment (wt% ^{235}U)/ burnup (GWd/MTU)**	**MOX lattice**	**MOX solution**	**LEU**	**HTC**	**CRC**	**Total**
21 PWR nominal configuration	2.0/ 0	0	0	37	0	4	41[a]
	3.0/ 0	0	0	37	1	5	43[a]
	3.0/ 15	17	0	0	145	56	218
	3.5/ 25	18	0	0	145	56	219
	4.0/ 30	18	1	0	145	56	220
	4.5/ 35	19	11	0	145	56	231
	5.0/ 40	18	1	0	145	56	220
21 PWR design-basis configuration	2.0/ 0	0	0	37	0	4	41[a]
	3.0/ 0	0	0	37	0	5	42[a]
	3.0/ 15	17	0	0	145	56	218
	3.5/ 25	18	0	0	145	56	219
	4.0/ 30	18	1	0	145	56	220
	4.5/ 35	19	2	0	145	56	222
	5.0/ 40	18	1	0	145	56	220
44 BWR nominal configuration	3.0/ 0	0	0	37	0	4	41[a]
	3.0/ 10	20	9	0	145	56	230
	4.0/ 0	0	0	37	0	4	41[a]
	4.0/ 20	21	17	0	145	51	234
	5.0/ 30	21	19	0	145	51	236
44 BWR design-basis configuration	3.0/ 0	0	0	37	0	4	41[a]
	3.0/ 10	19	9	0	145	56	229
	4.0/ 0	0	0	37	0	4	41[a]
	4.0/ 20	21	17	0	145	51	234
	5.0/ 30	21	21	0	145	51	238

[a]Only the applicable LEU LCEs with EALF values below 0.3882 (36 LEU LCEs) were used to calculate the LBTL values shown in Sections 6.5 and 7 since the EALF for the evaluated fresh fuel waste packages varies from 0.20 eV to 0.33 eV.

Figures 8 through 13 show the c_k values and illustrate the set of applicable critical experiments to bias and bias uncertainty determination for the 21-PWR waste packages containing CSNF of 3.0 wt% ^{235}U and 15-GWd/MTU burnup, CSNF of 5.0 wt% ^{235}U and 40-GWd/MTU burnup, and fresh fuel of 3.0 wt% ^{235}U initial enrichment, and the 44-BWR waste package containing CSNF of 3.0 wt% ^{235}U and 10-GWd/MTU burnup, CSNF of 5.0 wt% ^{235}U and 30-GWd/MTU burnup, and fresh fuel of 3.0 wt% ^{235}U initial enrichment, respectively. The critical experiments with c_k values above the red grid line, that is, $c_k \geq 0.8$, are at least marginally applicable, whereas the critical experiments with c_k values above the green grid line, that is, $c_k \geq 0.9$, are highly applicable. Critical experiments with c_k values ≥ 0.8 are used in the bias determination.

The direct perturbation method (refer to Appendix C for method description) is used to assess the quality of the sensitivity coefficients obtained in a TSUNAMI-3D calculation and provide confidence that sensitivities calculated by SCALE/TSUNAMI are consistent with what can be calculated with MCNP. Sensitivity coefficients from MCNP direct perturbation calculations were obtained for nuclides/elements for which k_{eff} exhibits significant sensitivities, such as H, ^{10}B, ^{235}U, ^{238}U, ^{239}Pu, and ^{149}Sm, in the waste package models. A comparison of direct perturbation and TSUNAMI-3D sensitivity coefficient calculations is presented in Table C-1, Appendix C. Note that the sensitivity coefficient estimates from the MCNP direct perturbation calculations have larger uncertainties than the TSUNAMI-3D sensitivity coefficients, although the estimated k_{eff} from each individual MCNP calculation had a very small standard deviation (0.00012). The two methods are in good agreement since the MCNP direct perturbation results differ from the TSUNAMI-3D results by less than ±10% for the majority of the calculations, with the rest of the direct perturbation calculations being within ±20% of the TSUNAMI-3D results. These results provide confidence that sensitivities calculated by SCALE/TSUNAMI are consistent with what can be calculated with MCNP. Hence, it is acceptable to use TSUNAMI for assessing applicability of experiments that will be used to validate MCNP.

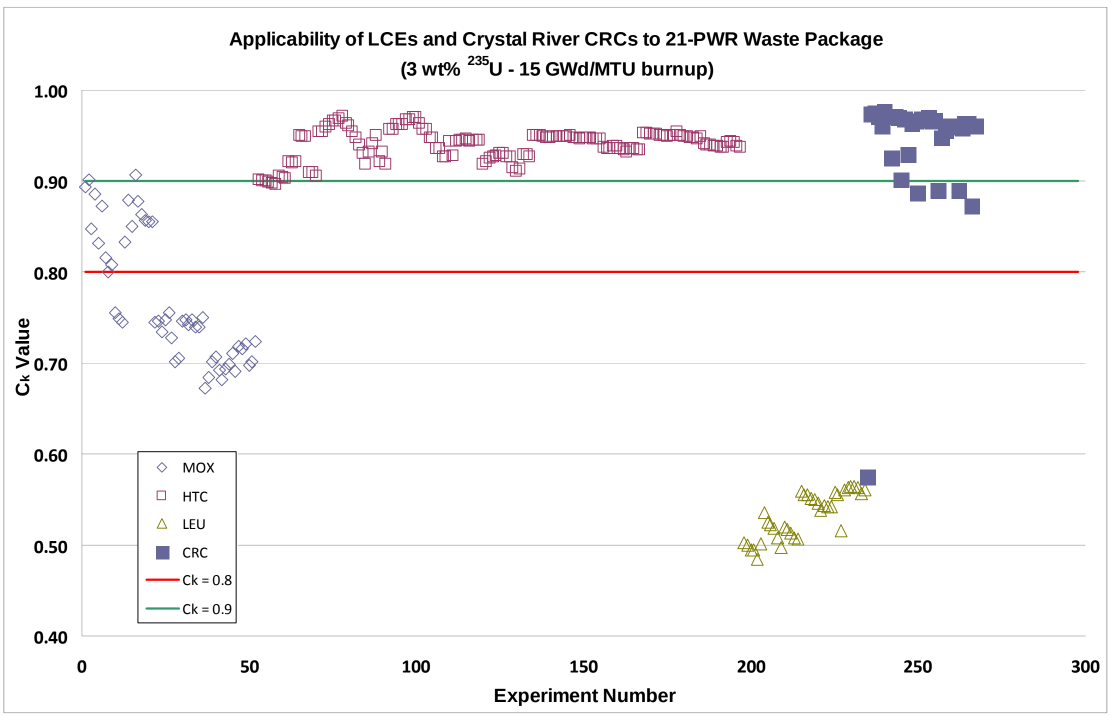


Fig. 8. c_k as a function of experiment number: 21-PWR waste package, CSNF of 3 wt% ^{235}U initial enrichment, and 15-GWd/MTU burnup.

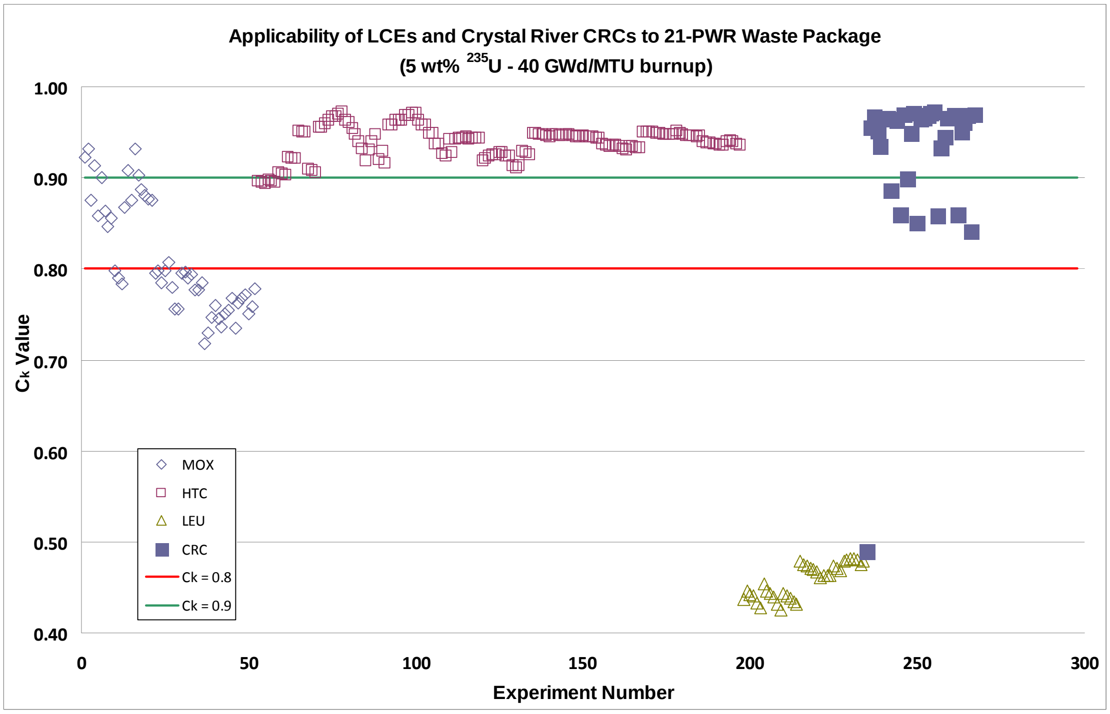


Fig. 9. c_k **as a function of experiment number: 21-PWR waste package, CSNF of 5 wt%** ^{235}**U initial enrichment, and 40-GWd/MTU burnup.**

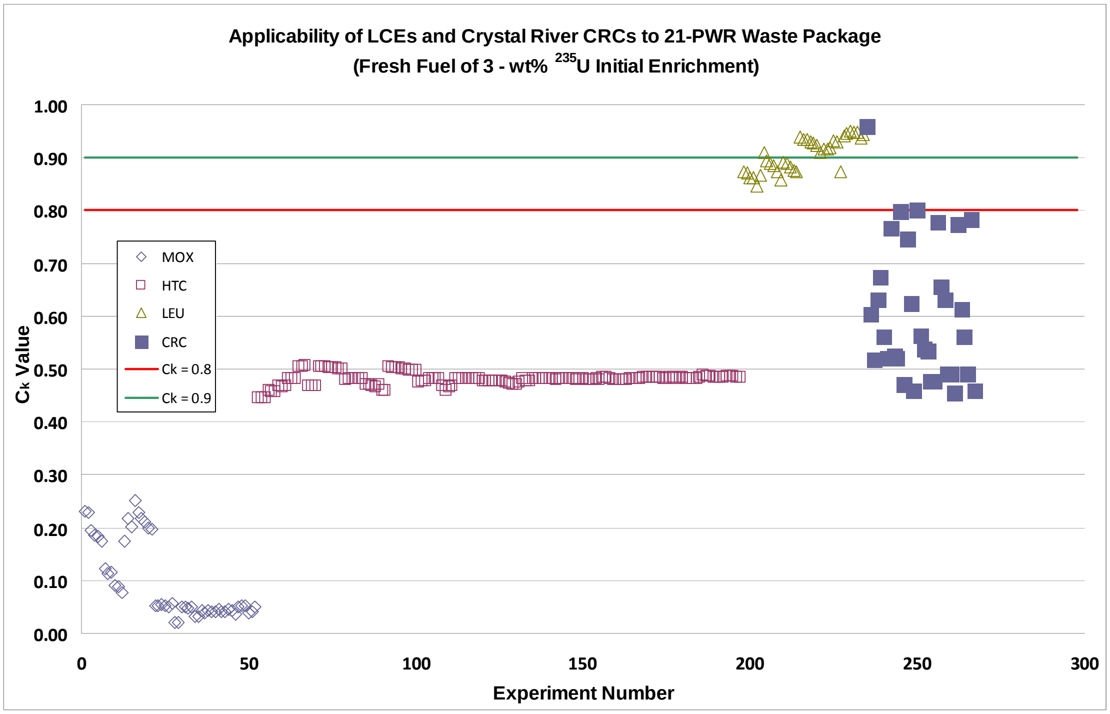


Fig. 10. c_k **as a function of experiment number: 21-PWR waste package, fresh fuel of 3 wt%** ^{235}**U initial enrichment.**

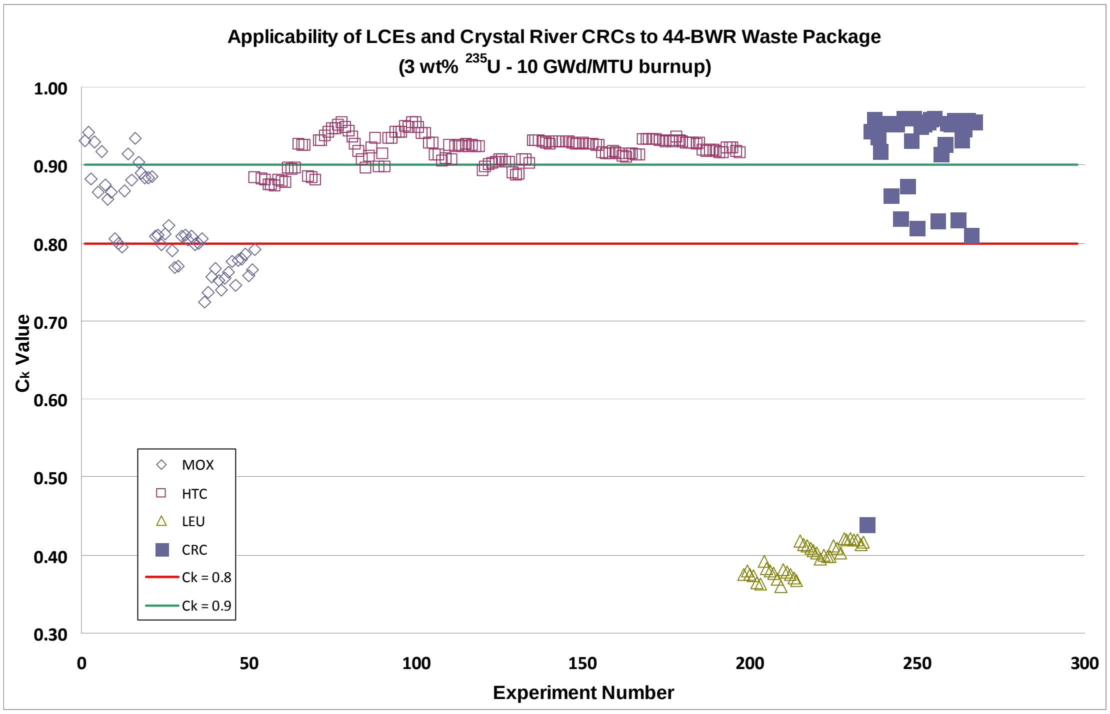


Fig. 11. c_k **as a function of experiment number: 44-BWR waste package, CSNF of 3 wt%** ^{235}**U initial enrichment, and 10-GWd/MTU burnup.**

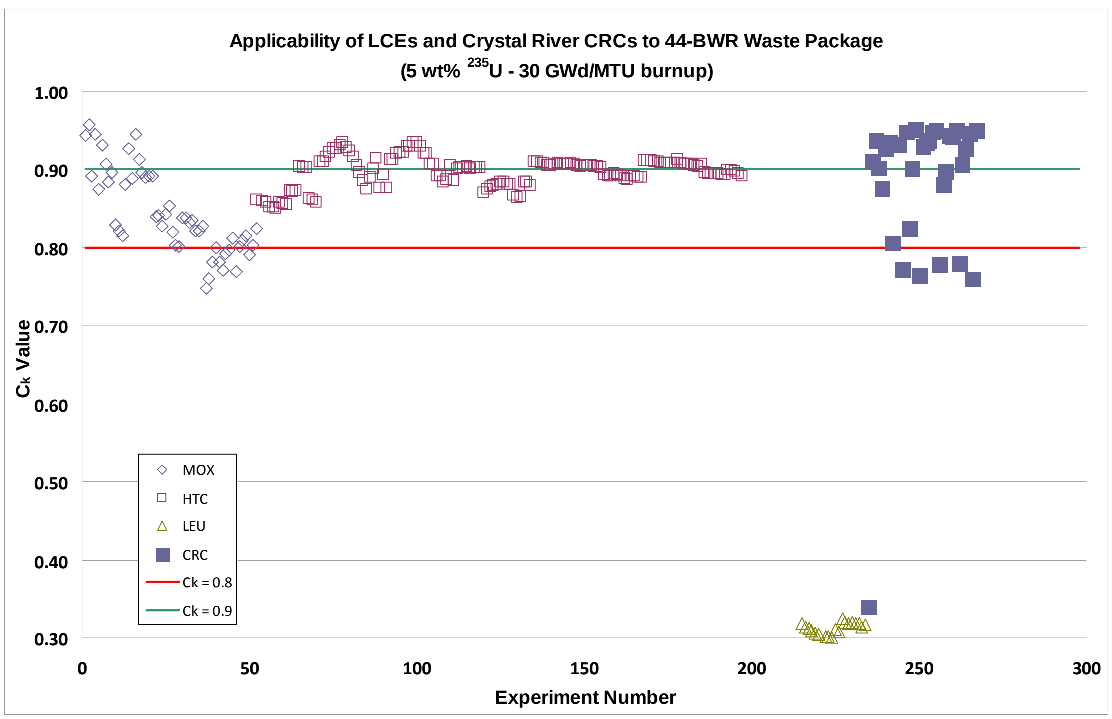


Fig. 12. c_k **as a function of experiment number: 44-BWR waste package, CSNF of 5 wt%** ^{235}**U initial enrichment, and 30-GWd/MTU burnup.**

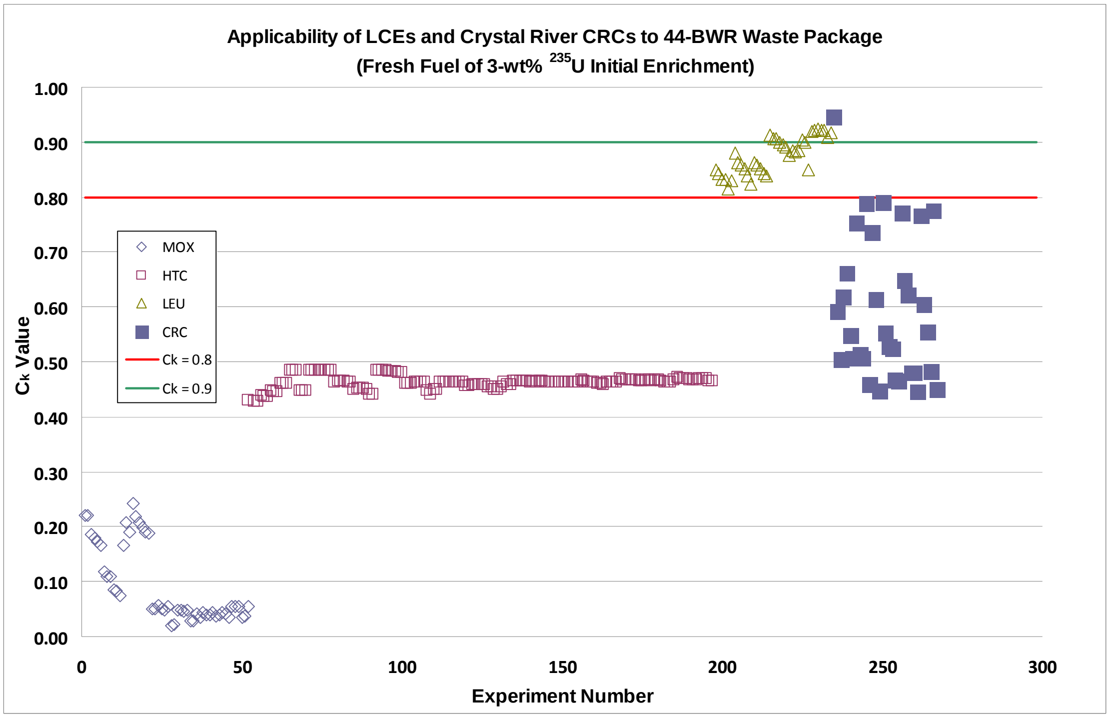


Fig. 13. c_k as a function of experiment number: 44-BWR waste package, fresh fuel of 3 wt% ^{235}U initial enrichment.

6.5 DETERMINATION OF BIAS AND BIAS UNCERTAINTY

This section describes the methods used to determine a lower bound tolerance limit for the applications evaluated in this calculation report and the calculation result analyses.

6.5.1 Methods

Bias and bias uncertainty over the area of applicability of critical experiments are determined using the guidance in ANSI/ANS-8.1-1998 and ANSI/ANS 8.17-2004. The accuracy of the computational method and cross-section data is established by evaluating critical experiments. Computational bias is the difference between calculated and experimental results. The uncertainty in bias is an allowance for uncertainties in the experiment conditions, the lack of accuracy and precision in the calculational method, and the extension of the area of applicability, if applicable. Generally, the bias and bias uncertainty are expected to be functions of various physical or neutronic parameters that can be determined using trending analyses. This technique can be applied to establish bias and bias uncertainty because k_{eff} values usually exhibit an increasing or decreasing trend as a function of parameters such as lattice pitch, ^{235}U or other fissile concentration, hydrogen-to-uranium ratio, EALF, etc., that can be distinguished from random behavior. Statistical techniques exist for evaluating the bias and bias uncertainty and for establishing limits that can reliably be used to predict subcriticality, such as tolerance band, single-sided tolerance limit, and distribution-free tolerance limit (nonparametric) methods.[1] These methods use bias and the bias uncertainty in combination with additional considerations (e.g., administrative margins, where applicable) to establish a critical limit (CL) (single value or a function, depending on the method applied) above which a desired fraction of the true population of k_{eff} values calculated for critical systems is expected to lie, with a prescribed confidence and within the area of applicability. The parametric methods require that the k_{eff} values for the applicable critical experiments form a normal distribution. When the k_{eff} values for the critical experiments are not normally distributed about a mean value, a nonparametric statistical treatment (i.e., distribution-free methods) should be used.

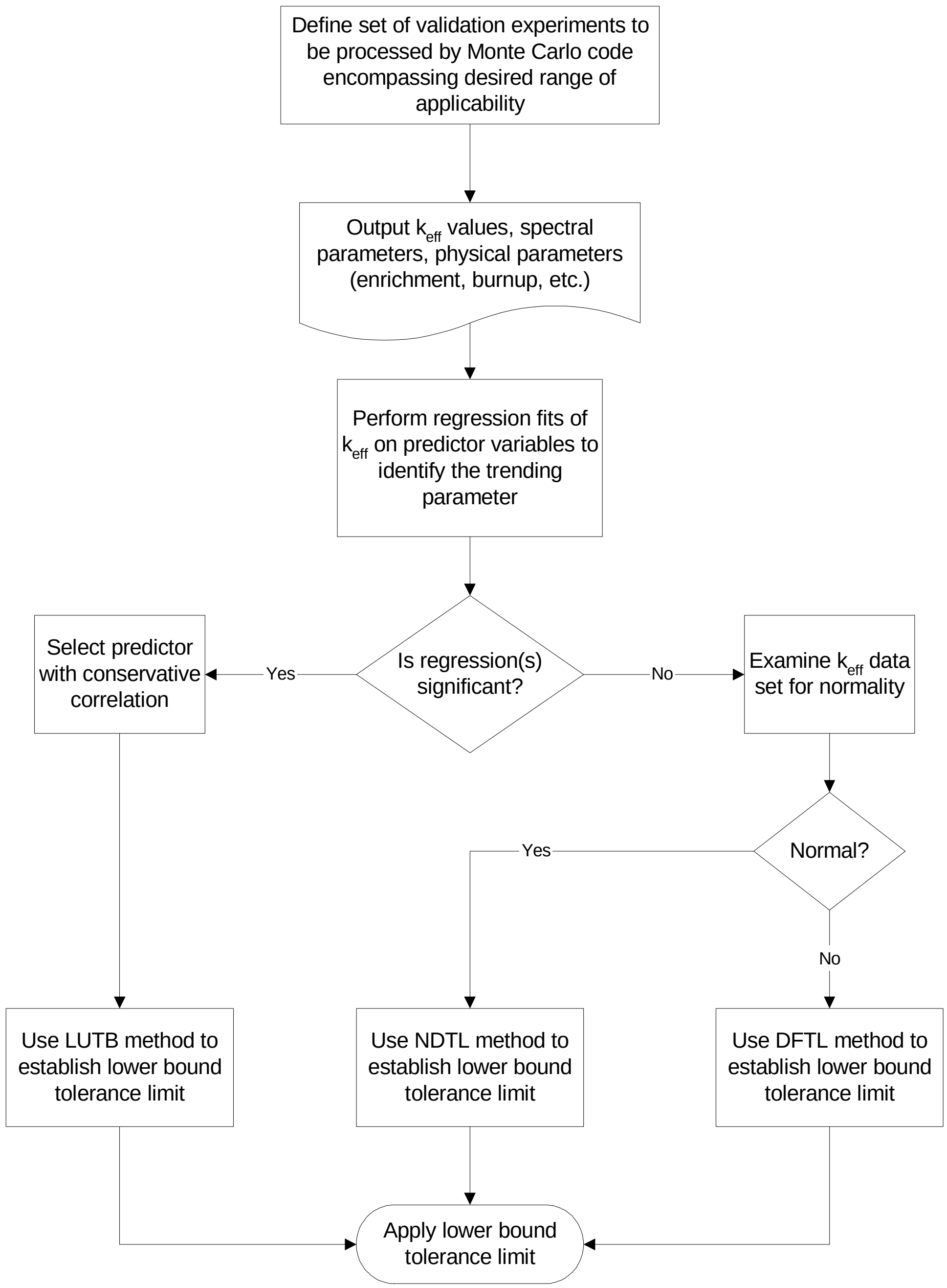
Based on Section 5 of ANSI/ANS 8.17-2004, the CL is represented as[1]

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

where

x	=	a neutronic parameter used for trending;
$f(x)$	=	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}	=	penalty for extending the range of applicability;
Δk_{ISO}	=	penalty for isotopic composition bias and uncertainty; and
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).

This calculation report determines only the LBTL and the penalty for extending the range of applicability, if applicable, using the process described in Section 3.5.3.2 of Ref. 1 and illustrated in Figure 14. Note that the penalty for isotopic composition bias and uncertainty component of the CL, that is the Δk_{ISO} term in the above equation, is not determined in this report (refer to Section 3.5.3.1 of Ref. 1 and Ref. 72 for the isotopic validation and the isotopic model, respectively). Linear regression, normal distribution tolerance limit (NDTL), and distribution-free tolerance limit (DFTL) methods are applied in this validation. For the linear regression models, statistical significance of trending is determined by the test of hypothesis that the slope differs from zero.



Note: LUTB = lower uniform tolerance band
NDTL = normal distribution tolerance limit
DFTL = distribution free tolerance limit

Fig. 14. Process for calculating lower bound tolerance limits.

6.5.1.1 Lower Uniform Tolerance Band Method

The statistical methods referred to as upper subcritical limit (USL) Method 2 in References 18 (Appendix C), 19, and 20 were implemented in a spreadsheet application using only native Excel functions. The USL Method 2 uses a single-sided uniform-width closed-interval approach, also referred to as a lower uniform tolerance band (LUTB) approach.[1, 18] LUTB is the preferred method for estimating a conservative LBTL provided a significant trend is identified with a single predictor variable.[1] The LBTL function is computed according to Eq. 1 (Ref. 18) and the equations for calculating the parameters in Eq. 1 are implemented in the spreadsheet application as described in Appendix E. The spreadsheet application also supports calculation of USLs based on extrapolation of similarity indices, such as c_k, to a value of 1.0, where the compared systems are considered to be identical for bias determination purposes. Regression fits, statistical significance of trending (refer to Eq. E-2, Appendix E), and the χ^2 normality test (refer to Eq. E-4, Appendix E) for the calculated k_{eff} values for the evaluated critical experiment sets were obtained using Microsoft Excel.

$$LBTL(x) = 1.0 - (C_{\alpha/P} \cdot S_P) + \beta(x) \,, \tag{1}$$

where x is a trending parameter, S_p is the pooled variance of k_{eff} values, and $\beta(x) = k_{eff}(x) - 1$. The term $C_{\alpha/P} \cdot S_P$ provides a band for which there is a probability P with a confidence α that an additional calculation of k_{eff} for a critical system will lie within the band. For example, a 95/95 multiplier produces a LBTL for which there is a 95% confidence that 950 out of 1000 future calculations of critical systems will yield a value of k_{eff} above the LBTL.

The following input parameters were used for the LUTB calculations described in Section 6.5.2:

P = proportion of population of critical experiments falling above lower tolerance level, 0.95,
$1 - \gamma$ = confidence on fit, 0.95, and
α = confidence on proportion P, 0.95.

6.5.1.2 Distribution-Free Tolerance Limit Method

The distribution-free tolerance limit method is typically used when trending is not appropriate and the k_{eff} values for the critical experiments do not pass a test for normality.[1] This method involves sorting all k_{eff} values for the applicable critical experiments in ascending order and determining the degree of confidence for the fraction of the true population that lies above the smallest observed value. The percent confidence that a fraction of the population of k_{eff} values calculated for critical systems is above the lowest observed value, $100\alpha\%$, can be determined using the following equation (Ref. 75):

$$\alpha = 1 - \sum_{j=0}^{m-1} \frac{n!}{j!(n-j)!} (1-p)^j \, p^{(n-j)} \,, \tag{2}$$

where

n = sample size,
m = rank order of the smallest k_{eff} value, and
p = the desired population fraction above the smallest k_{eff} value (normally 0.95).

The single-valued *LBTL* function for nonparametric data analysis is determined as follows:

$$LBTL = \text{smallest } k_{eff} \text{ value} - \text{uncertainty for smallest } k_{eff} \text{ value} - \text{nonparametric margin.} \quad (3)$$

Note that the confidence value determined by Eq. 2 increases with increasing sample size and the nonparametric margin is used to account for small sample size in Eq. 3 (e.g., the recommended margins are 0.0, 0.01, and 0.02 when confidence values are greater than 90%, from 80% to 90%, and from 70% to 80%, respectively) (Ref. 75).

6.5.1.3 Normal Distribution Tolerance Limit

The normal distribution tolerance limit method is used for conditions in which the values of k_{eff} for the critical experiments do not exhibit significant trends and form a normal distribution. A single-valued lower bound tolerance limit can be calculated as[1]

$$LBTL = k_{ave} - k\,(\gamma, P, n) \times S_P\,, \quad (4)$$

where

k_{ave}	= the average of the k_{eff} values, unless k_{eff} is greater than unity (1.0), in which instance the appropriate value for k_{ave} should be 1.0 to disallow positive uncertainty,
$k\,(\gamma, P, n)$	= a multiplier (Ref. 76) in which γ is the confidence level, P is the proportion of the population covered, and n is the sample size, and
S_P	= the square root of the sum of the inherent variance of the critical experiment data set plus the average of the criticality code variances for the critical experiment data set.

6.5.2 Analyses

The following analyses use the process for calculating lower bound tolerance limits illustrated in Figure 14 and the methods described in Sections 6.5.1.1, 6.5.1.2, and 6.5.1.3. The analyses and LBTL calculations required the following prerequisites. An additional uncertainty of 2% (two standard deviations, 95% level) in the k_{eff} values for the CRCs was included in the statistical evaluation for LBTL. The justification for this uncertainty value is provided in Section 6.3.3. The MCNP k_{eff} values for critical experiments with an experimental k_{eff} value different from unity (mainly the MOX LCEs; see Appendix A, Tables A-1 through A-4) were normalized to unity, that is, divided by the experimental k_{eff} value.

A first set of trending analyses focused on the LBTL determination using the LUTB method for the most reactive CSNF waste package configuration that contained burned fuel. This configuration is the design-basis 21-PWR waste package containing CSNF of 3.0 wt% ^{235}U and 15-GWd/MTU burnup (k_{eff} = 0.97166) (refer to Table 16 for k_{eff} values for the evaluated configurations). The trends in k_{eff} values for applicable critical experiments ($c_k \geq 0.8$) were examined as functions of predictor variables c_k, *EALF*, and burnup (where applicable), and the LBTL function was determined using Eq. 1. The results are summarized in Table 18. Figures 15 and 16 illustrate the LBTL trends as a function of burnup and *EALF* for cases 8 and 1 shown in Table 18, respectively. Note that the error bars in the graph reflect the k_{eff} uncertainties considered in trending analyses. The results in Table 18 show that the trending using *EALF* parameter yields lower LBTL values as compared with the trending using integral index c_k. Case 3 in Table 18 shows the LBTL values using the critical experiments that are highly similar to the application systems ($c_k \geq 0.9$) and *EALF* as the trending parameter. This selection mostly reduced the number of MOX LCEs and CRCs to be considered for bias determination. As seen in the table, the LBTL values based on highly similar critical experiments ($c_k \geq 0.9$) are less conservative than those based on similar and marginally similar critical experiments ($c_k \geq 0.8$).

As expected, trending analyses using only applicable CRCs produce the most limiting LBTL due to the additional uncertainty of 1% (one standard deviation) used in LBTL determination, whereas the combined sets of HTC and MOX critical experiments produce the least limiting LBTL since very small uncertainties are associated with these LCE sets. Note that the waste package k_{eff} has significant sensitivities to major actinides and the reactivity worth of minor actinides and fission product isotopes present in the application systems vary from approximately 5% to 8% (refer to the k_{eff} results included in /DVD/apps/21pwr/mcnp/rw and /DVD/apps/44bwr/mcnp/rw for fuel compositions containing only minor actinides and fission product isotopes). Therefore, the HTC LCEs and MOX LCEs should be included along with the CRCs in bias and bias uncertainty determination since significant correlation between the cross-section uncertainties in these LCEs and the application systems exists. The use of the applicable experiments ($c_k \geq 0.8$) from the combined HTC LCEs, MOX LCEs, and CRCs and trending analysis using the *EALF* parameter are the most appropriate for LBTL determination.

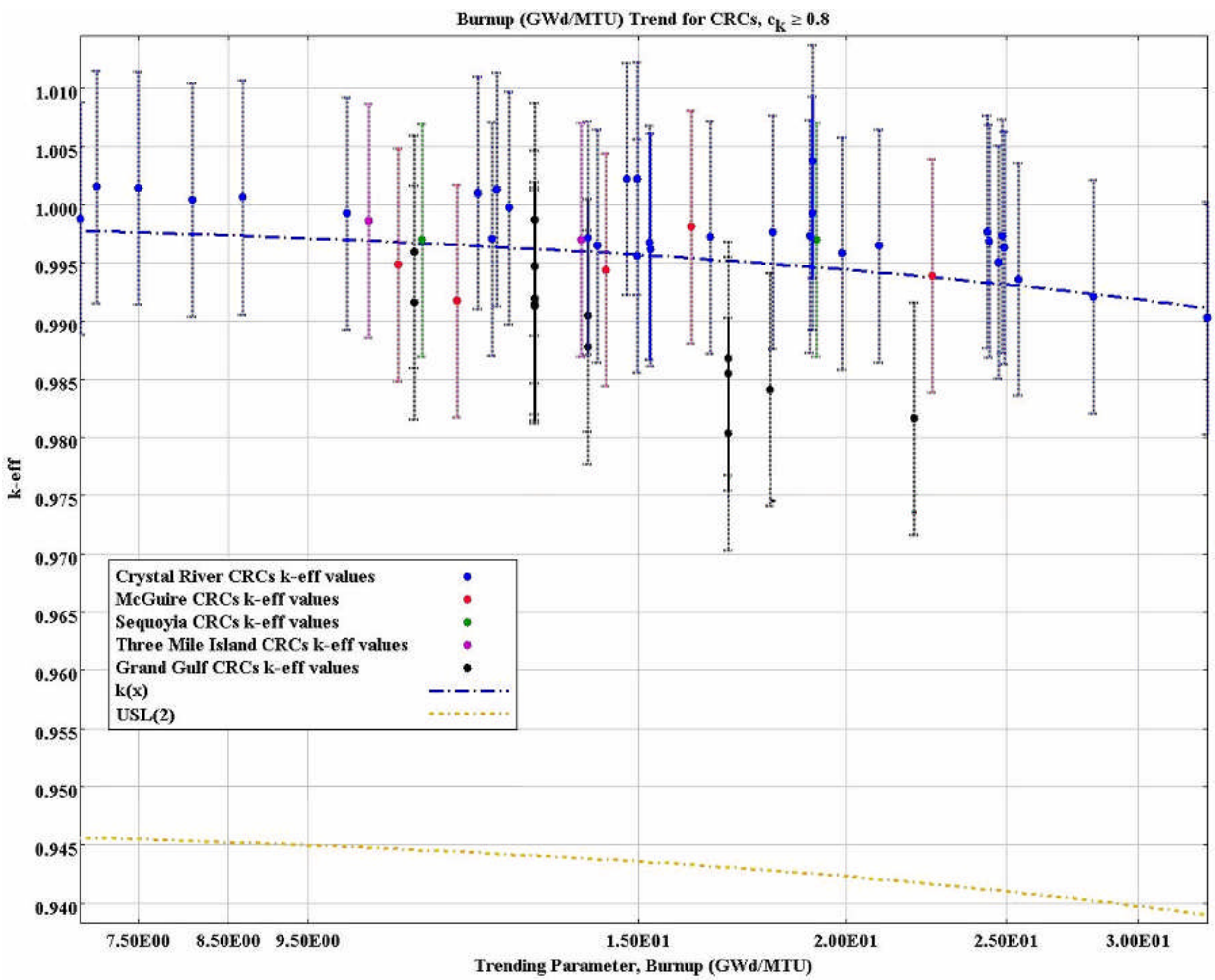
Table 18. LBTL functions from trending with *EALF*, c_k, and burnup using various sets of applicable critical experiments

Case no.	Excel file[a]	Trend parameter	Parameter value	LBTL value	LBTL function	Range of applicability
MOX, HTC & CRCs - $c_k \geq 0.8$						
1	case1	*EALF*[b]	0.3158	0.9800	0.9796+*EALF*·1.1973E-03	6.84E-02≤ *EALF*≤ 1.04E+00
2	case2	c_k	1.0000	0.9878	N/A[c]	N/A
MOX, HTC & CRCs - $c_k \geq 0.9$						
3	case3	*EALF*	0.3158	0.9835	0.9829+*EALF*·1.7352E-03	6.84E-02≤ *EALF*≤ 9.68E-01
MOX & HTC - $c_k \geq 0.8$						
4	case4	*EALF*	0.3158	0.9822	0.9838-*EALF*·4.9777E-03	6.84E-02≤ *EALF*≤ 8.89E-01
5	case5	c_k	1.0000	0.9928	N/A	N/A
CRCs - $c_k \geq 0.8$						
6	case6	*EALF*	0.3158	0.9639	0.9605+*EALF*·1.0702E-02	2.20E-01≤ *EALF*≤ 1.04E+00
7[d]	case7	c_k	1.0000	0.9704	N/A	N/A
8	case8	*BU*[e]	15.000	0.9639	0.9677-*BU*·2.551E-04	9.99E-01≤ *BU*≤ 3.30E+01

[a]Excel application included in the DVD attachment, path: /DVD/cl/Table18.
[b]*EALF* in eV.
[c]Not applicable.
[d]Only the c_k values for Crystal River CRCs were used.
[e]BU=burnup, in GWd/MTU.

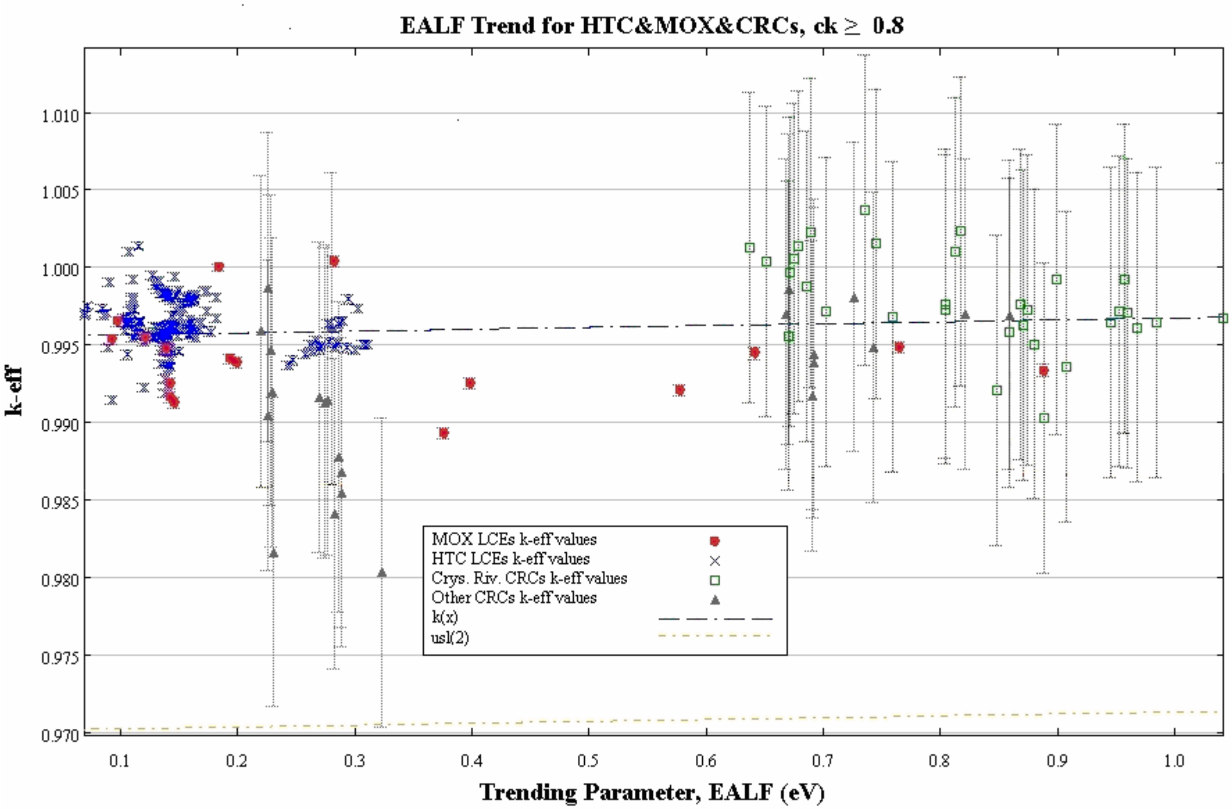
The analysis performed for the design-basis 21-PWR waste package containing CSNF of 3.0 wt% ^{235}U and 15-GWd/MTU burnup determined (1) use of the applicable experiments ($c_k \geq 0.8$) from the combined HTC LCEs, MOX LCEs, and CRCs and trending analysis using the *EALF* parameter are the most appropriate for LUTB determination, (2) the application system *EALFs* are within the area of applicability of the combined HTC LCEs, MOX LCEs, and CRCs, and (3) the regression analysis using the *EALF* parameter as the independent variable identifies a bias in k_{eff} results that distinguishes from statistical fluctuations. Note that the LBTL for this application system has a weak variation with *EALF* over the area of applicability and the statistical significance of trending with *EALF* is further determined using the test statistic in Eq. E-2, Appendix E, and $\alpha = .05$ level of significance in the spreadsheet /DVD/cl/Table18/case1.xls. The result of the hypothesis testing is that the null hypothesis that $\beta_1 = 0$ cannot be rejected at $\alpha = .05$ level of significance and the k_{eff} values of the applicable HTC LCEs, MOX LCEs, and CRCs do not exhibit a significant trend with the parameter *EALF*. The statistical significance of trending for all application systems was tested in the spreadsheets included in /DVD/cl/tests and showed that regression using the parameter *EALF* is not statistically significant. Figure 17 illustrates the LBTL trend with *EALF* for the fresh fuel 21-PWR and 44-BWR waste packages. As required by the criticality model illustrated in Figure 14, the k_{eff} values for applicable critical experiments will be further tested for normality.

The χ^2 test for normality was performed for all evaluated application systems using the test statistic in Eq. E-3, Appendix E, in the spreadsheets included in /DVD/cl/tests and showed that the k_{eff} values for the LEU LCEs (36 data points) that are applicable to the validation of criticality calculations for fresh fuel waste packages pass the normality test, whereas the k_{eff} values for the combined MOX LCE, HTC LCE, and CRC sets (~ between 218 and 238 data points, depending on the application), which are applicable to validation of criticality calculations for waste packages containing burned fuel, do not pass the normality test. For these sets, the distribution has a positive kurtosis, which indicates a relatively peaked distribution, and is negatively skewed, which indicates an asymmetric tail extending toward smaller k_{eff} values.



Note: The error bars on the k_{eff} values show a single standard deviation of 1% assigned to the CRC state-points.

Fig. 15. Burnup trend for CRC state-points.



Note: The error bars on the k_{eff} values for the CRC cases show a single standard deviation of 1% assigned to the CRC state-points.

Fig. 16. EALF trend for HTC LCEs, MOX LCEs, and CRCs.

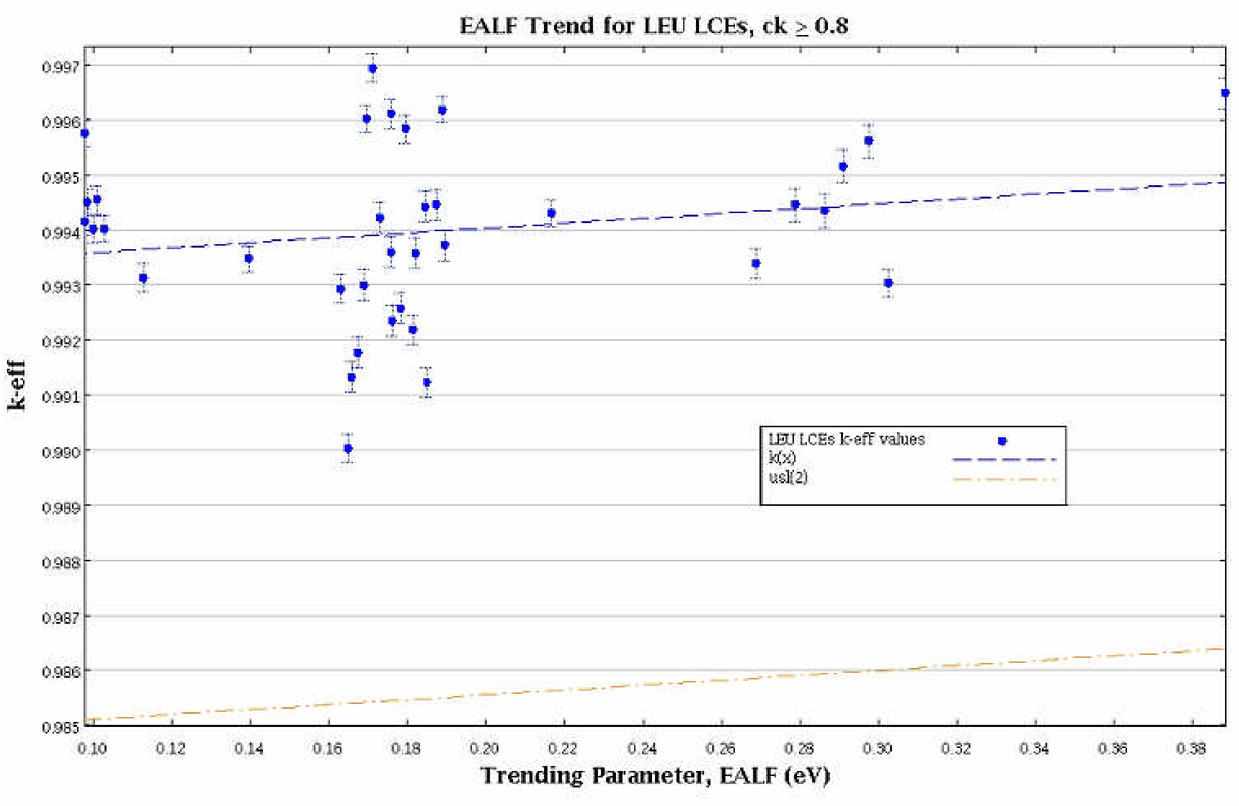


Fig. 17. EALF trend for the LEU LCEs applicable to the validation of criticality calculations for fresh fuel waste packages.

The k_{eff} values of the HTC, MOX, and CRC experiments ($c_k \geq 0.8$) that are applicable to validation of criticality calculations for waste packages containing burned fuel were further analyzed using the DFTL method since this combined set does not pass a normality test. Table 19 summarizes the results of the DFTL method based on Eqs. 2 and 3 (see Section 6.5.1.2), which are available in /DVD/cl/NDTL&DFTL.xls, worksheet DFTL-ptt15. The table shows the 1st- through the 7th-order statistics of the k_{eff} values for 218 applicable critical experiments (145 HTC LCEs, 56 CRCs, and 17 MOX LCEs), the percentage confidence that the k_{eff} population lies above each order statistic, $100\alpha\%$, and the LBTL obtained by subtracting analysis and MCNP calculation statistical uncertainties from the k_{eff} value. Note that these order statistics consist of k_{eff} values for Grand Gulf state-points. In the calculations, the desired percentage of the k_{eff} values from applicable critical experiments above the LBTL is 95% (Ref. 75). Based on the nonparametric analysis, the percentage confidence values that 95% of the k_{eff} population lies above 0.9703, 0.9716, 0.9741, 0.9755, 0.9768, 0.9778, and 0.9803 are 100%, 99.98%, 99.89%, 99.55%, 98.57%, 96.36%, and 92.25%, respectively. The 0.9778 value is used in this validation as a slightly conservative limit to ensure that 95% of the future calculations of CSNF waste packages containing burned fuel will yield a value above this limit at the 95% confidence level. The results of the nonparametric analysis apply to all application systems containing burned fuel since the first seven-order statistics for those systems consist of the k_{eff} values for Grand Gulf state-points provided in Table 19, second column.

Table 19. LBTL from the nonparametric method

Rank	k_{eff}	$100\alpha\%$	σ_a	σ_s	σ[a]	LBTL
1	0.9803	100.00	0.01	0.0001	0.0100	0.9703
2	0.9816	99.98	0.01	0.0001	0.0100	0.9716
3	0.9841	99.89	0.01	0.0001	0.0100	0.9741
4	0.9855	99.55	0.01	0.0001	0.0100	0.9755
5	0.9868	98.57	0.01	0.0001	0.0100	0.9768
6	0.9878	96.36	0.01	0.0001	0.0100	0.9778
7	0.9903	92.25	0.01	0.0001	0.0100	0.9803

[a] $\sigma = \sqrt{\sigma_a^2 + \sigma_s^2}$, where σ_a and σ_s are analysis and MCNP statistical calculation uncertainties, respectively.

The k_{eff} values of the 36 LEU LCEs ($c_k \geq 0.8$) (see Table 17) applicable to the validation of criticality calculations for fresh fuel waste packages were further analyzed using the normal distribution tolerance limit method (Eq. 4) since this set of critical experiments passes a normality test. The LBTL is determined in the spreadsheet available in /DVD/cl/NDTL&DFTL.xls, worksheet NDTL, and is applicable to all evaluated fresh fuel application systems. The applicable value for the multiplier $k(\gamma, P, n)$ in Eq. 4 is 2.166 for 36 data points, 95% confidence level, and a fraction of the k_{eff} population of 95% (Ref. 76). The LBTL for fresh fuel waste package applications is 0.9905.

7. CONCLUSIONS

The calculations and analyses documented in this report apply the criticality analysis methodology approach documented in Section 3.5 of the *Disposal Criticality Methodology Topical Report*[1] (refer to Sections 6.4 and 6.5 for the criticality model overview and the process for calculating lower bound tolerance limits, respectively) for validating the computational method used to perform postclosure criticality calculations, which is MCNP Version5/Revision 1.40 and nuclear data based primarily on the ENDF/B-VI library. The application systems for this validation consist of waste packages containing TAD canisters loaded with CSNF of varying assembly types, initial enrichments, and burnups that are expected from the waste stream and of varying degree of internal component degradation that may occur over the 10,000-year regulatory time period. The critical experiments considered for use in the validation process were selected based on physical characteristic similarities between the application systems and the critical experiments and include the following: proprietary HTC MOX LCEs, public MOX and LEU LCEs, and CRCs. Subsequently, S/U analyses were performed for these experiments, and neutronic similarity based on the integral index c_k value and published guidance was used to identify and select the critical experiments that are most applicable for this validation. Critical experiments having $c_k > 0.8$ (approximately 200 critical experiments for the CSNF waste packages containing irradiated fuel, depending on the actual configuration, and 36 critical experiments for the CSNF waste packages containing fresh fuel) were retained and used for determining the LBTL. The single-valued LBTL functions and the corresponding range of applicability for the evaluated applications are presented in Table 20.

Table 20. LBTL and corresponding range of applicability

Application systems	LBTL	Method[a]	Range of applicability; *EALF* in eV[b]
21-PWR waste packages containing fresh fuel	0.9905	NDTL	$0.0977 \leq EALF \leq 0.3882$
21-PWR waste packages containing burned fuel	0.9778	DFTL	$0.0684 \leq EALF \leq 1.0410$
44-BWR waste packages containing fresh fuel	0.9905	NDTL	$0.0977 \leq EALF \leq 0.3882$
44-PWR waste packages containing burned fuel	0.9778	DFTL	$0.0421 \leq EALF \leq 0.9679$

[a]Fraction of the k_{eff} population above the LBTL value is 95%; the confidence on population is 95%.

[b]This column shows the *EALF* range for the critical experiments used to determine the single-valued LBTL function.

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APPENDIX A: Results of Criticality Calculations

In this appendix, the results of criticality calculations for the selected HTC, MOX, and LEU LCEs and CRCs (refer to Section 6.3 for the section on critical experiments) are tabulated in Tables A-1 through A-4. All the results were obtained from jobs executed on the Dec Alpha workstations, unless otherwise noted.

Table A-1. Criticality calculation results for HTC LCEs

HTC (Experimental k_{eff} = 1.0000 for all)							
MCNP[a]				**SCALE[b]**			
Output filename	**k_{eff}**	**σ**	***EALF* (eV)**	**Filename[c]**	**k_{eff}**	**σ**	***EALF* (eV)**
ohtc1c01	0.99752	0.00020	7.15E-02	htc1c1sen	0.99889	0.00049	7.07E-02
ohtc1c02	0.99711	0.00021	6.85E-02	htc1c2sen	0.99616	0.00047	6.79E-02
ohtc1c03	0.99693	0.00020	6.84E-02	htc1c3sen	0.99740	0.00049	6.77E-02
ohtc1c04	0.99705	0.00024	8.78E-02	htc1c4sen	0.99718	0.00050	8.67E-02
ohtc1c05	0.99690	0.00024	8.56E-02	htc1c5sen	0.99717	0.00046	8.46E-02
ohtc1c06	0.99737	0.00024	8.47E-02	htc1c6sen	0.99737	0.00049	8.40E-02
ohtc1c07	0.99647	0.00025	1.06E-01	htc1c7sen	0.99675	0.00049	1.05E-01
ohtc1c08	0.99642	0.00026	1.04E-01	htc1c8sen	0.99599	0.00047	1.03E-01
ohtc1c09	0.99676	0.00027	1.03E-01	htc1c9sen	0.99608	0.00049	1.02E-01
ohtc1c10	0.99609	0.00028	1.47E-01	htc1c10sen	0.99498	0.00049	1.46E-01
ohtc1c11	0.99542	0.00027	1.42E-01	htc1c11sen	0.99313	0.00050	1.41E-01
ohtc1c12	0.99577	0.00027	1.40E-01	htc1c12sen	0.99400	0.00046	1.38E-01
ohtc1c13	0.99491	0.00029	2.71E-01	htc1c13sen	0.99113	0.00050	2.69E-01
ohtc1c14	0.99400	0.00029	2.47E-01	htc1c14sen	0.99064	0.00044	2.45E-01
ohtc1c15	0.99368	0.00028	2.43E-01	htc1c15sen	0.99138	0.00049	2.41E-01
ohtc1c16	0.99630	0.00026	1.05E-01	htc1c16sen	0.99618	0.00050	1.04E-01
ohtc1c17	0.99592	0.00025	1.03E-01	htc1c17sen	0.99582	0.00047	1.02E-01
ohtc1c18	0.99435	0.00027	1.05E-01	htc1c18sen	0.99333	0.00050	1.04E-01
ohtc2b01[d]	0.99504	0.00029	2.62E-01	htc2c1bsen	0.99371	0.00047	2.58E-01
ohtc2b02[d]	0.99441	0.00029	2.58E-01	htc2c2bsen	0.99215	0.00048	2.55E-01
ohtc2b03[d]	0.99471	0.00028	2.69E-01	htc2c3bsen	0.99205	0.00050	2.67E-01
ohtc2b04	0.99636	0.00028	2.78E-01	htc2c4bsen	0.99410	0.00049	2.75E-01
ohtc2b05	0.99657	0.00028	2.89E-01	htc2c5bsen	0.99404	0.00049	2.86E-01
ohtc2b06	0.99640	0.00028	2.86E-01	htc2c6bsen	0.99373	0.00043	2.83E-01
ohtc2b07	0.99793	0.00027	2.95E-01	htc2c7bsen	0.99456	0.00050	2.91E-01
ohtc2b08	0.99737	0.00028	3.03E-01	htc2c8bsen	0.99411	0.00047	2.99E-01
ohtc2b09	0.99854	0.00027	1.73E-01	htc2c9bsen	0.99713	0.00049	1.71E-01
ohtc2b10	0.99635	0.00027	1.68E-01	htc2c10bsen	0.99420	0.00047	1.66E-01
ohtc2b11	0.99801	0.00026	1.63E-01	htc2c11bsen	0.99593	0.00049	1.61E-01
ohtc2b12	0.99773	0.00027	1.57E-01	htc2c12bsen	0.99723	0.00046	1.54E-01
ohtc2b13	0.99685	0.00027	1.51E-01	htc2c13bsen	0.99447	0.00050	1.50E-01
ohtc2b14	0.99940	0.00027	1.46E-01	htc2c14bsen	0.99881	0.00050	1.45E-01
ohtc2b15	1.00104	0.00027	1.07E-01	htc2c15bsen	1.00017	0.00050	1.06E-01
ohtc2b16	0.99925	0.00026	1.11E-01	htc2c16bsen	0.99862	0.00050	1.10E-01
ohtc2b17	1.00140	0.00024	1.15E-01	htc2c17bsen	1.00013	0.00048	1.13E-01
ohtc2b18	0.99222	0.00026	1.20E-01	htc2c18bsen	0.99248	0.00050	1.19E-01
ohtc2b19	0.99717	0.00026	1.08E-01	htc2c19bsen	0.99789	0.00049	1.07E-01

Table A-1. Criticality calculation results for HTC LCEs (continued)

HTC (Experimental k_{eff} = 1.0000 for all)							
MCNP[a]				SCALE[b]			
Output filename	k_{eff}	σ	*EALF* (eV)	Filename[c]	k_{eff}	σ	*EALF* (eV)
ohtc2b20	0.99142	0.00025	9.27E-02	htc2c20bsen	0.99245	0.00048	9.14E-02
ohtc2b21	0.99481	0.00025	8.90E-02	htc2c21bsen	0.99451	0.00048	8.79E-02
ohtc2g01	0.99529	0.00029	2.67E-01	htc2c1gsen	0.99267	0.00048	2.66E-01
ohtc2g02	0.99460	0.00028	2.63E-01	htc2c2gsen	0.99225	0.00046	2.59E-01
ohtc2g03	0.99510	0.00029	2.85E-01	htc2c3gsen	0.99275	0.00050	2.82E-01
ohtc2g04	0.99485	0.00028	2.82E-01	htc2c4gsen	0.99217	0.00050	2.79E-01
ohtc2g05	0.99516	0.00028	2.77E-01	htc2c5gsen	0.99303	0.00049	2.75E-01
ohtc2g06	0.99464	0.00028	3.01E-01	htc2c6gsen	0.99251	0.00050	2.98E-01
ohtc2g07	0.99480	0.00028	2.93E-01	htc2c7gsen	0.99179	0.00048	2.91E-01
ohtc2g08	0.99504	0.00028	3.11E-01	htc2c8gsen	0.99189	0.00049	3.08E-01
ohtc2g09	0.99505	0.00028	3.08E-01	htc2c9gsen	0.99191	0.00046	3.05E-01
ohtc2g10	0.99587	0.00027	1.77E-01	htc2c10gsen	0.99389	0.00049	1.75E-01
ohtc2g11	0.99643	0.00027	1.69E-01	htc2c11gsen	0.99459	0.00049	1.67E-01
ohtc2g12	0.99598	0.00027	1.68E-01	htc2c12gsen	0.99559	0.00050	1.66E-01
ohtc2g13	0.99619	0.00027	1.61E-01	htc2c13gsen	0.99500	0.00046	1.59E-01
ohtc2g14	0.99662	0.00027	1.59E-01	htc2c14gsen	0.99528	0.00049	1.57E-01
ohtc2g15	0.99732	0.00028	1.54E-01	htc2c15gsen	0.99505	0.00049	1.52E-01
ohtc2g16	0.99747	0.00028	1.50E-01	htc2c16gsen	0.99526	0.00049	1.49E-01
ohtc2g17	0.99790	0.00026	1.10E-01	htc2c17gsen	0.99733	0.00048	1.09E-01
ohtc2g18	0.99904	0.00025	9.08E-02	htc2c18gsen	0.99867	0.00050	8.98E-02
ohtc2g19	0.99574	0.00026	1.18E-01	htc2c19gsen	0.99416	0.00049	1.17E-01
ohtc2g20	0.99806	0.00025	1.10E-01	htc2c20gsen	0.99641	0.00049	1.10E-01
ohtc3c01	0.99553	0.00028	1.29E-01	htc3c1sen	0.99412	0.00048	1.27E-01
ohtc3c03	0.99564	0.00028	1.35E-01	htc3c3sen	0.99504	0.00050	1.33E-01
ohtc3c04	0.99547	0.00027	1.29E-01	htc3c4sen	0.99545	0.00049	1.27E-01
ohtc3c05	0.99469	0.00027	1.41E-01	htc3c5sen	0.99498	0.00050	1.39E-01
ohtc3c07	0.99378	0.00028	1.34E-01	htc3c7sen	0.99187	0.00048	1.32E-01
ohtc3c09	0.99375	0.00027	1.39E-01	htc3c9sen	0.99454	0.00047	1.37E-01
ohtc3c10	0.99468	0.00026	1.35E-01	htc3c10sen	0.99484	0.00050	1.33E-01
ohtc3c11	0.99358	0.00027	1.43E-01	htc3c11sen	0.99394	0.00053	1.41E-01
ohtc3c12	0.99568	0.00027	1.17E-01	htc3c12sen	0.99576	0.00045	1.16E-01
ohtc3c13	0.99650	0.00026	1.16E-01	htc3c13sen	0.99584	0.00049	1.15E-01
ohtc3c14	0.99644	0.00027	1.16E-01	htc3c14sen	0.99501	0.00049	1.15E-01
ohtc3c15	0.99616	0.00025	1.15E-01	htc3c15sen	0.99421	0.00044	1.14E-01
ohtc3c16	0.99650	0.00026	1.15E-01	htc3c16sen	0.99476	0.00050	1.14E-01
ohtc3c17	0.99571	0.00026	1.13E-01	htc3c17sen	0.99525	0.00050	1.11E-01
ohtc3c18	0.99547	0.00027	1.11E-01	htc3c18sen	0.99543	0.00050	1.10E-01
ohtc3c19	0.99684	0.00026	1.08E-01	htc3c19sen	0.99530	0.00049	1.07E-01
ohtc3c20	0.99639	0.00025	1.06E-01	htc3c20sen	0.99538	0.00049	1.05E-01
ohtc3c21	0.99635	0.00026	1.09E-01	htc3c21sen	0.99654	0.00045	1.07E-01
ohtc3c22	0.99730	0.00026	1.11E-01	htc3c22sen	0.99653	0.00049	1.10E-01
ohtc3c23	0.99519	0.00027	1.20E-01	htc3c23sen	0.99555	0.00049	1.19E-01

Table A-1. Criticality calculation results for HTC LCEs (continued)

HTC (Experimental k_{eff} = 1.0000 for all)							
MCNP[a]				SCALE[b]			
Output filename	k_{eff}	σ	*EALF* (eV)	Filename[c]	k_{eff}	σ	*EALF* (eV)
ohtc3c24	0.99565	0.00026	1.58E-01	htc3c24sen	0.99514	0.00046	1.58E-01
ohtc3c25	0.99614	0.00026	1.32E-01	htc3c25sen	0.99498	0.00049	1.32E-01
ohtc3c26	0.99560	0.00026	1.20E-01	htc3c26sen	0.99612	0.00050	1.19E-01
ohtc4l02	0.99809	0.00027	1.55E-01	htc4pb02sen	0.99686	0.00049	1.55E-01
ohtc4l03	0.99774	0.00026	1.51E-01	htc4pb03sen	0.99656	0.00050	1.50E-01
ohtc4l04	0.99822	0.00026	1.48E-01	htc4pb04sen	0.99647	0.00050	1.47E-01
ohtc4l05	0.99784	0.00026	1.44E-01	htc4pb05sen	0.99645	0.00043	1.44E-01
ohtc4l06	0.99809	0.00027	1.39E-01	htc4pb06sen	0.99653	0.00048	1.38E-01
ohtc4l07	0.99833	0.00027	1.37E-01	htc4pb07sen	0.99699	0.00048	1.36E-01
ohtc4l08	0.99693	0.00026	1.43E-01	htc4pb08sen	0.99499	0.00050	1.42E-01
ohtc4l09	0.99629	0.00026	1.42E-01	htc4pb09sen	0.99445	0.00050	1.42E-01
ohtc4l10	0.99627	0.00027	1.41E-01	htc4pb10sen	0.99491	0.00044	1.40E-01
ohtc4l11	0.99602	0.00027	1.40E-01	htc4pb11sen	0.99495	0.00049	1.39E-01
ohtc4l15	0.99605	0.00028	1.35E-01	htc4pb15sen	0.99381	0.00049	1.34E-01
ohtc4l16	0.99569	0.00027	1.38E-01	htc4pb16sen	0.99513	0.00050	1.37E-01
ohtc4l18	0.99714	0.00027	1.48E-01	htc4pb18sen	0.99476	0.00049	1.47E-01
ohtc4l19	0.99812	0.00027	1.41E-01	htc4pb19sen	0.99453	0.00048	1.40E-01
ohtc4l20	0.99855	0.00027	1.38E-01	htc4pb20sen	0.99440	0.00049	1.37E-01
ohtc4l21	0.99620	0.00027	1.40E-01	htc4pb21sen	0.99247	0.00050	1.39E-01
ohtc4l22	0.99539	0.00027	1.39E-01	htc4pb22sen	0.99250	0.00050	1.38E-01
ohtc4l23	0.99481	0.00027	1.37E-01	htc4pb23sen	0.99244	0.00049	1.37E-01
ohtc4l24	0.99489	0.00027	1.37E-01	htc4pb24sen	0.99138	0.00049	1.35E-01
ohtc4l25	0.99835	0.00027	1.35E-01	htc4pb25sen	0.99580	0.00049	1.34E-01
ohtc4l26	0.99861	0.00027	1.32E-01	htc4pb26sen	0.99556	0.00050	1.32E-01
ohtc4l27	0.99803	0.00027	1.81E-01	htc4pb27sen	0.99775	0.00050	1.82E-01
ohtc4l28	0.99841	0.00026	1.73E-01	htc4pb28sen	0.99828	0.00048	1.74E-01
ohtc4l29	0.99826	0.00026	1.64E-01	htc4pb29sen	0.99598	0.00049	1.65E-01
ohtc4l30	0.99854	0.00026	1.50E-01	htc4pb30sen	0.99786	0.00050	1.50E-01
ohtc4l31	0.99831	0.00026	1.40E-01	htc4pb31sen	0.99750	0.00049	1.39E-01
ohtc4l32	0.99915	0.00026	1.33E-01	htc4pb32sen	0.99817	0.00050	1.34E-01
ohtc4l33	0.99884	0.00026	1.30E-01	htc4pb33sen	0.99843	0.00045	1.29E-01
ohtc4l34	0.99948	0.00026	1.28E-01	htc4pb34sen	0.99753	0.00050	1.27E-01
ohtc4l35	0.99791	0.00025	1.63E-01	htc4pb35sen	0.99702	0.00049	1.63E-01
ohtc4l36	0.99776	0.00026	1.62E-01	htc4pb36sen	0.99784	0.00047	1.62E-01
ohtc4l37	0.99817	0.00026	1.60E-01	htc4pb37sen	0.99709	0.00049	1.61E-01
ohtc4l38	0.99788	0.00026	1.59E-01	htc4pb38sen	0.99774	0.00048	1.60E-01
ohtc4s02	0.99601	0.00026	1.56E-01	htc4ss02sen	0.99579	0.00049	1.55E-01
ohtc4s03	0.99607	0.00026	1.52E-01	htc4ss03sen	0.99372	0.00049	1.52E-01
ohtc4s04	0.99620	0.00027	1.48E-01	htc4ss04sen	0.99568	0.00049	1.48E-01
ohtc4s05	0.99614	0.00027	1.45E-01	htc4ss05sen	0.99567	0.00048	1.44E-01
ohtc4s06	0.99446	0.00027	1.44E-01	htc4ss06sen	0.99440	0.00045	1.44E-01

Table A-1. Criticality calculation results for HTC LCEs (continued)

HTC (Experimental k_{eff} = 1.0000 for all)							
MCNP[a]				SCALE[b]			
Output filename	k_{eff}	σ	***EALF* (eV)**	**Filename[c]**	k_{eff}	σ	***EALF* (eV)**
ohtc4s07	0.99401	0.00027	1.43E-01	htc4ss07sen	0.99341	0.00048	1.42E-01
ohtc4s08	0.99415	0.00027	1.42E-01	htc4ss08sen	0.99316	0.00049	1.41E-01
ohtc4s09	0.99380	0.00027	1.41E-01	htc4ss09sen	0.99294	0.00049	1.40E-01
ohtc4s10	0.99562	0.00027	1.40E-01	htc4ss10sen	0.99543	0.00046	1.39E-01
ohtc4s11	0.99596	0.00028	1.38E-01	htc4ss11sen	0.99426	0.00049	1.37E-01
ohtc4s13	0.99455	0.00026	1.39E-01	htc4ss13sen	0.99389	0.00049	1.38E-01
ohtc4s15	0.99461	0.00026	1.49E-01	htc4ss15sen	0.99203	0.00050	1.49E-01
ohtc4s16	0.99479	0.00026	1.42E-01	htc4ss16sen	0.99275	0.00050	1.42E-01
ohtc4s17	0.99340	0.00026	1.41E-01	htc4ss17sen	0.99172	0.00049	1.41E-01
ohtc4s18	0.99235	0.00026	1.39E-01	htc4ss18sen	0.99014	0.00050	1.39E-01
ohtc4s19	0.99280	0.00027	1.38E-01	htc4ss19sen	0.99054	0.00050	1.37E-01
ohtc4s20	0.99191	0.00027	1.38E-01	htc4ss20sen	0.98996	0.00050	1.37E-01
ohtc4s21	0.99572	0.00027	1.39E-01	htc4ss21sen	0.99363	0.00050	1.38E-01
ohtc4s22	0.99674	0.00026	1.82E-01	htc4ss22sen	0.99805	0.00048	1.83E-01
ohtc4s23	0.99721	0.00027	1.73E-01	htc4ss23sen	0.99768	0.00049	1.73E-01
ohtc4s24	0.99549	0.00025	1.64E-01	htc4ss24sen	0.99663	0.00049	1.65E-01
ohtc4s25	0.99578	0.00027	1.63E-01	htc4ss25sen	0.99619	0.00040	1.63E-01
ohtc4s26	0.99580	0.00027	1.61E-01	htc4ss26sen	0.99655	0.00049	1.62E-01
ohtc4s27	0.99634	0.00026	1.60E-01	htc4ss27sen	0.99657	0.00049	1.61E-01
ohtc4s28	0.99603	0.00026	1.59E-01	htc4ss28sen	0.99626	0.00050	1.60E-01
ohtc4s29	0.99556	0.00026	1.49E-01	htc4ss29sen	0.99601	0.00046	1.49E-01
ohtc4s30	0.99611	0.00025	1.39E-01	htc4ss30sen	0.99682	0.00049	1.38E-01
ohtc4s31	0.99551	0.00026	1.33E-01	htc4ss31sen	0.99566	0.00050	1.32E-01
ohtc4s32	0.99619	0.00027	1.29E-01	htc4ss32sen	0.99610	0.00050	1.28E-01
ohtc4s33	0.99582	0.00026	1.27E-01	htc4ss33sen	0.99702	0.00049	1.26E-01

The input and output files are included in the DVD attachment, paths:
[a]DVD/exp/htc/mcnp.
[b]DVD/exp/htc/sens.
[c]Output file name is Filename.output.
[d]The results were obtained with MCNP jobs from CPILE2.

Table A-2. Criticality calculation results for MOX LCEs

MCNP[a]				SCALE[b]				Experimental k_{eff}
Output filename	k_{eff}	σ	*EALF* (eV)	Filename[c]	k_{eff}	σ	*EALF* (eV)	
oct02-01	0.99306	0.00038	5.78E-01	mct002-01sen	0.99118	0.00027	5.69E-01	1.0010
oct02-02	0.99577	0.00036	7.65E-01	mct002-02sen	0.99320	0.00029	7.57E-01	1.0009
oct02-03	0.99648	0.00028	1.94E-01	mct002-03sen	0.99642	0.00026	1.90E-01	1.0024
oct02-04	1.00277	0.00037	2.83E-01	mct002-04sen	1.00145	0.00024	2.77E-01	1.0024
oct02-05	0.99853	0.00037	1.39E-01	mct002-05sen	1.00021	0.00026	1.36E-01	1.0038
oct02-06	1.00289	0.00025	1.84E-01	mct002-06sen	1.00216	0.00022	1.80E-01	1.0029
oct03-01	0.99334	0.00041	8.89E-01	mct003-01sen	0.99161	0.00028	8.87E-01	1.0000
oct03-02	0.99478	0.00042	5.43E-01	mct003-02sen	0.99278	0.00028	5.37E-01	1.0000
oct03-03	0.99444	0.00042	6.42E-01	mct003-03sen	0.99214	0.00034	6.39E-01	1.0000
oct03-04	0.99560	0.00041	1.88E-01	mct003-04sen	0.99484	0.00032	1.85E-01	1.0000
oct03-05	0.99527	0.00039	1.56E-01	mct003-05sen	0.99559	0.00026	1.53E-01	1.0000
oct03-06	0.99861	0.00038	1.02E-01	mct003-06sen	0.99726	0.00025	9.99E-02	1.0000
oct04-01	0.99122	0.00036	1.46E-01	mct004-01sen	0.99132	0.00025	1.44E-01	1.0000
oct06-01	0.99089	0.00037	3.76E-01	mct006-01sen	0.98895	0.00026	3.70E-01	1.0016
oct07-02	0.99400	0.00034	1.43E-01	mct007-02sen	0.99428	0.00026	1.39E-01	1.0024
oct08-01	0.99223	0.00036	3.99E-01	mct008-01sen	0.99021	0.00028	3.92E-01	0.9997
oct08-02	0.99464	0.00035	2.00E-01	mct008-02sen	0.99277	0.00024	1.96E-01	1.0008
oct08-03	0.99481	0.00034	1.43E-01	mct008-03sen	0.99445	0.00023	1.40E-01	1.0023
oct08-04	0.99693	0.00033	1.21E-01	mct008-04sen	0.99840	0.00024	1.18E-01	1.0015
oct08-05	0.99869	0.00030	9.81E-02	mct008-05sen	0.99891	0.00025	9.60E-02	1.0022
oct08-06	0.99813	0.00028	9.30E-02	mct008-06sen	0.99906	0.00019	9.09E-02	1.0028
ost01-01	0.99226	0.00043	1.60E-01	mst001-01sen	0.99537	0.00031	1.57E-01	1.0000
ost01-02	0.99159	0.00044	1.61E-01	mst001-02sen	0.99537	0.00027	1.58E-01	1.0000
ost01-03	0.98652	0.00046	1.57E-01	mst001-03sen	0.99043	0.00029	1.54E-01	1.0000
ost01-04	0.99165	0.00044	1.70E-01	mst001-04sen	0.99486	0.00029	1.66E-01	1.0000
ost01-05	0.99500	0.00044	1.75E-01	mst001-05sen	0.99920	0.00032	1.71E-01	1.0000
ost01-06	0.99587	0.00045	1.68E-01	mst001-06sen	0.99813	0.00028	1.65E-01	1.0000
ost01-08	0.99688	0.00045	1.48E-01	mst001-08sen	1.00067	0.00032	1.46E-01	1.0000
ost01-09	0.99812	0.00043	9.18E-02	mst001-09sen	1.00029	0.00028	9.07E-02	1.0000
ost01-10	0.99742	0.00043	1.15E-01	mst001-10sen	1.00061	0.00027	1.13E-01	1.0000
ost01-11	1.00296	0.00041	1.11E-01	mst001-11sen	1.00552	0.00031	1.09E-01	1.0000
ost01-12	1.00445	0.00043	1.09E-01	mst001-12sen	1.00622	0.00025	1.07E-01	1.0000
ost01-13	0.99526	0.00041	8.37E-02	mst001-13sen	0.99742	0.00025	8.24E-02	1.0000
ost02-01	1.00188	0.00025	4.22E-02	mst002-01sen	1.00399	0.00021	4.20E-02	1.0000
ost02-02	1.00209	0.00024	4.21E-02	mst002-02sen	1.00412	0.00023	4.19E-02	1.0000
ost02-03	1.00171	0.00027	4.32E-02	mst002-03sen	1.00373	0.00021	4.29E-02	1.0000
ost04-01	0.99716	0.00045	7.10E-02	mst004-01sen	0.99796	0.00032	7.02E-02	1.0000
ost04-02	0.99566	0.00043	6.71E-02	mst004-02sen	0.99753	0.00029	6.63E-02	1.0000
ost04-03	0.99731	0.00043	6.97E-02	mst004-03sen	1.00017	0.00035	6.88E-02	1.0000
ost04-04	0.99838	0.00046	1.75E-01	mst004-04sen	1.00123	0.00029	1.72E-01	1.0000
ost04-05	0.99277	0.00047	1.59E-01	mst004-05sen	0.99561	0.00034	1.56E-01	1.0000
ost04-06	0.99314	0.00049	1.91E-01	mst004-06sen	0.99588	0.00035	1.88E-01	1.0000
ost04-07	0.99472	0.00049	3.51E-01	mst004-07sen	0.99696	0.00029	3.42E-01	1.0000

Table A-2. Criticality calculation results for MOX LCEs (continued)

MCNP[a]				SCALE[b]				Experimental k_{eff}
Output filename	k_{eff}	σ	***EALF* (eV)**	**Filename[c]**	k_{eff}	σ	***EALF* (eV)**	
ost04-08	0.99256	0.00047	2.65E-01	mst004-08sen	0.99632	0.00032	2.60E-01	1.0000
ost04-09	0.99484	0.00047	3.07E-01	mst004-09sen	0.99778	0.00030	3.00E-01	1.0000
ost05-01	0.99423	0.00045	7.09E-02	mst005-01sen	0.99390	0.00032	6.99E-02	1.0000
ost05-02	0.99848	0.00040	6.66E-02	mst005-02sen	0.99984	0.00028	6.57E-02	1.0000
ost05-03	0.99742	0.00047	1.54E-01	mst005-03sen	1.00009	0.00029	1.51E-01	1.0000
ost05-04	0.99619	0.00043	1.52E-01	mst005-04sen	0.99855	0.00032	1.49E-01	1.0000
ost05-05	0.98608	0.00047	1.94E-01	mst005-05sen	0.98815	0.00032	1.89E-01	1.0000
ost05-06	0.98564	0.00047	3.53E-01	mst005-06sen	0.98830	0.00033	3.44E-01	1.0000
ost05-07	0.99274	0.00045	2.53E-01	mst005-07sen	0.99665	0.00030	2.47E-01	1.0000

The input and output files are included in the DVD attachment, paths:
[a]DVD/exp/mox/mcnp.
[b]DVD/exp/mox/sens.
[c]Output file name is Filename.output.

Table A-3. Criticality calculation results for LEU LCEs

LEU [Experimental k_{eff} = 1.0000 for all except lct26c3 (1.0023)]							
MCNP[a]				SCALE[b]			
Output filename	k_{eff}	σ	*EALF* (eV)	Filename[c]	k_{eff}	σ	*EALF* (eV)
olct1005	0.99648	0.00028	3.88E-01	lct010c5	0.99547	0.00049	3.87E-01
olct1016	0.99561	0.00030	2.98E-01	lct010c16	0.99354	0.00049	2.93E-01
olct1017	0.99515	0.00030	2.91E-01	lct010c17	0.99362	0.00049	2.88E-01
olct1018	0.99434	0.00031	2.86E-01	lct010c18	0.99528	0.00049	2.83E-01
olct1019	0.99445	0.00030	2.79E-01	lct010c19	0.99210	0.00049	2.76E-01
olct1703	0.99576	0.00025	9.77E-02	lct017-03	0.99387	0.00049	5.59E-02
olct1704	0.99430	0.00024	2.17E-01	lct017-04	0.99350	0.00047	2.14E-01
olct1705	0.99618	0.00024	1.89E-01	lct017-05	0.99460	0.00049	1.87E-01
olct1706	0.99583	0.00025	1.80E-01	lct017-06	0.99434	0.00049	1.77E-01
olct1707	0.99602	0.00024	1.69E-01	lct017-07	0.99493	0.00050	1.67E-01
olct1708	0.99347	0.00024	1.40E-01	lct17c8	0.99184	0.00050	1.37E-01
olct1709	0.99313	0.00026	1.13E-01	lct017-09	0.99190	0.00049	1.11E-01
olct1710	0.99402	0.00024	1.03E-01	lct017-10	0.99381	0.00050	1.01E-01
olct1711	0.99454	0.00026	1.01E-01	lct017-11	0.99392	0.00049	9.92E-02
olct1712	0.99401	0.00025	9.99E-02	lct017-12	0.99305	0.00045	9.80E-02
olct1713	0.99450	0.00025	9.85E-02	lct017-13	0.99242	0.00048	9.65E-02
olct1714	0.99415	0.00025	9.77E-02	lct017-14	0.99271	0.00050	9.59E-02
olct1715	0.99122	0.00027	1.85E-01	lct017-15	0.99125	0.00050	1.82E-01
olct1716	0.99257	0.00028	1.78E-01	lct017-16	0.99164	0.00049	1.75E-01
olct1717	0.99422	0.00028	1.73E-01	lct17c17	0.99401	0.00048	1.70E-01
olct1719	0.99299	0.00028	1.69E-01	lct017-19	0.99274	0.00050	1.66E-01
olct1720	0.99177	0.00027	1.68E-01	lct017-20	0.98973	0.00049	1.64E-01
olct1721	0.99132	0.00028	1.66E-01	lct017-21	0.98884	0.00052	1.63E-01
olct1722	0.99003	0.00026	1.65E-01	lct017-22	0.98778	0.00048	1.62E-01
oclt1723	0.99611	0.00026	1.76E-01	lct017-23	0.99293	0.00049	1.74E-01
olct1724	0.99293	0.00026	1.71E-01	lct017-24	0.99339	0.00049	1.69E-01
olct1725	0.99303	0.00025	1.63E-01	lct017-25	0.98962	0.0004	1.61E-01
olct1728	0.99339	0.00026	3.03E-01	lct017-28	0.99066	0.0005	3.00E-01
olct1729	0.99576	0.00025	2.69E-01	lct017-29	0.99184	0.00049	2.65E-01
olct26c3	0.99789	0.00030	1.02E+00	lct26c3	0.99960	0.0005	9.48E-01
olct42c1	0.99235	0.00028	1.76E-01	lct42c1	0.99038	0.00049	1.73E-01

Table A-3. Criticality calculation results for LEU LCEs (continued)

LEU [Experimental k_{eff} = 1.0000 for all except lct26c3 (1.0023)]							
MCNP[a]				**SCALE**[b]			
Output filename	k_{eff}	**σ**	***EALF* (eV)**	**Filename**[c]	k_{eff}	**σ**	***EALF* (eV)**
olct42c2	0.99357	0.00028	1.82E-01	lct42c2	0.99085	0.00047	1.80E-01
olct42c3	0.99372	0.00028	1.90E-01	lct42c3	0.99304	0.00048	1.85E-01
olct42c4	0.99445	0.00028	1.87E-01	lct42c4	0.99277	0.00049	1.85E-01
olct42c5	0.99442	0.00028	1.85E-01	lct42c5	0.99320	0.00050	1.81E-01
olct42c6	0.99359	0.00028	1.76E-01	lct42c6	0.99190	0.00048	1.72E-01
olct42c7	0.99218	0.00027	1.82E-01	lct42c7	0.99054	0.00048	1.77E-01

The input and output files are included in the DVD attachment, paths:
[a]DVD/exp/leu/mcnp;
[b]DVD/exp/leu/sens.
[c]Output file name is Filename.output.

Table A-4. MCNP k_{eff} results for CRCs

Crystal River Unit 3 Experimental k_{eff} = 1.0000						
State-point	MCNP4B/ENDF/B-V[a]		MCNP 5.1.40/ENDF/B-VI			
	k_{eff}	σ	Output filename[b]	k_{eff}	σ	*EALF* (eV)
1	0.99601	0.00043	CR1o	0.99984	0.00028	5.79E-01
2	0.99285	0.00040	CR2o	1.00037	0.00030	6.52E-01
3	0.99502	0.00046	CR3o	1.00129	0.00029	6.38E-01
4	0.99282	0.00044	CR4o	1.00055	0.00028	6.75E-01
5	0.99408	0.00045	CR5o	1.00139	0.00028	6.78E-01
6	0.99304	0.00045	CR6o	0.99971	0.00027	6.72E-01
7	0.99073	0.00045	CR7o	0.99559	0.00027	6.70E-01
8	0.99134	0.00047	CR8o	0.99878	0.00027	6.86E-01
9	0.99152	0.00046	CR9o	0.99714	0.00028	7.02E-01
10	0.99603	0.00047	CR10o	1.00224	0.00028	6.90E-01
11	0.99479	0.00047	CR11o	1.00151	0.00028	7.46E-01
12	0.99805	0.00045	CR12o	1.00369	0.00027	7.36E-01
13	0.99561	0.00043	CR13o	1.00099	0.00028	8.13E-01
14	0.99579	0.00047	CR14o	1.00233	0.00021	8.17E-01
15	0.99273	0.00044	CR15o	0.99683	0.00028	7.60E-01
16	0.99324	0.00052	CR16o	0.99923	0.00029	8.99E-01
17	0.99083	0.00045	CR17o	0.99763	0.00028	8.68E-01
18	0.99222	0.00049	CR18o	0.99726	0.00029	8.74E-01
19	0.98993	0.00047	CR19o	0.99579	0.00030	8.59E-01
20	0.99321	0.00042	CR20o	0.99766	0.00029	8.04E-01
21	0.99247	0.00046	CR21o	0.99729	0.00028	8.05E-01
22	0.99039	0.00043	CR22o	0.99705	0.00029	9.59E-01
23	0.99021	0.00046	CR23o	0.99613	0.00030	9.68E-01
24	0.99063	0.00049	CR24o	0.99718	0.00029	9.53E-01
25	0.99054	0.00042	CR25o	0.99505	0.00029	8.80E-01
26	0.99067	0.00047	CR26o	0.99629	0.00030	8.70E-01
27	0.98772	0.00044	CR27o	0.99209	0.00031	8.49E-01
28	0.99208	0.00044	CR28o	0.99645	0.00029	9.85E-01
29	0.99311	0.0005	CR29o	0.99926	0.00028	9.58E-01
30	0.99078	0.00048	CR30o	0.99646	0.00029	9.46E-01
31	0.98837	0.00048	CR31o	0.99358	0.00029	9.08E-01
32	0.99164	0.00052	CR32o	0.99673	0.00029	1.04E+00
33	0.98725	0.00048	CR33o	0.99026	0.00031	8.89E-01

Table A-4. MCNP k_{eff} results for CRCs (continued)

State-point	MCNP4B/ENDF/B-V[a]		MCNP 5.1.40/ENDF/B-VI			
	k_{eff}	σ	Output filename[c]	k_{eff}	σ	*EALF* (eV)
Three Mile Island Unit 1 (Experimental k_{eff} = 1.0000)						
1	1.00141	0.00042	TM1o	1.00525	0.00029	6.17E-01
2	0.99088	0.00046	TM2o	0.99859	0.00028	6.70E-01
3	0.99162	0.00048	TM3o	0.99697	0.00028	6.68E-01
McGuire Unit 1 (Experimental k_{eff} = 1.0000)						
State-point	MCNP4B/ENDF/B-V[a]		MCNP 5.1.40/ENDF/B-VI			
	k_{eff}	σ	Output filename[d]	k_{eff}	σ	*EALF* (eV)
1	0.99946	0.00045	MG1o	1.00102	0.00029	6.37E-01
2	0.98541	0.00050	MG2o	0.99172	0.00030	6.91E-01
3	0.98771	0.00049	MG3o	0.99439	0.00028	6.92E-01
4	0.98954	0.00047	MG4o	0.99482	0.00029	7.42E-01
5	0.99175	0.00046	MG5o	0.99809	0.00028	7.26E-01
6	0.98723	0.00049	MG6o	0.99388	0.00029	6.92E-01
Sequoyah Unit 2 (Experimental k_{eff} = 1.0000)						
State-point	MCNP4B/ENDF/B-V[a]		MCNP 5.1.40/ENDF/B-VI			
	k_{eff}	σ	Output filename[e]	k_{eff}	σ	*EALF* (eV)
1	0.99631	0.00043	SE1o	0.99977	0.00028	6.10E-01
2	0.99158	0.00044	SE2o	0.99694	0.00029	8.58E-01
3	0.99180	0.00050	SE3o	0.99698	0.00029	8.21E-01
Grand Gulf Unit 1 (Experimental k_{eff} = 1.0000)						
State-point	MCNP4B/ENDF/B-V[a]		MCNP 5.1.40/ENDF/B-VI[f]			
	k_{eff}	σ	Output filename[g]	k_{eff}	σ	*EALF* (eV)
5	0.99554	0.0001	oGG5	0.99593	0.00010	2.20E-01
6	0.99324	0.0001	oGG6	0.99160	0.00010	2.69E-01
7	0.99296	0.0001	oGG7	0.99125	0.00009	2.74E-01
10	0.99461	0.0001	oGG10	0.99466	0.00010	2.28E-01
11	0.99810	0.0001	oGG11	0.99615	0.00010	2.80E-01
12	0.98685	0.0001	oGG12	0.98679	0.00010	2.89E-01
13	0.98551	0.0001	oGG13	0.98547	0.00009	2.88E-01
14	0.98295	0.0001	oGG14	0.98412	0.00009	2.83E-01
15	0.98309	0.0001	oGG15	0.98163	0.00010	2.30E-01
16	0.99875	0.0001	oGG16	0.99872	0.00010	2.26E-01
18	0.98993	0.0001	oGG18	0.99047	0.00010	2.26E-01
19	0.98249	0.0001	oGG19	0.98031	0.00010	3.23E-01
20	0.96644	0.0001	oGG20	0.96809	0.00009	3.07E-01
21	0.99211	0.0001	oGG21	0.99195	0.00010	2.29E-01
22	0.99380	0.0001	oGG22	0.99146	0.00010	2.77E-01
23	0.98986	0.0001	oGG23	0.98775	0.00010	2.86E-01

[a]Ref. 61.

The input and output files are included in the DVD attachment, paths:

[b]DVD/exps/CRC/CrystalRiver/mcnp.

[c]DVD/exps/CRC/TMI/mcnp.

[d]DVD/exps/CRC/McGuire/mcnp.

[e]DVD/exps/CRC/Sequoyah/mcnp.

[f]The results for Grand Gulf Unit 1 were obtained with MCNP jobs from CPILE2.

[g]DVD/exps/CRC/GrandGulf/mcnp.

APPENDIX B: Integral Index c_k

This appendix provides the definitions for sensitivity coefficients, S_k, and integral index c_k and the calculated c_k values for the application systems and critical experiments (Tables B-1 through B-12). Note that only sensitivity data files (*.sdf) for Crystal River state-points are available among all CRC state-points. These sensitivity files were obtained with a non-qualified version of SCALE5.1 and the 238-group ENDF/B-V SCALE library and NITAWL for resonance-cross section processing.

SENSITIVITY COEFFICIENTS, S_K

The sensitivity of k_{eff} to a particular nuclide-reaction pair macroscopic cross section Σ_x^n, referred to as sensitivity coefficient, provides a measure of the first-order effect of perturbations in nuclear reaction x for nuclide n upon k_{eff}. Nuclear data for which sensitivity coefficients are computed in a TSUNAMI calculation include total, scatter, capture, and fission cross sections, $\bar{\nu}$ (average number of neutrons per fission event), and χ (distribution function of fission neutrons). The sensitivity coefficient has been defined in Ref. 63 as

$$S_{k,\Sigma_x^n} = \frac{\delta k_{eff} / k_{eff}}{\delta \Sigma_x^n / \Sigma_x^n} \ .$$

A sensitivity coefficient is computed as the sum over all energy groups of the sensitivities of k_{eff} to group-wise cross-section data. The sensitivity coefficient expressed as a function of energy,

$$S_{k,\Sigma_{x,j}^n} = \frac{\delta k_{eff} / k_{eff}}{\delta \Sigma_{x,j}^n / \Sigma_{x,j}^n} \ ,$$

where j denotes an energy group, is referred to as an energy-dependent sensitivity profile. In addition to an explicit change in the affected nuclide reaction rate, perturbations of $\Sigma_{x,j}^n$ produce secondary effects on the resonance-shielded values of some cross sections, which in turn affect k_{eff}. Therefore, a complete sensitivity coefficient consists of two components referred to as explicit and implicit sensitivity coefficients. The implicit sensitivity component is the cumulative sensitivity of k_{eff} to all processes that are influenced by the perturbations in the value of Σ_x^n. TSUNAMI-3D computes sensitivity profiles in a SCALE energy group structure.

INTEGRAL INDEX c_k

The effects of uncertainties in nuclear data on the k_{eff} values of systems with the same materials and similar spectra are correlated. Integral index c_k is a measure of similarity of two systems in terms of their common components of uncertainty in k_{eff} due to cross-section uncertainties. A c_k value represents the correlation coefficient between sensitivity weighted uncertainties in the design system (application) and an experiment. The definition and intended use of the integral index c_k are documented in Refs.16 and 63.

Relative uncertainties in cross-section data can be represented as the elements of an $M \times M$ matrix, $C_{\alpha,\alpha} \equiv \left[\frac{cov(\alpha_n, \alpha_m)}{\alpha_n \alpha_m} \right]$, where M is the product of the number of nuclide-reaction pairs and the number of energy groups and $\alpha \equiv (\alpha_n)$ is a variable array containing the cross-sections of nuclide-reaction-energy group triplets. The $C_{\alpha,\alpha}$ matrix contains covariance data that provide a measure of how strong the correlation of uncertainty is between two nuclide-reaction-energy group triplets. An individual element of the covariance matrix, c_{nm}, is the ratio of the covariance of cross-section uncertainties to the product of cross-section expectation values for nuclide-reaction-energy group triplets *n* and *m*. In a TSUNAMI-IP calculation, the covariance data are propagated to relative changes in the calculated k_{eff} value of a given system via the sensitivity coefficients. An uncertainty matrix is computed for the system k_{eff} values, $C_{kk} = S_k C_{\alpha,\alpha} S_k^{\dagger}$, where S_k and $S_k^{\dagger}$ are the matrix and the transpose matrix, respectively, containing sensitivities of the calculated k_{eff} values of critical systems to the α parameters. S_k is an $I \times M$ matrix defined as

$$S_k \equiv \left[\frac{\alpha_m}{k_i} \frac{\partial k_i}{\partial \alpha_m} \right], \ i = 1, 2, \ldots, I; \ m = 1, 2, \ldots, M,$$

where *I* is the number of critical systems being considered.

The diagonal elements of the C_{kk} matrix represent the relative variance values, η_i^2, for each of the systems under consideration, and the off-diagonal elements, η_{ij}^2, represent the common variance between two systems. A correlation coefficient is defined as

$$c_k = \frac{\eta_{ij}^2}{(\eta_i \eta_j)},$$

such that the single c_k value represents the correlation coefficient between sensitivity weighted uncertainties in system *i* and system *j*. The interpretation of the correlation coefficient is the following: a value of 0.0 represents no correlation between the systems, a value of 1.0 represents full correlation between the systems, and a value of -1.0 represents a full anticorrelation.

Covariance data for some nuclide-reaction pairs are not available. In the TSUNAMI-IP calculations for this analysis, the default value of 0.05 was used for the fractional standard deviation in cross-section data for nuclide-reaction pairs for which covariance data are not available. This value is deemed to be a conservative estimation for fractional standard deviation in cross-section data in the thermal and ephithermal energy regions and is based on the fractional standard deviation in cross-section data for nuclide-reaction pairs for which covariance data are available.

Table B-1. Integral index c_k for nominal 21-PWR waste packages and HTC experiments

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tb2-0 c_k	tb3-0 c_k	tb15 c_k	tb25 c_k	tb30 c_k	tb35 c_k	tb40 c_k
htc1c1sen	0.4595	0.4484	0.9036	0.9094	0.9054	0.8945	0.8972
htc1c2sen	0.4587	0.4478	0.9021	0.9079	0.9039	0.8928	0.8959
htc1c3sen	0.4589	0.4480	0.9017	0.9075	0.9035	0.8923	0.8954
htc1c4sen	0.4709	0.4635	0.9026	0.9089	0.9054	0.8856	0.8998
htc1c5sen	0.4702	0.4628	0.9020	0.9083	0.9047	0.8850	0.8992
htc1c6sen	0.4700	0.4628	0.9008	0.9071	0.9036	0.8837	0.8980
htc1c7sen	0.4803	0.4734	0.9098	0.9160	0.9127	0.8912	0.9080
htc1c8sen	0.4795	0.4727	0.9086	0.9148	0.9116	0.8900	0.9069
htc1c9sen	0.4798	0.4730	0.9079	0.9140	0.9107	0.8890	0.9060
htc1c10sen	0.4951	0.4880	0.9258	0.9317	0.9289	0.9072	0.9249
htc1c11sen	0.4950	0.4879	0.9246	0.9304	0.9275	0.9057	0.9236
htc1c12sen	0.4951	0.4879	0.9257	0.9316	0.9287	0.9071	0.9246
htc1c13sen	0.5177	0.5096	0.9535	0.9588	0.9565	0.9379	0.9531
htc1c14sen	0.5167	0.5085	0.9524	0.9576	0.9553	0.9367	0.9519
htc1c15sen	0.5185	0.5101	0.9527	0.9578	0.9554	0.9367	0.9519
htc1c16sen	0.4809	0.4736	0.9140	0.9201	0.9168	0.8964	0.9118
htc1c17sen	0.4809	0.4736	0.9132	0.9193	0.9159	0.8956	0.9109
htc1c18sen	0.4809	0.4740	0.9106	0.9168	0.9135	0.8921	0.9087
htc2c1bsen	0.5171	0.5087	0.9575	0.9629	0.9607	0.9435	0.9572
htc2c2bsen	0.5166	0.5082	0.9578	0.9632	0.9610	0.9439	0.9575
htc2c3bsen	0.5159	0.5075	0.9617	0.9673	0.9653	0.9494	0.9617
htc2c4bsen	0.5148	0.5062	0.9653	0.9710	0.9691	0.9545	0.9654
htc2c5bsen	0.5144	0.5056	0.9684	0.9743	0.9724	0.9590	0.9685
htc2c6bsen	0.5143	0.5055	0.9685	0.9744	0.9725	0.9593	0.9686
htc2c7bsen	0.5128	0.5040	0.9709	0.9769	0.9751	0.9631	0.9712
htc2c8bsen	0.5124	0.5033	0.9732	0.9793	0.9775	0.9667	0.9735
htc2c9bsen	0.4914	0.4824	0.9651	0.9724	0.9701	0.9601	0.9648
htc2c10bsen	0.4932	0.4843	0.9621	0.9692	0.9668	0.9553	0.9617
htc2c11bsen	0.4944	0.4859	0.9567	0.9636	0.9611	0.9474	0.9562
htc2c12bsen	0.4950	0.4869	0.9502	0.9569	0.9543	0.9385	0.9496
htc2c13bsen	0.4952	0.4875	0.9427	0.9492	0.9465	0.9287	0.9421
htc2c14bsen	0.4953	0.4879	0.9346	0.9408	0.9380	0.9183	0.9338
htc2c15bsen	0.4821	0.4745	0.9230	0.9294	0.9262	0.9074	0.9211
htc2c16bsen	0.4820	0.4740	0.9345	0.9412	0.9382	0.9221	0.9327
htc2c17bsen	0.4809	0.4723	0.9429	0.9500	0.9470	0.9336	0.9412
htc2c18bsen	0.4790	0.4698	0.9511	0.9585	0.9557	0.9454	0.9494

Table B-1. Integral index c_k for nominal 21-PWR waste packages and HTC experiments (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tb2-0 c_k	tb3-0 c_k	tb15 c_k	tb25 c_k	tb30 c_k	tb35 c_k	tb40 c_k
htc2c19bsen	0.4821	0.4744	0.9246	0.9310	0.9278	0.9094	0.9226
htc2c20bsen	0.4714	0.4620	0.9335	0.9404	0.9371	0.9254	0.9302
htc2c21bsen	0.4720	0.4636	0.9213	0.9279	0.9245	0.9091	0.9182
htc2c1gsen	0.5158	0.5075	0.9597	0.9653	0.9632	0.9467	0.9597
htc2c2gsen	0.5155	0.5072	0.9597	0.9652	0.9632	0.9467	0.9596
htc2c3gsen	0.5139	0.5055	0.9645	0.9704	0.9685	0.9538	0.9649
htc2c4gsen	0.5137	0.5052	0.9646	0.9706	0.9687	0.9541	0.9651
htc2c5gsen	0.5131	0.5046	0.9650	0.9710	0.9691	0.9547	0.9654
htc2c6gsen	0.5107	0.5021	0.9693	0.9756	0.9738	0.9614	0.9701
htc2c7gsen	0.5106	0.5020	0.9691	0.9754	0.9737	0.9612	0.9699
htc2c8gsen	0.5082	0.4996	0.9719	0.9785	0.9769	0.9662	0.9731
htc2c9gsen	0.5086	0.5000	0.9720	0.9785	0.9769	0.9662	0.9731
htc2c10gsen	0.4869	0.4782	0.9641	0.9718	0.9696	0.9603	0.9645
htc2c11gsen	0.4901	0.4817	0.9592	0.9666	0.9643	0.9522	0.9594
htc2c12gsen	0.4895	0.4813	0.9587	0.9662	0.9639	0.9517	0.9591
htc2c13gsen	0.4928	0.4849	0.9505	0.9575	0.9550	0.9396	0.9504
htc2c14gsen	0.4928	0.4849	0.9503	0.9573	0.9548	0.9394	0.9502
htc2c15gsen	0.4945	0.4871	0.9395	0.9459	0.9432	0.9247	0.9390
htc2c16gsen	0.4942	0.4868	0.9397	0.9462	0.9435	0.9251	0.9393
htc2c17gsen	0.4801	0.4724	0.9299	0.9368	0.9338	0.9168	0.9285
htc2c18gsen	0.4715	0.4624	0.9289	0.9358	0.9324	0.9194	0.9258
htc2c19gsen	0.4784	0.4698	0.9451	0.9525	0.9497	0.9374	0.9439
htc2c20gsen	0.4808	0.4730	0.9313	0.9381	0.9350	0.9184	0.9297
htc3c1sen	0.4939	0.4847	0.9464	0.9526	0.9495	0.9341	0.9439
htc3c3sen	0.4942	0.4850	0.9480	0.9542	0.9511	0.9361	0.9455
htc3c4sen	0.4949	0.4854	0.9476	0.9536	0.9505	0.9354	0.9448
htc3c5sen	0.4938	0.4848	0.9488	0.9551	0.9521	0.9371	0.9466
htc3c7sen	0.4942	0.4849	0.9471	0.9532	0.9502	0.9350	0.9446
htc3c9sen	0.4944	0.4851	0.9480	0.9542	0.9512	0.9362	0.9456
htc3c10sen	0.4945	0.4851	0.9478	0.9540	0.9509	0.9360	0.9453
htc3c11sen	0.4944	0.4855	0.9475	0.9537	0.9508	0.9355	0.9453
htc3c12sen	0.4893	0.4817	0.9227	0.9286	0.9254	0.9049	0.9207
htc3c13sen	0.4903	0.4822	0.9255	0.9314	0.9281	0.9084	0.9232
htc3c14sen	0.4913	0.4827	0.9289	0.9346	0.9313	0.9126	0.9260
htc3c15sen	0.4920	0.4831	0.9300	0.9357	0.9323	0.9139	0.9269
htc3c16sen	0.4915	0.4824	0.9311	0.9368	0.9334	0.9156	0.9279
htc3c17sen	0.4923	0.4827	0.9332	0.9388	0.9354	0.9183	0.9296
htc3c18sen	0.4920	0.4820	0.9335	0.9389	0.9354	0.9189	0.9293

Table B-1. Integral index c_k for nominal 21-PWR waste packages and HTC experiments (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tb2-0 c_k	tb3-0 c_k	tb15 c_k	tb25 c_k	tb30 c_k	tb35 c_k	tb40 c_k
htc3c19sen	0.4880	0.4783	0.9294	0.9350	0.9314	0.9148	0.9253
htc3c20sen	0.4880	0.4782	0.9294	0.9350	0.9314	0.9150	0.9253
htc3c21sen	0.4839	0.4760	0.9183	0.9243	0.9210	0.9012	0.9158
htc3c22sen	0.4842	0.4770	0.9156	0.9216	0.9184	0.8973	0.9137
htc3c23sen	0.4874	0.4804	0.9178	0.9239	0.9208	0.8992	0.9164
htc3c24sen	0.4940	0.4865	0.9330	0.9391	0.9362	0.9164	0.9316
htc3c25sen	0.4914	0.4826	0.9329	0.9388	0.9355	0.9176	0.9300
htc3c26sen	0.4913	0.4828	0.9299	0.9357	0.9325	0.9138	0.9273
htc4pb02sen	0.4953	0.4861	0.9528	0.9591	0.9561	0.9422	0.9505
htc4pb03sen	0.4947	0.4853	0.9525	0.9588	0.9558	0.9420	0.9501
htc4pb04sen	0.4945	0.4850	0.9521	0.9584	0.9554	0.9416	0.9496
htc4pb05sen	0.4944	0.4848	0.9516	0.9578	0.9548	0.9410	0.9490
htc4pb06sen	0.4948	0.4852	0.9502	0.9563	0.9532	0.9391	0.9474
htc4pb07sen	0.4947	0.4850	0.9497	0.9558	0.9527	0.9384	0.9469
htc4pb08sen	0.4943	0.4848	0.9512	0.9574	0.9544	0.9405	0.9487
htc4pb09sen	0.4938	0.4843	0.9512	0.9574	0.9544	0.9405	0.9487
htc4pb10sen	0.4946	0.4851	0.9511	0.9572	0.9542	0.9401	0.9484
htc4pb11sen	0.4945	0.4850	0.9509	0.9571	0.9540	0.9399	0.9483
htc4pb15sen	0.4948	0.4846	0.9518	0.9579	0.9548	0.9415	0.9489
htc4pb16sen	0.4952	0.4849	0.9522	0.9582	0.9551	0.9418	0.9492
htc4pb18sen	0.4941	0.4846	0.9505	0.9567	0.9537	0.9399	0.9480
htc4pb19sen	0.4940	0.4844	0.9498	0.9560	0.9529	0.9390	0.9472
htc4pb20sen	0.4942	0.4846	0.9491	0.9552	0.9521	0.9379	0.9463
htc4pb21sen	0.4944	0.4847	0.9500	0.9561	0.9531	0.9391	0.9473
htc4pb22sen	0.4942	0.4845	0.9498	0.9560	0.9529	0.9388	0.9471
htc4pb23sen	0.4942	0.4845	0.9499	0.9560	0.9530	0.9389	0.9472
htc4pb24sen	0.4939	0.4842	0.9492	0.9553	0.9523	0.9380	0.9466
htc4pb25sen	0.4943	0.4847	0.9486	0.9546	0.9515	0.9372	0.9458
htc4pb26sen	0.4942	0.4846	0.9482	0.9543	0.9512	0.9368	0.9455
htc4pb27sen	0.4974	0.4895	0.9408	0.9468	0.9439	0.9257	0.9390
htc4pb28sen	0.4956	0.4876	0.9394	0.9454	0.9424	0.9245	0.9373
htc4pb29sen	0.4944	0.4860	0.9393	0.9452	0.9421	0.9248	0.9368
htc4pb30sen	0.4941	0.4848	0.9413	0.9470	0.9438	0.9279	0.9381
htc4pb31sen	0.4944	0.4848	0.9407	0.9464	0.9431	0.9273	0.9373
htc4pb32sen	0.4938	0.4843	0.9393	0.9450	0.9417	0.9255	0.9360
htc4pb33sen	0.4935	0.4843	0.9373	0.9430	0.9398	0.9230	0.9343
htc4pb34sen	0.4924	0.4835	0.9354	0.9412	0.9380	0.9207	0.9326
htc4pb35sen	0.4946	0.4861	0.9392	0.9451	0.9420	0.9247	0.9367

Table B-1. Integral index c_k for nominal 21-PWR waste packages and HTC experiments (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tb2-0 c_k	tb3-0 c_k	tb15 c_k	tb25 c_k	tb30 c_k	tb35 c_k	tb40 c_k
htc4pb36sen	0.4938	0.4854	0.9385	0.9445	0.9414	0.9240	0.9362
htc4pb37sen	0.4939	0.4855	0.9380	0.9440	0.9409	0.9233	0.9356
htc4pb38sen	0.4937	0.4853	0.9380	0.9440	0.9409	0.9233	0.9356
htc4ss02sen	0.4972	0.4881	0.9546	0.9608	0.9579	0.9437	0.9522
htc4ss03sen	0.4967	0.4875	0.9545	0.9607	0.9578	0.9437	0.9521
htc4ss04sen	0.4969	0.4875	0.9544	0.9605	0.9575	0.9436	0.9518
htc4ss05sen	0.4972	0.4877	0.9540	0.9600	0.9570	0.9430	0.9513
htc4ss06sen	0.4964	0.4869	0.9534	0.9596	0.9566	0.9426	0.9508
htc4ss07sen	0.4961	0.4866	0.9527	0.9588	0.9558	0.9417	0.9500
htc4ss08sen	0.4953	0.4858	0.9523	0.9585	0.9555	0.9414	0.9498
htc4ss09sen	0.4950	0.4855	0.9516	0.9578	0.9548	0.9406	0.9491
htc4ss10sen	0.4972	0.4877	0.9525	0.9585	0.9555	0.9411	0.9497
htc4ss11sen	0.4965	0.4871	0.9520	0.9581	0.9551	0.9406	0.9493
htc4ss13sen	0.4968	0.4860	0.9564	0.9623	0.9591	0.9473	0.9529
htc4ss15sen	0.4961	0.4868	0.9525	0.9586	0.9556	0.9417	0.9499
htc4ss16sen	0.4963	0.4869	0.9515	0.9576	0.9546	0.9403	0.9488
htc4ss17sen	0.4949	0.4854	0.9510	0.9572	0.9542	0.9400	0.9485
htc4ss18sen	0.4945	0.4849	0.9506	0.9568	0.9538	0.9396	0.9481
htc4ss19sen	0.4947	0.4850	0.9502	0.9564	0.9534	0.9391	0.9477
htc4ss20sen	0.4947	0.4851	0.9494	0.9555	0.9525	0.9380	0.9468
htc4ss21sen	0.4965	0.4870	0.9513	0.9573	0.9542	0.9399	0.9485
htc4ss22sen	0.5006	0.4928	0.9441	0.9499	0.9470	0.9288	0.9422
htc4ss23sen	0.4986	0.4907	0.9425	0.9483	0.9454	0.9273	0.9403
htc4ss24sen	0.4979	0.4897	0.9424	0.9481	0.9451	0.9275	0.9398
htc4ss25sen	0.4974	0.4892	0.9423	0.9481	0.9451	0.9275	0.9398
htc4ss26sen	0.4970	0.4888	0.9415	0.9474	0.9443	0.9267	0.9390
htc4ss27sen	0.4969	0.4887	0.9410	0.9468	0.9437	0.9260	0.9384
htc4ss28sen	0.4963	0.4881	0.9404	0.9463	0.9432	0.9255	0.9379
htc4ss29sen	0.4983	0.4893	0.9450	0.9507	0.9475	0.9312	0.9417
htc4ss30sen	0.4992	0.4898	0.9459	0.9514	0.9481	0.9322	0.9422
htc4ss31sen	0.4995	0.4901	0.9454	0.9509	0.9477	0.9314	0.9419
htc4ss32sen	0.4964	0.4873	0.9421	0.9478	0.9447	0.9279	0.9391
htc4ss33sen	0.4963	0.4876	0.9405	0.9463	0.9431	0.9257	0.9377

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/htc/sens, respectively.

Table B-2. Integral index c_k for design-basis 21-PWR waste packages and HTC experiments

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
htc1c1sen	0.4578	0.4453	0.9017	0.9081	0.9046	0.9011	0.8959
htc1c2sen	0.4570	0.4446	0.9002	0.9067	0.9032	0.8997	0.8945
htc1c3sen	0.4572	0.4447	0.8998	0.9063	0.9027	0.8993	0.8940
htc1c4sen	0.4685	0.4583	0.8982	0.9076	0.9050	0.9018	0.8973
htc1c5sen	0.4678	0.4576	0.8975	0.9070	0.9043	0.9012	0.8966
htc1c6sen	0.4676	0.4575	0.8963	0.9058	0.9032	0.9000	0.8954
htc1c7sen	0.4777	0.4679	0.9049	0.9147	0.9124	0.9094	0.9052
htc1c8sen	0.4769	0.4671	0.9037	0.9135	0.9113	0.9083	0.9041
htc1c9sen	0.4772	0.4674	0.9029	0.9127	0.9104	0.9074	0.9032
htc1c10sen	0.4925	0.4827	0.9210	0.9304	0.9286	0.9258	0.9221
htc1c11sen	0.4923	0.4825	0.9197	0.9291	0.9273	0.9245	0.9207
htc1c12sen	0.4925	0.4826	0.9209	0.9303	0.9284	0.9256	0.9218
htc1c13sen	0.5152	0.5052	0.9497	0.9575	0.9561	0.9538	0.9508
htc1c14sen	0.5141	0.5040	0.9485	0.9563	0.9549	0.9526	0.9495
htc1c15sen	0.5160	0.5057	0.9489	0.9564	0.9550	0.9526	0.9495
htc1c16sen	0.4784	0.4683	0.9094	0.9188	0.9165	0.9135	0.9092
htc1c17sen	0.4784	0.4683	0.9086	0.9180	0.9156	0.9126	0.9082
htc1c18sen	0.4783	0.4685	0.9057	0.9154	0.9131	0.9101	0.9059
htc2c1bsen	0.5147	0.5046	0.9541	0.9616	0.9602	0.9580	0.9550
htc2c2bsen	0.5141	0.5040	0.9543	0.9618	0.9605	0.9583	0.9553
htc2c3bsen	0.5135	0.5036	0.9586	0.9660	0.9647	0.9626	0.9596
htc2c4bsen	0.5125	0.5025	0.9625	0.9697	0.9684	0.9665	0.9635
htc2c5bsen	0.5121	0.5022	0.9660	0.9729	0.9717	0.9698	0.9668
htc2c6bsen	0.5121	0.5022	0.9661	0.9730	0.9718	0.9699	0.9669
htc2c7bsen	0.5107	0.5009	0.9688	0.9756	0.9744	0.9726	0.9696
htc2c8bsen	0.5103	0.5005	0.9714	0.9779	0.9767	0.9750	0.9720
htc2c9bsen	0.4895	0.4794	0.9635	0.9710	0.9692	0.9672	0.9634
htc2c10bsen	0.4912	0.4811	0.9601	0.9678	0.9660	0.9639	0.9601
htc2c11bsen	0.4922	0.4822	0.9541	0.9622	0.9604	0.9582	0.9544
htc2c12bsen	0.4927	0.4828	0.9469	0.9555	0.9537	0.9513	0.9476
htc2c13bsen	0.4928	0.4829	0.9389	0.9478	0.9460	0.9436	0.9398
htc2c14bsen	0.4928	0.4829	0.9303	0.9395	0.9376	0.9350	0.9312
htc2c15bsen	0.4797	0.4696	0.9189	0.9281	0.9258	0.9229	0.9186
htc2c16bsen	0.4798	0.4697	0.9311	0.9399	0.9376	0.9349	0.9306
htc2c17bsen	0.4788	0.4685	0.9403	0.9487	0.9464	0.9438	0.9394
htc2c18bsen	0.4772	0.4667	0.9494	0.9571	0.9548	0.9524	0.9481

Table B-2. Integral index c_k for design-basis 21-PWR waste packages and HTC experiments (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
htc2c19bsen	0.4797	0.4696	0.9206	0.9297	0.9274	0.9245	0.9202
htc2c20bsen	0.4695	0.4586	0.9314	0.9391	0.9363	0.9335	0.9287
htc2c21bsen	0.4699	0.4593	0.9181	0.9266	0.9239	0.9209	0.9162
htc2c1gsen	0.5134	0.5035	0.9564	0.9640	0.9627	0.9606	0.9575
htc2c2gsen	0.5131	0.5032	0.9564	0.9639	0.9626	0.9605	0.9575
htc2c3gsen	0.5116	0.5018	0.9617	0.9690	0.9678	0.9659	0.9629
htc2c4gsen	0.5114	0.5016	0.9619	0.9692	0.9680	0.9661	0.9631
htc2c5gsen	0.5108	0.5010	0.9623	0.9696	0.9685	0.9666	0.9636
htc2c6gsen	0.5085	0.4989	0.9671	0.9742	0.9731	0.9714	0.9684
htc2c7gsen	0.5084	0.4987	0.9669	0.9741	0.9730	0.9712	0.9683
htc2c8gsen	0.5061	0.4967	0.9702	0.9771	0.9761	0.9746	0.9717
htc2c9gsen	0.5065	0.4971	0.9702	0.9772	0.9761	0.9746	0.9717
htc2c10gsen	0.4850	0.4753	0.9626	0.9704	0.9688	0.9670	0.9633
htc2c11gsen	0.4881	0.4783	0.9569	0.9652	0.9635	0.9615	0.9578
htc2c12gsen	0.4875	0.4778	0.9565	0.9648	0.9632	0.9612	0.9574
htc2c13gsen	0.4905	0.4808	0.9474	0.9561	0.9544	0.9522	0.9484
htc2c14gsen	0.4905	0.4808	0.9472	0.9559	0.9542	0.9519	0.9482
htc2c15gsen	0.4921	0.4823	0.9354	0.9446	0.9428	0.9403	0.9366
htc2c16gsen	0.4918	0.4820	0.9357	0.9449	0.9431	0.9406	0.9369
htc2c17gsen	0.4778	0.4679	0.9263	0.9355	0.9332	0.9305	0.9263
htc2c18gsen	0.4695	0.4587	0.9264	0.9345	0.9318	0.9289	0.9242
htc2c19gsen	0.4764	0.4662	0.9428	0.9512	0.9490	0.9465	0.9422
htc2c20gsen	0.4785	0.4685	0.9277	0.9368	0.9345	0.9318	0.9275
htc3c1sen	0.4919	0.4808	0.9435	0.9514	0.9490	0.9463	0.9421
htc3c3sen	0.4923	0.4812	0.9452	0.9530	0.9507	0.9479	0.9437
htc3c4sen	0.4929	0.4816	0.9448	0.9524	0.9500	0.9472	0.9430
htc3c5sen	0.4919	0.4810	0.9460	0.9539	0.9516	0.9489	0.9448
htc3c7sen	0.4919	0.4808	0.9440	0.9518	0.9495	0.9468	0.9426
htc3c9sen	0.4921	0.4811	0.9450	0.9528	0.9505	0.9478	0.9437
htc3c10sen	0.4922	0.4810	0.9448	0.9526	0.9503	0.9476	0.9434
htc3c11sen	0.4922	0.4813	0.9444	0.9523	0.9501	0.9474	0.9433
htc3c12sen	0.4867	0.4764	0.9181	0.9273	0.9251	0.9222	0.9181
htc3c13sen	0.4877	0.4771	0.9212	0.9300	0.9277	0.9248	0.9207
htc3c14sen	0.4889	0.4779	0.9249	0.9333	0.9309	0.9279	0.9236
htc3c15sen	0.4896	0.4784	0.9261	0.9344	0.9319	0.9288	0.9246
htc3c16sen	0.4892	0.4778	0.9274	0.9355	0.9330	0.9300	0.9257
htc3c17sen	0.4899	0.4783	0.9297	0.9375	0.9349	0.9318	0.9275
htc3c18sen	0.4898	0.4777	0.9301	0.9376	0.9349	0.9317	0.9273

Table B-2. Integral index c_k for design-basis 21-PWR waste packages and HTC experiments (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
htc3c19sen	0.4858	0.4740	0.9260	0.9337	0.9309	0.9278	0.9233
htc3c20sen	0.4859	0.4739	0.9261	0.9337	0.9309	0.9278	0.9232
htc3c21sen	0.4815	0.4709	0.9140	0.9230	0.9206	0.9176	0.9133
htc3c22sen	0.4817	0.4716	0.9108	0.9203	0.9181	0.9151	0.9110
htc3c23sen	0.4847	0.4750	0.9129	0.9226	0.9205	0.9176	0.9136
htc3c24sen	0.4916	0.4817	0.9288	0.9379	0.9358	0.9330	0.9291
htc3c25sen	0.4892	0.4781	0.9292	0.9375	0.9351	0.9321	0.9278
htc3c26sen	0.4889	0.4780	0.9259	0.9344	0.9321	0.9291	0.9249
htc4pb02sen	0.4934	0.4825	0.9503	0.9578	0.9556	0.9529	0.9488
htc4pb03sen	0.4928	0.4818	0.9501	0.9576	0.9553	0.9526	0.9485
htc4pb04sen	0.4926	0.4815	0.9497	0.9572	0.9548	0.9522	0.9480
htc4pb05sen	0.4925	0.4813	0.9492	0.9566	0.9543	0.9516	0.9474
htc4pb06sen	0.4929	0.4816	0.9476	0.9551	0.9527	0.9500	0.9457
htc4pb07sen	0.4927	0.4814	0.9471	0.9546	0.9522	0.9494	0.9452
htc4pb08sen	0.4924	0.4812	0.9487	0.9562	0.9539	0.9512	0.9470
htc4pb09sen	0.4919	0.4807	0.9487	0.9562	0.9539	0.9512	0.9470
htc4pb10sen	0.4928	0.4815	0.9486	0.9560	0.9537	0.9510	0.9468
htc4pb11sen	0.4927	0.4814	0.9484	0.9559	0.9535	0.9508	0.9466
htc4pb15sen	0.4926	0.4809	0.9493	0.9565	0.9541	0.9513	0.9471
htc4pb16sen	0.4930	0.4812	0.9496	0.9568	0.9544	0.9517	0.9474
htc4pb18sen	0.4920	0.4809	0.9479	0.9554	0.9531	0.9504	0.9463
htc4pb19sen	0.4919	0.4807	0.9472	0.9546	0.9523	0.9496	0.9454
htc4pb20sen	0.4921	0.4808	0.9464	0.9538	0.9515	0.9488	0.9446
htc4pb21sen	0.4923	0.4810	0.9474	0.9548	0.9524	0.9497	0.9456
htc4pb22sen	0.4921	0.4807	0.9471	0.9546	0.9523	0.9496	0.9454
htc4pb23sen	0.4921	0.4807	0.9472	0.9547	0.9524	0.9497	0.9455
htc4pb24sen	0.4918	0.4804	0.9465	0.9540	0.9517	0.9490	0.9448
htc4pb25sen	0.4922	0.4808	0.9458	0.9533	0.9510	0.9482	0.9440
htc4pb26sen	0.4920	0.4807	0.9454	0.9530	0.9506	0.9479	0.9437
htc4pb27sen	0.4952	0.4850	0.9371	0.9456	0.9435	0.9407	0.9368
htc4pb28sen	0.4934	0.4831	0.9357	0.9441	0.9419	0.9391	0.9351
htc4pb29sen	0.4922	0.4816	0.9357	0.9440	0.9417	0.9388	0.9347
htc4pb30sen	0.4920	0.4807	0.9381	0.9458	0.9433	0.9404	0.9361
htc4pb31sen	0.4923	0.4807	0.9376	0.9451	0.9426	0.9396	0.9354
htc4pb32sen	0.4916	0.4801	0.9360	0.9437	0.9412	0.9383	0.9340
htc4pb33sen	0.4912	0.4799	0.9339	0.9417	0.9393	0.9364	0.9322
htc4pb34sen	0.4900	0.4790	0.9318	0.9399	0.9375	0.9346	0.9305
htc4pb35sen	0.4923	0.4817	0.9356	0.9439	0.9415	0.9386	0.9345

Table B-2. Integral index c_k for design-basis 21-PWR waste packages and HTC experiments (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
htc4pb36sen	0.4915	0.4810	0.9349	0.9432	0.9410	0.9381	0.9340
htc4pb37sen	0.4916	0.4811	0.9344	0.9427	0.9404	0.9375	0.9334
htc4pb38sen	0.4915	0.4809	0.9344	0.9427	0.9404	0.9375	0.9334
htc4ss02sen	0.4953	0.4846	0.9521	0.9595	0.9573	0.9546	0.9505
htc4ss03sen	0.4949	0.4840	0.9520	0.9594	0.9572	0.9545	0.9504
htc4ss04sen	0.4951	0.4841	0.9519	0.9593	0.9570	0.9543	0.9502
htc4ss05sen	0.4953	0.4843	0.9515	0.9588	0.9565	0.9537	0.9496
htc4ss06sen	0.4945	0.4834	0.9510	0.9583	0.9560	0.9533	0.9491
htc4ss07sen	0.4943	0.4831	0.9502	0.9576	0.9553	0.9525	0.9484
htc4ss08sen	0.4935	0.4823	0.9498	0.9573	0.9550	0.9523	0.9481
htc4ss09sen	0.4931	0.4819	0.9491	0.9566	0.9543	0.9516	0.9474
htc4ss10sen	0.4953	0.4842	0.9499	0.9573	0.9549	0.9521	0.9480
htc4ss11sen	0.4946	0.4835	0.9494	0.9569	0.9545	0.9517	0.9476
htc4ss13sen	0.4947	0.4826	0.9542	0.9608	0.9583	0.9556	0.9513
htc4ss15sen	0.4942	0.4832	0.9499	0.9573	0.9550	0.9523	0.9482
htc4ss16sen	0.4943	0.4832	0.9489	0.9563	0.9539	0.9512	0.9471
htc4ss17sen	0.4928	0.4817	0.9483	0.9558	0.9535	0.9508	0.9467
htc4ss18sen	0.4924	0.4812	0.9479	0.9554	0.9531	0.9504	0.9463
htc4ss19sen	0.4925	0.4812	0.9475	0.9550	0.9527	0.9500	0.9458
htc4ss20sen	0.4925	0.4812	0.9466	0.9542	0.9519	0.9491	0.9450
htc4ss21sen	0.4945	0.4833	0.9486	0.9560	0.9536	0.9508	0.9467
htc4ss22sen	0.4984	0.4885	0.9404	0.9487	0.9466	0.9438	0.9400
htc4ss23sen	0.4965	0.4864	0.9389	0.9471	0.9449	0.9421	0.9381
htc4ss24sen	0.4958	0.4855	0.9389	0.9469	0.9447	0.9417	0.9377
htc4ss25sen	0.4953	0.4849	0.9388	0.9469	0.9446	0.9417	0.9376
htc4ss26sen	0.4949	0.4845	0.9380	0.9462	0.9439	0.9409	0.9369
htc4ss27sen	0.4948	0.4844	0.9374	0.9456	0.9433	0.9403	0.9363
htc4ss28sen	0.4942	0.4838	0.9368	0.9450	0.9428	0.9398	0.9358
htc4ss29sen	0.4964	0.4854	0.9420	0.9495	0.9470	0.9440	0.9398
htc4ss30sen	0.4973	0.4860	0.9429	0.9502	0.9477	0.9446	0.9404
htc4ss31sen	0.4975	0.4863	0.9424	0.9497	0.9472	0.9442	0.9400
htc4ss32sen	0.4943	0.4832	0.9388	0.9466	0.9442	0.9412	0.9371
htc4ss33sen	0.4942	0.4833	0.9370	0.9450	0.9426	0.9397	0.9356

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/htc/sens, respectively.

Table B-3. Integral index c_k for 44-BWR waste packages and HTC LCEs

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	3	3	4	4	5	3	3	4	4	5
Burnup (GWd/MTU)	0	10	0	20	30	0	10	0	20	30
Filename[a]	tb3-0 c_k	tb3-10 c_k	tb4-0 c_k	tb4-20 c_k	tb5-30 c_k	tt3-0 c_k	tt3-10 c_k	tt4-0 c_k	tt4-20 c_k	tt5-30 c_k
htc1c1sen	0.4313	0.8846	0.4141	0.8693	0.8596	0.4292	0.8831	0.4124	0.8692	0.8606
htc1c2sen	0.4303	0.8829	0.4131	0.8675	0.8578	0.4281	0.8813	0.4114	0.8674	0.8588
htc1c3sen	0.4304	0.8824	0.4132	0.8670	0.8573	0.4283	0.8809	0.4115	0.8669	0.8583
htc1c4sen	0.4408	0.8773	0.4246	0.8604	0.8504	0.4379	0.8748	0.4220	0.8603	0.8521
htc1c5sen	0.4400	0.8766	0.4238	0.8598	0.8498	0.4371	0.8741	0.4212	0.8597	0.8514
htc1c6sen	0.4398	0.8753	0.4236	0.8584	0.8484	0.4368	0.8727	0.4210	0.8583	0.8500
htc1c7sen	0.4499	0.8831	0.4338	0.8659	0.8560	0.4466	0.8802	0.4308	0.8657	0.8576
htc1c8sen	0.4490	0.8818	0.4330	0.8647	0.8547	0.4457	0.8790	0.4299	0.8645	0.8564
htc1c9sen	0.4492	0.8808	0.4331	0.8635	0.8536	0.4458	0.8779	0.4300	0.8634	0.8553
htc1c10sen	0.4650	0.8990	0.4491	0.8817	0.8721	0.4614	0.8959	0.4456	0.8814	0.8735
htc1c11sen	0.4646	0.8974	0.4486	0.8800	0.8704	0.4609	0.8943	0.4451	0.8797	0.8718
htc1c12sen	0.4647	0.8987	0.4487	0.8814	0.8718	0.4611	0.8956	0.4452	0.8811	0.8732
htc1c13sen	0.4896	0.9290	0.4740	0.9124	0.9037	0.4857	0.9259	0.4700	0.9117	0.9042
htc1c14sen	0.4880	0.9276	0.4723	0.9109	0.9022	0.4841	0.9244	0.4684	0.9102	0.9027
htc1c15sen	0.4896	0.9275	0.4738	0.9106	0.9019	0.4856	0.9243	0.4698	0.9099	0.9024
htc1c16sen	0.4506	0.8881	0.4343	0.8710	0.8611	0.4473	0.8853	0.4314	0.8708	0.8627
htc1c17sen	0.4504	0.8871	0.4341	0.8700	0.8600	0.4471	0.8843	0.4311	0.8698	0.8616
htc1c18sen	0.4504	0.8838	0.4343	0.8666	0.8567	0.4470	0.8809	0.4312	0.8664	0.8582
htc2c1bsen	0.4892	0.9342	0.4737	0.9179	0.9094	0.4853	0.9310	0.4697	0.9172	0.9098
htc2c2bsen	0.4888	0.9346	0.4733	0.9184	0.9099	0.4849	0.9315	0.4693	0.9177	0.9103
htc2c3bsen	0.4890	0.9400	0.4737	0.9243	0.9160	0.4851	0.9370	0.4697	0.9235	0.9162
htc2c4bsen	0.4886	0.9450	0.4734	0.9298	0.9217	0.4848	0.9420	0.4695	0.9289	0.9217
htc2c5bsen	0.4889	0.9494	0.4738	0.9346	0.9267	0.4851	0.9465	0.4699	0.9337	0.9266
htc2c6bsen	0.4888	0.9496	0.4737	0.9348	0.9268	0.4850	0.9467	0.4698	0.9338	0.9267
htc2c7bsen	0.4882	0.9534	0.4733	0.9390	0.9313	0.4844	0.9505	0.4694	0.9380	0.9310
htc2c8bsen	0.4883	0.9568	0.4735	0.9428	0.9352	0.4846	0.9540	0.4697	0.9418	0.9349
htc2c9bsen	0.4671	0.9505	0.4519	0.9370	0.9288	0.4639	0.9481	0.4487	0.9362	0.9288
htc2c10bsen	0.4681	0.9458	0.4527	0.9317	0.9233	0.4648	0.9433	0.4494	0.9309	0.9235
htc2c11bsen	0.4682	0.9382	0.4526	0.9234	0.9148	0.4648	0.9356	0.4493	0.9228	0.9152
htc2c12bsen	0.4677	0.9295	0.4521	0.9141	0.9052	0.4643	0.9267	0.4487	0.9135	0.9059
htc2c13bsen	0.4669	0.9199	0.4512	0.9039	0.8948	0.4634	0.9171	0.4478	0.9034	0.8957
htc2c14bsen	0.4658	0.9097	0.4499	0.8931	0.8837	0.4623	0.9067	0.4465	0.8926	0.8848
htc2c15bsen	0.4526	0.8988	0.4365	0.8823	0.8726	0.4494	0.8961	0.4336	0.8820	0.8740
htc2c16bsen	0.4540	0.9132	0.4380	0.8975	0.8881	0.4509	0.9107	0.4351	0.8971	0.8892
htc2c17bsen	0.4541	0.9244	0.4382	0.9096	0.9005	0.4511	0.9221	0.4354	0.9091	0.9012
htc2c18bsen	0.4539	0.9360	0.4381	0.9220	0.9133	0.4510	0.9338	0.4354	0.9215	0.9137
htc2c19bsen	0.4528	0.9008	0.4366	0.8844	0.8747	0.4496	0.8981	0.4337	0.8841	0.8760
htc2c20bsen	0.4448	0.9161	0.4285	0.9014	0.8921	0.4421	0.9141	0.4262	0.9010	0.8929
htc2c21bsen	0.4437	0.9002	0.4274	0.8845	0.8748	0.4409	0.8979	0.4249	0.8842	0.8760

Table B-3. Integral index c_k for 44-BWR waste packages and HTC LCEs (continued)

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	3	3	4	4	5	3	3	4	4	5
Burnup (GWd/MTU)	0	10	0	20	30	0	10	0	20	30
Filename[a]	tb3-0 c_k	tb3-10 c_k	tb4-0 c_k	tb4-20 c_k	tb5-30 c_k	tt3-0 c_k	tt3-10 c_k	tt4-0 c_k	tt4-20 c_k	tt5-30 c_k
htc2c1gsen	0.4885	0.9373	0.4732	0.9215	0.9131	0.4846	0.9343	0.4692	0.9207	0.9134
htc2c2gsen	0.4881	0.9373	0.4728	0.9215	0.9131	0.4843	0.9342	0.4688	0.9207	0.9134
htc2c3gsen	0.4877	0.9442	0.4727	0.9291	0.9210	0.4839	0.9412	0.4688	0.9282	0.9211
htc2c4gsen	0.4875	0.9445	0.4724	0.9294	0.9213	0.4837	0.9415	0.4685	0.9285	0.9214
htc2c5gsen	0.4869	0.9451	0.4718	0.9301	0.9220	0.4831	0.9421	0.4679	0.9292	0.9221
htc2c6gsen	0.4858	0.9517	0.4711	0.9374	0.9298	0.4821	0.9488	0.4672	0.9365	0.9296
htc2c7gsen	0.4856	0.9515	0.4709	0.9372	0.9295	0.4819	0.9486	0.4670	0.9363	0.9294
htc2c8gsen	0.4844	0.9563	0.4700	0.9427	0.9353	0.4807	0.9535	0.4662	0.9417	0.9350
htc2c9gsen	0.4848	0.9562	0.4704	0.9426	0.9352	0.4811	0.9535	0.4665	0.9416	0.9349
htc2c10gsen	0.4629	0.9504	0.4480	0.9374	0.9294	0.4598	0.9480	0.4449	0.9366	0.9295
htc2c11gsen	0.4647	0.9426	0.4495	0.9287	0.9203	0.4614	0.9401	0.4463	0.9280	0.9207
htc2c12gsen	0.4642	0.9422	0.4491	0.9282	0.9199	0.4609	0.9396	0.4459	0.9276	0.9203
htc2c13gsen	0.4657	0.9305	0.4503	0.9154	0.9066	0.4624	0.9277	0.4470	0.9148	0.9073
htc2c14gsen	0.4657	0.9302	0.4502	0.9151	0.9063	0.4623	0.9274	0.4470	0.9145	0.9070
htc2c15gsen	0.4659	0.9159	0.4502	0.8998	0.8906	0.4624	0.9130	0.4468	0.8993	0.8916
htc2c16gsen	0.4656	0.9163	0.4499	0.9002	0.8911	0.4621	0.9134	0.4465	0.8998	0.8921
htc2c17gsen	0.4517	0.9079	0.4359	0.8922	0.8828	0.4486	0.9054	0.4330	0.8919	0.8839
htc2c18gsen	0.4439	0.9099	0.4276	0.8949	0.8855	0.4413	0.9079	0.4253	0.8946	0.8865
htc2c19gsen	0.4521	0.9279	0.4365	0.9136	0.9047	0.4492	0.9256	0.4337	0.9131	0.9054
htc2c20gsen	0.4524	0.9094	0.4364	0.8937	0.8843	0.4493	0.9069	0.4336	0.8934	0.8854
htc3c1sen	0.4659	0.9253	0.4493	0.9092	0.8998	0.4629	0.9228	0.4464	0.9088	0.9007
htc3c3sen	0.4665	0.9273	0.4500	0.9113	0.9020	0.4635	0.9249	0.4471	0.9110	0.9029
htc3c4sen	0.4668	0.9265	0.4501	0.9104	0.9010	0.4638	0.9241	0.4472	0.9100	0.9019
htc3c5sen	0.4665	0.9284	0.4501	0.9126	0.9033	0.4635	0.9260	0.4473	0.9122	0.9042
htc3c7sen	0.4655	0.9256	0.4489	0.9097	0.9004	0.4623	0.9231	0.4458	0.9092	0.9011
htc3c9sen	0.4660	0.9269	0.4495	0.9111	0.9018	0.4628	0.9244	0.4465	0.9106	0.9026
htc3c10sen	0.4658	0.9266	0.4492	0.9107	0.9014	0.4626	0.9241	0.4462	0.9102	0.9022
htc3c11sen	0.4664	0.9264	0.4500	0.9105	0.9013	0.4632	0.9239	0.4470	0.9101	0.9021
htc3c12sen	0.4587	0.8964	0.4424	0.8792	0.8694	0.4553	0.8935	0.4392	0.8789	0.8708
htc3c13sen	0.4597	0.8997	0.4432	0.8826	0.8728	0.4563	0.8969	0.4400	0.8823	0.8741
htc3c14sen	0.4608	0.9037	0.4440	0.8866	0.8768	0.4575	0.9010	0.4409	0.8863	0.8781
htc3c15sen	0.4615	0.9050	0.4446	0.8879	0.8781	0.4582	0.9023	0.4415	0.8876	0.8793
htc3c16sen	0.4611	0.9065	0.4441	0.8896	0.8798	0.4578	0.9039	0.4411	0.8893	0.8810
htc3c17sen	0.4618	0.9091	0.4447	0.8922	0.8824	0.4586	0.9065	0.4417	0.8919	0.8835
htc3c18sen	0.4615	0.9096	0.4441	0.8927	0.8829	0.4584	0.9072	0.4413	0.8924	0.8840
htc3c19sen	0.4577	0.9057	0.4405	0.8889	0.8791	0.4547	0.9033	0.4378	0.8887	0.8802
htc3c20sen	0.4576	0.9058	0.4404	0.8890	0.8791	0.4546	0.9034	0.4376	0.8887	0.8803
htc3c21sen	0.4535	0.8928	0.4370	0.8758	0.8659	0.4504	0.8901	0.4342	0.8755	0.8673

Table B-3. Integral index c_k for 44-BWR waste packages and HTC LCEs (continued)

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	3	3	4	4	5	3	3	4	4	5
Burnup (GWd/MTU)	0	10	0	20	30	0	10	0	20	30
Filename[a]	**tb3-0** c_k	**tb3-10** c_k	**tb4-0** c_k	**tb4-20** c_k	**tb5-30** c_k	**tt3-0** c_k	**tt3-10** c_k	**tt4-0** c_k	**tt4-20** c_k	**tt5-30** c_k
htc3c22sen	0.4537	0.8891	0.4375	0.8719	0.8621	0.4504	0.8862	0.4345	0.8717	0.8636
htc3c23sen	0.4569	0.8910	0.4408	0.8737	0.8640	0.4534	0.8880	0.4376	0.8735	0.8655
htc3c24sen	0.4660	0.9089	0.4500	0.8920	0.8824	0.4629	0.9062	0.4470	0.8917	0.8837
htc3c25sen	0.4624	0.9093	0.4456	0.8924	0.8827	0.4593	0.9067	0.4428	0.8922	0.8839
htc3c26sen	0.4611	0.9050	0.4444	0.8880	0.8783	0.4578	0.9023	0.4413	0.8878	0.8795
htc4pb02sen	0.4687	0.9335	0.4524	0.9178	0.9087	0.4658	0.9311	0.4496	0.9174	0.9095
htc4pb03sen	0.4679	0.9333	0.4515	0.9177	0.9085	0.4650	0.9309	0.4488	0.9173	0.9093
htc4pb04sen	0.4675	0.9328	0.4510	0.9171	0.9079	0.4646	0.9304	0.4483	0.9168	0.9087
htc4pb05sen	0.4672	0.9321	0.4506	0.9164	0.9072	0.4643	0.9298	0.4478	0.9161	0.9080
htc4pb06sen	0.4672	0.9301	0.4505	0.9142	0.9049	0.4642	0.9277	0.4477	0.9139	0.9057
htc4pb07sen	0.4669	0.9294	0.4501	0.9135	0.9042	0.4639	0.9271	0.4473	0.9132	0.9050
htc4pb08sen	0.4671	0.9316	0.4506	0.9159	0.9067	0.4642	0.9293	0.4478	0.9155	0.9075
htc4pb09sen	0.4667	0.9316	0.4501	0.9160	0.9068	0.4637	0.9293	0.4473	0.9156	0.9076
htc4pb10sen	0.4673	0.9313	0.4507	0.9155	0.9062	0.4644	0.9289	0.4479	0.9151	0.9070
htc4pb11sen	0.4672	0.9311	0.4506	0.9153	0.9060	0.4643	0.9288	0.4478	0.9149	0.9068
htc4pb15sen	0.4665	0.9318	0.4496	0.9162	0.9070	0.4631	0.9293	0.4464	0.9156	0.9075
htc4pb16sen	0.4668	0.9322	0.4500	0.9166	0.9074	0.4635	0.9297	0.4468	0.9160	0.9079
htc4pb18sen	0.4666	0.9307	0.4502	0.9152	0.9060	0.4635	0.9283	0.4473	0.9147	0.9067
htc4pb19sen	0.4660	0.9296	0.4494	0.9139	0.9047	0.4629	0.9272	0.4464	0.9135	0.9054
htc4pb20sen	0.4659	0.9285	0.4493	0.9128	0.9035	0.4628	0.9261	0.4463	0.9123	0.9042
htc4pb21sen	0.4663	0.9297	0.4497	0.9140	0.9048	0.4632	0.9273	0.4467	0.9135	0.9055
htc4pb22sen	0.4660	0.9295	0.4493	0.9137	0.9045	0.4628	0.9270	0.4463	0.9133	0.9052
htc4pb23sen	0.4660	0.9295	0.4493	0.9138	0.9046	0.4628	0.9271	0.4463	0.9133	0.9053
htc4pb24sen	0.4656	0.9287	0.4489	0.9129	0.9037	0.4624	0.9262	0.4459	0.9125	0.9044
htc4pb25sen	0.4658	0.9278	0.4491	0.9120	0.9027	0.4626	0.9253	0.4461	0.9115	0.9034
htc4pb26sen	0.4656	0.9273	0.4489	0.9115	0.9022	0.4624	0.9248	0.4458	0.9110	0.9029
htc4pb27sen	0.4703	0.9181	0.4542	0.9014	0.8919	0.4671	0.9154	0.4512	0.9011	0.8931
htc4pb28sen	0.4683	0.9167	0.4520	0.9001	0.8906	0.4652	0.9141	0.4492	0.8998	0.8918
htc4pb29sen	0.4669	0.9169	0.4505	0.9003	0.8908	0.4638	0.9143	0.4477	0.9000	0.8919
htc4pb30sen	0.4659	0.9193	0.4492	0.9029	0.8934	0.4629	0.9169	0.4464	0.9026	0.8944
htc4pb31sen	0.4655	0.9184	0.4485	0.9019	0.8923	0.4624	0.9159	0.4457	0.9016	0.8933
htc4pb32sen	0.4644	0.9165	0.4475	0.8999	0.8904	0.4613	0.9140	0.4445	0.8996	0.8914
htc4pb33sen	0.4639	0.9140	0.4471	0.8973	0.8877	0.4606	0.9114	0.4440	0.8970	0.8887
htc4pb34sen	0.4627	0.9118	0.4460	0.8951	0.8855	0.4594	0.9091	0.4429	0.8948	0.8866
htc4pb35sen	0.4669	0.9167	0.4505	0.9001	0.8905	0.4639	0.9142	0.4477	0.8998	0.8917
htc4pb36sen	0.4662	0.9161	0.4498	0.8995	0.8900	0.4631	0.9135	0.4470	0.8992	0.8911
htc4pb37sen	0.4662	0.9154	0.4498	0.8987	0.8892	0.4631	0.9128	0.4470	0.8985	0.8904
htc4pb38sen	0.4659	0.9154	0.4495	0.8987	0.8892	0.4629	0.9128	0.4467	0.8985	0.8904

Table B-3. Integral index c_k for 44-BWR waste packages and HTC LCEs (continued)

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	**3**	**3**	**4**	**4**	**5**	**3**	**3**	**4**	**4**	**5**
Burnup (GWd/MTU)	**0**	**10**	**0**	**20**	**30**	**0**	**10**	**0**	**20**	**30**
Filename[a]	**tb3-0** c_k	**tb3-10** c_k	**tb4-0** c_k	**tb4-20** c_k	**tb5-30** c_k	**tt3-0** c_k	**tt3-10** c_k	**tt4-0** c_k	**tt4-20** c_k	**tt5-30** c_k
htc4ss02sen	0.4716	0.9355	0.4553	0.9198	0.9106	0.4688	0.9333	0.4527	0.9195	0.9115
htc4ss03sen	0.4710	0.9355	0.4547	0.9198	0.9106	0.4682	0.9333	0.4521	0.9194	0.9114
htc4ss04sen	0.4709	0.9353	0.4545	0.9195	0.9103	0.4682	0.9331	0.4519	0.9192	0.9111
htc4ss05sen	0.4710	0.9347	0.4545	0.9188	0.9095	0.4683	0.9325	0.4520	0.9185	0.9104
htc4ss06sen	0.4699	0.9341	0.4533	0.9182	0.9090	0.4671	0.9319	0.4507	0.9179	0.9098
htc4ss07sen	0.4694	0.9331	0.4528	0.9173	0.9080	0.4666	0.9309	0.4502	0.9169	0.9088
htc4ss08sen	0.4685	0.9328	0.4520	0.9170	0.9078	0.4657	0.9305	0.4493	0.9167	0.9086
htc4ss09sen	0.4680	0.9319	0.4514	0.9161	0.9069	0.4651	0.9296	0.4487	0.9158	0.9077
htc4ss10sen	0.4707	0.9327	0.4541	0.9167	0.9074	0.4679	0.9305	0.4515	0.9164	0.9083
htc4ss11sen	0.4699	0.9323	0.4533	0.9163	0.9070	0.4671	0.9301	0.4507	0.9160	0.9079
htc4ss13sen	0.4689	0.9374	0.4518	0.9219	0.9128	0.4656	0.9350	0.4487	0.9213	0.9131
htc4ss15sen	0.4697	0.9331	0.4533	0.9174	0.9082	0.4668	0.9307	0.4505	0.9169	0.9089
htc4ss16sen	0.4693	0.9315	0.4527	0.9156	0.9064	0.4663	0.9292	0.4499	0.9152	0.9072
htc4ss17sen	0.4675	0.9310	0.4510	0.9153	0.9061	0.4644	0.9286	0.4481	0.9148	0.9068
htc4ss18sen	0.4668	0.9305	0.4502	0.9148	0.9056	0.4636	0.9280	0.4472	0.9143	0.9063
htc4ss19sen	0.4667	0.9299	0.4500	0.9141	0.9049	0.4635	0.9274	0.4470	0.9137	0.9056
htc4ss20sen	0.4665	0.9288	0.4498	0.9129	0.9037	0.4633	0.9263	0.4468	0.9125	0.9044
htc4ss21sen	0.4692	0.9310	0.4526	0.9151	0.9058	0.4662	0.9287	0.4498	0.9147	0.9066
htc4ss22sen	0.4747	0.9218	0.4587	0.9049	0.8955	0.4719	0.9193	0.4561	0.9047	0.8968
htc4ss23sen	0.4726	0.9203	0.4565	0.9034	0.8939	0.4699	0.9179	0.4540	0.9033	0.8953
htc4ss24sen	0.4718	0.9204	0.4555	0.9035	0.8940	0.4691	0.9181	0.4531	0.9034	0.8953
htc4ss25sen	0.4713	0.9204	0.4550	0.9036	0.8940	0.4686	0.9181	0.4526	0.9035	0.8953
htc4ss26sen	0.4707	0.9195	0.4544	0.9027	0.8931	0.4680	0.9171	0.4519	0.9025	0.8944
htc4ss27sen	0.4704	0.9187	0.4540	0.9018	0.8923	0.4676	0.9163	0.4515	0.9017	0.8936
htc4ss28sen	0.4697	0.9181	0.4534	0.9013	0.8917	0.4669	0.9157	0.4508	0.9011	0.8930
htc4ss29sen	0.4720	0.9237	0.4553	0.9069	0.8974	0.4695	0.9216	0.4530	0.9069	0.8986
htc4ss30sen	0.4724	0.9244	0.4556	0.9076	0.8979	0.4700	0.9224	0.4533	0.9075	0.8992
htc4ss31sen	0.4724	0.9236	0.4556	0.9066	0.8970	0.4699	0.9215	0.4533	0.9066	0.8983
htc4ss32sen	0.4684	0.9197	0.4517	0.9029	0.8933	0.4655	0.9173	0.4490	0.9027	0.8944
htc4ss33sen	0.4681	0.9175	0.4515	0.9007	0.8910	0.4652	0.9151	0.4488	0.9005	0.8922

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/44bwr/sens, and DVD/exps/htc/sens, respectively.

Table B-4. Integral index c_k for nominal 21-PWR waste packages and MOX LCEs

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tb2-0 c_k	tb3-0 c_k	tb15 c_k	tb25 c_k	tb30 c_k	tb35 c_k	tb40 c_k
mct002-01sen	0.2426	0.2323	0.8926	0.9217	0.9232	0.9337	0.9233
mct002-02sen	0.2394	0.2294	0.8994	0.9291	0.9309	0.9455	0.9311
mct002-03sen	0.2072	0.1979	0.8474	0.8769	0.8773	0.8833	0.8764
mct002-04sen	0.1962	0.1871	0.8821	0.9141	0.9151	0.9329	0.9134
mct002-05sen	0.1939	0.1849	0.8315	0.8612	0.8612	0.8673	0.8596
mct002-06sen	0.1838	0.1747	0.8695	0.9015	0.9019	0.9201	0.8991
mct003-01sen	0.1277	0.1240	0.8141	0.8529	0.8578	0.8748	0.8635
mct003-02sen	0.1189	0.1156	0.7985	0.8370	0.8413	0.8552	0.8468
mct003-03sen	0.1195	0.1162	0.8062	0.8452	0.8499	0.8654	0.8555
mct003-04sen	0.0958	0.0931	0.7549	0.7921	0.7952	0.8050	0.7989
mct003-05sen	0.0919	0.0892	0.7484	0.7854	0.7882	0.7979	0.7914
mct003-06sen	0.0826	0.0798	0.7437	0.7805	0.7825	0.7943	0.7840
mct004-01sen	0.1852	0.1773	0.8328	0.8658	0.8672	0.8764	0.8678
mct006-01sen	0.2301	0.2202	0.8779	0.9073	0.9084	0.9166	0.9084
mct007-02sen	0.2131	0.2030	0.8492	0.8783	0.8781	0.8850	0.8760
mct008-01sen	0.2664	0.2540	0.9049	0.9329	0.9336	0.9446	0.9324
mct008-02sen	0.2433	0.2318	0.8769	0.9054	0.9055	0.9133	0.9036
mct008-03sen	0.2304	0.2191	0.8622	0.8908	0.8905	0.8983	0.8880
mct008-04sen	0.2229	0.2117	0.8556	0.8842	0.8837	0.8924	0.8806
mct008-05sen	0.2131	0.2013	0.8532	0.8820	0.8810	0.8936	0.8766
mct008-06sen	0.2099	0.1978	0.8525	0.8813	0.8802	0.8945	0.8752
mst001-01sen	0.0533	0.0516	0.7426	0.7838	0.7887	0.8055	0.7951
mst001-02sen	0.0534	0.0554	0.7446	0.7858	0.7908	0.8078	0.7972
mst001-03sen	0.0568	0.0518	0.7327	0.7731	0.7780	0.7924	0.7846
mst001-04sen	0.0535	0.0512	0.7450	0.7864	0.7915	0.8085	0.7981
mst001-05sen	0.0530	0.0571	0.7536	0.7954	0.8005	0.8192	0.8069
mst001-06sen	0.0585	0.0193	0.7271	0.7674	0.7725	0.7853	0.7796
mst001-08sen	0.0187	0.0209	0.6997	0.7424	0.7482	0.7644	0.7562
mst001-09sen	0.0199	0.0502	0.7040	0.7458	0.7505	0.7665	0.7563
mst001-10sen	0.0519	0.0514	0.7446	0.7854	0.7897	0.8065	0.7947
mst001-11sen	0.0533	0.0484	0.7460	0.7867	0.7908	0.8073	0.7957
mst001-12sen	0.0503	0.0499	0.7396	0.7801	0.7842	0.8009	0.7891
mst001-13sen	0.0517	0.0314	0.7459	0.7861	0.7896	0.8067	0.7930
mst002-01sen	0.0330	0.0312	0.7361	0.7757	0.7772	0.8007	0.7758
mst002-02sen	0.0328	0.0443	0.7365	0.7761	0.7776	0.8013	0.7761
mst002-03sen	0.0471	0.0403	0.7465	0.7851	0.7863	0.8091	0.7844
mst004-01sen	0.0408	0.0446	0.6730	0.7108	0.7143	0.7224	0.7191
mst004-02sen	0.0450	0.0418	0.6839	0.7217	0.7251	0.7339	0.7295
mst004-03sen	0.0424	0.0428	0.7013	0.7403	0.7438	0.7551	0.7478

Table B-4. Integral index c_k for nominal 21-PWR waste packages and MOX LCEs (continued)

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	**0**	**0**	**15**	**25**	**30**	**35**	**40**
Filename[a]	**tb2-0** c_k	**tb3-0** c_k	**tb15** c_k	**tb25** c_k	**tb30** c_k	**tb35** c_k	**tb40** c_k
mst004-04sen	0.0434	0.0461	0.7055	0.7463	0.7519	0.7642	0.7599
mst004-05sen	0.0465	0.0426	0.6919	0.7316	0.7371	0.7470	0.7452
mst004-06sen	0.0432	0.0429	0.6823	0.7222	0.7279	0.7372	0.7367
mst004-07sen	0.0437	0.0461	0.6926	0.7338	0.7405	0.7527	0.7506
mst004-08sen	0.0467	0.0437	0.6981	0.7391	0.7454	0.7574	0.7550
mst004-09sen	0.0444	0.0380	0.7102	0.7521	0.7586	0.7728	0.7681
mst005-01sen	0.0391	0.0498	0.6901	0.7285	0.7319	0.7436	0.7360
mst005-02sen	0.0501	0.0517	0.7168	0.7554	0.7586	0.7718	0.7619
mst005-03sen	0.0519	0.0506	0.7148	0.7550	0.7604	0.7725	0.7678
mst005-04sen	0.0509	0.0394	0.7184	0.7587	0.7639	0.7772	0.7710
mst005-05sen	0.0405	0.0405	0.6963	0.7367	0.7423	0.7554	0.7506
mst005-06sen	0.0418	0.0504	0.7003	0.7417	0.7483	0.7634	0.7581
mst005-07sen	0.0508	0.4484	0.7213	0.7627	0.7687	0.7836	0.7773

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/mox/sens, respectively.

Table B-5. Integral index c_k for design-basis 21-PWR waste packages and MOX LCEs

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
mct002-01sen	0.2410	0.2302	0.8939	0.9190	0.9221	0.9266	0.9230
mct002-02sen	0.2380	0.2276	0.9017	0.9264	0.9297	0.9346	0.9312
mct002-03sen	0.2055	0.1953	0.8473	0.8743	0.8766	0.8803	0.8756
mct002-04sen	0.1951	0.1856	0.8851	0.9112	0.9138	0.9185	0.9139
mct002-05sen	0.1923	0.1824	0.8315	0.8586	0.8604	0.8639	0.8587
mct002-06sen	0.1828	0.1733	0.8726	0.8987	0.9006	0.9049	0.8997
mct003-01sen	0.1263	0.1222	0.8157	0.8499	0.8567	0.8651	0.8632
mct003-02sen	0.1174	0.1136	0.7994	0.8341	0.8405	0.8484	0.8462
mct003-03sen	0.1180	0.1143	0.8075	0.8423	0.8490	0.8572	0.8551
mct003-04sen	0.0942	0.0910	0.7548	0.7893	0.7946	0.8013	0.7979
mct003-05sen	0.0904	0.0872	0.7483	0.7826	0.7876	0.7941	0.7904
mct003-06sen	0.0813	0.0780	0.7442	0.7776	0.7818	0.7877	0.7833
mct004-01sen	0.1835	0.1748	0.8330	0.8631	0.8665	0.8715	0.8671
mct006-01sen	0.2284	0.2178	0.8785	0.9046	0.9075	0.9118	0.9078
mct007-02sen	0.2115	0.2004	0.8494	0.8756	0.8773	0.8805	0.8753
mct008-01sen	0.2648	0.2519	0.9064	0.9302	0.9326	0.9364	0.9322
mct008-02sen	0.2417	0.2293	0.8774	0.9028	0.9046	0.9080	0.9031
mct008-03sen	0.2287	0.2166	0.8627	0.8882	0.8896	0.8927	0.8874
mct008-04sen	0.2214	0.2093	0.8563	0.8816	0.8828	0.8857	0.8801
mct008-05sen	0.2119	0.1994	0.8550	0.8793	0.8799	0.8827	0.8766
mct008-06sen	0.2088	0.1962	0.8547	0.8786	0.8790	0.8817	0.8755
mst001-01sen	0.0530	0.0510	0.7445	0.7816	0.7888	0.7976	0.7954
mst001-02sen	0.0530	0.0511	0.7466	0.7836	0.7909	0.7996	0.7974
mst001-03sen	0.0569	0.0554	0.7344	0.7713	0.7785	0.7870	0.7849
mst001-04sen	0.0531	0.0513	0.7470	0.7842	0.7916	0.8005	0.7983
mst001-05sen	0.0527	0.0506	0.7559	0.7931	0.8005	0.8095	0.8073
mst001-06sen	0.0581	0.0565	0.7282	0.7654	0.7728	0.7814	0.7795
mst001-08sen	0.0183	0.0194	0.7012	0.7402	0.7484	0.7579	0.7563
mst001-09sen	0.0195	0.0204	0.7055	0.7436	0.7505	0.7590	0.7563
mst001-10sen	0.0515	0.0496	0.7466	0.7831	0.7897	0.7978	0.7950
mst001-11sen	0.0527	0.0507	0.7479	0.7843	0.7907	0.7988	0.7959
mst001-12sen	0.0499	0.0479	0.7416	0.7778	0.7842	0.7923	0.7894
mst001-13sen	0.0514	0.0494	0.7480	0.7838	0.7894	0.7969	0.7933
mst002-01sen	0.0325	0.0309	0.7397	0.7729	0.7761	0.7822	0.7766
mst002-02sen	0.0324	0.0307	0.7401	0.7733	0.7765	0.7826	0.7769
mst002-03sen	0.0467	0.0438	0.7500	0.7823	0.7852	0.7910	0.7852
mst004-01sen	0.0395	0.0388	0.6724	0.7084	0.7141	0.7212	0.7180
mst004-02sen	0.0443	0.0438	0.6840	0.7197	0.7253	0.7322	0.7289
mst004-03sen	0.0414	0.0407	0.7018	0.7379	0.7435	0.7507	0.7472

Table B-5. Integral index c_k for design-basis 21-PWR waste packages and MOX LCEs (continued)

Initial enrichment (wt% ^{235}U)	**2**	**3**	**3**	**3.5**	**4**	**4.5**	**5**
Burnup (GWd/MTU)	**0**	**0**	**15**	**25**	**30**	**35**	**40**
Filename[a]	**tt2-0** c_k	**tt3-0** c_k	**tt15** c_k	**tt25** c_k	**tt30** c_k	**tt35** c_k	**tt40** c_k
mst004-04sen	0.0425	0.0417	0.7061	0.7441	0.7520	0.7610	0.7594
mst004-05sen	0.0460	0.0454	0.6922	0.7298	0.7376	0.7462	0.7448
mst004-06sen	0.0418	0.0411	0.6819	0.7199	0.7280	0.7369	0.7357
mst004-07sen	0.0425	0.0416	0.6928	0.7315	0.7405	0.7504	0.7499
mst004-08sen	0.0461	0.0454	0.6987	0.7371	0.7458	0.7554	0.7546
mst004-09sen	0.0436	0.0427	0.7111	0.7498	0.7586	0.7685	0.7677
mst005-01sen	0.0380	0.0369	0.6904	0.7261	0.7317	0.7388	0.7354
mst005-02sen	0.0509	0.0503	0.7188	0.7540	0.7593	0.7661	0.7625
mst005-03sen	0.0524	0.0520	0.7164	0.7537	0.7613	0.7699	0.7682
mst005-04sen	0.0517	0.0512	0.7204	0.7575	0.7649	0.7734	0.7716
mst005-05sen	0.0395	0.0383	0.6968	0.7344	0.7424	0.7515	0.7501
mst005-06sen	0.0409	0.0396	0.7012	0.7394	0.7484	0.7584	0.7578
mst005-07sen	0.0516	0.0509	0.7235	0.7613	0.7697	0.7790	0.7780

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/mox/sens, respectively.

Table B-6. Integral index c_k for 44-BWR waste packages and MOX LCEs

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	3	3	4	4	5	3	3	4	4	5
Burnup (GWd/MTU)	0	10	0	20	30	0	10	0	20	30
Filename[a]	tb3-0 c_k	tb3-10 c_k	tb4-0 c_k	tb4-20 c_k	tb5-30 c_k	tt3-0 c_k	tt3-10 c_k	tt4-0 c_k	tt4-20 c_k	tt5-30 c_k
mct002-01sen	0.2233	0.9335	0.2121	0.9460	0.9439	0.2210	0.9308	0.2095	0.9448	0.9439
mct002-02sen	0.2219	0.9448	0.2111	0.9592	0.9581	0.2196	0.9422	0.2085	0.9577	0.9574
mct002-03sen	0.1877	0.8841	0.1773	0.8941	0.8901	0.1858	0.8815	0.1751	0.8936	0.8915
mct002-04sen	0.1807	0.9319	0.1711	0.9470	0.9451	0.1791	0.9299	0.1693	0.9459	0.9449
mct002-05sen	0.1749	0.8679	0.1648	0.8775	0.8731	0.1732	0.8654	0.1629	0.8772	0.8748
mct002-06sen	0.1683	0.9187	0.1588	0.9331	0.9304	0.1669	0.9169	0.1573	0.9322	0.9306
mct003-01sen	0.1189	0.8774	0.1140	0.9033	0.9060	0.1172	0.8743	0.1120	0.9020	0.9062
mct003-02sen	0.1100	0.8585	0.1055	0.8822	0.8836	0.1084	0.8554	0.1035	0.8813	0.8846
mct003-03sen	0.1110	0.8685	0.1065	0.8935	0.8955	0.1094	0.8655	0.1045	0.8924	0.8961
mct003-04sen	0.0874	0.8087	0.0837	0.8283	0.8273	0.0861	0.8059	0.0820	0.8279	0.8294
mct003-05sen	0.0836	0.8014	0.0800	0.8204	0.8190	0.0824	0.7987	0.0784	0.8201	0.8212
mct003-06sen	0.0746	0.7968	0.0710	0.8151	0.8130	0.0736	0.7945	0.0697	0.8149	0.8152
mct004-01sen	0.1673	0.8692	0.1581	0.8819	0.8793	0.1656	0.8667	0.1562	0.8816	0.8810
mct006-01sen	0.2106	0.9171	0.1997	0.9285	0.9256	0.2084	0.9143	0.1971	0.9276	0.9262
mct007-02sen	0.1924	0.8822	0.1813	0.8910	0.8867	0.1907	0.8798	0.1793	0.8906	0.8881
mct008-01sen	0.2442	0.9374	0.2311	0.9471	0.9444	0.2419	0.9348	0.2285	0.9461	0.9444
mct008-02sen	0.2209	0.9067	0.2084	0.9151	0.9112	0.2189	0.9042	0.2062	0.9145	0.9122
mct008-03sen	0.2082	0.8916	0.1960	0.8997	0.8954	0.2064	0.8893	0.1940	0.8993	0.8966
mct008-04sen	0.2010	0.8855	0.1889	0.8935	0.8891	0.1994	0.8833	0.1871	0.8932	0.8904
mct008-05sen	0.1917	0.8856	0.1797	0.8944	0.8900	0.1904	0.8840	0.1783	0.8940	0.8910
mct008-06sen	0.1888	0.8861	0.1767	0.8951	0.8908	0.1876	0.8846	0.1754	0.8948	0.8917
mst001-01sen	0.0494	0.8104	0.0473	0.8359	0.8370	0.0494	0.8083	0.0470	0.8359	0.8393
mst001-02sen	0.0495	0.8128	0.0474	0.8384	0.8395	0.0495	0.8107	0.0471	0.8384	0.8418
mst001-03sen	0.0552	0.7992	0.0533	0.8234	0.8241	0.0559	0.7974	0.0536	0.8239	0.8271
mst001-04sen	0.0497	0.8136	0.0477	0.8395	0.8408	0.0498	0.8115	0.0474	0.8395	0.8431
mst001-05sen	0.0489	0.8237	0.0468	0.8504	0.8519	0.0489	0.8216	0.0464	0.8502	0.8539
mst001-06sen	0.0552	0.7916	0.0533	0.8158	0.8166	0.0554	0.7894	0.0530	0.8160	0.8194
mst001-08sen	0.0200	0.7715	0.0206	0.7989	0.8006	0.0202	0.7693	0.0204	0.7990	0.8034
mst001-09sen	0.0210	0.7725	0.0215	0.7974	0.7978	0.0212	0.7705	0.0213	0.7977	0.8007
mst001-10sen	0.0480	0.8108	0.0460	0.8349	0.8351	0.0481	0.8088	0.0457	0.8350	0.8375
mst001-11sen	0.0489	0.8115	0.0469	0.8351	0.8351	0.0489	0.8095	0.0464	0.8353	0.8376
mst001-12sen	0.0463	0.8053	0.0443	0.8289	0.8288	0.0463	0.8033	0.0439	0.8291	0.8314
mst001-13sen	0.0478	0.8101	0.0458	0.8326	0.8321	0.0479	0.8083	0.0456	0.8328	0.8346
mst002-01sen	0.0292	0.7991	0.0279	0.8207	0.8194	0.0292	0.7980	0.0277	0.8206	0.8210
mst002-02sen	0.0291	0.7996	0.0277	0.8213	0.8200	0.0291	0.7986	0.0276	0.8212	0.8216
mst002-03sen	0.0413	0.8070	0.0389	0.8274	0.8258	0.0413	0.8059	0.0387	0.8274	0.8275
mst004-01sen	0.0363	0.7267	0.0354	0.7460	0.7446	0.0355	0.7240	0.0341	0.7462	0.7477
mst004-02sen	0.0428	0.7394	0.0419	0.7584	0.7569	0.0429	0.7373	0.0415	0.7590	0.7604
mst004-03sen	0.0389	0.7592	0.0379	0.7796	0.7785	0.0386	0.7569	0.0371	0.7798	0.7814
mst004-04sen	0.0399	0.7701	0.0388	0.7954	0.7966	0.0396	0.7676	0.0381	0.7953	0.7992

Table B-6. Integral index c_k for 44-BWR waste packages and MOX LCEs (continued)

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	**3**	**3**	**4**	**4**	**5**	**3**	**3**	**4**	**4**	**5**
Burnup (GWd/MTU)	**0**	**10**	**0**	**20**	**30**	**0**	**10**	**0**	**20**	**30**
Filename[a]	**tb3-0 c_k**	**tb3-10 c_k**	**tb4-0 c_k**	**tb4-20 c_k**	**tb5-30 c_k**	**tt3-0 c_k**	**tt3-10 c_k**	**tt4-0 c_k**	**tt4-20 c_k**	**tt5-30 c_k**
mst004-05sen	0.0446	0.7543	0.0436	0.7781	0.7789	0.0447	0.7520	0.0432	0.7784	0.7821
mst004-06sen	0.0385	0.7431	0.0375	0.7675	0.7687	0.0377	0.7402	0.0361	0.7673	0.7714
mst004-07sen	0.0390	0.7586	0.0378	0.7866	0.7896	0.0383	0.7556	0.0366	0.7861	0.7917
mst004-08sen	0.0443	0.7646	0.0431	0.7915	0.7940	0.0443	0.7620	0.0427	0.7915	0.7966
mst004-09sen	0.0409	0.7789	0.0397	0.8072	0.8102	0.0406	0.7762	0.0390	0.8069	0.8123
mst005-01sen	0.0348	0.7474	0.0337	0.7677	0.7664	0.0343	0.7450	0.0327	0.7679	0.7695
mst005-02sen	0.0527	0.7790	0.0516	0.7987	0.7973	0.0543	0.7780	0.0529	0.7999	0.8011
mst005-03sen	0.0538	0.7815	0.0528	0.8054	0.8062	0.0552	0.7801	0.0538	0.8063	0.8097
mst005-04sen	0.0535	0.7864	0.0524	0.8104	0.8110	0.0551	0.7851	0.0536	0.8114	0.8147
mst005-05sen	0.0363	0.7609	0.0350	0.7864	0.7877	0.0357	0.7582	0.0340	0.7863	0.7904
mst005-06sen	0.0375	0.7690	0.0360	0.7977	0.8008	0.0369	0.7661	0.0351	0.7973	0.8030
mst005-07sen	0.0529	0.7927	0.0517	0.8196	0.8218	0.0543	0.7912	0.0528	0.8203	0.8250

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/44bwr/sens, and DVD/exps/mox/sens, respectively.

Table B-7. Integral index c_k for nominal 21-PWR waste packages and LEU LCEs

Initial enrichment (wt% ^{235}U)	**2**	**3**	**3**	**3.5**	**4**	**4.5**	**5**
Burnup (GWd/MTU)	**0**	**0**	**15**	**25**	**30**	**35**	**40**
Filename[a]	**tb2-0** c_k	**tb3-0** c_k	**tb15** c_k	**tb25** c_k	**tb30** c_k	**tb35** c_k	**tb40** c_k
lct010c5	0.8654	0.8804	0.5196	0.4595	0.4517	0.3601	0.4453
lct010c16	0.8391	0.8730	0.5173	0.4606	0.4555	0.3608	0.4546
lct010c17	0.8318	0.8728	0.5126	0.4566	0.4515	0.3569	0.4506
lct010c18	0.8321	0.8575	0.5121	0.4559	0.4507	0.3562	0.4497
lct010c19	0.8168	0.9174	0.5023	0.4474	0.4421	0.3482	0.4413
lct017-03	0.8703	0.8748	0.5174	0.4557	0.4452	0.3555	0.4347
lct017-04	0.9229	0.9173	0.5510	0.4848	0.4733	0.3847	0.4603
lct017-05	0.9053	0.9024	0.5404	0.4759	0.4646	0.3754	0.4523
lct017-06	0.9009	0.8985	0.5378	0.4737	0.4624	0.3731	0.4503
lct017-07	0.8939	0.8925	0.5335	0.4700	0.4588	0.3694	0.4469
lct17c8	0.8796	0.8812	0.5236	0.4612	0.4504	0.3608	0.4392
lct017-09	0.8631	0.8677	0.5138	0.4528	0.4424	0.3525	0.4321
lct017-10	0.8962	0.9006	0.5347	0.4711	0.4605	0.3698	0.4496
lct017-11	0.8923	0.8966	0.5321	0.4687	0.4581	0.3675	0.4473
lct017-12	0.8876	0.8919	0.5290	0.4660	0.4554	0.3649	0.4446
lct017-13	0.8806	0.8850	0.5243	0.4619	0.4513	0.3609	0.4406
lct017-14	0.8774	0.8816	0.5220	0.4598	0.4492	0.3590	0.4385
lct017-15	0.9427	0.9455	0.5742	0.5074	0.4968	0.4062	0.4853
lct017-16	0.9373	0.9401	0.5705	0.5042	0.4935	0.4027	0.4820
lct17c17	0.9386	0.9406	0.5698	0.5033	0.4925	0.4017	0.4809
lct017-19	0.9354	0.9370	0.5670	0.5006	0.4898	0.3991	0.4781
lct017-20	0.9323	0.9340	0.5648	0.4987	0.4878	0.3970	0.4762
lct017-21	0.9283	0.9302	0.5619	0.4962	0.4853	0.3946	0.4739
lct017-22	0.9138	0.9168	0.5536	0.4892	0.4784	0.3876	0.4674
lct017-23	0.9220	0.9237	0.5582	0.4926	0.4818	0.3927	0.4703
lct017-24	0.9213	0.9231	0.5573	0.4918	0.4810	0.3916	0.4695
lct017-25	0.9239	0.9252	0.5579	0.4922	0.4813	0.3913	0.4697
lct017-28	0.9454	0.9391	0.5727	0.5053	0.4937	0.4053	0.4804
lct017-29	0.9414	0.9363	0.5696	0.5024	0.4909	0.4022	0.4779
lct26c3	0.8281	0.8809	0.5314	0.4763	0.4740	0.3840	0.4768
lct42c1	0.9444	0.9470	0.5748	0.5079	0.4971	0.4064	0.4854
lct42c2	0.9513	0.9526	0.5774	0.5096	0.4988	0.4086	0.4868
lct42c3	0.9542	0.9554	0.5791	0.5110	0.5002	0.4102	0.4882
lct42c4	0.9529	0.9539	0.5785	0.5105	0.4997	0.4096	0.4876
lct42c5	0.9516	0.9530	0.5774	0.5095	0.4987	0.4086	0.4868
lct42c6	0.9414	0.9431	0.5711	0.5041	0.4934	0.4030	0.4816
lct42c7	0.9494	0.9505	0.5756	0.5078	0.4970	0.4069	0.4850

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/leu/sens, respectively.

Table B-8. Integral index c_k for design-basis 21-PWR waste packages and LEU LCEs

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
lct010c5	0.8602	0.8733	0.5026	0.4618	0.4516	0.4338	0.4370
lct010c16	0.8348	0.8700	0.5000	0.4634	0.4562	0.4404	0.4461
lct010c17	0.8274	0.8622	0.4952	0.4592	0.4521	0.4365	0.4420
lct010c18	0.8276	0.8619	0.4946	0.4585	0.4513	0.4357	0.4411
lct010c19	0.8121	0.8460	0.4846	0.4498	0.4427	0.4273	0.4326
lct017-03	0.8665	0.8655	0.5015	0.4587	0.4462	0.4269	0.4275
lct017-04	0.9189	0.9098	0.5358	0.4877	0.4738	0.4532	0.4534
lct017-05	0.9013	0.8940	0.5249	0.4788	0.4653	0.4451	0.4453
lct017-06	0.8969	0.8900	0.5222	0.4765	0.4631	0.4430	0.4432
lct017-07	0.8900	0.8838	0.5178	0.4728	0.4596	0.4396	0.4398
lct17c8	0.8758	0.8722	0.5078	0.4641	0.4513	0.4317	0.4321
lct017-09	0.8593	0.8581	0.4977	0.4557	0.4434	0.4242	0.4248
lct017-10	0.8930	0.8924	0.5192	0.4743	0.4616	0.4418	0.4427
lct017-11	0.8889	0.8882	0.5165	0.4719	0.4592	0.4394	0.4403
lct017-12	0.8841	0.8832	0.5133	0.4691	0.4565	0.4368	0.4376
lct017-13	0.8770	0.8760	0.5085	0.4649	0.4523	0.4328	0.4335
lct017-14	0.8737	0.8725	0.5061	0.4628	0.4502	0.4307	0.4314
lct017-15	0.9398	0.9392	0.5596	0.5109	0.4979	0.4774	0.4787
lct017-16	0.9342	0.9333	0.5556	0.5076	0.4945	0.4742	0.4753
lct17c17	0.9353	0.9338	0.5549	0.5066	0.4935	0.4730	0.4741
lct017-19	0.9319	0.9299	0.5519	0.5038	0.4906	0.4703	0.4712
lct017-20	0.9288	0.9266	0.5495	0.5018	0.4886	0.4683	0.4692
lct017-21	0.9246	0.9226	0.5466	0.4992	0.4861	0.4659	0.4668
lct017-22	0.9099	0.9085	0.5379	0.4921	0.4792	0.4594	0.4602
lct017-23	0.9183	0.9164	0.5431	0.4956	0.4826	0.4626	0.4634
lct017-24	0.9175	0.9156	0.5421	0.4948	0.4818	0.4617	0.4626
lct017-25	0.9201	0.9176	0.5426	0.4952	0.4821	0.4619	0.4627
lct017-28	0.9415	0.9325	0.5580	0.5082	0.4941	0.4733	0.4736
lct017-29	0.9375	0.9295	0.5547	0.5054	0.4915	0.4707	0.4711
lct26c3	0.8242	0.8734	0.5158	0.4792	0.4744	0.4607	0.4687
lct42c1	0.9425	0.9416	0.5608	0.5120	0.4988	0.4783	0.4794
lct42c2	0.9484	0.9467	0.5630	0.5131	0.4998	0.4791	0.4803
lct42c3	0.9511	0.9495	0.5647	0.5144	0.5011	0.4805	0.4817
lct42c4	0.9498	0.9480	0.5640	0.5139	0.5006	0.4799	0.4810
lct42c5	0.9486	0.9470	0.5629	0.5130	0.4997	0.4790	0.4802
lct42c6	0.9382	0.9366	0.5563	0.5075	0.4943	0.4738	0.4749
lct42c7	0.9462	0.9444	0.5610	0.5112	0.4979	0.4773	0.4784

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/leu/sens, respectively.

Table B-9. Integral index c_k for 44-BWR waste packages and LEU LCEs

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	**3**	**3**	**4**	**4**	**5**	**3**	**3**	**4**	**4**	**5**
Burnup (GWd/MTU)	**0**	**10**	**0**	**20**	**30**	**0**	**10**	**0**	**20**	**30**
Filename[a]	**tb3-0 c_k**	**tb3-10 c_k**	**tb4-0 c_k**	**tb4-20 c_k**	**tb5-30 c_k**	**tt3-0 c_k**	**tt3-10 c_k**	**tt4-0 c_k**	**tt4-20 c_k**	**tt5-30 c_k**
lct010c5	0.8575	0.3792	0.8497	0.3052	0.2857	0.8491	0.3747	0.8424	0.3039	0.2851
lct010c16	0.8493	0.3837	0.8589	0.3133	0.2955	0.8421	0.3797	0.8526	0.3130	0.2961
lct010c17	0.8401	0.3789	0.8495	0.3091	0.2914	0.8326	0.3747	0.8428	0.3086	0.2918
lct010c18	0.8395	0.3779	0.8485	0.3080	0.2903	0.8319	0.3737	0.8417	0.3075	0.2906
lct010c19	0.8217	0.3687	0.8304	0.3001	0.2826	0.8138	0.3643	0.8233	0.2994	0.2828
lct017-03	0.8362	0.3665	0.8176	0.2907	0.2696	0.8303	0.3635	0.8128	0.2908	0.2705
lct017-04	0.8871	0.3953	0.8632	0.3152	0.2931	0.8806	0.3921	0.8575	0.3147	0.2931
lct017-05	0.8689	0.3859	0.8462	0.3072	0.2854	0.8626	0.3827	0.8407	0.3068	0.2857
lct017-06	0.8643	0.3836	0.8417	0.3051	0.2834	0.8580	0.3803	0.8363	0.3048	0.2837
lct017-07	0.8572	0.3798	0.8350	0.3019	0.2803	0.8509	0.3766	0.8298	0.3017	0.2808
lct17c8	0.8440	0.3716	0.8236	0.2949	0.2736	0.8380	0.3685	0.8187	0.2949	0.2743
lct017-09	0.8287	0.3636	0.8100	0.2883	0.2674	0.8228	0.3605	0.8053	0.2884	0.2683
lct017-10	0.8672	0.3835	0.8487	0.3055	0.2840	0.8624	0.3811	0.8449	0.3061	0.2853
lct017-11	0.8622	0.3807	0.8436	0.3031	0.2816	0.8573	0.3783	0.8398	0.3036	0.2829
lct017-12	0.8564	0.3776	0.8377	0.3003	0.2789	0.8513	0.3750	0.8337	0.3008	0.2801
lct017-13	0.8482	0.3731	0.8294	0.2963	0.2751	0.8427	0.3703	0.8251	0.2966	0.2762
lct017-14	0.8441	0.3707	0.8253	0.2943	0.2730	0.8386	0.3679	0.8208	0.2945	0.2741
lct017-15	0.9184	0.4203	0.9014	0.3391	0.3172	0.9137	0.4181	0.8972	0.3397	0.3182
lct017-16	0.9108	0.4160	0.8934	0.3351	0.3133	0.9059	0.4135	0.8890	0.3356	0.3142
lct17c17	0.9108	0.4145	0.8930	0.3335	0.3116	0.9055	0.4119	0.8882	0.3339	0.3124
lct017-19	0.9055	0.4108	0.8872	0.3301	0.3082	0.8998	0.4080	0.8821	0.3302	0.3087
lct017-20	0.9017	0.4085	0.8833	0.3280	0.3061	0.8957	0.4055	0.8780	0.3280	0.3066
lct017-21	0.8970	0.4057	0.8788	0.3256	0.3038	0.8909	0.4026	0.8732	0.3255	0.3042
lct017-22	0.8812	0.3981	0.8633	0.3191	0.2976	0.8747	0.3947	0.8576	0.3190	0.2980
lct017-23	0.8902	0.4027	0.8725	0.3232	0.3017	0.8837	0.3994	0.8665	0.3230	0.3018
lct017-24	0.8893	0.4017	0.8714	0.3223	0.3007	0.8828	0.3984	0.8655	0.3221	0.3009
lct017-25	0.8911	0.4016	0.8725	0.3218	0.3001	0.8846	0.3983	0.8667	0.3216	0.3003
lct017-28	0.9100	0.4147	0.8874	0.3331	0.3110	0.9032	0.4113	0.8810	0.3326	0.3106
lct017-29	0.9058	0.4116	0.8838	0.3303	0.3082	0.8992	0.4083	0.8776	0.3298	0.3080
lct26c3	0.8564	0.4068	0.8810	0.3402	0.3247	0.8484	0.4026	0.8730	0.3393	0.3241
lct42c1	0.9222	0.4222	0.9047	0.3405	0.3185	0.9184	0.4205	0.9015	0.3416	0.3200
lct42c2	0.9257	0.4219	0.9079	0.3400	0.3179	0.9206	0.4195	0.9033	0.3404	0.3186
lct42c3	0.9288	0.4234	0.9111	0.3413	0.3193	0.9235	0.4209	0.9063	0.3416	0.3198
lct42c4	0.9268	0.4226	0.9090	0.3406	0.3186	0.9215	0.4201	0.9042	0.3409	0.3191
lct42c5	0.9257	0.4217	0.9079	0.3398	0.3177	0.9205	0.4192	0.9032	0.3401	0.3183
lct42c6	0.9140	0.4157	0.8961	0.3345	0.3126	0.9086	0.4131	0.8913	0.3348	0.3132
lct42c7	0.9226	0.4197	0.9046	0.3379	0.3159	0.9173	0.4171	0.8998	0.3382	0.3164

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/44bwr/sens, and DVD/exps/leu/sens, respectively.

Table B-10. Integral index c_k for nominal 21-PWR waste packages and Crystal River CRCs

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	**0**	**0**	**15**	**25**	**30**	**35**	**40**
Filename[a]	**tb2-0** c_k	**tb3-0** c_k	**tb15** c_k	**tb25** c_k	**tb30** c_k	**tb35** c_k	**tb40** c_k
cr1r238	0.9587	0.9591	0.5854	0.5145	0.5058	0.4297	0.4938
cr2r238	0.6157	0.6042	0.9734	0.9650	0.9622	0.9494	0.9555
cr3r238	0.5338	0.5179	0.9740	0.9754	0.9733	0.9706	0.9673
cr4r238	0.6385	0.6304	0.9714	0.9608	0.9586	0.9428	0.9528
cr5r238	0.6807	0.6731	0.9614	0.9453	0.9426	0.9222	0.9361
cr6r238	0.5732	0.5611	0.9751	0.9725	0.9707	0.9634	0.9652
cr7r238	0.5338	0.5202	0.9705	0.9722	0.9708	0.9682	0.9658
cr8r238	0.7727	0.7665	0.9287	0.9004	0.8963	0.8634	0.8884
cr9r238	0.5393	0.5261	0.9702	0.9712	0.9697	0.9668	0.9646
cr10r238	0.5331	0.5198	0.9680	0.9696	0.9682	0.9656	0.9632
cr11r238	0.7979	0.7991	0.9053	0.8727	0.8692	0.8308	0.8624
cr12r238	0.4839	0.4708	0.9657	0.9732	0.9728	0.9772	0.9692
cr13r238	0.7439	0.7469	0.9318	0.9077	0.9057	0.8754	0.9010
cr14r238	0.6272	0.6253	0.9636	0.9546	0.9538	0.9390	0.9504
cr15r238	0.4711	0.4593	0.9635	0.9731	0.9733	0.9790	0.9709
cr16r238	0.7894	0.8006	0.8906	0.8589	0.8571	0.8175	0.8535
cr17r238	0.5650	0.5629	0.9682	0.9668	0.9672	0.9599	0.9652
cr18r238	0.5418	0.5387	0.9656	0.9669	0.9675	0.9632	0.9658
cr19r238	0.5376	0.5336	0.9684	0.9704	0.9710	0.9673	0.9692
cr20r238	0.4865	0.4779	0.9643	0.9722	0.9728	0.9762	0.9710
cr21r238	0.4857	0.4770	0.9650	0.9732	0.9738	0.9773	0.9721
cr22r238	0.7656	0.7781	0.8933	0.8645	0.8636	0.8272	0.8610
cr23r238	0.6492	0.6553	0.9480	0.9356	0.9359	0.9170	0.9344
cr24r238	0.6257	0.6303	0.9562	0.9472	0.9476	0.9316	0.9463
cr25r238	0.4951	0.4903	0.9594	0.9660	0.9672	0.9687	0.9664
cr26r238	0.4954	0.4908	0.9583	0.9648	0.9660	0.9673	0.9652
cr27r238	0.4636	0.4557	0.9568	0.9672	0.9684	0.9745	0.9676
cr28r238	0.7611	0.7747	0.8937	0.8655	0.8648	0.8285	0.8627
cr29r238	0.6093	0.6129	0.9589	0.9519	0.9525	0.9389	0.9513
cr30r238	0.5614	0.5621	0.9622	0.9610	0.9621	0.9552	0.9612
cr31r238	0.4956	0.4909	0.9614	0.9680	0.9692	0.9712	0.9684
cr32r238	0.7665	0.7829	0.8764	0.8468	0.8463	0.8081	0.8446
cr33r238	0.4676	0.4609	0.9581	0.9685	0.9699	0.9748	0.9696

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/CRC/CrystalRiver/sens-unqualified, respectively.

Table B-11. Integral index c_k for design-basis 21-PWR waste packages and Crystal River CRCs

Initial enrichment (wt% ^{235}U)	2	3	3	3.5	4	4.5	5
Burnup (GWd/MTU)	0	0	15	25	30	35	40
Filename[a]	tt2-0 c_k	tt3-0 c_k	tt15 c_k	tt25 c_k	tt30 c_k	tt35 c_k	tt40 c_k
cr1r238	0.9566	0.9593	0.5753	0.5183	0.5058	0.4862	0.4889
cr2r238	0.6144	0.6040	0.9734	0.9647	0.9613	0.9567	0.9549
cr3r238	0.5327	0.5175	0.9753	0.9745	0.9725	0.9702	0.9674
cr4r238	0.6371	0.6301	0.9708	0.9607	0.9577	0.9529	0.9519
cr5r238	0.6792	0.6732	0.9602	0.9455	0.9416	0.9355	0.9350
cr6r238	0.5720	0.5607	0.9757	0.9719	0.9697	0.9668	0.9650
cr7r238	0.5326	0.5198	0.9717	0.9714	0.9699	0.9681	0.9659
cr8r238	0.7711	0.7666	0.9256	0.9014	0.8955	0.8863	0.8864
cr9r238	0.5381	0.5259	0.9715	0.9703	0.9687	0.9668	0.9647
cr10r238	0.5320	0.5194	0.9693	0.9687	0.9672	0.9654	0.9633
cr11r238	0.7961	0.7991	0.9013	0.8740	0.8683	0.8585	0.8599
cr12r238	0.4829	0.4707	0.9680	0.9720	0.9718	0.9718	0.9698
cr13r238	0.7422	0.7468	0.9290	0.9084	0.9047	0.8974	0.8990
cr14r238	0.6258	0.6250	0.9630	0.9544	0.9528	0.9492	0.9494
cr15r238	0.4700	0.4589	0.9658	0.9718	0.9723	0.9731	0.9714
cr16r238	0.7875	0.8003	0.8862	0.8601	0.8561	0.8475	0.8506
cr17r238	0.5637	0.5625	0.9686	0.9663	0.9661	0.9646	0.9647
cr18r238	0.5405	0.5384	0.9665	0.9661	0.9664	0.9656	0.9655
cr19r238	0.5363	0.5332	0.9694	0.9696	0.9699	0.9692	0.9690
cr20r238	0.4854	0.4775	0.9663	0.9711	0.9718	0.9725	0.9713
cr21r238	0.4846	0.4766	0.9669	0.9720	0.9728	0.9735	0.9724
cr22r238	0.7637	0.7781	0.8895	0.8656	0.8625	0.8549	0.8583
cr23r238	0.6476	0.6553	0.9468	0.9357	0.9348	0.9311	0.9330
cr24r238	0.6242	0.6301	0.9554	0.9471	0.9465	0.9435	0.9450
cr25r238	0.4939	0.4899	0.9610	0.9650	0.9661	0.9668	0.9665
cr26r238	0.4943	0.4904	0.9599	0.9638	0.9649	0.9656	0.9653
cr27r238	0.4625	0.4554	0.9591	0.9659	0.9673	0.9689	0.9680
cr28r238	0.7592	0.7746	0.8898	0.8666	0.8637	0.8564	0.8600
cr29r238	0.6078	0.6127	0.9584	0.9517	0.9514	0.9489	0.9503
cr30r238	0.5600	0.5620	0.9628	0.9605	0.9609	0.9599	0.9607
cr31r238	0.4944	0.4907	0.9632	0.9669	0.9681	0.9688	0.9686
cr32r238	0.7645	0.7826	0.8721	0.8479	0.8451	0.8376	0.8417
cr33r238	0.4664	0.4603	0.9600	0.9671	0.9689	0.9705	0.9699

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/21pwr/sens, and DVD/exps/CRC/CrystalRiver/sens-unqualified, respectively.

Table B-12. Integral index c_k for 44-BWR waste packages and Crystal River CRCs

	Nominal configurations					Design-basis configurations				
Initial enrichment (wt% ^{235}U)	**3**	**3**	**4**	**4**	**5**	**3**	**3**	**4**	**4**	**5**
Burnup (GWd/MTU)	**0**	**10**	**0**	**20**	**30**	**0**	**10**	**0**	**20**	**30**
Filename[a]	**tb3-0 c_k**	**tb3-10 c_k**	**tb4-0 c_k**	**tb4-20 c_k**	**tb5-30 c_k**	**tt3-0 c_k**	**tt3-10 c_k**	**tt4-0 c_k**	**tt4-20 c_k**	**tt5-30 c_k**
cr1r238	0.9517	0.4417	0.9412	0.3621	0.3420	0.9457	0.4395	0.9348	0.3613	0.3404
cr2r238	0.5953	0.9447	0.5798	0.9209	0.9120	0.5914	0.9427	0.5756	0.9196	0.9101
cr3r238	0.5077	0.9598	0.4897	0.9451	0.9383	0.5044	0.9580	0.4862	0.9440	0.9367
cr4r238	0.6224	0.9383	0.6092	0.9127	0.9039	0.6182	0.9362	0.6047	0.9113	0.9019
cr5r238	0.6663	0.9191	0.6533	0.8885	0.8787	0.6618	0.9170	0.6485	0.8871	0.8766
cr6r238	0.5518	0.9542	0.5363	0.9360	0.9287	0.5482	0.9523	0.5323	0.9347	0.9270
cr7r238	0.5106	0.9565	0.4944	0.9424	0.9362	0.5072	0.9546	0.4907	0.9412	0.9346
cr8r238	0.7591	0.8624	0.7462	0.8200	0.8076	0.7541	0.8602	0.7408	0.8186	0.8055
cr9r238	0.5173	0.9561	0.5016	0.9415	0.9352	0.5139	0.9542	0.4979	0.9402	0.9334
cr10r238	0.5103	0.9543	0.4944	0.9402	0.9341	0.5070	0.9524	0.4907	0.9390	0.9324
cr11r238	0.7935	0.8336	0.7860	0.7879	0.7752	0.7879	0.8312	0.7800	0.7864	0.7728
cr12r238	0.4626	0.9623	0.4476	0.9544	0.9501	0.4595	0.9606	0.4443	0.9531	0.9484
cr13r238	0.7417	0.8749	0.7361	0.8373	0.8269	0.7364	0.8724	0.7303	0.8357	0.8245
cr14r238	0.6189	0.9339	0.6107	0.9106	0.9032	0.6144	0.9317	0.6059	0.9091	0.9011
cr15r238	0.4509	0.9623	0.4369	0.9564	0.9529	0.4478	0.9605	0.4335	0.9551	0.9513
cr16r238	0.7969	0.8219	0.7970	0.7779	0.7666	0.7908	0.8192	0.7906	0.7762	0.7640
cr17r238	0.5566	0.9522	0.5489	0.9365	0.9311	0.5525	0.9500	0.5444	0.9349	0.9290
cr18r238	0.5325	0.9541	0.5243	0.9410	0.9363	0.5285	0.9519	0.5201	0.9394	0.9342
cr19r238	0.5269	0.9574	0.5181	0.9448	0.9401	0.5231	0.9552	0.5139	0.9433	0.9381
cr20r238	0.4702	0.9612	0.4584	0.9540	0.9504	0.4668	0.9592	0.4548	0.9526	0.9486
cr21r238	0.4690	0.9618	0.4571	0.9548	0.9514	0.4657	0.9599	0.4535	0.9534	0.9496
cr22r238	0.7763	0.8318	0.7782	0.7911	0.7808	0.7703	0.8290	0.7717	0.7892	0.7780
cr23r238	0.6524	0.9163	0.6507	0.8911	0.8840	0.6474	0.9138	0.6452	0.8892	0.8814
cr24r238	0.6262	0.9293	0.6233	0.9069	0.9003	0.6214	0.9268	0.6181	0.9051	0.8979
cr25r238	0.4840	0.9562	0.4750	0.9484	0.9451	0.4804	0.9541	0.4711	0.9469	0.9431
cr26r238	0.4843	0.9547	0.4755	0.9468	0.9435	0.4807	0.9526	0.4716	0.9453	0.9415
cr27r238	0.4489	0.9584	0.4380	0.9540	0.9515	0.4456	0.9564	0.4345	0.9525	0.9497
cr28r238	0.7728	0.8333	0.7754	0.7933	0.7832	0.7667	0.8305	0.7689	0.7913	0.7805
cr29r238	0.6088	0.9354	0.6053	0.9150	0.9088	0.6041	0.9330	0.6003	0.9132	0.9065
cr30r238	0.5579	0.9486	0.5528	0.9338	0.9291	0.5537	0.9463	0.5482	0.9321	0.9267
cr31r238	0.4852	0.9588	0.4766	0.9512	0.9480	0.4817	0.9568	0.4727	0.9497	0.9459
cr32r238	0.7812	0.8134	0.7859	0.7723	0.7622	0.7749	0.8105	0.7791	0.7703	0.7594
cr33r238	0.4533	0.9583	0.4430	0.9537	0.9513	0.4498	0.9562	0.4392	0.9522	0.9495

Note: Cell shading identifies critical experiments applicable to bias and bias uncertainty determination.
[a]TSUNAMI-IP and TSUNAMI-3D input and output files for the applications and the experiments are included in the DVD attachment, paths: DVD/ip, DVD/apps/44bwr/sens, and DVD/exps/CRC/CrystalRiver/sens-unqualified, respectively.

APPENDIX C: Direct Perturbation Calculations

This appendix describes the direct perturbation method used to verify that the TSUNAMI-3D calculated sensitivity coefficient values are consistent with the sensitivity coefficients that MCNP would estimate. Sensitivity coefficients from MCNP direct perturbation calculations were obtained for nuclides/elements for which k_{eff} exhibits significant sensitivities, such as H, ^{10}B, ^{235}U, ^{238}U, ^{239}Pu, and ^{149}Sm. A comparison of direct perturbation and TSUNAMI-3D sensitivity coefficient calculations is presented in Table C-1. Note that the sensitivity coefficient estimates from the MCNP direct perturbation calculations have larger uncertainties than the TSUNAMI-3D sensitivity coefficients, although k_{eff} estimate from each individual MCNP calculation had a very small standard deviation (0.00012). The two methods are in good agreement since the MCNP direct perturbation results differ from the TSUNAMI-3D results by less than ±10% for the majority of the calculations, with the rest of the direct perturbation calculations being within ±20% of the TSUNAMI-3D results.

DIRECT PERTURBATION SENSITIVITY COEFFICIENTS

The direct perturbation method is used to assess the quality of the sensitivity coefficients obtained in a TSUNAMI-3D calculation that could be affected by the quality of the neutron fluxes from forward and adjoint Monte Carlo calculations with KENO V.a. Factors that determine the quality of neutron flux estimates are related to the number and quality of sample neutron tracks or to the size of the unit volumes used in a track-length estimation of the flux.

The macroscopic cross section of a nuclide-reaction pair can be perturbed by changing either the nuclide atom density or the microscopic cross section for the neutron reaction with the nuclide. The direct perturbation method employs variations of nuclide atom density that result in small k_{eff} variations consistent with the linear-perturbation approximation. Applications of this method require k_{eff} results for the nominal system and for the perturbed system, with the concentration of the nuclide of interest increased or decreased by the same percentage. The direct total perturbation sensitivity coefficient of k_{eff} to some input quantity is determined as

$$S_k = \frac{\alpha}{k} \times \frac{dk}{d\alpha} = \frac{\alpha}{k} \times \frac{k_{\alpha^+} - k_{\alpha^-}}{\alpha^+ - \alpha^-} \ ,$$

where α^+ and α^- represent the increased and decreased values of the input quantity, α, respectively, and k_{α^+} and k_{α^-} represent the corresponding values of k_{eff}. The standard deviation of a direct perturbation sensitivity coefficient is determined as

$$\sigma_S = \left(\left(\frac{\left(\sigma_{k^+}^2 + \sigma_{k^-}^2\right)}{\left(k^+ - k^-\right)^2} + \frac{\sigma_k^2}{k^2} \right) \times \left(\frac{k^+ - k^-}{k} \right)^2 \right)^{1/2} \times \frac{\alpha}{\alpha^+ - \alpha^-} \ .$$

The direct perturbation calculations provided in the Table C-1 were performed using Microsoft Excel (see DVD/dp/DP.xls). The names of the output files are described in spreadsheet *DP.xls*, worksheet *keff results*. The paths to the input and output files are indicated in the table endnotes.

Table C-1. Comparison of MCNP direct perturbation and TSUNAMI-3D sensitivity calculations

21-PWR waste package, initial enrichment = 3 wt% ^{235}U, burnup = 15 GWd/MTU: nominal configuration[a]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[b]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.94769	0.00012	0.94359	0.00012	2.17E-01	8.98E-03	2.16E-01	6.02E-03	-0.3
^{10}B	2	0.94488	0.00013	0.94579	0.00012	-2.41E-02	4.68E-03	-2.64E-02	2.90E-05	9.8
^{235}U	1	0.94623	0.00012	0.94288	0.00012	1.77E-01	8.98E-03	1.78E-01	3.27E-04	0.4
^{238}U	2	0.94245	0.00012	0.94662	0.00012	-1.10E-01	4.49E-03	-1.16E-01	2.73E-04	5.3
^{239}Pu	1	0.94541	0.00012	0.9436	0.00012	9.57E-02	8.98E-03	9.90E-02	1.77E-04	3.4
^{149}Sm	100			0.95873	0.00013	-1.43E-02	1.84E-04	-1.36E-02	1.23E-05	-4.5
21-PWR waste package, initial enrichment = 5 wt% ^{235}U, burnup = 40 GWd/MTU: nominal configuration[a]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[b]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.93955	0.00013	0.93468	0.00013	2.60E-01	9.81E-03	2.50E-01	8.61E-03	-3.9
^{10}B	5	0.93563	0.00013	0.93814	0.00013	-2.68E-02	1.96E-03	-2.54E-02	2.78E-05	-5.2
^{235}U	1	0.93711	0.00013	0.93425	0.00013	1.53E-01	9.81E-03	1.48E-01	2.80E-04	-2.8
^{238}U	1	0.93428	0.00013	0.9358	0.00013	-8.11E-02	9.81E-03	-8.85E-02	2.53E-04	9.1
^{239}Pu	1	0.93644	0.00013	0.93444	0.00013	1.07E-01	9.81E-03	9.90E-02	1.94E-04	-7.2
^{149}Sm	100			0.95127	0.00013	-1.52E-02	1.84E-04	-1.48E-02	1.34E-05	-2.5
21-PWR waste package, initial enrichment = 3 wt% ^{235}U, burnup = 15 GWd/MTU: design-basis configuration[a]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[b]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.9735	0.00012	0.9698	0.00012	1.90E-01	8.73E-03	1.96E-01	6.18E-03	2.9
^{10}B	5	0.97067	0.00012	0.97322	0.00012	-2.62E-02	1.75E-03	-2.61E-02	3.38E-05	-0.5
^{235}U	1	0.97291	0.00012	0.96917	0.00012	1.92E-01	8.73E-03	1.75E-01	3.49E-04	-9.0
^{238}U	1	0.96965	0.00012	0.97215	0.00012	-1.29E-01	8.73E-03	-1.19E-01	2.92E-04	-7.3
^{239}Pu	2	0.97282	0.00012	0.96899	0.00012	9.85E-02	4.37E-03	1.01E-01	1.91E-04	2.8
^{149}Sm	100			0.98506	0.00012	-1.38E-02	1.70E-04	-1.37E-02	1.33E-05	-0.5
21-PWR waste package, initial enrichment = 5 wt% ^{235}U, burnup = 40 GWd/MTU: design-basis configuration[a]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[b]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.96452	0.00013	0.96039	0.00013	2.15E-01	9.55E-03	2.33E-01	7.49E-03	8.6
^{10}B	2	0.96222	0.00013	0.96339	0.00013	-3.04E-02	4.78E-03	-2.48E-02	3.12E-05	-18.3
^{235}U	1	0.96243	0.00013	0.95982	0.00013	1.36E-01	9.55E-03	1.47E-01	2.90E-04	8.4
^{238}U	1	0.96042	0.00013	0.96209	0.00013	-8.68E-02	9.55E-03	-9.14E-02	2.62E-04	5.3
^{239}Pu	2	0.96322	0.00013	0.95923	0.00012	1.04E-01	4.60E-03	9.97E-02	2.00E-04	-3.8
^{149}Sm	100			0.97719	0.00013	-1.53E-02	1.84E-04	-1.49E-02	1.38E-05	-2.5
44-BWR waste package, initial enrichment = 3 wt% ^{235}U, burnup = 0 GWd/MTU: nominal configuration[c]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[d]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.84805	0.00013	0.84456	0.00013	2.06E-01	1.09E-02	1.76E-01	5.71E-03	-14.5
^{10}B	2	0.84547	0.00013	0.84710	0.00013	-4.82E-02	5.43E-03	-4.51E-02	4.46E-05	-6.3
^{235}U	1	0.84857	0.00013	0.84424	0.00013	2.56E-01	1.09E-02	2.65E-01	5.14E-04	3.4
^{238}U	1	0.8455	0.00013	0.84737	0.00013	-1.10E-01	1.09E-02	-1.12E-01	2.80E-04	1.1

Table C-1. Comparison of MCNP direct perturbation and TSUNAMI-3D sensitivity calculations (continued)

44-BWR waste package, initial enrichment = 5 wt% ^{235}U, burnup = 30 GWd/MTU: nominal configuration[c]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[d]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	σ_s	S	σ	
H	1	0.83484	0.00013	0.83159	0.00013	1.95E-01	1.10E-02	1.83E-01	4.48E-03	-6.3
^{10}B	5	0.83157	0.00013	0.83502	0.00013	-4.14E-02	2.21E-03	-4.31E-02	4.96E-05	4.1
^{235}U	1	0.83223	0.00013	0.83049	0.00013	1.04E-01	1.10E-02	1.16E-01	2.18E-04	10.7
^{238}U	4	0.82967	0.00013	0.83340	0.00013	-5.60E-02	2.76E-03	-5.96E-02	2.82E-04	6.5
^{239}Pu	1	0.83268	0.00013	0.83063	0.00013	1.23E-01	1.10E-02	1.24E-01	2.95E-04	0.6
^{149}Sm	100			0.86302	0.00014	-3.62E-02	1.91E-04	-3.44E-02	3.51E-05	-5.1
44-BWR waste package, initial enrichment = 3 wt% ^{235}U, burnup = 0 GWd/MTU: design-basis configuration[c]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[d]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	σ_s	S	σ	
H	1	0.89133	0.00013	0.88857	0.00013	1.55E-01	1.03E-02	1.48E-01	5.58E-03	-4.7
^{10}B	5	0.88823	0.00013	0.89188	0.00013	-4.10E-02	2.07E-03	-4.25E-02	4.86E-05	3.5
^{235}U	1	0.89228	0.00013	0.88736	0.00013	2.76E-01	1.03E-02	2.63E-01	5.03E-04	-4.9
^{238}U	2	0.88802	0.00013	0.89217	0.00013	-1.17E-01	5.16E-03	-1.16E-01	2.75E-04	-0.6
44-BWR waste package, initial enrichment = 5 wt% ^{235}U, burnup = 30 GWd/MTU: design-basis configuration[c]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[d]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	σ_s	S	σ	
H	1	0.8761	0.00013	0.87333	0.00013	1.58E-01	1.05E-02	1.60E-01	4.39E-03	1.0
^{10}B	5	0.87282	0.00013	0.8766	0.00013	-4.32E-02	2.10E-03	-3.97E-02	5.28E-05	-8.1
^{235}U	1	0.87407	0.00013	0.87211	0.00013	1.12E-01	1.05E-02	1.14E-01	2.15E-04	1.9
^{238}U	2	0.87179	0.00013	0.87419	0.00013	-6.86E-02	5.25E-03	-6.29E-02	2.77E-04	-8.3
^{239}Pu	1	0.87393	0.00013	0.87185	0.00013	1.19E-01	1.05E-02	1.23E-01	2.93E-04	3.1
^{149}Sm	100			0.90649	0.00014	-3.63E-02	1.91E-04	-3.47E-02	3.48E-05	-4.4
LEU LCEs; lct42c3 = unperturbed MCNP model[e]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[f]**		**% Differenc[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	σ_s	S	σ	
H	1	0.99661	0.00013	0.99161	0.00013	2.52E-01	9.25E-03	2.26E-01	1.19E-01	-10.2
^{235}U	1	0.99657	0.00013	0.99170	0.00013	2.45E-01	9.25E-03	2.48E-01	7.00E-04	1.1
^{238}U	2	0.99114	0.00013	0.99681	0.00013	-1.43E-01	4.62E-03	-1.44E-01	5.09E-04	1.1
MOX LCEs; mct08-01 = unperturbed MCNP model[g]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[h]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	σ_s	S	σ	
H	1	0.99491	0.00015	0.98964	0.00015	2.66E-01	1.07E-02	2.91E-01	2.20E-02	9.5
^{235}U	2	0.99307	0.00015	0.99148	0.00015	4.01E-02	5.34E-03	3.99E-02	8.67E-05	-0.4
^{238}U	2	0.99047	0.00015	0.99413	0.00015	-9.22E-02	5.34E-03	-9.13E-02	2.92E-04	-1.0
^{239}Pu	2	0.99465	0.00015	0.98986	0.00015	1.21E-01	5.34E-03	1.32E-01	3.37E-04	9.2

Table C-1. Comparison of MCNP direct perturbation and TSUNAMI-3D sensitivity calculations (continued)

HTC LCEs; htc1c01 = unperturbed MCNP model[i]										
Nuclide	Change (wt%)	+Change		-Change		Direct perturbation		TSUNAMI[j]		% Difference[p]
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	0.5	0.99641	0.0001	0.99829	0.0001	-1.88E-01	1.42E-02	-1.65E-01	5.96E-02	-12.5
^{235}U	1	0.99945	0.0001	0.99538	0.0001	2.04E-01	7.09E-03	1.96E-01	5.46E+00	-3.9
^{238}U	1	0.99667	0.0001	0.99824	0.0001	-7.87E-02	7.09E-03	-8.05E-02	3.31E-04	2.3
HTC LCEs; htc2b01 = unperturbed MCNP model[k]										
Nuclide	Change (wt%)	+Change		-Change		Direct perturbation		TSUNAMI[j]		% Difference[p]
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.99797	0.00013	0.99255	0.00013	2.72E-01	9.24E-03	2.68E-01	1.12E-02	-1.6
^{235}U	1	0.99627	0.00013	0.99377	0.00014	1.26E-01	9.60E-03	1.17E-01	1.99E-05	-6.9
^{238}U	2	0.99335	0.00013	0.99720	0.00014	-9.67E-02	4.80E-03	-1.10E-01	3.01E-04	13.9
^{10}B	1	0.99489	0.00013	0.99526	0.00013	-1.86E-02	9.24E-03	-1.72E-02	1.99E-05	-7.3
HTC LCEs; htc2g01 = unperturbed MCNP model[l]										
Nuclide	Change (wt%)	+Change		-Change		Direct perturbation		TSUNAMI[j]		% Difference[p]
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.99770	0.00013	0.99228	0.00013	2.72E-01	9.24E-03	2.63E-01	8.73E-03	-3.5
^{235}U	2	0.99760	0.00014	0.99219	0.00014	1.36E-01	4.98E-03	1.21E-01	2.39E-04	-11.0
^{238}U	1	0.99384	0.00014	0.99577	0.00014	-9.70E-02	9.95E-03	-1.09E-01	2.96E-04	12.5
^{157}Gd	5	0.99366	0.00013	0.99564	0.00014	-1.99E-02	1.92E-03	-2.14E-02	2.54E-04	7.7
HTC LCEs; htc301 = unperturbed model[m]										
Nuclide	Change (wt%)	+Change		-Change		Direct perturbation		TSUNAMI[j]		% Difference[p]
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	0.99716	0.00013	0.99426	0.00013	1.46E-01	9.23E-03	1.50E-01	1.15E-02	3.1
^{235}U	1	0.99694	0.00013	0.99436	0.00013	1.30E-01	9.23E-03	1.49E-01	2.83E-04	15.2
^{238}U	1	0.99476	0.00013	0.99694	0.00013	-1.10E-01	9.23E-03	-9.54E-02	2.55E-04	-12.9
HTC LCEs; htc4s01 = unperturbed model[n]										
Nuclide	Change (wt%)	+Change		-Change		Direct perturbation		TSUNAMI[j]		% Difference[p]
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	$σ_s$	S	σ	
H	1	1.00126	0.00012	0.99809	0.00012	1.59E-01	8.49E-03	1.58E-01	8.49E-03	-0.2
^{235}U	1	1.00116	0.00013	0.99814	0.00012	1.51E-01	8.85E-03	1.54E-01	2.29E-04	1.9
^{238}U	1	0.99889	0.00012	1.00077	0.00012	-9.40E-02	8.49E-03	-9.58E-02	2.55E-04	1.9

Table C-1. Comparison of MCNP direct perturbation and TSUNAMI-3D sensitivity calculations (continued)

HTC LCEs; htc4l01 = unperturbed model[o]										
Nuclide	**Change (wt%)**	**+Change**		**-Change**		**Direct perturbation**		**TSUNAMI[j]**		**% Difference[p]**
		k_{eff}+	σ+	k_{eff}-	σ-	S_k	σ_s	S	σ	
H	1	1.00328	0.00012	1.00011	0.00012	1.58E-01	8.47E-03	1.60E-01	8.49E-03	0.9
^{235}U	1	1.0032	0.00012	1.00035	0.00012	1.42E-01	8.47E-03	1.54E-01	2.25E-04	8.0
^{238}U	1	1.00074	0.00013	1.00248	0.00012	-8.68E-02	8.83E-03	-9.51E-02	2.23E-04	9.5

The input and output files are included in the DVD attachment, paths:
[a]DVD/dp/21pwr.
[b]DVD/apps/21pwr/sens.
[c]DVD/dp/44bwr.
[d]DVD/apps/44bwr/sens.
[e]DVD/dp/leu.
[f]DVD/exps/leu/sens.
[g]DVD/dp/mox.
[h]DVD/exps/mox/sens.
[i]DVD/dp/htc/htc1.
[j]DVD/exps/htc/sens.
[k]DVD/dp/htc/htc2/B.
[l]DVD/dp/htc/htc2/Gd.
[m]DVD/dp/htc/htc3.
[n]DVD/dp/htc/htc4/SS.
[o]DVD/dp/htc/htc4/Pb.
[p]$(S-S_k)/S_k*100$

APPENDIX D: Various CRC Calculations and Results

This appendix contains various CRC calculations needed for analyses presented in this report. Changes were made to the original MCNP input files (Ref. 53) to create new input files for MCNP 5.1.40 calculations with ENDF/B-VI. A change made to the input files for one-eighth symmetry CRC models consists of replacement of the original geometry cutting plane that defines a one-eighth symmetry core model with a cutting plane that defines a one-fourth symmetry core model. Note that the modeling for a one-fourth symmetry core was already implemented in the original MCNP 4B input files for these cases. The MCNP 4C k_{eff} results for one-fourth symmetry geometry and the MCNP 4B k_{eff} results for the one-eighth symmetry geometry provided in Ref. 52 are almost identical, as shown in Table D-1, which indicate that the two MCNP core models are identical. Note that the MCNP 4B version was not available for these calculations and the MCNP 4C version was used instead. Also note that the results of these calculations were not used in the validation calculations; they only confirm that the modified and original MCNP core geometry representations are equivalent.

Table D-1. One-fourth core symmetry MCNP calculations

	MCNP 4C[a]			Comparison calculations[b]	
State-point	**Output file**	k_{eff}	σ	k_{eff}	σ
1	CR1qo	0.9965	0.0005	0.9960	0.0004
10	CR10qo	0.9968	0.0004	0.9960	0.0005
11	CR11qo	0.9951	0.0005	0.9948	0.0005
12	CR12qo	0.9977	0.0004	0.9981	0.0005
13	CR13qo	0.9953	0.0005	0.9956	0.0004
14	CR14qo	0.9958	0.0005	0.9958	0.0005
15	CR15qo	0.9929	0.0005	0.9927	0.0004
16	CR16qo	0.9930	0.0005	0.9932	0.0005
17	CR17qo	0.9927	0.0004	0.9908	0.0005
18	CR18qo	0.9918	0.0005	0.9922	0.0005
19	CR19qo	0.9914	0.0005	0.9899	0.0005
20	CR20qo	0.9938	0.0004	0.9932	0.0004
21	CR21qo	0.9931	0.0004	0.9925	0.0005
32	CR32qo	0.9903	0.0005	0.9916	0.0005
33	CR33qo	0.9870	0.0005	0.9873	0.0005

[a]MCNP input and output files available in the DVD attachment, path: DVD/exps/CRC/CrystalRiver/mcnp/verc.
[b]MCNP criticality calculations for Crystal River Unit 3 are provided in Ref. 52.

CSAS25/KENO V.a modeling was performed for Crystal River Unit 3 CRC state-points for use in TSUNAMI-3D calculations. Generally, the CSAS25 k_{eff} results are in good agreement with the results described in the referenced document (±0.3%), as shown in Table D-2, indicating that the mixture compositions and geometry models are consistent between the CSAS25 and MCNP calculations. Only the results for the last two Crystal River state-points are significantly lower than the comparison MCNP calculation results. However, the impact on sensitivity coefficients is expected to be less important because these coefficients are defined in terms of relative values (see Appendix B). Note that the results of these calculations were not used directly in the validation calculations; they only confirm that the CSAS/KENO V.a and MCNP model representations (Ref. 53) are equivalent.

Table D-2. k_{eff} results for Crystal River CRC state-points

State point	Case identifier	EALF (eV)	CSAS25[a]		Comparison calculations[b]		% Difference[c]
			k_{eff}	σ	k_{eff}	σ	
1	CR3SP1	5.58E-01	0.9938	0.0004	0.9960	0.0004	0.22
2	CR3SP2	6.28E-01	0.9925	0.0004	0.9929	0.0004	0.04
3	CR3SP3	6.09E-01	0.9946	0.0005	0.9950	0.0005	0.04
4	CR3SP4	6.28E-01	0.9920	0.0004	0.9928	0.0004	0.08
5	CR3SP5	6.58E-01	0.9924	0.0004	0.9941	0.0005	0.17
6	CR3SP6	6.46E-01	0.9919	0.0004	0.9930	0.0005	0.11
7	CR3SP7	6.43E-01	0.9893	0.0005	0.9907	0.0005	0.14
8	CR3SP8	6.62E-01	0.9915	0.0004	0.9913	0.0005	-0.02
9	CR3SP9	6.35E-01	0.9890	0.0004	0.9915	0.0005	0.25
10	CR3SP10	6.64E-01	0.9956	0.0004	0.9960	0.0005	0.04
11	CR3SP11	7.24E-01	0.9952	0.0004	0.9948	0.0005	-0.04
12	CR3SP12	7.08E-01	0.9960	0.0004	0.9981	0.0005	0.21
13	CR3SP13	7.88E-01	0.9940	0.0004	0.9956	0.0004	0.16
14	CR3SP14	7.80E-01	0.9948	0.0004	0.9958	0.0005	0.10
15	CR3SP15	7.36E-01	0.9899	0.0003	0.9927	0.0004	0.28
16	CR3SP16	8.74E-01	0.9923	0.0004	0.9932	0.0005	0.09
17	CR3SP17	8.40E-01	0.9902	0.0003	0.9908	0.0005	0.06
18	CR3SP18	8.46E-01	0.9906	0.0003	0.9922	0.0005	0.16
19	CR3SP19	8.27E-01	0.9895	0.0004	0.9899	0.0005	0.04
20	CR3SP20	7.78E-01	0.9912	0.0005	0.9932	0.0004	0.20
21	CR3SP21	7.83E-01	0.9899	0.0003	0.9925	0.0005	0.26
22	CR3SP22	9.39E-01	0.9905	0.0004	0.9904	0.0004	-0.01
23	CR3SP23	9.42E-01	0.9903	0.0004	0.9902	0.0005	-0.01
24	CR3SP24	9.34E-01	0.9916	0.0004	0.9906	0.0005	-0.10
25	CR3SP25	8.52E-01	0.9910	0.0005	0.9905	0.0004	-0.05
26	CR3SP26	8.37E-01	0.9910	0.0005	0.9907	0.0005	-0.03
27	CR3SP27	8.20E-01	0.9873	0.0004	0.9877	0.0004	0.04
28	CR3SP28	9.60E-01	0.9895	0.0004	0.9921	0.0004	0.26
29	CR3SP29	9.32E-01	0.9919	0.0004	0.9931	0.0005	0.12
30	CR3SP30	9.23E-01	0.9897	0.0004	0.9908	0.0005	0.11
31	CR3SP31	8.81E-01	0.9861	0.0004	0.9884	0.0005	0.23
32	CR3SP32	1.04E+00	0.9811	0.0005	0.9916	0.0005	1.06
33	CR3SP33	8.60E-01	0.9807	0.0005	0.9873	0.0005	0.67

[a]CSAS25 input and output files are available in the DVD attachment, path: DVD/exps/CRC/CrystalRiver/csas.
[b]MCNP criticality calculations for Crystal River Unit 3 are provided in Ref. 61.
[c]100x(Comparison calculation k_{eff} – CSAS25 k_{eff})/Comparison calculation k_{eff}.

Figure D-1 shows the distribution histogram plot for PWR and BWR Grand Gulf CRC k_{eff} values that pass χ^2 normality test in /DVD/cl/Table18/case8.xls, worksheet normality test.

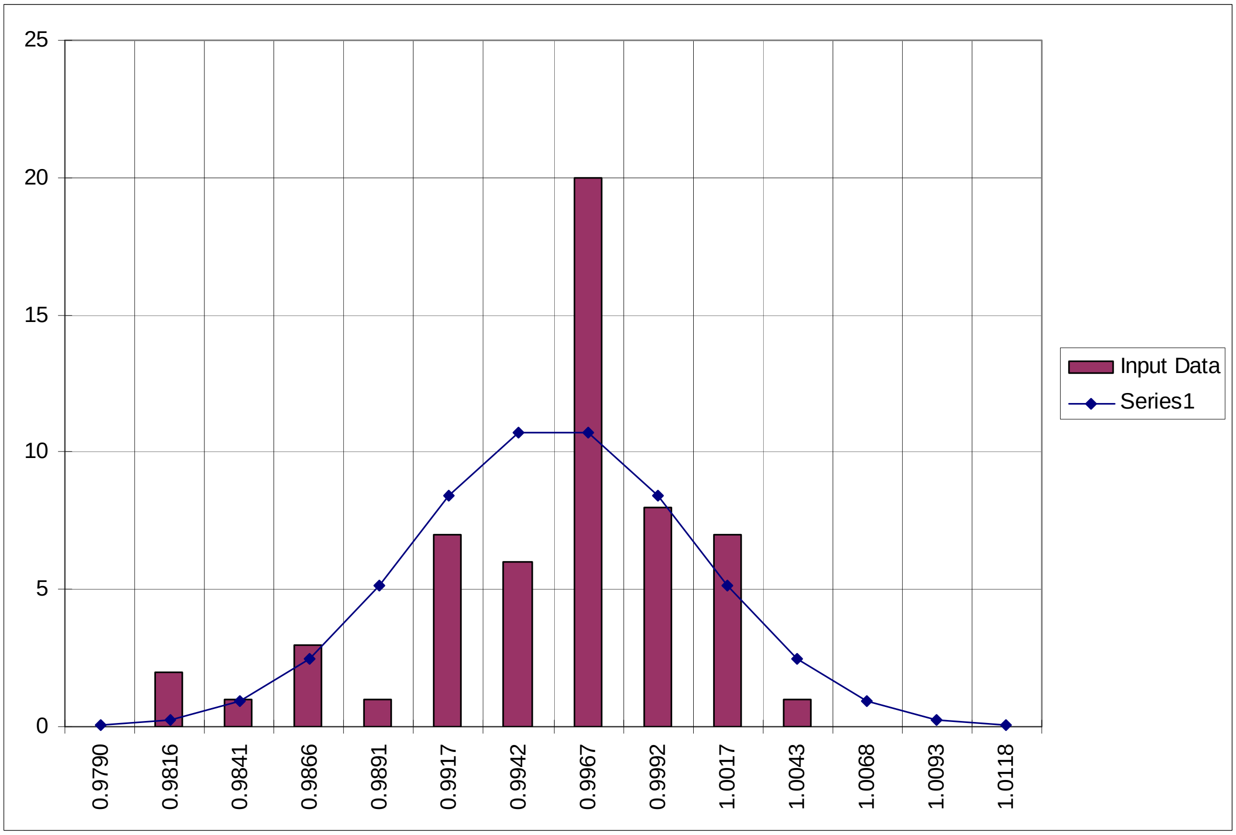

Fig. D-1. CRC k_{eff} frequency histogram

APPENDIX E: Statistical Methods for LBTL Determination

This appendix describes the equations for applying the lower uniform tolerance band method, the regression fit significance test, and the χ^2 normality test.

Lower Uniform Tolerance Band Method

The *LBTL* function from the LUTB method is computed as[18]

$$LBTL(x) = 1.0 - (C_{\alpha/P} \cdot s_P) + \beta(x),$$

where x is a trending parameter, s_p is the pooled variance of k_{eff} values, and $\beta(x) = k_{eff}(x) - 1$. The term $C_{\alpha/P} \cdot s_P$ provides a band for which there is a probability P with a confidence α that an additional calculation of k_{eff} for a critical system will lie within the band. For example, a C95/95 multiplier produces a USL for which there is a 95% confidence that 950 out of 1000 future calculations of critical systems will yield a value of k_{eff} above the USL.

The analysis is over the closed interval from $x = a$ to $x = b$ that includes n data points. $C_{\alpha/P}$ is calculated according to the following equations:

$$g = \sqrt{\frac{1}{n} + \frac{(a - \bar{x})^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2}}$$

$$h = \sqrt{\frac{1}{n} + \frac{(b - \bar{x})^2}{\sum_{i=1}^{n} (x_i - \bar{x})^2}}$$

$$\rho = \frac{1}{gh} \bullet \left\{ \frac{1}{n} + \frac{(a - \bar{x})(b - \bar{x})}{\sum_{i=1}^{n} (x_i - \bar{x})^2} \right\}$$

$$A = \frac{g}{h}$$

A, ρ, and $(n - 2)$ are used to determine the value of D (refer to Eq. E-1) from Table 3 in Ref. 19, which covers values of $0.5 \leq A \leq 1.5$. The procedure to follow when A is in this range is

$$C^* = D \cdot A \cdot g$$

When A is outside the above range, A is replaced by $1/A$ for the determination of D, and C^* is given by

$$C^* = D \cdot A \cdot h$$

Next,

$$C_{\alpha/P} = C^* + z_P \bullet \sqrt{\frac{n-2}{\chi^2}} ,$$

where

z_P is the Student *t* statistic depending on *n* and *P*, and

$\chi 2$ is the chi square distribution, a function of $(n-2)$ and α.

Parameter D is the solution to the following equation:

$$\int_{-D}^{D}\int_{-AD}^{AD} \frac{1}{2\pi(1-\rho^2)^{1/2}}\left[1+\frac{u^2-2\rho uw+v^2}{(n-2)(1-\rho^2)}\right]^{-n/2} dudv = 1-\gamma , \qquad \text{Eq. E-1}$$

where $1-\gamma$ is the confidence coefficient.

The pooled standard deviation is obtained from the pooled variance ($s_p = \sqrt{s_p^2}$), where s_p^2 is given as

$$s_p^2 = s_{k(x)}^2 + s_w^2 ,$$

where $s_{k(x)}^2$ is the variance (or mean-square error) of the regression fit, and is given by:

$$s_{k(x)}^2 = \frac{1}{(n-2)}\left[\sum_{i=1,n}(k_i-\bar{k})^2 - \frac{\left\{\sum_{i=1,n}(x_i-\bar{x})(k_i-\bar{k})\right\}^2}{\sum_{i=1,n}(x_i-\bar{x})^2}\right] ,$$

and s_w^2 is the within-variance of the data:

$$s_w^2 = \frac{1}{n}\sum_{i=1,n}\sigma_i^2 ,$$

where σ_i is the standard deviation associated with k_i for a Monte Carlo calculation. For best results, it is recommended that the individual standard deviations for the Monte Carlo calculations be roughly uniform in value. For deterministic codes that do not have a standard deviation associated with a computed value of *k*, the standard deviation is zero. However, this term could be used as a mechanism to include known uncertainties in experimental data.

Statistical Significance of Trending

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. 77. The statistical model is a linear relationship between an independent variable predictor variable, *x* (e.g., *EALF*, burnup, etc.) and the dependent variable, *y(x)* (e.g., LBTL):

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

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

$$T = \frac{\hat{\beta}_1 - \beta_{10}}{S\sqrt{c_{11}}}, \qquad \text{Eq. E-2}$$

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,

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

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

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

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

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

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

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:	$\lvert t \rvert > t_{\alpha/2}$ (two-tailed alternative), where α is the level of significance.

Chi2 Normality Test

The χ^2 normality test is applied to binned k_{eff} values using the following statistic[76]

$$\chi^2 = \sum_{i=1}^{k} (n_i^2 / nP_i) - n, \qquad \text{Eq. E-3}$$

where k is the number of bins, n_i is the number of k_{eff} values in each bin, nP_i is the expected number of k_{eff} values in each bin, and n is the sample size.

The Test of Hypothesis for the normality test is:

H_0:	The k_{eff} values follow a normal distribution
H_a:	The k_{eff} values do not follow a normal distribution
Rejection:	$\chi^2 \geq \chi^2_{1-\alpha}$ for *k-1* degrees of freedom, where α is the significance level.

APPENDIX E REFERENCE

77. D. D. Wackerly, W. Mendenhall III, and R. L. Scheaffer, *Mathematical Statistics with Applications,* 5th Edition, Belmont, CA, Wadsworth Publishing Company, 1996.

APPENDIX F: Electronic Data Specifications

This appendix contains a listing and description of files contained in the Digital Versatile/Video Discs (DVD+R format) that are attached to the calculation report *Range of Applicability and Bias Determination for Postclosure Criticality of Commercial Spent Nuclear Fuel*. The operating system used to create the electronic data on the DVDs was Microsoft Windows Vista Enterprise, Version 6.0.6000 Build 6000. The files stored on the electronic media consist of MCNP or SCALE input and output files (text format), Microsoft Excel files, and a Mathematica file. 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 electronic data for the calculation is provided on seven DVDs and the folder contents are listed below. Hierarchical directory structure and name, size, date, and time for each electronic file are listed in the text file *overall_listing* included in DVD-7.

Table F-1. DVD content summary

DVD no.	Folder/file name	Size	Number of files	File time[b]	Description
DVD-1	DVD/exps/CRC/CrystalRiver/csas/	4.33 GB	36	7:27:25 a.m.	Crystal River, state-points 1 through 18, CSAS25 files
DVD-2	DVD/exps/CRC/CrystalRiver/csas/	4.12 GB	30	8:04:12 a.m.	Crystal River, state-points 19 through 33, CSAS25 files
DVD-3	DVD/exps/CRC/CrystalRiver/mcnp/	832 MB	96	8:31:06 a.m.	Crystal River, MCNP files
	DVD/exps/CRC/CrystalRiver/sens-unqualified/	244 MB	94	8:35:36 a.m.	Crystal River, TSUNAMI sensitivity files
	DVD/exps/CRC/GrandGulf/mcnp/	1.77 GB	6	8:36:55 a.m.	Grand Gulf, state-points 5, 6 & 7, MCNP files
DVD-4	DVD/exps/CRC/GrandGulf/mcnp/	4.31 GB	14	8:49:31 a.m.	Grand Gulf, state-points 10 through 16, MCNP files
DVD-5	DVD/exps/CRC/GrandGulf/mcnp/	3.82 GB	12	9:15:32 a.m.	Grand Gulf, state-points 18 through 23, MCNP files
DVD-6	DVD/exps/CRC/McGuire/	842 MB	13	10:29:17 a.m.	MCNP files for McGuire CRCs
	DVD/exps/CRC/Sequoyah/	46.6 MB	6	10:33:49 a.m.	MCNP files for Sequoyah CRCs
	DVD/exps/CRC/TMI/	43.5 MB	6	10:34:04 a.m.	MCNP files for TMI CRCs
	DVD/exps/leu/	168 MB	186	10:34:18 a.m.	MCNP and TSUNAMI-3D files for LEU LCEs
	DVD/exps/mox/	2.17 GB	2,175	10:35:15 a.m.	MCNP and TSUNAMI-3D files for MOX LCEs
	DVD/apps/	472 MB	6,872	10:15:43 a.m.	MCNP, CSAS25, and TSUNAMI-3D files for waste packages
	DVD/dp	439 MB	299	10:26:44 a.m.	MCNP files for direct perturbation calculations
	DVD/cl	12.5 MB	21	10:26:39 a.m.	Excel and Mathematica files
	LoadingCurve_v344.xls	7.96 MB	1	10:15:35 a.m.	Calculation output file
	Tables.xls	903 KB	1	10:15:43 a.m.	Summary results Excel file

Table F-1. DVD content summary (continued)

DVD no.	Folder/file name	Size	Number of files	File time[b]	Description
DVD-7	DVD/exps/htc/ [a]	1.54 GB	791	10:57:46 a.m.	MCNP and TSUNAMI-3D files for HTC LCEs
	DVD/ip/	1.69 GB	25,182	11:07:04 a.m.	TSUNAMI-IP files
	separate_DVD_trees.out	8.68 KB	1	11:48:25 a.m.	Separate DVD trees
	DVDtree.out	5.95 KB	1	11:48:24 a.m.	DVD tree
	overall_listing	2.63 MB	1	11:48:24 a.m.	File name, size, date, and time for all files
	DVD-1_listing	2.86 KB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-1
	DVD-2_listing	2.47 KB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-2
	DVD-3_listing	13.1 KB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-3
	DVD-4_listing	1.30 KB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-4
	DVD-5_listing	1.24 KB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-5
	DVD-6_listing	694 KB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-6
	DVD-7_listing	1.94 MB	1	11:48:23 a.m.	File name, size, date, and time for all files on DVD-7

[a]Limited Rights Data (French HTC Experimental Data).
[b]All DVDs were created on October 9, 2007 by D. E. Mueller.

EXTERNAL DISTRIBUTION

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